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Nonequilibrium stationary states of rotor and oscillator chains

États stationnaires hors-équilibre de chaînes de rotateurs et oscillateurs

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Résumé

La mécanique statistique relie la description macroscopique d'un système, basée sur des paramètres thermodynamiques, à la dynamique microscopique de ses composants. Les valeurs assumées par les paramètres macroscopiques tels que la température ou la pression, sont le résultat du comportement collectif des composants du système, dont les positions et les vitesses évoluent à l'échelle moléculaire suivant les lois de la dynamique hamiltonienne sur l'espace des phases. Il y a bien évidemment quelques problèmes liés à cette description microscopique (Balian (2007), Schwabl (2006)). Premièrement, il est impossible de connaître exactement l'état d'un système possédant un tel nombre de degrés de liberté à tout instant. Deuxièmement, de très petites différences dans les conditions initiales sont généralement exponentiellement amplifiées dans le temps en raison de la nature chaotique de la dynamique hamiltonienne sous-jacente. Troisièmement, considérer l'évolution de tous les degrés de liberté est inutile, puisque dans de nombreuses situations, nous ne sommes intéressés que par quelques propriétés moyennes, comme la densité d'énergie. Pour toutes ces raisons, un système est mieux décrit par un ensemble thermodynamique, c'est-à-dire une loi de probabilité définie sur l'espace des phases, et ses caractéristiques macroscopiques sont calculées comme des moyennes par rapport à cette loi.

Le concept d'équilibre est apparenté au sens empirique utilisé en thermodynamique : un système est à l'équilibre lorsque son état thermodynamique ne change pas dans le temps et reste stable sous des petites perturbations. Il existe d'autres particularités qui caractérisent les systèmes à l'équilibre : leur évolution est conservative et invariante par inversion temporelle ; leur état macroscopique est indépendant des détails de l'évolution de leurs composantes et l'ensemble thermodynamique qui les décrit est ergodique par rapport à leur dynamique microscopique. Cependant, les états d'équilibre sont, en quelque sorte, une idéalisation. En effet, dans notre expérience quotidienne, nous traitons principalement des processus irréversibles et non conservatifs, qui caractérisent les systèmes hors d'équilibre, dont l'évolution macroscopique dépend fortement des détails de la dynamique microscopique.

Il existe deux grandes catégories de problèmes qui peuvent être considérés. La première traite de la relaxation à l'équilibre d'un système qui a subi une perturbation. À titre d'exemple, on peut considérer un système qui a été partiellement chauffé par une source externe : la chaleur circule naturellement de la partie la plus chaude à la partie la plus froide jusqu'à ce que tout le système atteigne une température uniforme. Cela se produit sauf si le processus de réchauffement a

profondément modifié certaines des caractéristiques physiques ou chimiques du système, l'éloignant trop de son état initial d'équilibre. La deuxième catégorie de problèmes concerne les systèmes constamment soumis à un forçage mécanique ou thermique externe, qui les maintient hors équilibre. C'est la catégorie de systèmes que je considère dans ce travail de thèse. Sous certaines conditions, la dynamique de ces systèmes peut évoluer vers un état stationnaire hors-équilibre décrit par une mesure de probabilité invariante et caractérisé par des courants constants de quantités conservées. En effet, deux des principaux problèmes théoriques dans l'étude des systèmes hors-équilibre consistent à établir l'existence et l'unicité de l'état stationnaire hors-équilibre et à estimer le taux de convergence vers cet état.

L'état stationnaire hors-équilibre d'un système composé de nombreuses particules en interaction présente des comportements inattendus et parfois imprévisibles, qui le rendent remarquablement différent des immuables états d'équilibre. De plus, ses propriétés thermodynamiques sont encore mal comprises, surtout dans des conditions qui gardent le système très loin de l'équilibre. Le cadre classique d'étude de l'état stationnaire hors-équilibre est celui d'un système en contact avec deux thermostats à températures différentes et idéalement infinis, et isolé partout ailleurs : un courant thermique circule dans le système, du thermostat le plus chaud au thermostat le plus froid et l'état stationnaire est atteint lorsque la chaleur fournie au système par le thermostat dont la température est la plus élevée est égal à la chaleur absorbée par le thermostat dont la température est la moins élevée. Dans ce cas, le flux de chaleur devient stable et le profil de température à l'intérieur du système devient constant dans le temps. Un autre cadre est celui d'un système soumis à des forces mécaniques non conservatives, effectuant un travail qui injecte de l'énergie dans le système et augmente l'énergie cinétique de chaque particule. Il est évident qu'aucun état stationnaire ne peut être atteint dans ce cas sans un certain mécanisme de dissipation, qui permet un flux sortant d'énergie sous forme de chaleur absorbée par l'environnement ; sans ce mécanisme, l'énergie interne augmenterait indéfiniment. L'état stationnaire est atteint lorsque l'énergie thermique dissipée est égale au travail effectué par la force non conservative qui agit sur le système, ce qui comporte la stationnarité des flux thermiques et des profils de température.

Dans le contexte du transfert de chaleur spontané d'une région chaude à une région froide dans un solide, une loi empirique macroscopique définissant la conduction thermique a été proposée par Joseph Fourier en 1808. La loi de Fourier établit que le courant thermique est proportionnel au gradient de température, la constante de proportionnalité étant la conductivité thermique, une propriété physique intrinsèque du système qui dépend des paramètres d'équilibre tels que la température et la densité. Au cours des dernières décennies, de nombreux efforts ont été déployés dans la compréhension et la validation microscopique de la loi de Fourier, à la fois dans un contexte de relaxation à l'équilibre et dans le cadre dynamique (voir *e.g.* Bonetto et al. (2000), Lepri et al. (2003), Dhar (2008)). Cependant, ceci reste un problème ouvert et difficile. Alors que dans les matériaux tridimensionnels, la conductivité thermique a été entièrement caractérisée et mesurée, dans certains systèmes de faible dimension conservant le

moment, elle dépend de la taille du système et elle diverge dans la limite thermodynamique. Ce comportement anormal n'est pas seulement déroutant du point de vue théorique : il a également des implications pertinentes en science des matériaux, en ingénierie et dans les applications pratiques (nanotubes de carbone, graphène, nanofils, etc.).

Cette thèse se compose de deux parties, qui sont précédées d'un chapitre d'introduction. La première partie, composée des Chapitres 2 et 3, contient les résultats de l'étude théorique sur le modèle à un rotateur et la deuxième partie, composée des Chapitres 4 et 5, contient les résultats de l'étude numérique des modèles de chaînes d'atomes.

Chapitre 1 : Introduction

Ce premier chapitre contient le cadre théorique du travail, cadre que j'ai voulu présenter de façon synthétique et en même temps la plus complète possible.

Je rappelle brièvement, dans la section 1.1, quelques concepts classiques en mécanique statistique comme ceux d'ensemble thermodynamique et d'observable et les principales caractéristiques de la description microscopique hamiltonienne du système. J'introduis de façon générale les processus de diffusion de Markov et les semigroupes qui y sont associés, je décris leurs lois d'évolution et je rappelle brièvement leurs propriétés. J'introduis ensuite la mesure invariante, j'énonce les conditions de son existence et de son unicité et je donne la caractérisation des mesures invariantes hors-équilibre. En effet, dans le cas hors-équilibre, la mesure invariante dépend de façon non banale des détails de la dynamique microscopique du système, laquelle est irréversible, contrairement au cas à l'équilibre.

Dans la section 1.2, je m'intéresse à l'analyse du comportement de long terme de la dynamique et en particulier de sa convergence vers l'état stationnaire. Je considère séparément le cas hypoelliptique et le cas elliptique, en introduisant la dynamique de Langevin générale et la dynamique de Langevin suramortie (*overdamped*), respectivement hypoelliptique et elliptique. En particulier, je présente de façon succincte quelques méthodologies pour une analyse plus ou moins quantitative des taux de convergence, notamment les méthodologies qui s'appuient sur des inégalités fonctionnelles pour le cas elliptique et celles qui s'appuient sur des estimations hypocoércives pour le case hypoelliptique. Dans le cas elliptique, les inégalités fonctionnelles considérées sont celle de Poincaré et celle de Sobolev logarithmique. La première permet d'obtenir une convergence dans l'espace L^2 des fonctions à carré intégrable (éventuellement par rapport à une mesure de référence), tandis que la seconde permet d'obtenir une convergence dans un espace plus grand, l'espace $L^1 \log L^1$.

Dans la section 1.3, j'introduis l'approche typique aux problèmes hors-équilibre. Il est supposé que le système initialement à l'équilibre soit entraîné et maintenu hors-équilibre par un forçage externe. La perturbation engendre des courants stationnaires qui parcourent le système et restent constants dans le temps. Ces courants représentent la réponse du système à la perturbation et, d'un point

de vue physique, ils constituent l'expression de l'irréversibilité de la dynamique sous-jacente. Évidemment, le type de courant (par exemple thermique ou électrique) dépendra du système en examen et du type de perturbation considéré. La définition des coefficients de transport repose généralement sur l'analogie avec les équations d'évolution macroscopique. Par conséquent, dans le régime de réponse linéaire, c'est-à-dire dans le cas de petites perturbations de la dynamique de Langevin générale, l'amplitude de la réponse moyenne est proportionnelle à l'amplitude du forçage externe et la constante de proportionnalité est appelée le coefficient de transport. J'introduis les deux perturbations paradigmatiques de la dynamique d'équilibre que je considère par la suite : une mécanique et l'autre thermique. La perturbation mécanique est introduite par l'application au système d'une force aux bords qui ne peut pas être obtenue comme le gradient d'un potentiel. La perturbation thermique est en revanche obtenue en ajoutant aux bords des termes de fluctuation de températures différentes.

Le problème central du transport thermique, à savoir la validité de la loi de Fourier, est présenté de manière concise dans la section 1.4. Cette loi permet d'étudier aussi bien la relaxation à l'équilibre d'un système isolé que les propriétés de transport en régime stationnaire d'un système mis en contact avec deux réservoirs (supposés infinis) de températures différentes. Dans ce cas, il y a un flux d'énergie constant net du réservoir le plus chaud vers le réservoir le plus froid qui, à l'état stationnaire, a une divergence nulle. Il faut remarquer que l'énoncé même de la loi de Fourier implique de pouvoir définir une température locale, ce qui à son tour implique que l'hypothèse d'équilibre local soit satisfaite. Comme je l'ai mentionné plus haut, la loi de Fourier a été validée dans les solides tridimensionnels pour des gradients de température pas trop importants, alors qu'elle n'a pas été validée dans le cas unidimensionnel. Des études récentes (voir Spohn (2014)) suggèrent l'universalité de la valeur de l'exposant qui contrôle la divergence de la conductivité par rapport à la longueur du système.

L'approche par simulation à l'étude des propriétés des états hors-équilibre est introduite dans la section 1.5, où je présente le cadre général de l'étude numérique des dynamiques stochastiques et du calcul des propriétés de transport. Étant donné un observable, sa moyenne canonique est estimée numériquement par la discrétisation de sa moyenne temporelle calculée sur une réalisation d'une dynamique stochastique qui soit ergodique par rapport à la mesure cible. Nous pouvons mesurer la qualité de cette approximation grâce aux deux types d'erreurs engendrées par ce procédé : une erreur statistique et une erreur systématique. La première est due au fait que la réalisation de la dynamique stochastique sur laquelle nous calculons la moyenne temporelle a une durée finie. La deuxième est due à la discrétisation et implique que la mesure associée à la dynamique discrète soit différente de celle associée à la dynamique continue (cependant toutes les deux doivent être ergodiques, chacune par rapport à sa propre dynamique). L'erreur statistique domine l'erreur systématique et peut être réduite en augmentant la durée de la simulation. Je termine la section en introduisant les schémas numériques pour l'intégration de la dynamique de Langevin, avec leur propriétés.

Enfin, dans la section 1.6, je présente synthétiquement les contributions de ce

travail de thèse, dont les détails font le sujet des chapitres 2 à 5.

Première partie : Contributions théoriques

Nous considérons dans cette partie une dynamique de Langevin en dimension d dans un espace des positions compact. Physiquement, cette dynamique peut être considérée comme la dynamique d'un système à une seule particule dans un espace d-dimensionnel ou comme celle d'un ensemble de n particules dans un espace de dimension d' tel que $d = nd'$. Les particules sont soumises à une force constante τF, de direction F telle que $|F| = 1$. Le système est en équilibre thermique avec un thermostat de Langevin à une température fixée β^{-1} et, en l'absence de forçage thermique, il est maintenu hors équilibre par le terme de dérive non-gradient donné par la force. L'interaction avec le thermostat est modélisée par la dynamique stochastique habituelle, c'est-à-dire un terme de fluctuation aléatoire et un terme de friction d'intensité ξ, liés par un mécanisme de fluctuation-dissipation. Cette dynamique est donc une perturbation stochastique de la dynamique hamiltonienne. La partie hamiltonienne de la dynamique est régie par un potentiel d'interaction $U(q)$ lisse et périodique. Il en résulte une dynamique dégénérée dont le générateur est hypoelliptique.

En l'absence de forçage externe ($\tau = 0$), le système a une mesure stationnaire d'équilibre, qui est donnée par la mesure canonique, c'est-à-dire une mesure de Gibbs relative à l'Hamiltonien du système et correspondante à la température β^{-1}. La dynamique d'équilibre est bien comprise, alors que les propriétés du système hors-équilibre ont été moins explorées. Quand $\tau \neq 0$, il peut être démontré par les techniques décrites dans les sections 1.1.5.1 et 1.2.3 qu'il existe une unique mesure stationnaire hors-équilibre, dont la forme explicite reste cependant inconnue, et que la dynamique y converge exponentiellement vite.

Chapitre 2 : Perturbations de la dynamique de Langevin

Avec S. Olla et G. Stoltz (Iacobucci et al. (2017)), nous étudions la convergence exponentielle à l'état stationnaire de la dynamique de Langevin hors-équilibre que je viens de décrire, à travers l'analyse du comportement à long terme de la solution d'équation de Fokker-Planck stationnaire associée. Notre but est d'obtenir une expression du taux de convergence qui puisse montrer une dépendance des paramètres physiques (en particulier du paramètre de friction) plus explicite que celle obtenue par les techniques de Lyapunov (voir Section 1.2.3). Les résultats de ce travail et quelques éléments complémentaires font l'objet du chapitre 2.

La dynamique de Langevin est un modèle couramment utilisé pour décrire l'évolution des systèmes à température constante, c'est-à-dire en contact avec un thermostat à l'équilibre à une température donnée. Il peut être utilisé pour échantillonner des configurations d'un système physique à l'équilibre, selon l'ensemble canonique, ce qui permet d'estimer numériquement les propriétés macroscopiques moyennes ; voir par exemple Leimkuhler and Matthews (2015) pour

une introduction à la dynamique moléculaire du point de vue des mathématiques. La dynamique de Langevin est maintenant bien comprise, tant pour ses propriétés théoriques que pour sa discrétisation (voir par exemple l'article de revue de Lelièvre and Stoltz (2016)). D'autre part, les propriétés de la dynamique de Langevin hors-équilibre, telle que celle obtenue par l'addition d'un terme de dérive non gradient, ont été moins étudiées. La dynamique est paramétrée par plusieurs constantes : la masse $m > 0$ des particules (pour simplifier, nous considérons une masse unique m, bien que nos résultats puissent être étendus pour tenir compte de matrices de masse plus générales), la température inverse $\beta > 0$, la friction $\xi > 0$ et la magnitude de la force externe $\tau \in \mathbb{R}$, avec une direction constante donnée. Soulignons que le forçage externe est en effet non gradient puisqu'il est induit par une force qui n'est pas le gradient d'une fonction périodique lisse. Mentionnons aussi que notre analyse pourrait être étendue à des forçages non gradients plus généraux $F(q)$ dépendant de la variable de position, tant que la fonction F est suffisamment lisse.

Nous suivons une approche perturbative basée sur des techniques hypocoércives développées pour la dynamique de Langevin à l 'équilibre. Deux régimes limites intéressants peuvent être considérés : (i) la limite $\xi \to 0$, qui correspond à la limite hamiltonienne ; (ii) la limite $m \to 0$ ou $\xi \to +\infty$ (avec, dans ce dernier cas, un rééchelonnement temporel d'un facteur ξ), ce qui correspond à une limite suramortie. Nous étudions ces deux limites en détail. En particulier, la grandeur maximale des perturbations admissibles est quantifiée en fonction du paramètre de friction. Les résultats numériques, basés sur une discrétisation de Galerkin du générateur de la dynamique, confirment les bornes inférieures théoriques sur le trou spectral.

Nous discutons d'abord de l'état stationnaire en rappelant quelques résultats antérieurs (Mattingly and Stuart (2002), Rey-Bellet (2006*a*)), relatifs en particulier à l'existence et l'unicité de la mesure stationnaire (section 2.2.1) et au fait que la mesure hors-équilibre et bien définie en tant que produit de la mesure d'équilibre de Gibbs μ et d'une densité de probabilité lisse h_τ qui est fonction de l'intensité τ de la perturbation. L'expression analytique explicite est inconnue. Les les résultats à la Rey-Bellet (2006*a*), présentés dans la section 1.2.3, assurent bien la convergence de la loi du processus à la mesure stationnaire, mais il est difficile de quantifier cette convergence en terme des paramètres de la dynamique, tels que la friction et l'amplitude du potentiel, ou de l'intensité du forçage externe.

Nous obtenons, dans la section 2.2.2, quelques propriétés qualitatives simples de l'état stationnaire par des calculs formels (c'est-à-dire des calculs qui peuvent être faits sans connaître l'expression explicite de la mesure stationnaire), comme l'expression de la vitesse moyenne, la relation de conservation de l'énergie, la positivité de la production d'entropie et la validité de la relation d'Einstein.

Nous donnons ensuite la forme explicite du développement de h_τ en série de puissances de τ (section 2.2.3) et montrons que la borne supérieure de τ pour que l'expansion converge est de l'ordre de $\min(1, \xi)$. Ceci est compatible avec l'intuition physique : lorsque le terme de fluctuation-dissipation est faible, les forçages externes qui peuvent être supportés par le système sont au mieux du même ordre

de grandeur que le mécanisme de dissipation ; tandis que pour des grandes valeurs du terme de fluctuation-dissipation, les forçages externes du même ordre de grandeur que ∇U peuvent être supportés par le système. Pour des forçages extrêmement grands, nous nous attendons à ce que la mesure invariante soit très différente de la mesure d'équilibre et que donc l'approche perturbative échoue en tant que tel.

Les résultats théoriques de ce travail sont contenus dans la section 2.3 et concernent la convergence exponentielle de la loi du processus vers la solution stationnaire de l'équation de Fokker-Planck associée, c'est-à-dire vers l'état stationnaire. Ils sont obtenus par deux techniques hypocoércives et présentés dans trois théorèmes principaux. Comme je l'ai spécifié, nous analysons les deux régimes limites, Hamiltonien et suramorti, correspondant respectivement aux valeurs du paramètre de friction ξ allant à zéro ou à l'infini. Ces deux techniques hypocoércives, développées, je le rappelle, pour la dynamique de Langevin à l'équilibre, sont basées sur des estimations en $L^2(\mu)$, où μ est la mesure d'équilibre de Gibbs. Elles sont plus quantitatives que la technique qui repose sur les fonctions de Lyapunov qui a été introduite dans la section 1.2.3. Dans les deux cas, nous trouvons une estimation du trou spectral λ_τ de l'ordre de $\min(\xi, \xi^{-1})$, ce qui est cohérent avec ce qui est reporté dans d'autres travaux (voir Hairer and Pavliotis (2008), Leimkuhler et al. (2015), Lelièvre and Stoltz (2016)).

Dans la première approche, nous appliquons la technique d'hypocoércivité standard à la Villani (2009), que je présente dans la section 1.2.2.1. Nous choisissons la forme dégénérée de la norme H^1 modifiée proposée par Villani (2009), car elle permet de calculer des bornes sur le trou spectral du générateur qui sont plus explicites par rapport à celle obtenues avec la norme non dégénérée. Aussi, le choix de cette norme dégénérée permet d'obtenir un résultat de convergence sans préfacteur, ce qui n'est pas le cas pour d'autres résultats de convergence en $H^1(\mu)$ avec préfacteur, dans lesquels ce dernier dépend de ξ et peut donc devenir grand dans les limites $\xi \to 0$ ou $\xi \to +\infty$.

Le résultat de convergence obtenu dans $H^1(\mu)$ est «transféré» dans $L^2(\mu)$ par régularisation hypoelliptique, en suivant la procédure décrite dans Hairer and Pavliotis (2008) et basée sur un résultat présenté dans Hérau (2007). L'approche $H^1(\mu)$ modifiée permet de traiter des forçages hors-équilibre de l'ordre de $\tau = \mathcal{O}\Big(\min(\xi, \xi^{-1})\Big)$. Dans le cas de grands forçages, ce résultat n'est donc pas optimal, car il n'est pas cohérent avec la borne supérieure $\min(1, \xi)$ de l'expansion en série de la mesure stationnaire.

Dans la seconde approche, nous appliquons la technique d'estimation directe en $L^2(\mu)$ proposée par Dolbeault et al. (2009, 2015) et introduite dans la section 1.2.2.3. Cette approche facilite l'expression quantitative du taux de convergence et permet un choix plus large de la densité initiale. Elle permet aussi d'obtenir des expressions très explicites du préfacteur et du taux de convergence en terme des paramètres physiques. Plus précisément, elle donne une borne supérieure sur τ de l'ordre de $\min(1, \xi)$, en accord avec la borne supérieure du développement en série de la mesure invariante.

Une troisième technique d'analyse de la convergence à l'état stationnaire est considérée : celle utilisant l'approche d'hypocoércivité entropique décrite dans la section 1.2.2.2. L'un des principaux intérêts des estimations entropiques est qu'elles permettent de prendre en compte des densités initiales plus générales et, plus important encore, qu'elles ont généralement un meilleur comportement d'échelle par rapport à la dimension. Les estimations d'entropie hypocoércives sont déjà présentes dans Villani (2009), mais sont rendues plus explicites dans Olla and Letizia (2017). Par le biais de cette technique, il est possible de préciser la dépendance des préfacteurs et des taux de convergence du paramètre de friction, voir l'Annexe 2.6.3.

Cependant, alors que dans le cas à l'équilibre ($\tau = 0$) il est possible de démontrer la convergence et d'en estimer le taux, l'estimation par hypocoércivité entropique ne peut pas fournir un résultat de convergence explicite dans le cas hors-équilibre, car une inégalité log-Sobolev pour la mesure stationnaire $h_\tau \, \mathrm{d}\mu$ est nécessaire afin d'estimer explicitement la borne inférieure du taux exponentiel. Or, puisque l'expression analytique de h_τ reste inconnue, cette estimation explicite semble être impossible. En effet, à notre connaissance, aucun résultat de convergence au sens entropique n'a été obtenu jusqu'à présent, même pas dans un cadre perturbatif.

Malgré cela, nous arrivons à prouver par un calcul formel que la dérivée temporelle de l'entropie relative de la loi de la diffusion par rapport à la densité stationnaire a une expression miraculeusement simple en fonction de l'information de Fisher dégénérée. Ceci est le résultat de simplifications algébriques qui cachent vraisemblablement une structure intéressante, laquelle mériterait d'ultérieures investigations.

Dans le cas d'un seul rotateur en une dimension, nous confirmons numériquement les résultats théoriques obtenus, en estimant le trou spectral du générateur de la dynamique par le biais d'une discrétisation de Galerkin. Cette estimation est faite pour différentes valeurs des paramètres τ et ξ et de l'intensité du potentiel. Pour ce faire, nous utilisons une base orthonormale de fonctions de Fourier à poids pour les positions et une décomposition en polynômes d'Hermite dans les moments. Le générateur de la dynamique est exprimé dans cette base par une matrice dont les éléments sont facilement calculables grâce aux propriétés des polynômes d'Hermite et des modes de Fourier. Le trou spectral du générateur est ainsi approximé par le trou spectral de cette matrice.

Afin de valider notre procédé, nous vérifions la cohérence du trou spectral calculé par la méthode de Galerkin avec sa valeur analytique dans le cas d'équilibre à potentiel nul, calculée dans la section 2.6.1 d'après le résultat de Kozlov (1989). Nous trouvons un accord parfait entre le résultat analytique et l'estimation numérique. Dans le cas hors-équilibre, nous étudions le trou spectral en fonction du paramètre de friction ξ pour différentes valeurs du forçage τ et de l'amplitude du potentiel U_0, à température et masse unitaires fixées. Nous trouvons que l'effet de la perturbation n'est pas détectable pour des petites valeurs de U_0 ni pour des grandes. Ceci est lié au fait que le trou spectral est indépendant de τ quand $U_0 = 0$ (voir Section 3.2), une caractéristique qui persiste approximative-

ment pour des valeurs petites mais non nulles de U_0. Pour des grandes valeurs de U_0, la perturbation est dominée par la partie gradient de la force ; elle a donc moins d'impact sur le trou spectral.

L'effet de la perturbation est cependant visible pour des valeurs intermédiaires de U_0. En augmentant τ, nous avons pu calculer le trou spectral uniquement pour les valeurs du paramètre de friction au-dessus d'un certain seuil, approximativement $\xi \geqslant |\tau|$. Les forçages doivent cependant être suffisamment forts pour que la perturbation ait un impact non négligeable sur le comportement du trou spectral en fonction de ξ. Enfin, on observe que le trou spectral décroît comme $\sim 1/\xi$ pour des grandes valeurs de ξ et ceci quelle que soit la valeur de τ considérée. Les résultats des simulations confirment donc notre estimation théorique des bornes inférieures du trou spectral.

Chapitre 3 : Dynamique de Langevin hors-équilibre avec un potentiel faible

Dans ce chapitre, je considère la version unidimensionnelle du modèle de rotateur étudié dans le chapitre 2, composé d'un seul rotateur en équilibre avec un thermostat à une température donnée et soumis à un moment de torsion constant.

Je commence par calculer formellement, dans la section 3.1, l'expression explicite du noyau de transition du processus de Markov. Pour ce faire, je pars de la solution explicite de la dynamique stochastique dégénérée sur un domaine non-borné. Pour cette dynamique, le moment est un processus d'Ornstein-Uhlenbeck standard (puisque le terme de force constante n'est rien d'autre qu'un terme de décalage de la vitesse) et le bruit est transféré sur la position via l'équation hamiltonienne. Il en résulte que la position et la vitesse du système sont deux variables gaussiennes corrélées, dont on connaît explicitement la matrice de variance-covariance et, par conséquent, la probabilité jointe. Grace à une procédure de «wrapping», qui consiste à calculer la transformée de Fourier de la probabilité jointe dans la variable position et puis calculer la transformée de Fourier inverse discrète sur des valeurs entières de la fréquence, j'obtiens l'expression du noyaux de la probabilité de transition recherchée.

J'utilise cette probabilité de transition dans la section 3.2 pour l'estimation du trou spectral du générateur du processus à l'équilibre. Comme dans le cas de la validation de l'application de la méthode de Galerkin présentée dans la section 2.4.2.1, le résultat est comparé avec celui calculé analytiquement dans Kozlov (1989) et présenté dans la section 2.6.1.

Dans la section 3.3, je considère le système à l'équilibre perturbé par un potentiel faible U. En exprimant la mesure stationnaire hors-équilibre comme un développement en puissances de $\|U\|_{L^\infty}$, par un simple argument perturbatif j'arrive à estimer une borne supérieure explicite en $L^2(\mu)$ pour le rayon de convergence de la série. On remarque que cette borne supérieure ne dépend pas de l'intensité τ de la force constante.

Les résultats du travail avec G. Gallavotti et S. Olla (Gallavotti et al. (2013)) sont présentés dans la section 3.4. Ce travail donne un exemple de l'effort technique qui peut être nécessaire pour les constructions réelles d'états stationnaires dans le cas apparemment simple mais étonnamment non banal d'un pendule forcé en présence de bruit.

Nous étudions le comportement du système composé d'un unique rotateur pour de petites valeurs de l'énergie potentielle U, que l'on contrôle par le paramètre g. Notre but est d'obtenir une expression explicite pour la mesure stationnaire, en cherchant à exprimer explicitement les coefficients du développement en puissances de g. Pour ce faire, nous supposons d'abord que la solution $F(q,p;g)$ de l'équation de Fokker-Planck stationnaire relative à l'adjoint en $L^2(\mathrm{d}q,\mathrm{d}p)$ du générateur du processus puisse être exprimée comme le produit d'une loi gaussienne de moyenne nulle et variance égale à l'inverse de la température pour le moment mécanique, et d'une densité $f(q,p;g)$ lisse. Ensuite, nous supposons que cette densité $f(q,p;g)$ admette une expansion en polynômes d'Hermite avec des coefficients $\rho_n(q,g)$ dépendants de la position et du paramètre g. Enfin, nous supposons que ces coefficients soient des fonctions de classe C^∞ en q et g, et que les dérivées en q, p et g de la solution F puissent être obtenues en différenciant terme à terme le développement de F, de sorte que nous obtenons des séries convergentes.

Sous ces hypothèses, nous obtenons notre résultat principal : un développement formel en puissances de g de la densité F avec des coefficients ρ_n tels que leurs transformées de Fourier puissent être déterminées par un algorithme constructif (voir section 3.4.4) et qui s'annulent pour des fréquences $|k| > R$. En outre, nous estimons des bornes supérieures pour ces transformées de Fourier, en fonction des paramètres physiques du problème.

Deuxième partie : Simulations numériques

Dans cette deuxième partie, j'analyse les propriétés de l'état stationnaire et les propriétés de transport de deux systèmes unidimensionnels de N atomes interagissants par un potentiel lisse, dont les extrémités sont mises en contact avec deux thermostats à températures différentes. Le premier modèle est une chaîne de rotateurs qui, en plus du forçage thermique, est soumise à un forçage mécanique en forme d'un moment de rotation constant appliqué au dernier rotateur sur la droite. Le deuxième modèle est une chaîne d'oscillateurs qui interagissent par le potentiel de Toda et qui sont soumis à une perturbation stochastique qui conserve l'énergie et le moment totaux.

Chapitre 4 : Rotateurs

Ce chapitre contient les résultats de l'étude numérique de la chaîne de rotateurs soumise à un forçage thermique avec une différence de température aux bords égale à $\Delta T = T_\mathrm{L} - T_\mathrm{R}$ et à un forçage mécanique d'intensité constante F (Iacobucci

et al. (2011)).

Les propriétés thermodynamiques des états stationnaires hors équilibre sont très peu comprises. Ces états sont généralement caractérisés par des courants de quantités conservées (telles que l'énergie), qui circulent dans le système. Lorsque les états stationnaires sont proches des états d'équilibre, c'est-à-dire quand les perturbations sont de faible intensité, la théorie de la réponse linéaire est efficace et explique les phénomènes macroscopiques communs tels que la loi de Fourier. Ainsi, dans un système en contact avec deux thermostats à températures différentes, si la différence entre les deux températures est faible, le flux de chaleur est proportionnel au gradient thermique. D'autre part, il n'y a pas de théorie générale pour décrire les systèmes dans un état stationnaire loin de l'équilibre, et les propriétés macroscopiques correspondantes semblent dépendre des détails spécifiques de la dynamique.

Dans le problème que nous sommes en train de considérer, si $F = 0$ et $T_L = T_R = T$, le système est à l'équilibre, et la mesure stationnaire unique est donnée par la mesure de Gibbs à la température T, associée à la Hamiltonienne du système. Quand $F = 0$ et $T_L \neq T_R$, le système n'est plus à l'équilibre et les propriétés de son état stationnaire ont été étudiées numériquement par différents auteurs, voir par exemple Giardiná et al. (2000), Gendelman and Savin (2000), Yang and Hu (2005), Gendelman and Savin (2005). La conductivité thermique, définie comme le courant stationnaire d'énergie multiplié par la taille du système et divisé par la différence de température (Bonetto et al. (2000)), a une limite finie pour des tailles du système de plus en plus grandes, et ce même si la chaîne de rotateurs est un système unidimensionnel qui conserve le moment total (Basile et al. (2006, 2009)). En outre, il est montré par Giardiná et al. (2000), que la conductivité thermique diminue considérablement lorsque la température moyenne T augmente au-dessus de la valeur 0.5 .

Si $F \neq 0$, le système est hors équilibre quelles que soient les valeurs des températures des thermostats, même si $T_L = T_R$. Ceci à cause du fait que F est une force non-gradient. À l'état stationnaire, la force induit un courant d'énergie vers la gauche. L'état stationnaire ne peut pas être calculé explicitement et, comme on l'a dit, si la valeur de F est grande, la théorie de la réponse linéaire ne peut pas être utilisée pour obtenir des informations sur la conductivité du système.

Dans le cas $T_L < T_R$, il y a deux mécanismes séparés qui génèrent un courant d'énergie vers la gauche du système : la force mécanique F et la force thermique donnée par le gradient de température. Il semble cependant difficile de séparer les contributions de chaque mécanisme. Les expériences numériques rapportées au chapitre 4 montrent que ces deux mécanismes ne sont pas nécessairement additifs et que l'effet combiné de ces deux forces généralisées peut réduire le courant au lieu de l'augmenter. Cet effet est observé pour des grandes valeurs du forçage mécanique F, quand la température T_R du thermostat de droite est augmentée alors que celle du thermostat de gauche T_L reste fixe. Puisque le forçage mécanique induit toujours un courant de la droite vers la gauche (négatif dans notre référentiel), lorsque la température de droite T_R est augmentée alors que T_L reste fixe on s'attendrait logiquement à ce que le forçage thermique négatif soit

plus important, et donc que le courant total soit plus grand en valeur absolue. Contrairement à ce à quoi on s'attend dans ce cas, nous observons que le courant est réduit. En revanche, cet effet n'apparaît pas si la température de gauche T_L est baissée et celle de droite T_R est maintenue fixe. En effet, dans ce cas, le courant devient plus grand en valeur absolue.

Il nous semble évident que de tels comportements montrent la complexité des états stationnaires dans les cas très loin de l'équilibre, et suggèrent également que la loi de Fourier n'est valide que près de l'équilibre. Par conséquent, une extension naïve de la définition de conductivité thermique à des contextes qui sont fortement hors équilibre, peut donner suite à des valeurs négatives pour cette quantité (d'où le titre provocateur de l'article Iacobucci et al. (2011)).

Dans la section 4.2, nous donnons la description du système et de sa dynamique et introduisons le schéma numérique utilisé dans les simulations. Le système évolue suivant les lois de la dynamique hamiltonienne, perturbée aux bords par des processus d'Ornstein-Uhlenbeck. Nous considérons des conditions aux bords fixes à gauche et libres à droite, tout en vérifiant la robustesse de nos résultats par rapport à ce choix. Aussi, nous ne considérons pas l'impact du paramètre de couplage avec le thermostat, qui reste fixé à 1 dans toutes les simulations. L'intégration numérique de la dynamique est effectuée en utilisant une stratégie de «splitting» selon laquelle la partie hamiltonienne de l'évolution est intégrée par le schéma de Verlet (1967). Les parties de fluctuation-dissipation, avec l'inclusion de la force non-gradient, sont des processus d'Ornstein-Uhlenbeck et peuvent donc être intégrées analytiquement. Le choix du pas de temps a été effectué de façon à assurer la conservation de l'énergie : même s'il peut y avoir un biais, qualitativement les conclusions de notre étude sont robustes en ce qui concerne ce choix.

Les propriétés du système hors-équilibre sont considérées dans la section 4.3. Nous discutons d'abord de l'existence d'une mesure stationnaire pour la dynamique. Nous sommes convaincus qu'il existe une mesure stationnaire lisse unique, cependant, à notre connaissance, il n'y a pas de résultat rigoureux en cette direction pour les chaînes de rotateurs, même dans le cas $F = 0$. En effet, les techniques standard (voir par exemple Rey-Bellet (2006*b*), Carmona (2007)) utilisées pour prouver l'existence et l'unicité d'une mesure invariante pour les chaînes d'oscillateurs sous forçage thermique ne s'appliquent pas au cas en examen.

Une pathologie possible pour les chaînes de rotateurs, qui pourrait empêcher l'atteinte de l'état stationnaire, est que l'énergie interne se concentre localement sur un ou plusieurs rotateurs, lesquels tournent de plus en plus vite. Puisque les forces d'interaction sont limitées, il pourrait ne pas être possible d'empêcher cette rotation rapide en dissipant suffisamment vite l'énergie en excès de certains rotateurs, laquelle pourrait augmenter indéfiniment. En pratique, nous n'avons pas observé de telles catastrophes dans le régime de paramètres que nous avons considérés, mais les profils de température cinétique présentés dans le panneau en haut à gauche de la figure 4.1 sont assez inattendus et montrent que l'énergie interne tend à être plus grande au milieu de la chaîne[1]. Les résultats présentés

[1] Ce résultat peut être relié au comportement de la solution du problème diffusif correspon-

dans cette figure permettent également de comprendre ce qui se passe lorsque les températures imposées aux extrémités droite et gauche changent : la température maximale dans la chaîne est presque inchangée, mais la position du maximum est déplacée. Cela montre que la correction de réponse linéaire à la mesure stationnaire est nécessairement non locale. De tels effets non locaux ont déjà été observés dans le processus d'exclusion hors-équilibre par Derrida et al. (2002*a*,*b*). La figure en question montre aussi que le profil des moments moyens (panneau en bas à gauche) est fortement non linéaire, et que sa dérivée est maximale là où la température est maximale. Nous observons également que le profil semble devenir plus raide dans la limite thermodynamique.

Sous l'hypothèse que la mesure stationnaire existe, des relations intéressantes et compatibles avec l'intuition physique peuvent néanmoins être obtenues, comme nous le montrons dans la section 4.3.1.

Malgré les caractéristiques non locales que nous venons de souligner, nous montrons dans la section 4.3.2 que localement l'équilibre est atteint. La question de l'équilibre local a été traitée par Mai et al. (2007) dans le cas de systèmes soumis à des forçages thermiques. Dans notre étude, nous vérifions en trois étapes l'hypothèse d'équilibre local en présence du seul forçage mécanique. La première étape consiste à étudier l'accord entre la température cinétique locale et la température potentielle locale. La première est définie comme la variance des vitesses et la dernière est la valeur pour laquelle la moyenne canonique de l'énergie potentielle est à peu près égale à sa moyenne temporelle, estimée numériquement le long de la trajectoire solution des équations de la dynamique (voir section 4.3.2). Le résultat (voir figure 4.2 en haut à gauche) montre que les deux températures locales sont assez différentes pour des petits systèmes, mais deviennent pratiquement identiques pour des systèmes plus grands. En outre, au fur et à mesure que la longueur du système augmente, les deux profils deviennent plus symétriques.

Dans la deuxième étape, nous vérifions que les distributions individuelles des moments et des positions sont en accord avec un équilibre de Gibbs local. À cette fin, nous traçons les histogrammes des moments et des distances relatifs au site $i_{\max}$ où la température locale est maximale, puisque c'est l'endroit dans lequel le désaccord entre les températures locales cinétique et potentielle est le plus fort. Les résultats présentés dans la figure 4.2 (panneaux du bas) montrent que les distributions empiriques des moments et des positions sur le site choisi sont en excellent accord avec les distributions de Gibbs correspondant au même ensemble de paramètres (moment moyen $\overline{p}_i$, température locale $T_{i_{\max}}$), sauf pour les plus petits systèmes.

Enfin, dans la troisième étape, nous vérifions que les moments et les distances sont indépendants. À cette fin, nous comparons leur loi jointe avec la loi produit obtenue à partir du produit tensoriel des distributions individuelles des deux variables, en définissant un paramètre de distance entre les deux distributions, qui dépend de la longueur de la chaîne considérée. Le résultat de nos simulations montre que cette distance décroît de façon inversement proportionnelle à la racine carrée de la longueur de la chaîne. Ce résultat semble montrer que même des

dant, voir Komorowski et al. (2016).

systèmes fortement perturbés peuvent être localement très proches de l'équilibre.

Le comportement du courant d'énergie stationnaire en fonction de F, T_L et T_R est discuté dans la section 4.3.3. Nous considérons les situations suivantes : (i) mêmes températures sur la gauche et sur la droite ; (ii) extrémité gauche chaude et extrémité droite froide ; (iii) extrémité gauche froide et extrémité droite chaude. Les courants sont calculés en fonction de l'intensité F du terme de forçage non gradient pour les systèmes de différentes longueurs. Puisque l'hypothèse d'équilibre local est vérifiée à l'ordre dominant, le courant d'énergie est induit par les corrections du premier ordre en l'inverse de la longueur de la chaîne. En comparant les courants lorsque la température à l'extrémité droite est fixée, nous observons que (voir figure 4.3, panneaux du haut) le courant négatif induit par le forçage mécanique est réduit par le courant thermique positif, comme attendu. Nous comparons ensuite les courants à différence de température fixée $T_R - T_L$, pour différentes températures moyennes (voir figure 4.3, panneaux du bas). Dans ce cas, on observe que, pour de forts forçages mécaniques, le courant augmente lorsque la température moyenne diminue, tandis que le contraire se produit lorsque le forçage mécanique est petit.

Nous passons enfin à la situation la plus intéressante. La température à l'extrémité gauche est fixé et la température à l'extrémité droite varie (voir figure 4.4). Dans ce cas, des résultats contre-intuitifs sont observés pour de grands forçages mécaniques : le courant total augmente lorsque T_R diminue, même si, dans une telle situation, le gradient thermique est dans la direction opposée. Le forçage mécanique induit un courant négatif, tandis que le gradient thermique induit un courant positif, en l'absence de forçage mécanique. L'effet combiné des forçages mécaniques et thermiques induit un courant négatif plus grand (en valeur absolue) que celui en l'absence de tout gradient thermique.

Comme nous observons dans la section 4.4, nous sommes incapables de fournir une explication précise et convaincante aux phénomènes ci-décrits. Une interprétation possible est basée sur le fait que, comme nous le verrons plus tard, la conductivité thermique de ce système est une fonction décroissante de la température lorsque F est grand. Il est donc possible qu'en baissant la température T_R du thermostat de droite, et donc en augmentant la conductivité à l'extrémité droite, on rende le système plus sensible au forçage mécanique, lui aussi appliqué à droite. L'augmentation du courant mécanique peut donc contrebalancer celle du courant thermique qui passe en direction opposée. C'est le phénomène de l'«ami bordélique» (cit. Stefano Olla), celui qui se propose pour aider à ranger et qui, tout en étant plein de bonne volonté, met un tel bazar qu'il rend le processus de rangement plus lent que ce qu'il l'aurait été s'il n'avait pas «aidé».

Chapitre 5 : La chaîne de Toda

Ce chapitre contient les résultats présentés dans Iacobucci et al. (2010). Nous étudions la conductivité thermique d'une chaîne d'oscillateurs interagissants par un potentiel de Toda, perturbée par une dynamique stochastique préservant l'énergie et le moment. L'intensité du bruit stochastique est contrôlée par un paramètre

γ. Nous montrons que le transport de chaleur est anormal et que la conductivité thermique diverge avec la longueur n de la chaîne comme $\kappa(n) \sim n^{\alpha}$, avec $0 < \alpha \leqslant 1/2$. En particulier, la conduction balistique de la chaleur, qu'on observe dans la chaîne Toda non perturbée, est détruite et l'exposant α de la divergence dépend de γ.

Dans la section 5.1 nous définissons la conductivité thermique, qui fera l'objet principale de notre étude, et rappelons les résultats de la littérature. Pour un système unidimensionnel de longueur L, la conductivité thermique peut être définie par le flux stationnaire d'énergie induit en connectant le système à deux thermostats à différentes températures T_l et T_r. Ce flux d'énergie J_L est proportionnel au rapport entre la différence de température $\Delta T = T_l - T_r$ et la longueur de la chaîne, et nous définissons la conductivité thermique κ_L comme la constante de proportionnalité. Si la limite $\lim_{L\to\infty}\lim_{\Delta T\to 0} \kappa_L = \kappa$ existe et est finie, alors la conductivité est normale et le système est censé satisfaire la loi de Fourier (voir Bonetto et al. (2000)). La limite κ est la conductivité thermique, propriété intrinsèque du système.

Il est bien connu, par des expériences numériques et certaines considérations analytiques, que la conductivité thermique diverge dans le cas de systèmes unidimensionnels d'oscillateurs dont la dynamique conserve le moment total (Lepri et al. (2003, 1997)). Ceci est également compatible avec certains résultats expérimentaux sur la dépendance de la longueur de la conductance thermique des nanotubes de carbone (voir par exemple les travaux de Wang et al. (2007) et de Chang et al. (2008)). Dans le cas d'une chaîne d'oscillateurs harmoniques, J_L peut être calculé explicitement (Rieder et al. (1967)) et ne diminue pas lorsque la taille L du système augmente. Cela est dû au transport balistique de l'énergie portée par les phonons non-interagissants. Le même phénomène se produit pour les chaînes harmoniques optiques dont les atomes sont accrochés (*pinned*), dans lesquelles le moment total n'est pas conservé. Un transport balistique de l'énergie est attendu pour tous les systèmes dont la dynamique est complètement intégrable (Zotos (2002)), comme pour la chaîne Toda (Toda (1979), Hatano (1999)).

L'évidence numérique montre que la non-intégrabilité (quelle que soit la définition que l'on considère de ce concept) n'est pas une condition suffisante pour une conductivité normale, en particulier pour les chaînes anharmoniques d'oscillateurs non accrochés comme c'est le cas du modèle FPU étudié par Lepri et al. (1997). Une superdiffusion d'énergie est attendue dans les systèmes conservant le moment, dans lesquels la conductivité thermique diverge comme $\kappa_L \sim L^{\alpha}$, pour des valeurs de $\alpha \in (0,1)$. Il existe un large débat dans la littérature en physique sur l'existence ou la non-existence d'une (ou plusieurs) valeur universelle de α, comme le mentionnent Narayan and Ramaswamy (2002) et Lepri et al. (2003).

Des perturbations stochastiques de la dynamique ont été introduites pour comprendre ces phénomènes. Un modèle dans lequel des thermostats de Langevin sont attachés à chaque oscillateur dans une chaîne harmonique a été introduit par Bolsterli et al. (1970). Ce bruit détruit tous les types de lois de conservation, y compris celles de l'énergie, et la conductivité correspondante est finie (voir Bonetto et al. (2004) et Bonetto et al. (2009) pour le cas anharmonique). Aussi, des

perturbations stochastiques qui ne conservent que l'énergie du système donnent une conductivité thermique finie (Bernardin and Olla (2005)).

La situation change radicalement si la perturbation stochastique conserve à la fois l'énergie et le moment, comme l'ont montré Basile et al. (2006). De telles perturbations stochastiques conservatives modélisent l'effet chaotique des non linéarités. Ces systèmes peuvent alors être vus comme complètement non-intégrables, puisque les seules quantités conservées sont l'énergie et le moment. Dans ce cas, au moins pour les interactions harmoniques, la conductivité thermique peut être explicitement calculée par la formule Green-Kubo. Pour les modèles de chaînes non accrochées, elle reste finie seulement en dimension $d \geq 3$, alors qu'elle diverge quand $d = 1$ ou 2. Plus précisément $\kappa_L \sim \sqrt{L}$ quand $d = 1$, et $\kappa_L \sim \log L$ quand $d = 2$ (Basile et al. (2006, 2009)). Certaines considérations analytiques pour les mêmes systèmes harmoniques stochastiques dans un contexte hors équilibre donnent les mêmes résultats pour la conductivité thermique, voir Lepri et al. (2009). Pour les interactions anharmoniques, des bornes supérieures rigoureuses peuvent être établies, toujours par la formule de Green-Kubo. Dans le cas unidimensionnel cela conduit à $\kappa_L \leqslant C\sqrt{L}$ (Basile et al. (2009)).

Ces résultats rigoureux nous ont motivés à analyser l'effet des perturbations stochastiques sur un autre système complètement intégrable : la chaîne d'oscillateurs de Toda. La conductivité thermique des treillis de Toda a déjà été étudiée par Hatano (1999), qui a montré que le transport balistique d'énergie est détruit dans le cas d'un système diatomique. Différemment du cas harmonique, pour lequel de nombreux calculs peuvent être réalisés analytiquement, la dynamique non-linéaire considérée ici ne peut qu'être résolue par le biais de simulations numériques. Nous avons considéré une chaîne dans un état stationnaire hors-équilibre, couplée avec deux thermostats de Langevin à différentes températures attachées à ses extrémités. Nous avons choisi la perturbation stochastique la plus simple possible conservant à la fois le moment et l'énergie : chaque couple de particules voisines échange le moment à des instants aléatoires distribués selon une loi exponentielle de paramètre $\gamma > 0$.

La dynamique que nous considérons est présentée dans la section 5.2. Nous introduisons l'Hamiltonien, avec le potentiel de Toda, et spécifions les conditions aux bords, qui sont fixes à gauche et libres à droite. Le générateur de la dynamique est constitué par le générateur Hamiltonien, les générateurs de Langevin relatifs aux deux thermostats et le générateur du bruit stochastique ; nous définissons le courant d'énergie comme la somme du courant Hamiltonien et du courant dû au mécanisme stochastique d'échange de moments.

Nous discutons ensuite de l'état stationnaire, qui est explicitement connu à l'équilibre ($T_l = T_r = T$) alors que pour $T_l \neq t_r$ il n'a pas une forme analytique connue. Pour certaines classes de potentiels anharmoniques, les résultats de Rey-Bellet (2006*b*), Carmona (2007) montrent qu'il existe une mesure de probabilité stationnaire unique. Les hypothèses sur le potentiel contenues par exemple dans Carmona (2007) ne sont pas satisfaites par le potentiel de Toda (en particulier, la croissance à l'infini est trop lente dans la limite $r \to +\infty$). Cependant, il est possible que ces techniques puissent être étendues pour traiter aussi le cas de la

chaîne de Toda. Sous l'hypothèse que la mesure stationnaire existe, nous pouvons obtenir l'expression qualitative du courant moyen, dans laquelle nous remarquons que la contribution directe du courant stochastique reste bornée dans la limite de chaîne infinie. Par conséquent, la divergence de la conductivité ne peut qu'être due au courant hamiltonien.

Les simulations numériques que nous avons réalisées sont décrites en détail dans la section 5.3. Pour la discrétisation en temps de la dynamique, nous adoptons une stratégie de «splitting» standard, qui considère la partie de bruit stochastique séparément du reste, c'est-à-dire la dynamique hamiltonienne et les deux dynamiques de Langevin aux bords. Le terme de bruit est simulé en échangeant les moments de deux oscillateurs voisins à des instants aléatoires distribués exponentiellement, alors que l'intégration numérique de la partie Hamiltonienne de la dynamique et de l'action des thermostats sur les deux extrémités de la chaîne est faite par une discrétisation de BBK (Brünger et al. (1984)). Le conditions initiales sont choisies en imposant un profil de température linéaire obtenu à partir de la moyenne temporelle de l'énergie cinétique locale. Après un temps de thermalisation, que l'on peut définir au sens large comme le temps après lequel les variations du courant instantané se stabilisent, nous calculons la conductivité comme le rapport entre la moyenne temporelle du courant hamiltonien multipliée par le nombre d'oscillateurs, et la différence de température aux bords. Les différentes sources d'erreur dans les simulations ont été considérées avec attention et leur effet sur les résultats estimé avec soin.

Enfin, dans la section 5.4, nous tirons les conclusions des résultats numériques. Nos principaux résultats sont les suivants :

A) dès qu'un bruit est présent, c'est-à-dire dès que $\gamma > 0$, le transport balistique est immédiatement détruit, comme dans le cas harmonique, et le transport d'énergie devient superdiffusif, avec $\kappa_L \sim L^\alpha$ pour $0 < \alpha \leqslant 1/2$;

B) l'exposant α semble dépendre de la force du bruit γ, de façon monotonement croissante.

Si le premier résultat était attendu, le deuxième est assez surprenant. Il peut s'expliquer par le fait que le bruit détruit certains phénomènes diffusifs dus à des non-linéarités, comme les «breathers» localisées. Il en résulte que la corrélation courant-courant décroît plus vite quand le terme de bruit est plus important (voir aussi Basile et al. (2007) où ce phénomène a aussi été observé). En outre, le résultat B suggère que toute théorie revendiquant l'existence d'un paramètre universel α doit être correctement circonstanciée.

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Mai dire gatto.
Anonymous, 20th century

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Statistical mechanics connects the macroscopic description of a system, based on thermodynamic parameters, to the microscopic dynamics of its components. The values assumed by the macroscopic parameters like temperature or pressure, are the result of the collective behavior of the system components, whose positions and velocities evolve at the molecular scale following the laws of Hamiltonian dynamics on the phase-space. There are obviously some issues related to the handling of a microscopic description (Balian (2007), Schwabl (2006)). First, it is impossible to exactly know the state of a system with so many degrees of freedom at all times. Second, very small discrepancies in the initial conditions are usually exponentially magnified in time due to the chaotic nature of the underlying Hamiltonian dynamics. Third, considering the evolution of so many degrees of freedom is unnecessary, since in many situations we are only interested in a few average properties, like energy density. For all these reasons, a system is better described by a probability law (also called thermodynamic ensemble) defined on the phase-space and its macroscopic features are computed as averages with respect to this law.

The concept of equilibrium is related to the empirical sense used in thermodynamics: a system is at equilibrium when its thermodynamic state does not change with time and is stable under small perturbations. There are other features that characterize equilibrium systems: their evolution is conservative and invariant under time reversal; their macroscopic state is independent of the details of the particles evolution and it is described by a probability measure (or thermodynamic ensemble), which is ergodic with respect to the microscopic dynamics. On the other hand, equilibrium states are somehow an idealization. As a matter of fact, in our daily experience we mainly deal with irreversible, non-conservative processes which characterize out-of-equilibrium systems, whose macroscopic evolution strongly depends on the details of the microscopic dynamics.

There are two broad classes of problems which can be considered. The first one deals with the relaxation to equilibrium of a perturbed equilibrium system. As an example one may consider a system who has been partially heated by an external source: the heat naturally flows from the hottest to the coldest part until the whole system attains a uniform temperature. This happens unless the heating process has dramatically modified some of the physical or chemical features of the system, taking it too far from its initial equilibrium state. The second class of problems concerns systems constantly subjected to an external mechanical or thermal forcing which maintains them out of equilibrium. This is the class of systems I consider in this work. Under certain conditions, the dynamics of these systems may evolve towards a nonequilibrium stationary state (NESS) described by an invariant probability measure and characterized by steady currents of conserved quantities. Indeed, two of the main theoretical issues in the study of nonequilibrium systems are those of establishing the existence and uniqueness of the NESS and of estimating the rate of convergence to it.

The NESS of a system composed of many interacting particles displays unexpected and sometimes unpredictable behaviors that makes it strikingly different from the immutable equilibrium states and its thermodynamic properties are still poorly understood, especially in the far-from-equilibrium case. The classical framework for studying a NESS is that of a system in contact with two ideally infinite thermostats at different temperatures and isolated elsewhere: a heat current flows through the system from the hottest to the coldest thermostat and the stationary state is attained when the heat entering the system from the thermo-

stat at higher temperature equals the heat absorbed by the thermostat at lower temperature. In this case the heat flux becomes steady and the temperature profile inside the system becomes constant. Another framework is that of a system subjected to mechanical, non-conservative forces that perform work which injects energy into the system, increasing each particle's kinetic energy. Of course, no stationary state can be attained without some dissipation mechanism, that allows an outgoing flux of energy in the form of heat which is absorbed by the environment, otherwise the internal energy would increase indefinitely. The stationary state is reached when the dissipated thermal energy equals the work done by the non conservative force acting on the system, resulting in stationary heat flows and temperature profiles.

In the context of spontaneous heat transfer from a hot to a cold region in a solid, a macroscopic empirical law of heat conduction was proposed by Joseph Fourier in 1808. Fourier's law states that the heat current is proportional to the temperature gradient, the proportionality constant being the thermal conductivity, an intrinsic physical property of the system which depends on its equilibrium parameters such as temperature and density. In the last decades many efforts have been put in the microscopic understanding of the Fourier law, both in a relaxation to equilibrium context and in a dynamical framework (see *e.g.* Bonetto et al. (2000), Lepri et al. (2003), Dhar (2008)). However, it remains an open and challenging problem. While in three-dimensional materials, the thermal conductivity has been fully characterized and measured, in some low-dimensional momentum-conserving systems it depends on the system size, and it diverges in the thermodynamic limit. This anomalous behavior is not only puzzling from the theoretical point of view, but has also some relevant implications in materials science, engineering and real-world applications (carbon nanotubes, graphene, nanowires, etc.).

This introduction provides the theoretical framework for the work contained in the following chapters. In Section 1.1, I briefly recall some classical concepts like that of ensembles and the main features of the microscopic Hamiltonian description of the system. I introduce general Markov processes and semigroups, describe their evolution laws and briefly recall their properties. I then introduce the invariant measure, state the conditions for its existence and uniqueness and give the characterization of nonequilibrium invariant measures. In Section 1.2, I deal with the general convergence of the dynamics towards the steady state. I distinguish the elliptic and hypoelliptic case and summarize some methodologies for a more or less quantitative anaysis of the convergence rates. In Section 1.3, I introduce two paradigmatic perturbation of the equilibrium dynamics, a mechanical and a thermal one. Then, I rapidly sketch the linear response approach in the nonequlibrium case and recall the Green-Kubo formula for transport coefficients. In Section 1.4, I concisely discuss the main issue in thermal transport, namely the validity of the Fourier's law. In Section 1.5, I present the general framework for the numerical study of stocastic dynamics and for the computation of transport properties. Finally, in Section 1.6, I present the original contributions of this thesis.

1.1 Microscopic description and evolution

The microscopic state of a system composed of N point-like particles in d dimensions is completely determined at time t by a set of Nd canonical coordinates $q_1,\dots,q_{Nd} \in \mathcal{D}$ and their conjugate momenta $p_1,\dots,p_{Nd} \in \mathbb{R}^{Nd}$. The configuration space $\mathcal{D}$ of dimension Nd is a connected closed set whose properties depend on the boundary conditions imposed on the system. Free boundary conditions are chosen for isolated systems for which $\mathcal{D} = \mathbb{R}^{Nd}$. When periodic boundary conditions are chosen, $\mathcal{D} = (L\mathbb{T})^{Nd}$, with $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ the one dimensional torus.

A mathematical description of the interactions between the system and its environment is needed, as in the case of a system in contact with a thermal bath, with which it exchanges energy in the form of heat (see Section 1.1.2). In this case, a decision has to be made on the number of degrees of freedom we are willing to study in details. Ideally, one should consider the global Hamiltonian dynamics of all the particles composing the system and its environment, but this is unfeasible for obvious reasons. In practice, the choice is between stochastic or deterministic thermostat models. In the first case, one "averages out" the information about the dynamics of the thermal bath particles and model their interaction with the system by a stochastic dynamics at the boundaries. In the second case, the thermostat is modeled by a global variable whose evolution is deterministic. While deterministic thermostats are more appropriate to describe the real physical thermostats and ideally they might be considered more suited to study the dynamics of the relaxation towards equilibrium, their convergence properties are unclear and they may display a non-ergodic behavior (Legoll et al. (2007, 2009)). This motivates our choice of a stochastic approach: throughout this work the action of the thermostats will be modeled by a Langevin process, whose ergodic properties can be proved.

The state of the system is represented by a point (q,p) in the phase space $\mathcal{E} = \mathcal{D} \times \mathbb{R}^{Nd}$, which is the space of all the possible microscopic states that are compatible with a given macroscopic state. The physical content of the model is determined by the nature of the interaction among the particles, which is encoded in the potential energy function $U(q)$. Since we do not consider the subatomic structure of the particles composing the systems, the function $U(q)$ is actually an appropriately chosen empirical potential function describing the interaction among point-like particles. Only potentials $U \in C^\infty$ are considered in the following.

The total internal energy of this system is the sum of its total kinetic energy and its total potential energy and is given by the Hamiltonian $H(p,q)$, which is a function of the particle positions q_i and momenta p_i

$$H(q,p) = \frac{1}{2} p^T M^{-1} p + U(q) = K(p) + U(q), \qquad q \in \mathcal{D}, \qquad p \in \mathbb{R}^{Nd}. \tag{1.1}$$

The quantity $M = \mathrm{diag}(m_1 \mathrm{Id}_\mathrm{d},\dots,m_N \mathrm{Id}_\mathrm{d})$ with $m_i > 0$ is the mass matrix. The Hamiltonian (1.1) is separable in a kinetic part $K(p)$ and a potential one $U(q)$. Most of the Hamiltonians encountered in applications are separable, but there are examples of non-separable Hamiltonians, like that of a system whose masses depend on positions. In this work, we will only deal with separable Hamiltonians.

1.1.1 Hamiltonian evolution

The microscopic dynamics of the system is governed by the following system of Hamiltonian equations

$$\begin{cases} \dfrac{\mathrm{d}q(t)}{\mathrm{d}t} = \nabla_p H(q,p) = M^{-1}p\,, \\ \\ \dfrac{\mathrm{d}p(t)}{\mathrm{d}t} = -\nabla_q H(q,p) = -\nabla U(q)\,, \end{cases} \qquad q \in \mathcal{D}, \qquad p \in \mathbb{R}^{Nd}, \tag{1.2}$$

with initial conditions $(q(0), p(0)) = (q_0, p_0)$. The local in time existence and uniqueness of the trajectories typically follows from the Cauchy-Lipschitz (local in time) theorem, once we impose the sufficient condition that $\nabla H(q,p)$ is locally Lipschitz continuous. We will always assume in the sequel that the previous Cauchy problem is well-posed.

The Hamiltonian flow ϕ_t is defined as the application $(q(t), p(t)) = \phi_t(q^0, p^0)$. Since (1.2) is an autonomous system, the flow is a semi-group: $\phi_{t+s} = \phi_t \circ \phi_s$ for all $t, s \in \mathbb{R}$. It is easy to see that the Hamiltonian flow has the property of preserving volumes in the phase space, that is $\int_{\phi_t(B)} \mathrm{d}q\,\mathrm{d}p = \int_B \mathrm{d}q\,\mathrm{d}p$. The time derivative of $t \mapsto f(q(t), p(t))$ with $f \in C^1(\mathcal{E})$ is

$$\frac{\mathrm{d}}{\mathrm{d}t} f = \mathcal{L}_{\mathrm{ham}} f\,, \quad \mathcal{L}_{\mathrm{ham}} \doteq p^T M^{-1} \nabla_q - \nabla U(q)^T \nabla_p\,.$$

The linear differential operator $\mathcal{L}_{\mathrm{ham}}$ can be considered as the infinitesimal generator of the Hamiltonian dynamics in the sense that

$$u(q(t), p(t)) = (u \circ \phi_t)(q_0, p_0) = (\mathrm{e}^{t\mathcal{L}_{\mathrm{ham}}} u)(q_0, p_0)\,.$$

1.1.2 Thermodynamic ensembles

As I mentioned earlier, it is convenient to describe a macroscopic system with a probability measure on the phase space. In the equilibrium case, the macroscopic state of a system is represented by an invariant probability measure μ, which is also called a thermodynamic or statistical ensemble, a concept introduced in 1902 by the American physicist J. W. Gibbs. A statistical ensemble is an abstraction useful to mathematically represent the configuration of a dynamical system at time t when there is no precise knowledge of the initial conditions: it can be seen as a very large number of virtual copies of the system considered, corresponding to each possible microscopic state compatible with a given macroscopic state. The choice of the ensemble depends on the given physical context, that is the set of macroscopically observed variables which are appropriate for the description of the system. These variables are invariant quantities of the dynamics: number of particles (N), chemical potential (ζ), volume (V), pressure (P), energy (E) or temperature (T). Gibbs defined three main thermodynamic ensembles, which are equivalent in the thermodynamic limit $N \to \infty$ and whose related probability measures are explicitly known :

– the microcanonical ensemble (NVE), describing an isolated system at equilibrium, for which the probability measure is proportional to the normalized projection of the Lebesgue measure on the manifold defined by constant (NVE);

– the canonical ensemble (NVT), describing a system in contact with a thermostat at temperature T;

– the grand-canonical ensemble (ζVT), describing a system in thermal and chemical equilibrium with a larger system with which it exchanges energy and mass (particles), thus fixing its temperature and chemical potential ζ.

We will focus exclusively on the canonical ensemble, since we only deal with systems whose volume, temperature and number of particles are kept fixed. We suppose the system to be in contact with a thermal bath (*i.e.* a much larger system, ideally infinite, whose temperature T is constant), so that it spontaneously relaxes to an equilibrium state at the same temperature as the thermal bath.

The canonical measure, also called the Boltzmann-Gibbs distribution corresponding to the Hamiltonian H, reads

$$\mu(\mathrm{d}q\,\mathrm{d}p) = Z_\mu^{-1} \mathrm{e}^{-\beta H(p,q)}\,\mathrm{d}q\,\mathrm{d}p\,, \qquad Z_\mu = \int_{\mathcal{E}} \mathrm{e}^{-\beta H(p,q)}\,\mathrm{d}q\,\mathrm{d}p\,, \tag{1.3}$$

where H is the Hamiltonian given in (1.1), $\beta^{-1} = (k_B T)$ is proportional to the temperature via the Boltzmann's constant k_B and the normalization constant Z_μ is called the *partition function*, which is positive and finite if we assume that $\mathrm{e}^{-\beta U(q)} \in L^1(\mathcal{D})$. Since the Hamiltonian is separable, the measure μ_β is a product measure $\mu_\beta(\mathrm{d}q\,\mathrm{d}p) = \nu_\beta(\mathrm{d}q)\kappa_\beta(\mathrm{d}p)$: the positions and the momenta are independent random variables of laws

$$\nu(\mathrm{d}q) = Z_\nu^{-1}\,\mathrm{e}^{-\beta U(q)}\,\mathrm{d}q\,, \qquad Z_\nu \doteq \int_{\mathcal{D}} \mathrm{e}^{-\beta U(q)}\,\mathrm{d}q\,, \tag{1.4}$$

and

$$\kappa(\mathrm{d}p) = \prod_{i=1}^{3N} \left(\frac{\beta}{2\pi m_i}\right)^{1/2} \mathrm{e}^{-\frac{\beta}{2m_i}p_i^2}\,\mathrm{d}p_i\,. \tag{1.5}$$

Note that every component of the momenta is independent of the others, each following a normal distribution with variance $m_i\beta^{-1}$.

1.1.3 Observables and ergodicity

We assume that a system is characterized by a specific set of observables, whose values represent its physical state. Mathematically, an observable is by definition a bounded and continuous function of the microscopic state $\varphi(q,p)$. A measurement on this observable is a quantitative experiment of a certain duration T, which may be viewed as a process of averaging over the microscopic dynamics

$$\overline{\varphi}_T = \frac{1}{T}\int_0^T \varphi(q_t,p_t)\,\mathrm{d}t\,, \tag{1.6}$$

where (q_t,p_t) is the solution of the Hamiltonian equations (1.2). Note that $\overline{\varphi}_T$ is a random variable, since it depends on the random initial conditions. The "true" value φ_∞ of the observable $\varphi(p,q)$ may be obtained either in the limit of $T \to +\infty$

$$\varphi_\infty = \lim_{T\to+\infty} \overline{\varphi}_T \tag{1.7}$$

or by repeating the experiment an infinite number of time and averaging over the results. This is equivalent to averaging over all the possible microscopic configuration of the system in the given unknown state, *i.e.* to averaging with respect to the appropriate thermodynamic ensemble

$$\varphi_\pi \doteq \mathbb{E}_\pi(\varphi) = \int_{\mathcal{E}} \varphi(q,p)\,\pi(\mathrm{d}p\,\mathrm{d}q). \tag{1.8}$$

The two averaging procedures (1.7) and (1.8) are equivalent, that is

$$\varphi_\infty = \varphi_\pi\,, \qquad \pi-\text{almost everywhere}\,,$$

if the measure π of the ensemble average (1.8) is ergodic with respect to the dynamics generating the trajectory on which we compute the time average (1.6).

1.1.4 The stochastic dynamics

Let us consider the following generic set of time-homogeneous stochastic differential equations (SDE)

$$\mathrm{d}x_t = b(x_t)\,\mathrm{d}t + \sigma(x_t)\,\mathrm{d}W_t \tag{1.9}$$

where $x_t \in \mathcal{X}$, $W_t \in \mathbb{R}^k$ is a k-dimensional standard Brownian motion with independent normally distributed increments ($W_{t+s} - W_t \sim \mathcal{N}(0,s)$), $\mathrm{d}W_t$ is the Itō differential, $b : \mathcal{X} \to \mathbb{R}^n$ is the drift vector and $\sigma : \mathcal{X} \to \mathbb{R}^{n\times k}$ is the diffusion matrix. These functions are assumed to be such that, given an initial condition $x_{t=0} = x \in \mathcal{X}$, there exists a unique solution to the system (1.9), see Section 1.1.4.1.

Two paradigmatic versions of (1.9) are considered in the following, namely that describing Langevin dynamics ($n = 2Nd$; $\mathcal{X} = \mathcal{E}$)

$$\begin{cases} \mathrm{d}q_t = \dfrac{p}{m}\,\mathrm{d}t, \\ \mathrm{d}p_t = -\nabla U(q_t)\,\mathrm{d}t - \dfrac{\xi(q_t)}{m}p_t\,\mathrm{d}t + \sqrt{2\xi(q_t)\beta^{-1}}\,\mathrm{d}W_t, \end{cases} \qquad q \in \mathcal{D},\ p \in \mathbb{R}^{Nd}, \tag{1.10}$$

where $\xi(q_t) > 0$ is the damping (or friction) function and $m > 0$ is the mass of each particle; and that describing the so-called overdamped Langevin dynamics ($n = Nd$)

$$\mathrm{d}q_t = -\nabla U(q_t)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t\,, \qquad q \in \mathcal{D}. \tag{1.11}$$

Langevin dynamics is actually a modification of the Hamiltonian dynamics with two added components: a term $\xi(q_t)m^{-1}p_t\,\mathrm{d}t$ that provides dissipation and a random forcing term $\sqrt{2\xi(q_t)\beta^{-1}}\,\mathrm{d}W_t$. The effects of the two terms compensate each other in such a way that the value of the system average temperature remains fixed at a $T = (k_B\beta)^{-1}$.

We remark that, in the case of constant $\xi(q) = \xi_*$, the overdamped Langevin dynamics can be obtained from the Langevin dynamics (1.10) by taking either the large friction limit $\xi \to \infty$ with time rescaled as ξt, or the small mass limit $m \to 0$, see Lelièvre et al. (2010, Section 2.2.4) for details and a rigorous proof.

1.1.4.1 Existence and uniqueness of solutions of the SDE

The classical setting for the existence and uniqueness of a global in time solution of the equation (1.9) with initial condition $x_{t=0} = x_0$, defined on a generic space $\mathcal{X} \subset \mathbb{R}^n$, is to assume that b and σ are locally Lipschitz (see *e.g.* Øksendal (2013))

$$|b(x) - b(y)| + |\sigma(x) - \sigma(y)| \leqslant C|x - y|, \quad \forall x, y \in \mathcal{X}.$$

and that one of the following hypotheses are satisfied (Rey-Bellet (2006*a*))

(i) existence of a linear bound

$$|b(x)| + |\sigma(x)| \leqslant D(1 + |x|), \quad \forall x \in \mathcal{X},$$

or :

(ii) existence of a Lyapunov function $W(x)$, with $W(x) \geq 1$ and $\lim_{|x|\to+\infty} W(x) = +\infty$, such that

$$\mathcal{L}W(x) \leqslant cW(x), \tag{1.12}$$

for some positive constant c. The differential operator $\mathcal{L}$ in (1.12) is the infinitesimal generator of the dynamics of x_t defined hereafter (see eq. (1.15)). In this case the unique solution of (1.9) exists and is such that

$$\mathbb{E}_x[W(x_t)] \leqslant W(x)\mathrm{e}^{ct},$$

where $\mathbb{E}_x[\cdot]$ represents the average on all the realizations of (1.9) starting from x at $t = 0$.

Both Langevin and overdamped Langevin dynamics satisfy the conditions of existence and uniqueness of the solution, because of the supposed smoothness of the potential. As we shall see in Section 1.1.5.1, a stronger Lyapunov condition implying (1.12) is needed to prove the existence and uniqueness of the stationary law of the process x_t.

1.1.4.2 Density kernel and semigroup

The solution to (1.9) is a Markov diffusion process, since it may be thought of as the mathematical description of the motion of a small particle in a moving fluid. We define the probability kernel of the Markov process x_t as the probability of a transition in a time t from a point x to a set $Q \subset \mathcal{X}$, that is the conditional probability

$$P_t(x, Q) = \mathbb{P}\{x_t \in Q \,|\, x_0 = x\}; \qquad \int_{\mathcal{X}} P_t(x, \mathrm{d}y) = 1, \qquad \forall t \in \mathbb{R}^+,$$

for μ-almost every $x \in \mathcal{X}$, with P_t satisfying the Chapman-Kolmogorov equation

$$P_{t+s}(x, \mathrm{d}y) = \int_{z\in\mathcal{X}} P_t(x, \mathrm{d}z)\, P_s(z, \mathrm{d}y). \tag{1.13}$$

It follows that the average over all the realizations of the Brownian motion starting from a given point $x \in \mathbb{R}^n$ is

$$\mathbb{E}_x[\varphi(x_t)] = \int_{\mathcal{X}} \varphi(y) P_t(x, \mathrm{d}y) = T_t\varphi(x), \tag{1.14}$$

where $\varphi(x)$ is a measurable function on $\mathbb{R}^n$ representing the physical observable. On the rightmost side of the previous expression, I have introduced the operator T_t associated to the Markov process x_t, which is evidently a semigroup because of (1.13). The Markov semigroup has also other properties: it preserves positivity

$$T_t f \geq 0, \quad \forall f \geq 0,$$

and mass

$$T_t(\mathbb{1}) = \mathbb{1}.$$

It is also bounded

$$\|T_t\varphi(x)\|_{L^\infty(\mathcal{X})} = \int_{\mathcal{X}} |P_t(x, \mathrm{d}y)\varphi(y)| \leqslant \|\varphi(x)\|_{L^\infty(\mathcal{X})},$$

and in fact contractive.

Considering a generic Banach space E, we define the Banach space $\mathscr{B}(E)$ of bounded operators on E, endowed with the operator norm

$$\|A\|_{\mathscr{B}(E)} = \sup_{\phi \in E\setminus\{0\}} \frac{\|A\phi\|_E}{\|\phi\|_E}.$$

The contractivity of the Markov semigroup can thus be reformulated by means of this norm as $\|T_t\|_{\mathscr{B}(L^\infty(\mathcal{X}))} \leqslant 1$.

1.1.4.3 The generator of the dynamics

The properties of probability conservation and contractivity of the semigroup ensure the existence of the bounded time derivative of the function $T_t\varphi$ at $t = 0$, for well-behaved test functions φ (by Hille-Yosida theorem, see *e.g.* Bakry et al. (2014)). This allows the following definition of the infinitesimal generator $\mathcal{L}$ of the diffusion process

$$\mathcal{L}\varphi(x) \doteq \lim_{h\to 0} \frac{T_h\varphi(x) - \varphi(x)}{h} \equiv \left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}_x[\varphi]\right)\Big|_{t=0}, \tag{1.15}$$

for every function φ defined on the core $C_0^\infty(\mathcal{X})$ of smooth compactly suppported functions. [(1)]. We can compute the expression of the generator of the Markov process $(x_t)_{t\geq 0}$ solution of (1.9) by direct application of the Itō formula to $\varphi(x_t)$, obtaining

$$\mathcal{L} = b \cdot \nabla + \frac{1}{2}\sigma\sigma^T : \nabla^2, \tag{1.16}$$

where the symbol : in (1.16) denotes the Frobenious product[(2)].

(1) Following Ethier and Kurtz (2005) and Bakry et al. (2014), we can introduce the notion of *core* for a linear differential operator $\mathcal{L}$. A core for $\mathcal{L}$ is a subset $\mathcal{S}$ of the domain of $\mathcal{L}$ composed of all functions $\varphi \in C^\infty(\mathcal{E})$ for which, for any $s \in \mathbb{N}^n$ there exists $m \in \mathbb{N}$ such that $\partial^s\varphi \in L^\infty_{W_m}(\mathcal{E})$, where W_m are the Lyapunov functions introduced in Section 1.1.4.1 and further discussed below (see Section 1.1.5.1). Thus a core for $\mathcal{L}$ is the space $C_0^\infty(\mathcal{X})$ of smooth compactly supported functions.

(2) More explicitly, the action of $\mathcal{L}$ on φ is

$$\mathcal{L}\varphi = \sum_{i=1}^n b_i \partial_{x_i}\varphi + \frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n\sum_{h=1}^k \sigma_{i,h}\sigma^T_{h,j}\partial_{x_i x_j}\varphi. \tag{1.17}$$

Setting

$$b(x) = \begin{pmatrix} \dfrac{p}{m} \\ -\nabla U - \dfrac{\xi}{m} p \end{pmatrix}, \qquad \sigma(x) = \sigma \begin{pmatrix} 0 & 0 \\ 0 & \mathrm{Id}_{Nd} \end{pmatrix}$$

with

$$\sigma = \sqrt{2\xi\beta^{-1}}, \tag{1.18}$$

the explicit expression of the generator of the Langevin dynamics reads

$$\mathcal{L} = \frac{p}{m} \cdot \nabla_q - \nabla U(q) \cdot \nabla_p + \xi \left(\beta^{-1} \nabla_p^2 - \frac{p}{m} \cdot \nabla_p \right) = \mathcal{L}_{\mathrm{ham}} + \xi \mathcal{L}_{\mathrm{FD}}, \tag{1.19}$$

while, in the overdamped case one obtains

$$\mathcal{L}_{\mathrm{ovd}} = -\nabla U(q) \cdot \nabla_q + \beta^{-1} \Delta. \tag{1.20}$$

We shall see in what follows that the so-called fluctuation-dissipation relation (1.18) plays an essential role in the ergodicity properties of the Langevin dynamics (1.10).

1.1.4.4 Hypoellipticity and regularity property

The generator of the overdamped dynamics is elliptic, since the matrix of the coefficients of the highest-order derivatives $M = \beta^{-1}\mathrm{Id}_n$ is positive definite. By the regularization property of elliptic operators, the solution of the equation $\mathcal{L}_{\mathrm{ovd}} f = g$ on a compact subset of the phase-space $V \in \mathcal{D}$ when $g \in H^s(V)$ is in $H^{s+2}(V)$.

The generator of Langevin dynamics fails to be elliptic, since the rank of the matrix $M = \begin{pmatrix} 0 & 0 \\ 0 & \xi\beta^{-1}\mathrm{Id}_{Nd} \end{pmatrix}$ is not maximum in this case. Nevertheless it can be shown (see *e.g.* Rey-Bellet (2006*a*)) that, if the generator satisfies the Hörmander condition (see below), then the solution of $\mathcal{L} f = g$ on a compact subset of the phase-space $V \in \mathcal{E}$ when $g \in H^s(V)$ is in $H^{s+\varepsilon}(V)$ for some $\varepsilon > 0$. In particular, if $g \in C^\infty(\mathcal{X})$ then $f \in C^\infty(\mathcal{X})$, which is the definition of a hypoelliptic operator. The same property is shared by $\mathcal{L}^\dagger$, $\partial_t - \mathcal{L}$ and $\partial_t - \mathcal{L}^\dagger$.

Let $A_i = \sum_{j=1}^M A_i^j(x)\partial_{x_j}$, $1 = 1 \ldots, D$ be C^∞ vector fields on an D-dimensional space $\mathscr{X}$, denote by $A_i^\dagger$ the formal adjoint of A_i on $L^2(\mathscr{X})$ and consider operators of the form

$$\mathcal{A} = A_0 + \sum_{i=1}^{D} A_i^\dagger A_i .$$

Furthermore, denote by $[S, B] = SB - BS$ is the commutator between two operators.

Definition 1 (*parabolic Hörmander condition)*. The family of vector fields $\{A_i\}$ satisfies the Hörmander condition if the Lie algebra spanned by

$$\{A_i\}_{i=1,\ldots,M}, \quad \{[A_i, A_k]\}_{i,k=0,\ldots,M}, \quad \{[[A_i, A_k], A_l]\}_{i,k,l=0,\ldots,M}, \quad \ldots$$

has maximal rank D at every point $x \in \mathscr{X}$.

It is easy to see that the Langevin generator ($M = 2Nd$, $D = Nd$) satisfies this condition with

$$A_0 = \mathcal{L}_{\text{ham}} - \xi \frac{p}{m} \cdot \nabla_p , \qquad A_i = \sqrt{\xi \beta^{-1}} \partial_{p_i} .$$

This implies

$$[A_i, A_0] = \frac{1}{m} \sqrt{\xi \beta^{-1}} (\partial_{q_i} - \partial_{p_i}), \qquad \forall i = 1, \dots, D$$

and so the family of vector field $\{[A_i, [A_i, A_0]]\}_{i=0,\dots,M}$ as maximum rank $M = 2Nd$.

Theorem 1 (Hörmander)**.** *If the family of vector fields $\{A_i\}$ satisfies the parabolic Hörmander condition, then $\mathcal{L}$, $\mathcal{L}^\dagger$, $\partial_t - \mathcal{L}$ and $\partial_t - \mathcal{L}^\dagger$ are hypoelliptic.*

In addition to regularity, hypoellipticity implies other interesting and useful properties, among them the fact that, the transition kernel admits a smooth density with respect to the Lebesgue measure

$$P_t(x, \mathrm{d}y) = p_t(x, y) \, \mathrm{d}y . \tag{1.21}$$

This means that the invariant measure, if it exists, has a smooth density with respect to the Lebesgue measure.

1.1.4.5 Evolution of observables

Let us define $u(x, t) \doteq T_t \varphi(x)$. Applying T_t on both sides of (1.15), by the definition of derivative as the limit of the difference quotient, one obtains the Kolmogorov backward equation

$$\partial_t u(x, t) = T_t \mathcal{L} \varphi(x) = \mathcal{L} u(x, t), \tag{1.22}$$

where the last equality holds since $[T_t, \mathcal{L}] = 0$ (as proved *e.g.* in Øksendal (2013), Theorem 8.1.1). A formal integration of the previous equation with initial condition $u(x, 0) = \varphi(x)$ gives

$$u(x, t) = \mathrm{e}^{t\mathcal{L}} \varphi(x)$$

from which we get the expression of the semigroup

$$T_t = \mathrm{e}^{t\mathcal{L}} .$$

1.1.4.6 Evolution of the law of the process

If we suppose that the initial condition x is not given precisely but is a random variable distributed following a probability law π on $\mathcal{X}$, we may compute the average of (1.14) over all possible initial conditions

$$\mathbb{E}_\pi[\varphi(x_t)] = \int_{\mathcal{X}} \int_{\mathcal{X}} \varphi(y) \, P_t(x, \mathrm{d}y) \, \pi(x) \, \mathrm{d}x = \int_{\mathcal{X}} T_t \varphi(x) \, \pi(x) \, \mathrm{d}x .$$

When (1.21) holds, the integration of this equality with respect to y leads to

$$\mathbb{E}_\pi[\varphi(x_t)] = \int_{\mathcal{X}} \int_{\mathcal{X}} \varphi(y) \, p_t(x, y) \, \pi(x) \, \mathrm{d}x \, \mathrm{d}y = \int_{\mathcal{X}} S_t \pi(y) \varphi(y) \, \mathrm{d}y ,$$

thus giving a definition of the semigroup S_t related to the evolution of the initial conditions density. Note that $S_t = T_t^\dagger$, where the dagger denote the adjoint in $L^2(\mathrm{d}x)$. Defining $\psi(y,t) = S_t\pi(y)$, the dual equation of (1.22) is

$$\partial_t \psi(x,t) = \mathcal{L}^\dagger \psi(x,t), \tag{1.23}$$

more commonly known in mathematical physics as the Fokker-Planck equation. Integrating the previous equation with the initial condition $\psi(x,0) = \psi_0(x)$ one gets

$$\psi(x,t) = \mathrm{e}^{t\mathcal{L}^\dagger}\psi_0(x),$$

which is the time evolution of the probability density of the process x_t.

1.1.5 The invariant measure

The characterization of the invariant measure can be derived by the definition of the generator (1.15). Indeed, integrating both members with respect to the distribution π of all initial conditions, for $\varphi \in C_0^\infty(\mathcal{X})$ we get

$$\int_{\mathcal{X}} \mathcal{L}\varphi \,\mathrm{d}\pi = \lim_{h\to 0} \frac{\mathbb{E}_\pi[\varphi(x_h)] - \mathbb{E}_\pi[\varphi(x_0)]}{h}.$$

If π is the invariant measure for the dynamics generated by $\mathcal{L}$ we have $\mathbb{E}_\pi[\varphi(x_h)] = \mathbb{E}_\pi[\varphi(x_0)]$, thus

$$\int_{\mathcal{X}} \mathcal{L}\varphi \,\mathrm{d}\pi = 0, \tag{1.24}$$

which is the sought characterization. The invariant measure can also be obtained by duality as a solution of the stationary Fokker-Planck equation

$$\mathcal{L}^\dagger \psi = 0. \tag{1.25}$$

As a matter of fact, the solution of (1.25) is such that $T_t^\dagger \psi = \psi$.

If we consider π as a reference measure, it is sometimes useful to consider the adjoint $\mathcal{L}^*$ of $\mathcal{L}$ in $L^2(\pi)$

$$\int_{\mathcal{X}} \phi(\mathcal{L}\varphi)\,\mathrm{d}\pi = \int_{\mathcal{X}} (\mathcal{L}^*\phi)\varphi \,\mathrm{d}\pi.$$

Considering $\phi = \mathbb{1}$ in (1.24), the expression of the invariance of π reads

$$\mathcal{L}^*\mathbb{1} = 0,$$

thus the uniqueness of the reference invariant measure π implies that $\mathrm{Ker}(\mathcal{L}^*) = \mathrm{Span}(\mathbf{1})$.

One can intuitively say that stationary measures describe the long-time behavior of a stochastic process. This can be shown by the following formal reasoning (Rey-Bellet (2006*a*), Ethier and Kurtz (2005, Theorem 9.3)): suppose that the law of x_t with initial distribution π converges in some sense to a distribution which a priori depends on π and which we call γ_π, *i.e.*

$$\lim_{t\to\infty} \mathbb{P}_\pi\{x_t \in Q\} = \gamma_\pi(Q).$$

Then we have, formally,

$$\gamma_\pi(Q) = \lim_{t\to\infty} \int_{\mathcal{X}} \pi(\mathrm{d}x) P_t(x,Q) = \lim_{t\to\infty} \int_{\mathcal{X}} \pi(\mathrm{d}x) \int_{\mathcal{X}} P_{t-s}(x,\mathrm{d}y) P_s(y,Q)$$
$$= \int_{\mathcal{X}} \gamma_\pi(\mathrm{d}y) \int_{\mathcal{X}} P_s(y,Q) = S_s\gamma_\pi(Q). \tag{1.26}$$

This shows that γ_π is an invariant measure.

It is easy to prove that an invariant (equilibrium) measure of the Langevin dynamics (1.10) is the Gibbs measure relative to the Hamiltonian $H(p,q)$, while, for the overdamped dynamics, the Gibbs measure relative to the potential $U(q)$ is also an invariant measure. The invariance of the Gibbs measure under Langevin dynamics, and the ergodicity of the former with respect to the latter, stems from the fluctuation-dissipation relation (1.18), which relates the diffusion coefficient σ to the friction parameter ξ.

1.1.5.1 Existence and uniqueness of the invariant measure

Let us now consider the semigroup T_t and its associated transition kernel $P_t(x,\mathrm{d}y)$ defined in (1.14), both acting on smooth functions $\varphi \in C_0^\infty(\mathcal{X})$. To state the existence and uniqueness of the invariant measure with its smooth density with respect to the Lebesgue measure (and eventually the exponential decay to this invariant measure), the following assumptions can be considered (see Rey-Bellet (2006*a*)):

H1 (*irreducibility*): there exist a reference time $t_0 > 0$ such that

$$P_{t_0}(x,Q) > 0,$$

for all $x \in \mathcal{X}$ and all open sets $Q \subset \mathcal{X}$;

H2 (*regularity*): the transition kernel $P_t(x,\mathrm{d}y)$ has a smooth density $p_t(x,y)$ in both variables;

H3 (*Lyapunov condition*): there exists a Lyapunov function $W : \mathcal{X} \to [1,+\infty)$, and two constants $a > 0$ and $b \geq 0$ such that

$$(\mathcal{L}W)(x) \leqslant -aW(x) + b, \qquad \forall x \in \mathcal{X}. \tag{1.27}$$

The first assumption guarantees the ergodicity of the invariant measure with respect to the dynamics. Note that, since the kernel satisfy the Chapman-Kolmogorov equation (1.13), **H1** holds for all $t > t_0$. The second assumption implies hypoellipticity, thus it ensures the regularity of the invariant measure (and also of the solutions of both the parabolic problems (Kolmogorov backward and forward)). Assumptions **H1** and **H2** are sufficient for stating the existence and uniqueness of the stationary measure in the case of a compact phase-space $\mathcal{X}$ (*e.g.* the overdamped Langevin problem with a bounded potential), while in the case of unbounded phase-space such as overdamped dynamics with unbounded potential or generic Langevin dynamics (momentum variables are always defined in $\mathbb{R}^{Nd}$) they do not prove the existence, but only ensure that $S_t\pi = \pi$ has "at most" one smooth solution.

For proving the existence and uniqueness theorem in the case of unbounded phase-spaces, assumption **H3** is needed to guarantee stability. Recall that a Lyapunov function is also involved in the existence and uniqueness problem for the process x_t (see (1.12)). The role of this assumption is that of ensuring the existence of a compact subset in $\mathcal{X}$, characterized by not too large values of the Lyapunov function, where the process spends most of its time.

As of the analytical form of the Lyapunov functions, in the case of overdamped Langevin dynamics on a compact configuration space, the condition in **H3** trivially holds for $W_n(q) = \mathbf{1}$, while $W_n(q) = |q|^n$, with $n \geq 2$ is the standard choice in the unbounded case. For Langevin dynamics on a phase space $\mathcal{E} = \mathcal{D} \times \mathbb{R}^{Nd}$ with compact configuration space $\mathcal{D}$, one can easily check that Lyapunov condition (1.27) is satisfied by functions of the form $W_n(q,p) = 1 + |p|^n$, with $n \geq 2$ (the compactness of $\mathcal{D}$ accounts for the constant part). For Langevin dynamics on an unbounded position space, a possible choice for the Lyapunov function is given (Mattingly et al. (2002)) by

$$W_n(q,p) = \left(1 + H(q,p) - U_- + \frac{\xi}{2m} p \cdot q + \frac{\xi^2}{m} q^2\right)^n , \tag{1.28}$$

where it is assumed that the potential energy function $U(q)$ is bounded from below by $U_- < +\infty$ and that there exist $a, b > 0$ and $c \in \mathbb{R}$ such that

$$\frac{q}{m} \nabla U(q) \geq a\, U(q) + b\, \frac{q^2}{m} + c\,, \forall q \in \mathcal{D}.$$

One remarks the presence in (1.28) of a mixed term in p and q which, just like Hörmander commutators (and a modified H^1 scalar product that will be introduced in Section 1.2.2), allows for the retrieval of some dissipation in the position variable.

The existence and uniqueness result can be stated as follows:.

Theorem 2 (Existence and uniqueness of the invariant measure)**.** *Let $(x_t)_{t\geq 0}$ be a Markov process on a phase space $\mathcal{X}$ with generator $\mathcal{L}$. Then, if*

(i) $\mathcal{X}$ is compact and assumptions **H1** *and* **H2** *are satisfied ,*

or

(ii) $\mathcal{X} \equiv \mathbb{R}^{2Nd}$ and assumptions **H1**, **H2** *and* **H3** *are satisfied ,*

there exists a unique stationary measure π for $(x_t)_{t\geq 0}$.

I refer to Rey-Bellet (2006*a*) and Hairer and Mattingly (2011) for proofs and a more in-depth analysis. Given the fair generality of the assumptions **H1**-**H3**, this procedure can be applied to a wide variety of problems, included those involving nonequilibrium dynamics (see Section 2.2.1).

As we shall see in Section 1.2.3, there is a second part of Theorem 2 that states the exponential convergence of the semigroup under the same assumptions.

1.1.5.2 Equilibrium *vs.* nonequilibrium invariant measures

Nonequilibrium invariant measures are physically characterized by the existence of non-zero currents flowing from side to side, created and maintained by some

external forcings. The steady-state is reached thanks to the dissipation mechanism, which prevents the external forcing to cause an uncontrolled growth of the internal energy of the system.

From a mathematical viewpoint, the reversibility of the dynamics of an equilibrium system translates into the self-adjointness of the generator $\mathcal{L}$ on the weighted Hilbert space $L^2(\pi)$, where π is the (unique) invariant measure :

$$\int_{\mathcal{X}} \mathcal{L}f\, g \,\mathrm{d}\pi = \int_{\mathcal{X}} f\, \mathcal{L}g \,\mathrm{d}\pi. \tag{1.29}$$

In some cases, such a reversibility property holds only up to a one-to-one transformation preserving the invariant measure. For example, for the Langevin dynamics (1.10) reversibility is valid only upon momentum reversal $S(q,p) = (q,-p)$:

$$\int_{\mathcal{E}} \mathcal{L}f\, g \,\mathrm{d}\pi = \int_{\mathcal{E}} (f\circ S)\mathcal{L}(g\circ S) \,\mathrm{d}\pi. \tag{1.30}$$

Reversibility properties such as (1.29) or (1.30) do not hold for nonequilibrium dynamics.

An important property of nonequilibrium systems is that their invariant measures in general depend non-trivially on the details of the dynamics. This is not the case for equilibrium dynamics. Indeed, consider for instance the overdamped Langevin dynamics (1.11) on the compact configuration space $\mathcal{D} = \mathbb{T}^{Nd} = (\mathbb{R}\backslash\mathbb{Z})^{Nd}$ for a smooth periodic potential U, reported here for clarity

$$\mathrm{d}q_t = -\nabla U(q_t)\,\mathrm{d}t + \sqrt{\frac{2}{\beta}}\,\mathrm{d}W_t. \tag{1.11}$$

Its unique invariant probability measure is the canonical measure $\nu(\mathrm{d}q)$. Now, if the dynamics (1.11) is perturbed by a smooth gradient modification of the drift term as

$$\mathrm{d}q_t = -\Big(\nabla U(q_t) + \nabla\widetilde{U}(q_t)\Big)\mathrm{d}t + \sqrt{\frac{2}{\beta}}\,\mathrm{d}W_t,$$

then the unique invariant probability measure becomes $\mathrm{e}^{-\beta(U(q)-\widetilde{U}(q))}\,\mathrm{d}q$ up to a normalizing constant. In particular, the invariant measure is modified only on the support of the perturbation $\widetilde{U}$.

For nonequilibrium dynamics (*e.g.* in the case of a non-gradient perturbation), the invariant measure is in general modified everywhere even if the perturbation is restricted to a small domain. This is due to long-range correlations which are generically present in nonequilibrium systems (see for instance Derrida et al. (2002*b*)). Let us illustrate these physical considerations by a simple analytical example (taken from Reimann (2002, Section 2.5)). Consider the dynamics (1.11) for $\beta = 1$ in the one-dimensional case, perturbed by a force which is not the gradient of a periodic potential

$$\mathrm{d}q_t = \Big(-U'(q_t) + F\Big)\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t, \tag{1.31}$$

where $F \in \mathbb{R}\backslash\{0\}$ is a constant force. The generator of (1.35) is

$$\mathcal{L}_F = -(\nabla U - F)\cdot\nabla + \Delta.$$

The standard techniques sketched in Section 1.1.5.1 (based on Rey-Bellet (2006*a*)) allow to show the existence and uniqueness of an invariant probability measure $\psi_F(x)\,\mathrm{d}x$, which satisfies the stationary Fokker-Planck equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((U'-F)\psi_F+\frac{\mathrm{d}\psi_F}{\mathrm{d}x}\right)=0. \tag{1.32}$$

In fact, it can be checked that the periodic function

$$\psi_F(x)=Z_{\psi_F}^{-1}\mathrm{e}^{-\mathrm{U(x)+Fx}}\int_{\mathrm{x}}^{\mathrm{x+1}}\mathrm{e}^{\mathrm{U(y)-Fy}}\,\mathrm{dy}=Z_{\psi_\mathrm{F}}^{-1}\int_0^1\mathrm{e}^{\mathrm{U(x+y)-U(x)-Fy}}\,\mathrm{dy},$$

indeed satisfies (1.32). It is clear from the expression of ψ_F that, when $F\neq 0$, the invariant measure depends on the values of U everywhere on $\mathbb{T}$.

Rewriting the invariant measure in a more general way as $\psi_F(q)=\mathrm{e}^{-U_F(q)}$ and computing the adjoint of $\mathcal{L}_F$ in $L^2(\psi_F)$ it is straightforward to check that $\mathcal{L}_F^*=\mathcal{L}_F$ if and only if $\nabla(U_F-U)+F=0$. This condition can be satisfied only when F is a gradient force.

The dynamics in (1.31) is one of the rare cases in which the invariant measure of a nonreversible diffusion has an explicit analytic form.

1.2 Long-time analysis of the dynamics

We tackle in this section the issue of the convergence of the law of the Markov process to the invariant measure $\pi(\mathrm{d}x)$, under the hypothesis of hypoellipticity of its generator, which, as mentioned earlier, ensures the existence of smooth probability kernel densities $\psi(x,t)\,\mathrm{d}x$ or $f(x,t)\pi(\mathrm{d}x)$. For normalized initial densities $\psi(x,0)=\psi_0(x)$ and $f(x,0)=f_0(x)$ such that $\int_{\mathcal{X}}\psi_0(x)\,\mathrm{d}x=1$ and $\int_{\mathcal{X}}f_0(x)\pi(\mathrm{d}x)=1$, the convergence is expressed as

$$\mathrm{e}^{t\mathcal{L}^\dagger}\psi_0(x)\xrightarrow{t\to\infty}\pi,\qquad\text{or}\qquad\mathrm{e}^{t\mathcal{L}^*}f_0(x)\xrightarrow{t\to\infty}\mathbb{1},$$

and, by duality, the convergence of observables reads

$$\mathbb{E}_x[\varphi(x_t)]=\left(\mathrm{e}^{t\mathcal{L}}\varphi\right)(x)\xrightarrow{t\to\infty}\int_{\mathcal{X}}\varphi\,\mathrm{d}\pi.$$

We recall that a dagger denotes the L^2-adjoint with respect to the Lebesgue measure, while a star denotes the adjoint in $L^2(\pi)$. There are different approaches to the analysis of the convergence of the law and I will discuss some of them in the remainder of this section.

In a Banach space $E\subset\left\{\phi\in L^1(\pi)\,\middle|\,\int_{\mathcal{X}}\phi\,\mathrm{d}\pi=0\right\}$ (for instance $E=L^2_0(\pi)$), the generic convergence result provides an exponential convergence rate:

$$\|\mathrm{e}^{t\mathcal{L}}\|_{\mathscr{B}(E)}\leqslant C\mathrm{e}^{-\lambda t}.$$

This allows the definition of the inverse operator $\mathcal{L}^{-1}$ and the estimation of its bound. Indeed, the following proposition holds (see Lelièvre and Stoltz (2016)).

Proposition 1. *If* $\|\mathrm{e}^{t\mathcal{L}}\|_{\mathscr{B}(E)} \leqslant C\mathrm{e}^{-\lambda t}$ *holds, then the operator* $\mathcal{L}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$ *is a well-defined operator on* E *and admits the following bound:*

$$\|\mathcal{L}^{-1}\|_{\mathscr{B}(E)} \leqslant \frac{C}{\lambda}. \tag{1.33}$$

1.2.1 Convergence in the elliptic case (overdamped Langevin dynamics)

We have seen that the canonical measure $\nu(\mathrm{d}q) = Z_\nu^{-1}\exp\left(-\beta U(q)\right)\mathrm{d}q$ with $q \in \mathcal{X} \equiv \mathcal{D}$ is the solution of the stationary Fokker-Planck equation $\mathcal{L}^\dagger\psi = 0$, with $\mathcal{L} = \mathcal{L}_{\mathrm{ovd}}$ given by (1.20). A straightforward calculation proves that the generator of the overdamped dynamics is symmetric (and also self-adjoint, see Bakry et al. (2014, Section 3.3)) in $L^2(\nu)$ and can be written as

$$\mathcal{L} = -\beta^{-1}\nabla_q^*\cdot\nabla_q, \qquad \nabla_q^* = -\nabla_q + \beta\nabla U(q) \tag{1.34}$$

Note that we automatically have $\mathcal{L}^*\mathbb{1} = 0$, since in this case $\mathrm{Ker}(\mathcal{L}^*) = \mathrm{Span}(\mathbf{1})$.

Let us now consider the issue of the convergence to the invariant measure. Writing the law of the process as $\psi(q,t)\,\mathrm{d}q = f(q,t)\nu(\mathrm{d}q)$, it is easy to prove that the density f satisfies $\partial_t f = \mathcal{L}f$ and can thus be expressed as $f(t) = \mathrm{e}^{t\mathcal{L}}f_0$, with $f_0 \in L^1(\nu)$ such that $\int_{\mathcal{D}} f_0\,\mathrm{d}\nu = 1$. The convergence to equilibrium reads

$$\mathrm{e}^{t\mathcal{L}}(f_0 - \mathbb{1}) \xrightarrow{t\to\infty} 0. \tag{1.35}$$

We remark that, because of the symmetry of the generator, this problem is analogous to the convergence $\mathrm{e}^{t\mathcal{L}}\left(\varphi - \int_{\mathcal{D}}\varphi\,\mathrm{d}\nu\right) \xrightarrow{t\to\infty} 0$ of an observable.

In order to state quantitative convergence results involving exponential rates, we resort to Poincaré and logarithmic Sobolev inequalities. As we shall see, to make use of these functional inequalities, we need to restrict the class of initial densities f_0 under consideration.

1.2.1.1 Establishing convergence by Poincaré inequalities

Definition 2 (*Poincaré inequality*)**.** The measure ν is said to satisfy a Poincaré inequality with constant $R > 0$ if

$$\forall\varphi \in H^1(\nu)\cap L_0^2(\nu), \qquad \|\varphi\|_{L^2(\nu)}^2 \leqslant \frac{1}{2R}\|\nabla\varphi\|_{L^2(\nu)}^2 \tag{1.36}$$

where

$$L_0^2(\nu) = \left\{\varphi \in L^2(\nu)\;\middle|\;\int_{\mathcal{D}}\varphi\,\mathrm{d}\nu = 0\right\}$$

and

$$H^1(\nu) = \left\{\varphi \in L^2(\nu)\;\middle|\;\partial_i\varphi \in L^2(\nu),\, i \in [1, Nd]\right\}.$$

For the overdamped generator one has

$$\langle -\mathcal{L}\varphi, \varphi\rangle_{L^2(\nu)} = \beta^{-1}\|\nabla\varphi\|^2_{L^2(\nu)}. \tag{1.37}$$

If (1.36) holds, then

$$\langle -\mathcal{L}\varphi, \varphi\rangle_{L^2(\nu)} \geq 2R\beta^{-1}\|\varphi\|^2_{L^2(\nu)}, \qquad \forall \varphi \in L^2_0(\nu), \tag{1.38}$$

thus the fulfillment of a Poincaré inequality implies the coercivity of the operator with respect to the scalar product in $L^2(\mu)$. Since formally one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\|^2_{L^2(\nu)}\right) = \langle \mathrm{e}^{t\mathcal{L}}\varphi, \mathcal{L}\,\mathrm{e}^{t\mathcal{L}}\varphi\rangle_{L^2(\nu)},$$

by a Gronwall inequality, (1.38) in turn implies the contractivity of the associated semigroup.

Proposition 2. *The semigroup $\mathrm{e}^{t\mathcal{L}}$ is contractive with exponential bound*

$$\|\mathrm{e}^{t\mathcal{L}}\|_{\mathscr{B}(L^2_0(\nu))} \leqslant \mathrm{e}^{-2Rt/\beta}$$

if and only if the measure ν satisfies a Poincaré inequality of constant $R > 0$. When a Poincaré inequality holds, the operator $\mathcal{L}$ is invertible, with inverse $\mathcal{L}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$, and

$$\|\mathcal{L}^{-1}\|_{\mathscr{B}(L^2_0(\nu))} \leqslant \frac{\beta}{2R}.$$

The constant R depends on the inverse temperature β^{-1}, the potential and the domain $\mathcal{D}$. A sharp estimate of R can be given only in very specific cases and usually the best one can obtain is an upper bound. For example, when the domain $\mathcal{D}$ is a bounded connected domain such as $\mathcal{D} = (2\pi\mathbb{T})^{Nd}$, one can prove that the canonical measure ν satisfies a Poincaré inequality with the following upper bound:

$$R_\nu < R_{PW}\,\mathrm{e}^{-\beta(U_{\max}-U_{\min})}, \tag{1.39}$$

with $U_{\max} = \max_{q\in\mathcal{D}} U(q)$ and $U_{\min} = \min_{q\in\mathcal{D}} U(q)$ and where R_{PW} is the constant of the standard Poincaré-Wirtinger inequality on $\mathcal{D}$, that is

$$\|\varphi - \varphi_{\mathcal{D}}\|^2_{L^2(\mathcal{D})} \leqslant \frac{1}{2R_{PW}}\|\nabla\varphi\|^2_{L^2(\mathcal{D})}, \quad \varphi_{\mathcal{D}} = \frac{1}{|\mathcal{D}|}\int_{\mathcal{D}} \varphi(q)\,\mathrm{d}q.$$

I refer to Bakry et al. (2014) and Lelièvre and Stoltz (2016) for more details and the proof.

When we deal with product measures, as we will in the Langevin case, a useful result is that Poincaré inequalities can be "tensorized". Indeed, the following proposition holds.

Proposition 3. *When a probability measure is the product of m probability measures each satisfying a Poincaré inequality with constant R_i, $i = 1,\dots,m$, then the product measure also satisfies a Poincaré inequality with constant $R_* = \min\{R_1,\dots,R_m\}$.*

I refer to Section 2.6.2 for the proof.

1.2.1.2 Establishing convergence by logarithmic Sobolev inequalities

Let us start by defining some quantities that will be needed in what follows and let us consider two probability measures π_1 and π_2 defined on $\mathcal{D}$.

Definition 3 (*Relative entropy and Fisher information)*. Given two probability measures π_1 and π_2 such that $\pi_1 \ll \pi_2$, the entropy of π_1 with respect to π_2 is given by

$$\mathcal{H}(\pi_1|\pi_2) \doteq \int_{\mathcal{D}} \ln\left(\frac{\mathrm{d}\pi_1}{\mathrm{d}\pi_2}\right) \mathrm{d}\pi_1 \,,$$

while the Fisher information is given by

$$\mathcal{I}(\pi_1|\pi_2) \doteq \int_{\mathcal{D}} \left|\nabla \ln\left(\frac{\mathrm{d}\pi_1}{\mathrm{d}\pi_2}\right)\right|^2 \mathrm{d}\pi_1 \,.$$

Both functionals are non-negative, and null if and only if $\pi_1 = \pi_2$. Let $f > 0$ be the smooth density of π_1 with respect to π_2. Then we have

$$\mathcal{H}(\pi_1|\pi_2) = \mathrm{Ent}_{\pi_2}(f) = \int_{\mathcal{D}} f \ln f \,\mathrm{d}\pi_2 \,,$$
$$\mathcal{I}(\pi_1|\pi_2) = \mathcal{I}_{\pi_2}(f) = \int_{\mathcal{D}} \nabla f \cdot \nabla \ln f \,\mathrm{d}\pi_2 \,.$$

Note that these integrals might not be finite. We next introduce the total variation norm, which estimates the distance between two probability measures.

Definition 4 (*Total variation norm)*. Given two probability measures π_1 and π_2 their total variation norm is denoted by $\|\cdot\|_{TV}$ and is given by

$$\|\pi_1 - \pi_2\|_{TV} = \sup_{\|\varphi\|_{L^\infty} \leqslant 1} \left| \int_{\mathcal{D}} \varphi \,\mathrm{d}\pi_1 - \int_{\mathcal{D}} \varphi \,\mathrm{d}\pi_2 \right| .$$

If both measures π_1, π_2 have densities $f_1, f_2 \in L^1(\rho)$ with respect to a reference measure ρ, then setting $\varphi = |f_1 - f_2|/(f_1 - f_2)$ we obtain

$$\|\pi_1 - \pi_2\|_{TV} = \int_{\mathcal{D}} |f_1 - f_2| \,\rho(\mathrm{d}q) = \|f_1 - f_2\|_{L^1(\rho)} . \tag{1.40}$$

The log-Sobolev inequality that is about to be introduced relates the relative entropy to the Fisher information.

Definition 5 (*logarithmic Sobolev inequality)*. A probability measure π_2 satisfies a log-Sobolev inequality of constant $R > 0$ (LSI(R)) if

$$\mathcal{H}(\pi_1|\pi_2) \leqslant \frac{1}{2R} \mathcal{I}(\pi_1|\pi_2), \qquad \forall \pi_1 \ll \pi_2 \,, \quad \pi_1 \in L^1(\pi_2)$$

Note that the LSI has some very formal analogies with the Poincaré inequality and one can prove that if a measure ν satisfies an LSI(R) then it satisfies a Poincaré inequality with the same constant $R > 0$. Indeed the Poincaré inequality can be seen as the linearisation of the corresponding LSI, which is thus a stronger inequality. We can now state the convergence result:

Proposition 4. *The solution $\psi(t)$ to the Fokker-Plank equation* (1.23) *satisfies*

$$\mathcal{H}(\psi(t)|\nu) \leqslant \mathcal{H}(\psi_0|\nu)\,\mathrm{e}^{-2Rt/\beta}, \qquad \forall t \geq 0$$

for any initial condition ψ_0 such that $\int_{\mathcal{D}} \psi_0 \,\mathrm{d}q = 1$ and $\mathcal{H}(\psi_0|\nu) < +\infty$ if and only if the measure ν satisfies an LSI(R).

Once the previous convergence result is proved for the problem under consideration, the estimated bound can be transferred to the distance between $\psi(t)$ and ν by the Pinsker-Csiszàr-Kullback inequality $\|\pi_1 - \pi_2\|_{TV}^2 \leqslant 2\mathcal{H}(\pi_1|\pi_2)$ giving

$$\|\psi(t) - \nu\|_{TV}^2 \leqslant 2\mathcal{H}(\psi_0|\nu)\mathrm{e}^{-2Rt/\beta}.$$

If $\psi(t)$ has a density $f(t)$ with respect to the canonical measure ν then by (1.40) we have $\|\psi(t) - \nu\|_{TV} = \|f(t) - \mathbb{1}\|_{L^1(\nu)}$ and

$$\|f(t) - \mathbb{1}\|_{L^1(\nu)}^2 \leqslant 2\,\mathrm{Ent}_\nu(f_0)\,\mathrm{e}^{-2Rt/\beta}.$$

Note that the condition $\mathcal{H}(\psi_0|\nu) < +\infty$ in Proposition 4 becomes in this case $\mathrm{Ent}_\nu(f_0) < +\infty$ and it is satisfied for all initial densities of finite entropy ($f_0 \in (L^1 \log L^1)(\nu)$) which is a larger space than $L^2(\nu)$.

There are several ways to obtain LSIs for measures of the form of the canonical measure ν. In the case of a measure which is a product of m measures all satisfying an LSI, an exact equivalent of Proposition 3 can be stated: the LSI can be "tensorized" and and $R_* = \min\{R_1, \ldots, R_m\}$ (see Gross (1975)).

When the measure ν is not defined on a compact space ($\mathcal{D} = \mathbb{R}^{Nd}$) but the potential $U(q)$ satisfies a strict convexity condition of the form $\nabla^2 U > \widetilde{U}\,\mathrm{Id}$, the Bakry-Emery criterion (Bakry and Émery (1985)) ensures that an LSI($\beta\widetilde{U}$) holds.

Finally, the following result, analogous to (1.39), holds.

Theorem 3 (Holley-Stroock)**.** *If a measure π satisfies an LSI(R) and if $U : \mathcal{D} \to \mathbb{R}$ is a bounded function then $\widetilde{\nu} = \pi\nu$ satisfies an LSI($\widetilde{R}$) with $\widetilde{R} = R\mathrm{e}^{-\beta(\sup U - \inf U)}$.*

1.2.2 Convergence in the hypoelliptic case (Langevin dynamics)

In this section some methods for the study of the convergence of the law of the dynamics of the Langevin type are outlined. These methods can be extended to other dynamics whose generator is hypoelliptic. The generator $\mathcal{L}$ is given by (1.19) and it is rewritten here in a more convenient form as

$$\mathcal{L} = \mathcal{L}_{\mathrm{ham}} - \xi\beta^{-1}\nabla_p^* \cdot \nabla_p, \tag{1.41}$$

where $\nabla_p^* = -\nabla_p + \frac{\beta}{m}p$ is the adjoint of ∇_p with respect to the canonical measure $\mu(\mathrm{d}q, \mathrm{d}p) = Z_\mu^{-1} \exp^{-\beta H(q,p)}$. Let us recall here that μ is a product measure (cfr. (1.3)-(1.5)) and is invariant under the dynamics generated by $\mathcal{L}$ (*i.e.* $\mathcal{L}^\dagger \mu = 0$).

Since the Hamiltonian part of the generator is antisymmetric, the adjoint of $\mathcal{L}$ in $L^2(\mu)$ is

$$\mathcal{L}^* = -\mathcal{L}_{\text{ham}} - \xi\beta^{-1}\nabla_p^* \cdot \nabla_p .$$

Analogously to what is done in the overdamped case, we consider $\psi(t) = f(t)\mu$. The Fokker-Planck equation for f is $\partial_t f = \mathcal{L}^* f$ and its formal solution is $f(t) = \mathrm{e}^{t\mathcal{L}^*} f_0$, with $f(0) = f_0$ such that $\int_{\mathcal{E}} f_0 \mu = 1$, which is defined if $f_0 \in L^1(\mu)$. We want to study the convergence

$$\mathrm{e}^{t\mathcal{L}^*}(f_0 - \mathbb{1}) \xrightarrow{t\to\infty} 0 .$$

In order to state quantitative convergence results involving exponential rates, we consider some functional frameworks for which we need to restrict the class of initial densities f_0 under consideration.

It is important to emphasize that Langevin dynamics becomes singular both in the limit $\xi \to 0$, where it reduces to the Hamiltonian dynamics (with respect to which the canonical measure is not ergodic), and in the limit $\xi \to \infty$, where it converges to the overdamped dynamics. It is therefore expected that the convergence rate degrades in both these cases. The techniques sketched in this section allow to quantify the degradation of the convergence rate for very small or very large values of the friction parameter ξ. A careful application of the general framework of hypocoercivity in $H^1(\mu)$ can be found in Hairer and Pavliotis (2008) for the Hamiltonian limit and in Leimkuhler et al. (2015) for the overdamped limit.

1.2.2.1 Establishing convergence by hypocoercivity estimates

As we saw in Section 1.1.4.4, the Langevin generator fails to be elliptic. This is due to the fact that the rank of the matrix of the coefficients of the second-order derivative terms in $\mathcal{L}$ is not maximum, which is another way of acknowledging the fact that the noise term is degenerate (it acts only on the momentum variables). Nevertheless, by Hörmander theorem, we are able to recover hypoellipticity (*i.e.* ellipticity in the space spanned by the appropriate commutators).

Unlike the overdamped case (see (1.37)), the absence of second-order derivatives in the position variables also prevents the Langevin generator from being coercive. To retrieve some dissipation in q, we need a method that plays the role of the Hörmander condition which "reshuffles" the derivative terms by means of commutators and makes up for the ones that are missing, henceforth leading to some coercivity.

The main ingredient of hypocoercive estimates, which corresponds to the Hörmander condition for hypoellipticity, is a modified scalar product which introduces mixed derivatives in q and p and retrieves coercivity (dissipation) in q through some commutators identities. This idea was already present in Talay (2002) and has been later generalised in Villani (2009). It is reminiscent of the introduction of a mixed term in q and p in the Lyapunov function (1.28). More precisely, in the approach abstracted in Villani (2009) the following scalar product is introduced on $H^1(\mu)$:

$$\langle\langle f, g\rangle\rangle = \langle f, g\rangle + a\langle\nabla_p f, \nabla_p g\rangle + c\langle\nabla_q f, \nabla_q g\rangle + b\Big(\langle\nabla_p f, \nabla_q g\rangle + \langle\nabla_q f, \nabla_p g\rangle\Big), \quad (1.42)$$

where $\langle\cdot,\cdot\rangle$ denotes the standard scalar product in $L^2(\mu)$ and a, b, c are such that

$$a, c > 0, \qquad \text{and} \qquad ac - b^2 > 0,$$

so that the positivity of the bilinear form $s(u,v) = \langle (\nabla v)^T, S\nabla u\rangle$, with $S = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$, is guaranteed.

The scalar product (1.42) is different from, but equivalent to the canonical scalar product in $H^1(\mu)$. The modified H^1 scalar product (1.42) allows to obtain coercivity in the Hilbert space $H^1(\mu) \cap L^2_0(\mu)$, where, analogously to what done in the overdamped case, we have introduced the following space:

$$L^2_0(\mu) = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \,\mathrm{d}\mu = 0 \right\}. \tag{1.43}$$

If $\nu(\mathrm{d}q)$ satisfies a Poincaré inequality (and thanks to the equivalence of the norms), this allows to obtain an exponential decay estimate in $H^1(\mu)$ with rate κ_ξ. The result is then "transferred" in $L^2(\mu)$ by hypoelliptic regularization (see Hérau (2007), Hairer and Pavliotis (2008), Villani (2009), Lelièvre and Stoltz (2016)).

By choosing $(a,b,c) = \xi(\bar a, \bar b, \bar c)$ which gives the correct norm in the Hamiltonian limit, and $(a,b,c) = \xi^{-1}(\bar a, \bar b, \bar c)$ which gives the correct norm in the overdamped limits, we can make explicit the dependence of the decay rate κ_ξ from the friction parameter. A careful analysis of the scaling of κ_ξ shows that there exists a $\bar\kappa > 0$ such that

$$\kappa_\xi = \bar\kappa \min(\xi, \xi^{-1}).$$

The overall convergence result is thus the following:

Theorem 4 (Hypocoercive decay estimate)**.** *Assume either that the domain $\mathcal{D}$ is bounded, or that there exists $\rho > 0$ such that $|\nabla^2 U| \leqslant \rho(1 + |\nabla U(q)|)$ for all $q \in \mathcal{D}$. Assume also that a Poincaré inequality holds for $\nu(\mathrm{d}q)$. Then, there exist $C, \bar\kappa > 0$ such that, for any $\xi > 0$*

$$\forall t \geq 0, \qquad \forall f \in L^2_0(\mu), \qquad \|\mathrm{e}^{t\mathcal{L}^*} f\|_{L^2(\mu)} \leqslant C\,\mathrm{e}^{-\bar\kappa \min(\xi,\xi^{-1})t} \|f\|_{L^2(\mu)}. \tag{1.44}$$

It follows that $\mathcal{L}^*$ is invertible in $L^2_0(\mu)$, with

$$(\mathcal{L}^*)^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}^*}\,\mathrm{d}t, \qquad \|(\mathcal{L}^*)^{-1}\|_{\mathscr{B}(L^2_0(\mu))} \leqslant \frac{C}{\bar\kappa \min(\xi, \xi^{-1})},$$

where the equality on the left holds in $\mathscr{B}(L^2_0(\mu))$.

It emerges very clearly from (1.44) that in both the Hamiltonian and overdamped limits, the decay is apparent only at long time scales, namely t/ξ in the Hamiltonian case (the fluctuation/dissipation mechanism acts so slowly that energy diffusion is observable only at long times) and ξt in the overdamped case (the fluctuation/dissipation mechanism acts so fast that the momenta are continuously randomized so that the noise manages to act on the positions only at long times).

With some careful computations, the exponential decay rate can be made explicit also in terms of the other physical constants and for intermediate values of ξ. These calculations become somewhat simpler if we adopt the degenerate norm $a = b = c$ so that

$$\langle\langle f, f\rangle\rangle_a = \|f\|^2_{L^2(\mu)} + a\|(\nabla_p + \nabla_q) f\|^2_{L^2(\mu)}, \tag{1.45}$$

instead of the norm induced by (1.42). Decay estimates by means of this degenerate norm are provided in Chapter 2 for a perturbed Langevin dynamics.

All the results obtained for $e^{t\mathcal{L}^*}$ can be adapted to $e^{t\mathcal{L}}$, by changing the sign of b in (1.42) and considering observables in $L^2_0(\mu)$, the space of $L^2(\mu)$ functions with zero mean defined in (1.43). An application of this technique to the convergence of $e^{t\mathcal{L}}$ in the nonequililbrium case is presented in Section 2.3.1.

The hypocoercive estimate of the exponential decay relies on the fulfillment of the Poincaré inequality by $\nu(\mathrm{d}q)$. Indeed, one could see it as an "extension" of the Poincaré inequality in the case of hypoelliptic operators. By analogy, an entropy functional is introduced to make use of log-Sobolev inequalities for hypoelliptic operators, as recalled in the next section.

1.2.2.2 Establishing convergence by hypocoercive entropy estimates

The computations performed in $H^1(\mu)$ can be adapted to prove the decay of an entropy functional similar to the one used for LSIs.

As in the elliptic case, the interest of the entropic approach is that one can consider initial conditions in larger functional spaces. The general strategy is presented in Villani (2009) (Section 6). These computations can be simplified for Langevin-type dynamics (see Olla and Letizia (2017), Appendix D).

We introduce the entropy functional

$$\mathscr{E}(f) = \int_{\mathcal{E}} f \ln f \, \mathrm{d}\mu + \int_{\mathcal{E}} \frac{\nabla f^T S \nabla f}{f} \, \mathrm{d}\mu,$$

where $S \in \mathbb{R}^{2Nd\times 2Nd}$ is a constant non-negative symmetric matrix. The functional $\mathscr{E}(f)$ combines the relative entropy and a generalization of the Fisher information. Since $\mathscr{E}(\mathbb{1}) = 0$, it is expected that $\mathcal{E}(f)$ converges to 0 for $t \to \infty$. The convergence result is the following:

Theorem 5. *Assume that $\nabla^2 U$ is a bounded and measurable function on $\mathcal{D}$. Then there exist a non-negative symmetric matrix $S \in \mathbb{R}^{2Nd\times 2Nd}$ and a constant $\alpha > 0$ such that, for all $t \geq 0$*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathscr{E}(f(t))\right] \leqslant -\alpha \int_{\mathcal{E}} \frac{|\nabla f(t)|^2}{f(t)} \, \mathrm{d}\mu.$$

If in addition $\nu(\mathrm{d}q)$ satisfies an LSI, then there exists $\kappa = \bar{\kappa}\min(\xi, \xi^{-1}) > 0$, $\bar{\kappa} > 0$, such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathscr{E}(f(t))\right] \leqslant -\kappa \, \mathscr{E}(f(t)), \qquad \forall t \geq 0.$$

Thus for all initial densities $f_0 \in L^1(\mu)$ such that $\int_{\mathcal{E}} f_0 \, \mathrm{d}\mu = 1$ and $\mathscr{E}(f_0) < +\infty$, it holds

$$0 \leqslant \mathscr{E}(f(t)) \leqslant \mathscr{E}(f_0) \mathrm{e}^{-\bar{\kappa}\min(\xi,\xi^{-1})t}, \qquad \forall t \geq 0. \tag{1.46}$$

An application of this methodology can be found in Appendix 2.6.3. We wish to stress that the convergence result (1.46) relies crucially on the fulfillment of an LSI by the measure $\nu(\mathrm{d}q)$. This requirement may be hard to met in some cases, rendering difficult (if not impossible, see *e.g.* Section 2.3.3) the application of this convergence result.

1.2.2.3 Direct $L^2(\pi)$ estimates

Explicit results on exponential convergence rates for the semigroup $e^{t\mathcal{L}}$ can be obtained by an approach introduced in Dolbeault et al. (2009), Dolbeault et al. (2015) and more recently revisited by Grothaus and Stilgenbauer (2014). Presenting this approach for Langevin dynamics and considering all operators as defined on $L^2(\mu)$ allows to simplify several arguments in the procedure.

The approach is based on the introduction of a modified scalar product on $L^2(\mu)$ (see (1.47) below), which is such that $\mathcal{L}$ is dissipative in all variables, whereas it would be dissipative only in the p variables with the standard $L^2(\mu)$ scalar product. To define this new functional, we consider the decomposition of the operator $\mathcal{L}$ as in (1.41), namely as the sum of a Hamiltonian part and a fluctuation/dissipation part. We introduce the orthogonal projector $\Pi : L^2(\mu) \to L^2(\nu)$ on the subspace of functions depending only on positions, defined as

$$(\Pi g)(q) = \int_{\mathbb{R}^{Nd}} g(q,p)\, \kappa(\mathrm{d}p),$$

which maps $L^2_0(\mu)$ functions into $L^2_0(\nu)$ functions. We also introduce the operator

$$A \doteq [1 + (\mathcal{L}_{\mathrm{ham}}\Pi)^*(\mathcal{L}_{\mathrm{ham}}\Pi)]^{-1}(\mathcal{L}_{\mathrm{ham}}\Pi)^* = \beta^{-1}\left(1 - \frac{1}{m}\mathcal{L}_{\mathrm{ovd}}\right)^{-1}(-\Pi\mathcal{L}_{\mathrm{ham}})$$

where $\mathcal{L}_{\mathrm{ovd}}$ is the generator of the overdamped dynamics in (1.34). Note that $\Pi A = A$ by construction. Given $a(\xi) \in (0,1)$, the modified norm is defined as

$$\mathcal{E}(g) = \frac{1}{2}\|g\|_{L^2(\mu)} + a(\xi)\langle Ag, g\rangle_{L^2(\mu)}. \tag{1.47}$$

It is proved by Lemma 2 in Section 2.5.3 that, for all $\varphi \in L^2(\mu)$, the operator A is such that

$$\|A\varphi\|_{L^2(\mu)} \leqslant \frac{1}{2}\|(1-\Pi)\varphi\|^2_L(\mu), \quad \|\mathcal{L}_{\mathrm{ham}}A\varphi\|_{L^2(\mu)} \leqslant \|(1-\Pi)\varphi\|^2_L(\mu).$$

The first on the left of the above inequalities implies that the operator A is bounded in $L^2(\mu)$ with $\|A\|_{\mathscr{B}(L^2(\mu))} \leqslant 1$. Therefore, the equivalence between the scalar product induced by polarization from (1.47) and the canonical scalar product on $L^2(\mu)$ immediately follows, provided $|a(\xi)| < 1/2$.

We assume that the potential $U(q)$ is a smooth function defined on a compact space $\mathcal{D}$, hence the measure $\nu(\mathrm{d}q)$ satisfies a Poincaré inequality. Considering the time-derivative of $\mathcal{E}(e^{t\mathcal{L}}f)$, by means of some careful computation and thanks to a coercivity property, one proves an inequality relating the entropy and its time derivative along the trajectory of the process. Then, by a Gronwall inequality and the equivalence of the norms, one obtains the following exponential convergence result:

Theorem 6. *Assume that $U(q)$ is a smooth function defined on a compact space $\mathcal{D}$. Then there exist $C, \bar{\kappa} > 0$ such that for all $t \geq 0$*

$$\forall \varphi \in L^2_0(\mu), \qquad \|e^{t\mathcal{L}}\varphi\|_{L^2(\mu)} \leqslant Ce^{-\bar{\kappa}\min(\xi,\xi^{-1})t}\|\varphi\|_{L^2(\mu)}.$$

It follows that the inverse of the generator $\mathcal{L}^{-1} = -\int_0^{+\infty} \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$ *is well-defined on* $L^2_0(\mu)$ *and has the following upper bound:*

$$\|\mathcal{L}^{-1}\|_{\mathscr{B}(L^2_0(\mu))} \leqslant \frac{C}{\bar{\kappa}} \max(\xi, \xi^{-1}).$$

Note that this result can be extended by duality to the case of the semigroup $\mathrm{e}^{t\mathcal{L}^*}$. In this case, the convergence result reads

$$\forall f \in L^2_0(\mu), \qquad \|\mathrm{e}^{t\mathcal{L}^*} f\|_{L^2(\mu)} \leqslant C\mathrm{e}^{-\bar{\kappa}\min(\xi,\xi^{-1})}\|f\|_{L^2(\mu)},$$

and, if f_0 is such that $\int_{\mathcal{E}} f_0\,\mathrm{d}\mu = 1$, it can be rewritten as

$$\|\mathrm{e}^{t\mathcal{L}^*} f - \mathbb{1}\|_{L^2(\mu)} \leqslant C\mathrm{e}^{-\bar{\kappa}\min(\xi,\xi^{-1})}\|f - \mathbb{1}\|_{L^2(\mu)}.$$

An extension of this methodology to the nonequilibrium case is presented in Sections 2.3.2 and 2.5.3.

1.2.3 Convergence in weighted L^∞-spaces

As anticipated at the end of Section 1.1.5.1, another tool for the analysis of the long-time behavior of general SDEs is based on Lyapunov functions. Indeed, the present section has to be seen as a follow-up of Section 1.1.5.1.

Consider the dynamics (1.9) generated by the operator $\mathcal{L}$, the associated semigroup T_t defined in (1.14) and the Lyapunov functions W_n we introduced in Section 1.1.5.1 (see (1.28) and the preceding discussion). In the Lyapunov functional framework, the convergence of the process to its stationary state is measured in the following weighted spaces:

$$L^\infty_W(\mathcal{X}) = \left\{ \varphi \in \mathcal{X} \;\middle|\; \|\varphi\|_{L^\infty_W} < +\infty \right\},$$

where we introduced the weighted norm

$$\|\varphi\|_{L^\infty_W} = \left\| \frac{\varphi}{W} \right\|_{L^\infty},$$

and

$$L^\infty_{W,0}(\mathcal{X}) = \left\{ \varphi \in L^\infty_W(\mathcal{X}) \;\middle|\; \int_{\mathcal{X}} \varphi\,\mathrm{d}\pi = 0 \right\}.$$

The convergence result is the following:

Theorem 7 (Convergence in L^∞_W)**.** *Under the hypotheses of Theorem 2, the semigroup* T_t *admits a unique invariant probability measure* π*. This measure is such that*

$$\int_{\mathcal{X}} W_n\,\mathrm{d}\pi < +\infty, \qquad \forall n \leqslant 0.$$

Moreover, there exist $C, \kappa > 0$ *such that*

$$\|\mathrm{e}^{t\mathcal{L}}\varphi\|_{L^\infty_W} \leqslant C\mathrm{e}^{-\kappa t}\|\varphi\|_{L^\infty_W}, \qquad \forall \varphi \in L^\infty_{W,0}(\mathcal{X}).$$

As a consequence, the inverse of the generator, $\mathcal{L}^{-1} = -\int_0^{+\infty} \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$ *is well-defined on* $L^\infty_{W,0}(\mathcal{X})$ *and admits the following bound:*

$$\|\mathcal{L}^{-1}\|_{\mathscr{B}(L^\infty_{W,0}(\mathcal{X}))} \leqslant \frac{C}{\kappa}.$$

We refer to Hairer and Mattingly (2011) for the proof and to Lelièvre and Stoltz (2016) for more insights[3].

Since the invariant measure integrates all the Lyapunov functions, by duality we deduce that similar convergence results can be obtained with analogous procedures for the Fokker-Planck semigroup S_t, since the exponential decay of T_t is equivalent to that of S_t.

The main interest of the weighted L^∞ estimates is that they do not require specific assumptions on the type of dynamics considered and can thus be applied in many contexts, included those of nonequilibrium. An example is outlined in Section 2.2.1.

1.3 Nonequilibrium perturbations of equilibrium dynamics

We study in this section the effects of the application of some external forcings to the system, supposing that they perturb the equilibrium dynamics and keep the system in a nonequilibrium stationary state. We have discussed the mathematical definition of irreversibility in Section 1.1.5.2. From a physical viewpoint, the irreversibility of the evolution manifests itself through the presence of currents, which are constant in average at the stationary state and represent the response of the system to the perturbation. This response is defined on the basis of the physical context of the problem, in analogy with macroscopic thermodynamics.

In the linear response regime, *i.e.* for small forcings, the magnitude of the average response is proportional to the magnitude of the external forcing by the transport coefficient α, also called susceptibility. The definition of transport coefficients usually relies on an analogy with the macroscopic evolution equations. Therefore, the introduction of the (small) perturbations in the general Langevin dynamics allows the computation of α as the ratio of the average response to the the magnitude of the perturbation.

We will consider two main types of techniques for the computation of transport properties:

(i) *equilibrium techniques* based on Green-Kubo formulas, which are integrated correlation functions of the general form

$$\alpha = \int_0^{+\infty} \mathbb{E}_\pi\Big(\phi(x_t)\psi(x_0)\Big)\,\mathrm{d}t. \tag{1.48}$$

[3] In fact, these authors prove the discrete version of Theorem 7. In this case the evolution is observed at integer multiples of a reference time t_0. The proof in the continuous case follows quite straightforwardly.

Here, ϕ and ψ are two appropriately chosen observables with zero average with respect to π. The expectation is taken with respect to initial conditions distributed according to the equilibrium probability measure π and for all realizations of this dynamics;

(ii) *steady-state nonequilibrium techniques* where a forcing mechanism is permanently applied to the system. In this framework we may distinguish two subcategories: boundary driven techniques, where the external forcing is imposed only on boundary regions, and bulk driven dynamics, where the perturbation is experienced by all the particles of the system. In both cases, an appropriate flux is measured, and the transport coefficient is obtained as the ratio of the average flux to the magnitude of the external forcing. However, it is in general impossible to prove the existence and uniqueness of an invariant probability measure for boundary driven dynamics, except for very simple geometries such as one dimensional atom chains.

In what follows, we consider two paradigmatic perturbations of the Langevin dynamics (1.10): a mechanical forcing, through the application of a non-gradient force, and a thermal forcing, by taking into account models of chains whose edges are in contact with two thermostats at different temperatures T_L and T_R.

1.3.1 Non-gradient drift terms

Consider the following perturbed Langevin dynamics for a system subjected to a periodic potential U:

$$\begin{cases} \mathrm{d}q_t = M^{-1} p_t \, \mathrm{d}t, \\ \mathrm{d}p_t = \Big(-\nabla U(q_t) + \tau F \Big) \mathrm{d}t - \xi M^{-1} p_t \, \mathrm{d}t + \sqrt{\dfrac{2\xi}{\beta}} \, \mathrm{d}W_t, \end{cases} \tag{1.49}$$

where $(q_t, p_t) \in \mathbb{T}^d \times \mathbb{R}^d$, $F \in \mathbb{R}^d$, with $|F| = 1$ and $\xi > 0$ is the intensity of the coupling with the thermostats. Note that the constant force of magnitude $\tau > 0$ does not derive from a periodic potential. The existence and uniqueness of the invariant measure can be proved in this case by the general method of Section 1.1.5.1 as outlined in Section 2.2.1.

Physically it is expected that the application of a non-zero constant force in a given direction induces a non-zero velocity in this direction. The response of the system is therefore the observable

$$V_{\|}(q,p) = F \cdot M^{-1} p \,, \tag{1.50}$$

which is the average projected velocity in the direction of the force. The transport coefficient, called the mobility in this framework, is defined as as the ratio of the average of $V_{\|}$ with respect to the stationary measure to the magnitude τ of the force, in the limit of small values of τ (see (1.61) below).

1.3.2 Fluctuation terms with different temperatures

Consider a one dimensional chain of N atoms of unitary masses, with positions $q = (q_1, \ldots, q_N)$ and momenta $p = (p_1, \ldots, p_N)$. The right end is free, while the left

end of the chain is attached to a wall ($q_0 = 0$ and $p_0 = 0$ at all times), to remove the translation invariance of the whole system. Denoting by u the nearest-neighbor interaction potential, the Hamiltonian reads

$$H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + U(q), \qquad U(q) = u(q_1) + \sum_{i=1}^{N-1} u(q_{i+1} - q_i). \tag{1.51}$$

The evolution is governed by Hamiltonian dynamics in the bulk ($i \in \{2,\dots,N-1\}$), while Langevin dynamics at both edges impose the temperatures $T_{\mathrm{L}}, T_{\mathrm{R}}$ at the left and right boundaries respectively:

$$\begin{cases} \mathrm{d}q_i = p_i \,\mathrm{d}t, \\ \mathrm{d}p_i = \Big(u'(q_{i+1} - q_i) - u'(q_i - q_{i-1})\Big)\mathrm{d}t, \qquad i \neq 1, N, \\ \mathrm{d}p_1 = \Big(u'(q_2 - q_1) - u'(q_1)\Big)\mathrm{d}t - \xi p_1 \,\mathrm{d}t + \sqrt{2\xi T_{\mathrm{L}}}\,\mathrm{d}W_t^1, \\ \mathrm{d}p_N = -u'(q_N - q_{N-1})\,\mathrm{d}t - \xi p_N \,\mathrm{d}t + \sqrt{2\xi T_{\mathrm{R}}}\,\mathrm{d}W_t^N. \end{cases} \tag{1.52}$$

The existence and uniqueness of a smooth invariant probability measure for the dynamics (1.52) can be proved under appropriate assumptions on the interaction potential u. In particular, some (super)quadratic growth at infinity is required to allow the compactness of the resolvent of the generator of the dynamics, which implies the existence of a spectral gap and the consequent exponential decay to the stationary state (see Eckmann et al. (1999*b*), Rey-Bellet and Thomas (2002*a*,*b*), Carmona (2007). There are also situations where the existence of a stationary measure cannot be proved. An interesting example of model for which the resolvent fails to be compact is studied in Hairer and Mattingly (2009). In this case, the system does not relax exponentially fast to the stationary state.

At equilibrium, that is when $T_{\mathrm{L}} = T_{\mathrm{R}} = T$, the dynamics (1.52) reduces to a standard Langevin dynamics, whose invariant measure is the Gibbs measure relative to the Hamiltonian (1.51), at inverse temperature $\beta^{-1} = k_{\mathrm{B}}T$. When $T_{\mathrm{L}} \neq T_{\mathrm{R}}$, there is in general no simple expression of the invariant measure. In this case, one expects that some energy in the form of heat flows through the system from the hot to the cold region, with a consequent entropy production (Eckmann et al. (1999*a*), Bernardin and Olla (2014)). The local conservation of energy in the bulk is expressed by the following equation:

$$d\varepsilon_i + \Big(j_i - j_{i-1}\Big)\mathrm{d}t = 0\,, \qquad 2 \leqslant i \leqslant N-1\,,$$

where

$$\varepsilon_i(q,p) = \frac{p_i^2}{2} + \frac{1}{2}\Big(u(q_{i+1} - q_i) + u(q_i - q_{i-1})\Big), \qquad 2 \leqslant i \leqslant N-1\,,$$

is the total energy of the particle at site i and the quantity j_i is the energy flux from site i to site $i+1$. A simple computation (see *e.g.* Lepri et al. (2003)) shows that this quantity is given by the following expression:

$$j_i(q,p) = -u'(q_{i+1} - q_i)\frac{p_i + p_{i+1}}{2}\,.$$

The response of the system in this case is the sum J of the local currents j_i

$$J(q,p) = \sum_{i=1}^{N-1} j_i(q,p). \tag{1.53}$$

The transport coefficient, called the thermal conductivity in this case, is defined as the energy flux J divided by the temperature difference $\Delta T = T_L - T_R$ (see (1.62) below).

1.3.3 Linear response for nonequilibrium dynamics

We present in this section a formal study of the stationary properties of the nonequilibrium dynamics (1.49) and (1.52). The various assumptions we make need to be justified for the particular dynamics considered in applications.

We denote by

$$\mathcal{L}_\eta = \mathcal{L}_0 + \eta \widetilde{\mathcal{L}}$$

the generator of the nonequilibrium dynamics on the state-space $\mathcal{X}$, where $\mathcal{L}_0$ is the generator of the reference equilibrium dynamics and $\widetilde{\mathcal{L}}$ is the generator of the perturbation. We assume that the reference dynamics has a unique invariant measure ψ_0.

Let us give the expressions of the above quantities for the two examples presented in Sections 1.3.1 and 1.3.2.

(i) For the case $\eta = \tau$ in (1.49), the generator of the reference dynamics (obtained by setting $F = 0$) and that of the perturbation respectively read

$$\mathcal{L}_0 = M^{-1} p \cdot \nabla_p - \nabla U \cdot \nabla_p - \xi \left(M^{-1} p \cdot \nabla_p - \frac{1}{\beta} \Delta_p \right), \qquad \widetilde{\mathcal{L}} = F \cdot \nabla_p, \tag{1.54}$$

while the invariant probability measure ψ_0 is the following Gibbs measure:

$$\psi_0(q,p)\, \mathrm{d}q\, \mathrm{d}p = Z^{-1} \exp\left(-\beta \left[\frac{1}{2} p^T M^{-1} p + U(q) \right] \right) \mathrm{d}q\, \mathrm{d}p.$$

(ii) As for the dynamics (1.52) with $T_\mathrm{L} = T + \Delta T$ and $T_\mathrm{R} = T - \Delta T$, we set $\eta = \Delta T$. The reference equilibrium dynamics is the Langevin dynamics (1.52) with the two thermostats at the boundaries at the same temperature T. Its generator reads

$$\mathcal{L}_0 = \sum_{i=1}^{N} \left[p_i \partial_{q_i} - \left(\partial_{q_i} U \right) \partial_{p_i} \right] - \xi \left(p_1 \partial_{p_1} + p_N \partial_{p_N} \right) + \xi T \left(\partial_{p_1}^2 + \partial_{p_N}^2 \right),$$

and the invariant probability measure has a density $\psi_0(q,p) = Z^{-1} \mathrm{e}^{-H(q,p)/T}$, where H is given by (1.51). The generator of the perturbation is

$$\widetilde{\mathcal{L}} = \xi (\partial_{p_1}^2 - \partial_{p_N}^2).$$

1.3.3.1 Invariant measure of the nonequilibrium dynamics

We denote by ψ_η the density of the invariant measure of the nonequilibrium dynamics with respect to the Lebesgue measure. The existence and uniqueness of the invariant measure for both the dynamics (1.49) and (1.52) have been proved in Section 2.2.1 and in Carmona (2007), respectively. The smoothness of ψ_η stems from the hypoellipticity of $\mathcal{L}_\eta^\dagger$, that can be proved by Hörmander theorem, see Section 1.1.4.4.

The function ψ_η can be defined through the following requirement:

$$\int_{\mathcal{E}} \left(\mathcal{L}_0 + \eta\widetilde{\mathcal{L}}\right)\varphi\,\psi_\eta = 0\,, \tag{1.55}$$

for $\varphi \in C_0^\infty(\mathcal{E})$, or, equivalently, it can be defined as the solution of the stationary Fokker-Planck equation $\mathcal{L}_\eta^\dagger \psi_\eta = 0$, see Section 1.1.5.

Denoting by ψ_0 the reference measure, we write ψ_η as

$$\psi_\eta = f_\eta\,\psi_0,$$

where f_η is a positive smooth function, which is, by (1.55), the unique solution of the stationary Fokker-Planck equation

$$\mathcal{L}_\eta^* f_\eta = \left(\mathcal{L}_0^* + \eta\widetilde{\mathcal{L}}^*\right) f_\eta = 0, \qquad \int_{\mathcal{E}} f_\eta \psi_0 = 1. \tag{1.56}$$

It is convenient to work in the Hilbert space $L^2(\psi_0)$ endowed with the scalar product

$$\langle f, g\rangle_{L^2(\psi_0)} = \int_{\mathcal{E}} f(x) g(x)\,\psi_0(x)\,\mathrm{d}x.$$

and to consider its subspace

$$L_0^2(\psi_0) = \left\{ f \in L^2(\psi_0) \;\middle|\; \int_{\mathcal{E}} f\,\psi_0 = 0 \right\}.$$

Under appropriate assumptions on the perturbation $\widetilde{\mathcal{L}}$, the following result gives the expression of the function f_η as a power series in η when η is sufficiently small.

Theorem 8. *Assume that* (1.56) *has a unique solution, and that*

(a) $\mathcal{L}_0$ *is such that* $\mathrm{Ker}(\mathcal{L}^*) = \mathrm{Span}(\mathbf{1})$ *and* $\mathcal{L}_0^*$ *is invertible on* $L_0^2(\psi_0)$*;*

(b) $\widetilde{\mathcal{L}}$ *is such that* $\mathrm{Ran}(\widetilde{\mathcal{L}}^*) \subset L_0^2(\psi_0)$ *and* $\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^*$ *is bounded on* $L_0^2(\psi_0)$*.*

Denote by r the spectral radius of the bounded operator $\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^* \in \mathcal{B}(L_0^2(\psi_0))$*, i.e.*

$$r = \lim_{n\to+\infty} \left\| \left(\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^* \right)^n \right\|^{1/n}_{\mathcal{B}(L_0^2(\psi_0))}.$$

Then, for $|\eta| < r^{-1}$, *the unique solution of* (1.56) *can be written as*

$$f_\eta = \left(1 + \eta\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^*\right)^{-1}\mathbf{1} = \left(1 + \sum_{n=1}^{+\infty}(-\eta)^n\left[\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^*\right]^n\right)\mathbf{1}. \tag{1.57}$$

We refer to Lelièvre and Stoltz (2016) for the proof of Theorem 8 and make here a few comments.

We remark that the measure ψ_η is indeed a probability measure. In particular, the normalization constant of ψ_η does not depend on η. This is due to the fact that $f_\eta - \mathbf{1} \in L^2_0(\psi_0)$ and thus

$$\int_{\mathcal{E}} \psi_\eta = \int_{\mathcal{E}} \psi_0 = 1.$$

The first assumption in the above theorem ensures that the equilibrium dynamics has good ergodic properties. In fact, by Proposition 1, the invertibility of the generator is a consequence of the exponential decay to the "existing and unique" stationary measure, and the uniqueness of the measure implies its ergodicity, as discussed *e.g.* in Rey-Bellet (2006*a*, Section 3.2). The second assumption ensures that the perturbation has the right regularity properties and it is not too strong.

The solution of (1.56), which is unique by hypothesis, is provided by (1.57) when the series on the right-hand side of (1.57) converges. Indeed

$$\mathcal{L}_\eta^* f_\eta = (\mathcal{L}_0^* + \eta\widetilde{\mathcal{L}}^*)f_\eta = \mathcal{L}_0^*\left[1 + \eta\,(\mathcal{L}_0^*)^{-1}\,\widetilde{\mathcal{L}}^*\right]f_\eta = 0 \quad \Rightarrow \quad \left[1 + \eta\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^*\right]f_\eta = \mathbf{1}$$

The convergence of the series is guaranteed by the convergence in $\mathcal{B}(L^2_0(\psi_0))$ of the series

$$\sum_{n=1}^{+\infty}(-\eta)^n\left[\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^*\right]^n,$$

which is ensured by the condition $|\eta| r < 1$.

1.3.3.2 Linear response and correlation functions

Linear response properties are first order deviations (in η) of average properties computed in the nonequilibrium steady state, that are compared to the same average property computed at equilibrium. Averages in the nonequilibrium steady state are obtained by the integration of an observable h with respect to the measure ψ_η

$$\mathbb{E}_\eta[h] = \int_{\mathcal{E}} h(x)\,\psi_\eta(x)\,\mathrm{d}x = \langle h, f_\eta\rangle_{L^2(\psi_0)},$$

while equilibrium averages, denoted by $\mathbb{E}_0[h]$, correspond to an integration with respect to ψ_0.

Given a perturbation of magnitude η, and denoting by R the generic response of the systems (so that R stands for $V_\parallel$ or J according to the context) transport

coefficients are defined as

$$\alpha = \lim_{\eta \to 0} \frac{\mathbb{E}_\eta(R) - \mathbb{E}_0(R)}{\eta}. \tag{1.58}$$

This is the definition of the transport coefficient based on the linear response of nonequilibrium dynamics. Note that $\mathbb{E}_0[R] = 0$ in both our paradigmatic examples. Substituting the series expansion of f_η in (1.58) one automatically obtains

$$\alpha = \lim_{\eta \to 0} \frac{\mathbb{E}_\eta[R]}{\eta} = \int R \mathrm{f}_1 \psi_0, \tag{1.59}$$

where

$$\mathrm{f}_1 = -\left(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1}\right)^* \mathbf{1}.$$

is the linear term in η in the expansion (1.57) of f_η.

In practice, if $\mathbb{E}_0(R) = 0$, an estimate of α can be obtained by choosing a value of η sufficiently small, approximating $\mathbb{E}_\eta[R]$ by a very long time average over one realization of the dynamics (to approximate (1.7)), and dividing this quantity by η. In order to check that the value of η is indeed small enough to neglect higher order contributions, it is possible for instance to check the linearity of the response by computing approximations of $\mathbb{E}_\eta[R]$ with η replaced by, say, $\eta/2$ or 2η.

1.3.3.3 The Green-Kubo formula for transport coefficients

Using $-(\widetilde{\mathcal{L}}\mathcal{L}_0^{-1})^*$ and $-\mathcal{L}_0^{-1}$ defined by[4]

$$-\mathcal{L}_0^{-1} = \int_0^{+\infty} \mathrm{e}^{t\mathcal{L}_0} \, \mathrm{d}t,$$

both seen as operators on $L_0^2(\psi_0)$, linear response properties can be rephrased using correlation functions. In fact, introducing the conjugate response function, formally defined as

$$S = \widetilde{\mathcal{L}}^* \mathbf{1},$$

we obtain

$$\alpha = \int_{\mathcal{E}} R \mathrm{f}_1 \, \psi_0 = -\int_{\mathcal{E}} \left[\mathcal{L}_0^{-1} R\right]\left[\widetilde{\mathcal{L}}^* \mathbf{1}\right] \psi_0 = \int_0^{+\infty} \mathbb{E}_0\Big(R(x_t) S(x_0)\Big) \mathrm{d}t, \tag{1.60}$$

where the expectation is taken over all initial conditions distributed according to ψ_0, and over all realizations of the reference equilibrium dynamics. Note that the expression of the conjugate response function S is determined by the applied perturbation $\widetilde{\mathcal{L}}$, not by the response function R.

Equation (1.60) expresses the equivalence between the transport coefficient obtained by the linear response of nonequilibrium dynamics and the one obtained by the Green-Kubo formula (1.48).

[4] The fact that $-\mathcal{L}_0^{-1}$ is well-defined is justified by the existence and uniqueness of ψ_0 for the reference equilibrium dynamics, and the exponential decay towards it, see Proposition 1.

The autocorrelation of R is recovered for perturbations such that $S \propto R$. For the two examples presented in Sections 1.3.1 and 1.3.2, and studied in greater detail below (see Section 2.2.2 and Chapters 4 and 5), $S(q,p) = \beta R(q,p) = \beta F \cdot M^{-1} p$ for (1.49), while $S(q,p) = \xi \beta^2 (p_1^2 - p_N^2)$ for (1.52). In the latter case, S is not directly related to the response function defined in (1.53) and the corresponding Green-Kubo formula is a time integrated correlation between two different quantities.

Note that the implication of the Green-Kubo formula is remarkable, in that it shows that a nonequilbirium property (*i.e.* the transport coefficient) can be obtained by equilibrium simulations.

1.3.3.4 Applications

We apply the general definitions provided in Section 1.3.3.2 to the two prototypical examples introduced in Sections 1.3.1 and 1.3.2, and obtain the definition of the mobility of a system described by a Langevin equation with a mechanical forcing term, and that of the thermal conductivity of one dimensional chains.

Considering the dynamics (1.49), the linear response of the projected velocity (1.50) allows to define the mobility in terms of the autocorrelation of $V_{\|}$ for a system evolving according to the reference dynamics with generator $\mathcal{L}_0$ defined in (1.54):

$$\alpha = \lim_{\tau \to 0} \frac{\mathbb{E}_\tau \left[F \cdot M^{-1} p \right]}{\tau} = \beta \int_0^{+\infty} \mathbb{E}_0 \Big((F \cdot M^{-1} p_t)(F \cdot M^{-1} p_0) \Big) \, \mathrm{d}t. \tag{1.61}$$

As of the dynamics (1.52), the thermal conductivity is defined by the linear response of the energy current :

$$\kappa = \lim_{\Delta T \to 0} \frac{\mathbb{E}_{\Delta T}[J]}{\Delta T} = -\beta^2 \xi \int_0^{+\infty} \int_{\mathcal{E}} \left(\mathrm{e}^{-t\mathcal{L}_0} J \right) (p_1^2 - p_N^2) \psi_0 \, \mathrm{d}t. \tag{1.62}$$

Some (non trivial) manipulations allow to rewrite the above correlation in terms of the energy current autocorrelation (see for instance Bernardin and Olla (2005), Kundu et al. (2009)):

$$\kappa = 2\beta^2 \int_0^{+\infty} \mathbb{E} \Big(j_{i+1,i}(q_t, p_t) J(q_0, p_0) \Big) \, \mathrm{d}t = \frac{2\beta^2}{N-1} \int_0^{+\infty} \mathbb{E} \Big(J(q_t, p_t) J(q_0, p_0) \Big) \, \mathrm{d}t, \tag{1.63}$$

where the equalities hold for any $i = 1, \ldots, N-1$.

1.4 Thermal transport

Fourier's law is an empirical law, which is assumed to hold close to equilibrium. It was first proposed by Joseph Fourier in 1808 in an attempt to describe the spontaneous transfer of thermal energy from a hot to a cold region in a solid to reach a uniform distribution of heat. It thus allows to discuss the relaxation to equilibrium of isolated systems through the diffusive behavior of the energy. In a nonequilibrium framework, it can also be used to describe transport properties

in the steady state of a system put in contact with two (infinite) reservoirs at different temperatures. In this case, there is a net energy flow j from the hotter to the colder reservoir which, at the stationary state, satisfies the homogeneous equation $\nabla \cdot j = 0$.

Denoting by $T = T(x,t)$ the function that expresses the temperature of the system at a given location x and a given time t (*i.e.* its local temperature), its evolution follows a macroscopic continuity equation

$$c_v(T)\,\partial_t T = \nabla \cdot j\,,$$

where c_v is the heat capacity and j is the energy current density, *i.e.* the amount of heat transported through the unit surface per unit time. The energy current density, or flow, is expressed by Fourier's law, which relates it to the temperature gradient by a constant κ, that depends on the temperature and is an intrinsic physical property of the system

$$j = -\kappa(T)\nabla T\,. \tag{1.64}$$

We stress that the definition of the quantities in (1.64) relies on the possibility of defining a local temperature $T(x,t)$ for a macroscopically small but microscopically large volume at each site x for each time t (local equilibrium hypothesis).

1.4.1 Validity of Fourier's law and thermodynamic limit of the conductivity

In actual materials, when the temperature varies slowly on the microscopic scale, Fourier's Law has been largely confirmed by experiments. For common three dimensional solids, it is observed by numerical simulations that Fourier's law appropriately describes the behavior of the system. In particular, the thermal conductivity does not depend on the system size, and so, it is a well-defined thermodynamic quantity.

On the contrary, the validity of Fourier's law is questionable in one dimensional systems. Indeed, despite many attempts to derive it from microscopic dynamics, both numerical and analytical results from a number of studies over the last 50 years suggest that Fourier's law may not be universally valid in low-dimensional systems, which may display anomalous transport properties (see *e.g.* Lepri et al. (2003), Dhar (2008)). In particular, there is often no thermodynamic limit for the thermal conductivity in these models, as we shall briefly discuss below. This finding is consistent with some experimental results on the length dependence of the thermal conductance of carbon nanotubes Wang et al. (2007), Chang et al. (2008).

It is still unclear which are the necessary and/or sufficient conditions for anomalous thermal transport. In a recent work Komorowski and Olla (2017) provide a rigorous result of a normal diffusion of energy in a non acoustic[(5)] chain of harmonic oscillators whose dynamics is perturbed by a random local exchange of momentum that conserves both energy and momentum. A normal conductivity has also been numerically observed and indisputably confirmed in the case

[(5)] In non-acoustic chains, the interaction potential depends only on the bending of the chain which is defined as $-\Delta q_x = -[(q_{x+1} - q_x) - (q_x - q_{x-1})]$.

of interacting rotor chains, where the interaction depends only on the relative angles between consecutive atoms, so that the total (angular) momentum is conserved (Gendelman and Savin (2000), Yang and Hu (2005), Gendelman and Savin (2005)). On the other hand, in many numerical experiments on one-dimensional momentum-conserving anharmonic chains it has been observed that $j \sim N^{-(1-\alpha)}$ with $\alpha > 1$ (see Dhar (2008) and reference therein).

Beyond diverging finite-size thermal conductivity, anomalous transport in low-dimensional systems manifests itself by a number of features such as slow decay in the equilibrium time correlation functions like the integrand in (1.63), superdiffusive propagation of small energy perturbations or nonlinear temperature profiles. While it is expected that the exponent controlling the decay of the current-current correlation $t^{1-\delta}$ and the one controlling the divergence of the thermal conductivity N^{α} are equal, it is also expected that the all exponents describing these processes (which are different but share a common physical origin), are related to each other and independent of the microscopic details of the dynamics. This suggests the their value could be dictated by a scaling of the underlying dynamics and that the exponents could be universal. In particular the conductivity divergence exponent could be 1/3. Recently, Spohn (2014) developped an approach to make precise by formal computations how the space time correlations of the conserved quantities should decay in time. He considered a system governed by Euler equations in the hydrodynamic limit and heuristically derived the equations for fluctuations around this limit. He explained how the possibly anomalous decay, slower than diffusive, is to be related to the anomalous transport properties as quantified by the divergence of the thermal conductivity.

1.4.2 Some facts on the thermodynamic limit of the conductivity in one dimensional systems

We define the thermal conductivity for a one-dimensional chain of oscillators of size N as the average energy current (*i.e.* the quantity (1.53) divided by the length of the chain) divided by the temperature gradient $\Delta T/N$, assuming a linear temperature profile (see (1.62) and (1.63)):

$$\begin{aligned}\kappa_N &= \lim_{\Delta T\to 0} \frac{\langle J/(N-1)\rangle_{\Delta T}}{\Delta T/N} = \lim_{\Delta T\to 0} \frac{N}{N-1}\frac{\langle J\rangle_{\Delta T}}{\Delta T} \\ &= 2\beta^2 \frac{N}{N-1}\int_0^{+\infty}\sum_{i=1}^{N-1}\mathbb{E}_0\Big(j_{2,1}(q_t,p_t)j_{i+1,i}(q_0,p_0)\Big)\,\mathrm{d}t. \end{aligned} \tag{1.65}$$

Fourier's law is satisfied if κ_N has a finite limit as the system size goes to infinity, that is

$$\overline{\kappa} = \lim_{N\to+\infty} \kappa_N < +\infty. \tag{1.66}$$

The limit (1.66) is often studied using numerical experiments, except in simple analytical cases corresponding to harmonic potentials (see Basile et al. (2016) and references therein). The following facts have been established to date, by theoretical or numerical arguments:

(i) for harmonic systems, it was proved by Rieder et al. (1967) (even in the presence of a harmonic pinning potentials), that $\kappa_N = cN$. This is established by an analytical proof showing that the value of J is independent of N. It is also expected that $\kappa_N \sim N$ for integrable systems, which posses as many invariants of the dynamics as the number of degrees of freedom (see Zotos (2002)). A famous example of such a system is the Toda lattice (see Toda (1979)), which corresponds to a chain of oscillators with the interaction potential ($b > 0$)

$$v(r) = \frac{\mathrm{e}^{-br} + br - 1}{b^2}.$$

For this potential, it is observed numerically that J is constant, thus $\kappa_N \sim N$ (see *e.g.* Hatano (1999) for a study of the thermal conductivity of a diatomic Toda chain).

(ii) the limit (1.66) is numerically observed for rotor chains, which are systems like (1.52) with an interaction potential given by $u(r) = u_0(1 - \cos(r))$ (see the references in Chapter 4). It is also observed for systems with pinning potentials for which the interaction potential and/or the pinning potential is anharmonic. This can be rigorously proved for systems subjected to specific random perturbations for which the momentum of the system is not conserved while energy is (typically, changing the sign of the velocities at random times) as shown in Bernardin and Olla (2011, 2014).

(iii) for chains with generic anharmonic potentials (non-integrable systems) and no pinning potentials, the conductivity is observed to diverge as N^α with $0 < \alpha < 1$. The addition of a stochastic perturbation preserving both the total momentum and the energy (such as exchanging the velocities of neighboring atoms) does not change qualitatively the picture. Such perturbations, introduced in Olla et al. (1993), aim at modeling the effect of the nonlinearities of the potential, and also ensure that the only invariants of the dynamics are the energy and the total momentum. For harmonic interactions, it can be proved theoretically that $\kappa_N \sim \sqrt{N}$ (Basile et al. (2006)), while for anharmonic interactions $\kappa_N \leqslant C\sqrt{N}$ (Basile et al. (2009)).

(iv) another stochastic perturbation is that of assigning random masses to the atoms of the systems. This type of perturbation has been introduced by Rubin and Greer (1971) in the case of harmonic systems with free boundary conditions. It has been proved that $\kappa_N \sim N^{-1/2}$ for fixed boundary conditions (Casher and Lebowitz (1971), Ajanki and Huveneers (2011)) while it decreases exponentially when some harmonic pinning potential is considered. Depending on the boundary conditions, other scaling regimes can be obtained (Dhar (2001)). There are also several studies on the influence of mass disorder on anharmonic chains (see *e.g.* Dhar and Lebowitz (2008)), but the general conclusion is that mass disorder *per se* is not sufficient to prevent the divergence of the thermal conductivity.

A question related to the convergence (1.66) is whether the dynamics of infinite dimensional chains of oscillators is such that the energy current autocorrelation (an appropriate generalization of the integrand in the rightmost term of (1.65)) is an integrable function of time or not. Bernardin and Olla (2011) prove the existence of the limit (1.66) for an anharmonic chain perturbed by independent random flips of the sign of the velocities. In a more recent article,

Bernardin et al. (2015) extended the result to three different models, namely: a chain of coupled pinned anharmonic oscillators, a chain of rotors and a harmonic chain with random (positive) pinnings.

1.5 Numerical aspects

Computing very high dimensional integrals like those referring to dynamic (1.14) or thermodynamic (1.8) quantities is a significant mathematical challenge: analytical integration being definitely out of the picture, the only possible approach is numerical estimation.

Given the high number of dimensions, deterministic quadrature methods based on tensorized sets of one-dimensional quadrature points are impossible to apply. In fact, if we denote by N_{1D} the number of one-dimensional grid points, the total number of quadrature nodes typically is of the order of N_{1D}^{Nd}, with N as large as possible (ideally $N \sim 10^{23}$, in real simulation a record value is 10^9) and Δt as small as possible (see below), so these methods might be too expensive already for small systems composed of only a handful of particles. Purely stochastic methods are very difficult to apply too. In fact, because of the potential U, the canonical measure typically have highly concentrated modes, separated by large areas of very low probability, thus i.i.d. sampling is typically impossible. Therefore, both ensemble averages (1.8) and path averages (1.14) are approximated by ergodic averages over a collection of samples which are realizations of random variables distributed according to a target probability measure.

Sampling configurations (q, p) according to the canonical measure μ (1.3) can be performed by independently sampling positions according to ν given by (1.4) and momenta according to κ given by (1.5). Sampling momenta is straightforward, since they constitute a vector of n i.i.d. normal variables of variance $m\beta^{-1}$. The actual issue is therefore to sample positions from ν.

Given an observable φ and an initial condition x_0, the typical estimator of its canonical average is the time average over a realization of a stochastic dynamics (1.9) with respect to which the target probability measure is ergodic[6], that is

$$\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(x_s)\,\mathrm{d}s. \tag{1.67}$$

When the generator of the stochastic dynamics is elliptic or hypoelliptic and the invariant measure of the process π admits a positive density with respect to the Lebesgue measure (which is the case for Langevin and overdamped Langevin dynamics (see Section 1.1.4.4),) a result by Kliemann (1987) ensures the existence of the following ergodic limit for the continuous dynamics:

$$\widehat{\varphi}_t \xrightarrow[t\to+\infty]{\text{a. s.}} \mathbb{E}_\pi[\varphi] = \int_{\mathcal{X}} \varphi(x)\pi(\mathrm{d}x),$$

for any initial condition $x_0 \in \mathcal{X}$ and the consequent uniqueness of the invariant measure π.

[6] Linking up with the discussion in Section 1.1.3, the average (1.67) is the stochastic analogous of (1.6) for the Hamiltonian dynamics.

Note that the configurations of the continuous dynamics on the right end side of (1.67) are in general not independent. This can be seen by comparing the expression of the asymptotic variance of the estimator $\widehat{\varphi}_t$ with that of the asymptotic variance of the estimator $\widehat{\varphi}_N^{\text{i.i.d.}} = \frac{1}{N}\sum_{n=1}^N \varphi(x^n)$ computed on a sample of i.i.d. random variables distributed according to π. These expressions are

$$\begin{aligned} \zeta_\varphi^2 &\doteq \lim_{t\to+\infty} t\,\mathrm{Var}_\pi(\widehat{\varphi}_t) &&= -2\int_{\mathcal{X}} (\mathcal{L}^{-1}\Pi\varphi)\Pi\varphi\,\mathrm{d}\pi, \\ \zeta_{\varphi,i.i.d.}^2 &\doteq \lim_{t\to+\infty} N\,\mathrm{Var}_\pi(\widehat{\varphi}_N^{\text{i.i.d.}}) &&= \int_{\mathcal{X}} (\Pi\varphi)^2\,\mathrm{d}\pi, \end{aligned} \tag{1.68}$$

where $\Pi\varphi = \varphi - \int_{\mathcal{X}} \varphi\,\mathrm{d}\pi$ and the expectation in (1.68) is computed with respect to an initial condition $x_0 \sim \pi$. For ζ_φ^2 to be well-defined one must have that the Poisson equation

$$-\mathcal{L}\Phi = \Pi\varphi$$

has a solution in $L^2(\pi)$, thus that $\varphi \in L^2(\pi)$ and $\mathcal{L}^{-1}$ is well-defined in $L_0^2(\pi)$, see Proposition 1. In this case, a central limit theorem holds

$$\sqrt{t}\,\widehat{\Pi\varphi_t} \xrightarrow[t\to+\infty]{d} \mathcal{N}(0,\zeta_\varphi^2), \tag{1.69}$$

for every initial condition distributed following π. An identical result is obtained by Bhattacharya (1982) for initial conditions not distributed according to the invariant measure.

We can compare the two variances through the quantity $\theta_{\text{corr}} = \zeta_\varphi^2/\zeta_{\varphi,i.i.d.}^2$, which can be interpreted as a correlation time. This correlation time is bounded by the inverse of the spectral gap of $-\mathcal{L}$ that is $\theta_{\text{corr}} \leqslant 1/\lambda$, thus the larger the spectral gap, the faster the convergence of $\widehat{\varphi}_t$ to $\mathbb{E}_\pi[\varphi]$ (see *e.g.* Lelièvre and Stoltz (2016, Sect. 3.1.2) for details). Because of the metastability of the underlying dynamics, the correlation time is often very large.

1.5.1 Discretization of the continuous dynamics

In order to numerically evaluate the estimator (1.67), a time discretization of the stochastic dynamics (1.9) is required. We fix a time step $\Delta t > 0$ and denote by x^n the approximation of the continuous solution $x_{n\Delta t}$ at time $t_n = n\Delta t$. We consider an explicit numerical scheme, where the solution at time t_{n+1} is obtained from the approximate solution at time t_n as

$$x^{n+1} = \phi_{\Delta t}(x^n, G^n). \tag{1.70}$$

Here G^n is a sequence of i.i.d. random Gaussian variables with covariance matrix Id_{Nd} and $\phi_{\Delta t}$ is a one-step explicit numerical scheme for the generic dynamics (1.9), such as the Euler-Maruyama scheme

$$x^{n+1} = x^n + b(x^n)\,\Delta t + \sqrt{\Delta t}\,\sigma(x^n)\,G^n.$$

The one-step transition operator associated with the generic scheme (1.70) is defined as

$$(P_{\Delta t}\varphi)(x) = \mathbb{E}(\varphi(x^{n+1}) \mid x^n = x),$$

and it constitutes the discrete counterpart of the semigroup $\mathrm{e}^{\Delta t \mathcal{L}}$.

The time average $\widehat{\varphi}_t$ in (1.67) is then approximated by

$$\widehat{\varphi}_{N_{\mathrm{iter}},\Delta t} = \frac{1}{N_{\mathrm{iter}}} \sum_{n=0}^{N_{\mathrm{iter}}-1} \varphi(x^n), \tag{1.71}$$

where the sample $(x^n)_{n\in[0,N_{\mathrm{iter}}-1]}$ is constructed from a given initial condition $x^0 = x_0$ by iteratively applying the numerical scheme $\phi_{\Delta t}$.

For the estimator (1.71) to be a good estimator, there must be a probability measure $\pi_{\Delta t}$ which is ergodic with respect to the discrete dynamics,

$$\widehat{\varphi}_{N_{\mathrm{iter}},\Delta t} \xrightarrow[N_{\mathrm{iter}}\to+\infty]{\text{a. s.}} \int_{\mathcal{X}} \varphi \,\mathrm{d}\pi_{\Delta t}. \tag{1.72}$$

The measure $\pi_{\Delta t}$ depends on the discretization and must be sufficiently close to the invariant measure of the associated continuous dynamics. Moreover, the discrete dynamics must be consistent, in the sense that

$$\int_{\mathcal{X}} \varphi \,\mathrm{d}\pi_{\Delta t} \xrightarrow[\Delta t\to 0]{} \mathbb{E}_\pi[\varphi]. \tag{1.73}$$

Given a numerical scheme $\phi_{\Delta t}$, the first issue is therefore to prove the validity of (1.72), that is the existence of an invariant measure $\pi_{\Delta t}$ which is ergodic with respect to the numerical scheme[7]. This can be done by resorting to results such as Theorem 2 (see also the review in Lelièvre and Stoltz (2016, § 3.2.2) and references therein), while the discrete version of Theorem 7 (see Meyn and Tweedie (2009) and Hairer and Mattingly (2011)) ensures the exponential convergence of the law of x^n to $\pi_{\Delta t}$, for almost all initial conditions $x^0 \in \mathcal{X}$.

Once one proves the existence of a $\pi_{\Delta t}$ and its ergodicity with respect to $\phi_{\Delta t}$, another property to consider is the variance of the scheme. Indeed, considering the variance-bias trade-off, the best scheme among those satisfying (1.72) and (1.73) is the one that represents the best compromise between a sufficiently small value of the variance and not too large a value of the bias.

It can be proved (see Meyn and Tweedie (2009, Chapter 17) and Lelièvre and Stoltz (2016, § 3.2.2)) that the expression of the asymptotic variance in the discrete case for all initial conditions $x^0 \in \pi_{\Delta t}$ is

$$\begin{aligned}\zeta^2_{\varphi,\Delta t} &\doteq \lim_{N_{\mathrm{iter}}\to+\infty} N_{\mathrm{iter}} \mathrm{Var}_{\pi_{\Delta t}}\left(\widehat{\varphi}_{N_{\mathrm{iter}},\Delta t}\right) \\ &= 2\int_{\mathcal{X}} (\Pi_{\Delta t}\varphi)(\mathrm{Id} - P_{\Delta t})^{-1}(\Pi_{\Delta t}\varphi)\,\mathrm{d}\pi_{\Delta t} - \zeta^2_{\varphi,i.i.d.,\Delta t},\end{aligned} \tag{1.74}$$

where $\Pi_{\Delta t}\varphi = \varphi - \int_{\mathcal{X}} \varphi \,\mathrm{d}\pi_{\Delta t}$ and $\zeta^2_{\varphi,i.i.d.,\Delta t} = \int_{\mathcal{X}} (\Pi_{\Delta t}\varphi)^2 \,\mathrm{d}\pi_{\Delta t}$ is the asymptotic variance of an i.i.d. sample from $\pi_{\Delta t}$. If the Poisson equation

$$(\mathrm{Id} - P_{\Delta t})\Phi = \Pi_{\Delta t}\varphi \tag{1.75}$$

[7] The ergodicity of π with respect to the continuous dynamics does not guarantee that of $\pi_{\Delta t}$ with respect to the the numerical scheme.

has a solution Φ in $L^2(\pi_{\Delta t})$, then the asymptotic variance (1.74) is well-defined. A typical way for ensuring that $\Phi \in L^2(\pi_{\Delta t})$ is to prove that it belongs to some subspace B of $L^2(\pi_{\Delta t})$, a property which is implied by the well-posedness of (1.75) in the functional space B. A sufficient condition for the well-posedness of (1.75) is that $\mathrm{Id} - P_{\Delta t}$ is invertible on B and φ belongs to B (hence *a fortiori* the right hand side $\Pi_{\Delta t}\varphi \in B$). One convenient functional space to this end is $B \equiv L^{(\Delta t),\infty}_{W,0}(\mathcal{X})$, where

$$L^{(\Delta t),\infty}_{W,0}(\mathcal{X}) = \left\{ f \in L^{\infty}_{W}(\mathcal{X}) \;\middle|\; \int_{\mathcal{X}} f \, d\pi_{\Delta t} = 0 \right\},$$

which is indeed a subspace of $L^2(\pi_{\Delta t})$ when $W \in L^2(\pi_{\Delta t})$. In fact, $\mathrm{Id} - P_{\Delta t}$ is invertible in this space, as one can prove by a result similar to that contained in Corollary 2.26 of Lelièvre and Stoltz (2016).

When the variance is well-defined, analogously to (1.69), the following central limit theorem holds

$$\sqrt{T}\,\widehat{\Pi\varphi}_{N_{\mathrm{iter}},\Delta t} \xrightarrow[T\to+\infty]{d} \mathcal{N}(0, \zeta^2_{\varphi,\Delta t}), \tag{1.76}$$

where $T = N_{\mathrm{iter}}\Delta$, see Meyn and Tweedie (2009, Theorem 17.4.4). The comparison between two variances is interpreted as a measure of correlation as in the continuous case. We may write

$$\zeta^2_{\varphi,\Delta t} = N^{\mathrm{corr}}_{\mathrm{iter}}\, \zeta^2_{\varphi,i.i.d.,\Delta t} \ , \tag{1.77}$$

where the parameter $N^{\mathrm{corr}}_{\mathrm{iter}}$ indicates the number of iterations to be performed to have a new configuration sufficiently decorrelated from the previous. This parameter depends on the time step and the observable φ. A relationship holds between the correlation measures of the continuous and discrete dynamics and, in the limit of small Δt it can be proved that

$$\theta_{\mathrm{corr},\varphi} = N^{\mathrm{corr}}_{\mathrm{iter}}\Delta t + \mathcal{O}(\Delta t^2), \tag{1.78}$$

as discussed after (1.80).

1.5.1.1 Error analysis on time averages

There are three main commonly-used notions to be considered when evaluating the quality of a scheme. A numerical scheme is :

– *consistent*, if the local discretization error (error over one time step) converges to zero for $\Delta t \to 0$ with at least $\mathcal{O}(\Delta t)$;

– *convergent*, if the global discretization error over a fixed time interval $[0, T]$ converges to 0 in some sense as $\Delta t \to 0$;

– *stable*, if it reproduces qualitatively the long-time behavior of the exact solution.

These notions are used also in the deterministic case. In the stochastic case, they all have a weak and a strong form, which deals respectively with probability distributions and trajectories convergence. On a finite time-horizon T, one

considers weak and strong convergence based on the definition of two types of errors

$$\varepsilon^{\text{weak}}_{\Delta t,T,\varphi} \doteq \sup_{0\leqslant n\leqslant T/\Delta t} |\mathbb{E}(\varphi(x^n)) - \mathbb{E}(\varphi(x_{n\Delta t}))| \leqslant C_\varphi(T)\,\Delta t^\alpha\,,$$
$$\varepsilon^{\text{strong}}_{\Delta t,T;p} \doteq \sup_{0\leqslant n\leqslant T/\Delta t} \mathbb{E}\Big(|x^n - x_{n\Delta t}|^p\Big)^{1/p} \leqslant C_\varphi(T)\,\Delta t^\beta\,.$$

and it can be proved that $\alpha \geq \beta$, see *e.g.* Kloeden and Platen (1999).

Given a numerical scheme, the weak order α is determined by the formal equality

$$P_{\Delta t} = \mathrm{e}^{\Delta t\mathcal{L}} + \mathcal{O}(\Delta t^{\alpha+1}), \tag{1.79}$$

for a small enough Δt.

The error bound on a finite time horizon T depends not only on the time step, but also on a constant C which diverges as $T \to +\infty$. Thus, in the computation of long-time averages, what matters more is the stability of a given numerical scheme.

Two types of errors measure the quality of the approximation $\widehat{\varphi}_{N_{\text{iter}},\Delta t}$ of $\mathbb{E}_\pi[\varphi]$: a statistical and a systematic error. In fact we may write

$$\widehat{\varphi}_{N_{\text{iter}},\Delta t} - \mathbb{E}_\pi(\varphi) \;=\; [\widehat{\varphi}_{N_{\text{iter}},\Delta t} - \mathbb{E}_{\pi_{\Delta t}}(\varphi)] + [\mathbb{E}_{\pi_{\Delta t}}(\varphi) - \mathbb{E}_\pi(\varphi)]. \tag{1.80}$$

The first term in square brackets represents the statistical error due to the finiteness of the number of iterations. By the central limit theorem (1.76), in the asymptotic regime $N_{\text{iter}} \to +\infty$ the statistical error behaves like a Gaussian random variable of zero mean. Since this error is of order $T^{-1/2}$, where $T = N_{\text{iter}}\Delta t$ is the physical simulation time, it can thus be reduced by increasing N_{iter}. In practice, the asymptotic regime is attained when $N_{\text{iter}} \gg N^{\text{corr}}_{\text{iter}}$. Nevertheless the correlation number can be so large that the asymptotic regime may not be attained within the values of N_{iter} which are achievable by computer simulations.

The second term in square brackets in (1.80) represents the systematic error (or bias) and is due to discretization. It decreases for $\Delta t \to 0$, while it persists for $N_{\text{iter}} \to +\infty$. The bias is essentially a measure of the difference between π and $\pi_{\Delta t}$. Typically,

$$\int_{\mathcal{X}} \varphi\,\mathrm{d}\pi_{\Delta t} = \int_{\mathcal{X}} \varphi\,(1+\Delta t^p f)\,\mathrm{d}\pi + \mathcal{O}(\Delta t^{p+1}), \tag{1.81}$$

for some smooth function f, some integer $p \geq 1$ and a sufficiently small Δt. It usually holds that $p \geq \alpha$, where α is defined in (1.79) as the weak error of the numerical scheme.

Let us now compare the magnitudes of the two errors. The statistical error can be expressed as a standard deviation, which in the asymptotic regime is

$$\widehat{\varphi}_{N_{\text{iter}},\Delta t} - \mathbb{E}_{\pi_{\Delta t}}(\varphi) \sim \frac{\zeta_{\varphi,\Delta t}}{\sqrt{N_{\text{iter}}}}\,G, \qquad G \sim \mathcal{N}(0,1),$$

by the central limit theorem (1.76). Hence, for the bias to be of order of the statistical error, one must have that

$$N_{\text{iter}} \sim \frac{\zeta^2_{\varphi,\Delta t}}{\Delta t^{2p}}.$$

This estimation and the fact that the asymptotic regime is difficult to attain, imply that the statistical error often dominates the bias in actual simulations.

By (1.77) and (1.78), we have that

$$\frac{\zeta_{\varphi,\Delta t}}{\sqrt{N_{\text{iter}}}} = \frac{\sqrt{N_{\text{iter}}^{\text{corr}}}}{\sqrt{N_{\text{iter}}}}\,\zeta_{\varphi,i.i.d.\,,\Delta t} = \frac{\zeta_{\varphi,i.i.d.\,,\Delta t}}{\sqrt{N_{\text{iter}}\Delta t/\theta_{\text{corr},\varphi}}} + \mathcal{O}(\sqrt{\Delta t}),$$

which shows how the effect of correlation is basically that of decreasing the integration time. Thus the greater the correlation, the higher the number of iterations to attain a certain level of precision.

Finally, we remark that the asymptotic variance $\zeta^2_{\varphi,\Delta t}$ of time averages computed by the discrete dynamics is related to first order in Δt to the asymptotic variance ζ^2_φ of time averages computed on the continuous process. In fact, to ensure weak consistency, the one-step numerical scheme $P_{\Delta t}$ must be such that

$$\frac{\mathrm{Id} - \mathrm{P}_{\Delta \mathrm{t}}}{\Delta t}\varphi = -\mathcal{L}\varphi + \mathcal{O}(\Delta t),$$

so that substituting in (1.74), one has $\lim_{\Delta t\to 0}\Delta t\,\zeta^2_{\varphi,\Delta t} = \zeta^2_\varphi$ (see Lelièvre and Stoltz (2016, Theorem 5.6)). Linking up to the discussion before (1.74), this implies that the value of the variance can be decreased by a judicious choice of the continuous model while a good choice of the numerical scheme can improve the bias.

1.5.1.2 Nonequilibrium: error analysis on the transport coefficient

In presence of a perturbation $\eta \neq 0$, the expansion in (1.81) is a two-parameters expansion. A result proved in Leimkuhler et al. (2015, Theorem 3.4) in the case of mechanical forcing states that

$$\int_{\mathcal{X}} \varphi \,\mathrm{d}\pi_{\eta,\Delta t} = \int_{\mathcal{X}} \varphi \left(1 + \eta f_{0,1} + \Delta t^p f_{p,0} + \eta \Delta t^p f_{p,1}\right) \mathrm{d}\pi + \mathcal{O}(n^2, \Delta t^{p+1}),$$

where $f_{p,0}$ and $f_{p,1}$ are smooth functions, $f_{0,1}$ is the unique solution of the Poisson equation

$$\mathcal{L}_0^* f_{0,1} = -\widetilde{\mathcal{L}}^* \mathbf{1},$$

and Δt and η are sufficiently small. This result holds also for other forms of perturbation, namely thermal forcing. Note that $f_{0,1}$ is the linear response term of the invariant measure when $\eta \neq 0$, that is the function f_1 defined in (1.59), while $f_{p,0}$ is the function f in (1.81) and accounts for the effects of discretization.

As for the transport coefficient (1.58), its discrete counterpart is given by

$$\alpha_{\Delta t} = \lim_{\eta\to 0} \frac{\mathbb{E}_{\eta,\Delta t}(R) - \mathbb{E}_{0,\Delta t}(R)}{\eta},$$

where $\mathbb{E}_{\eta,\Delta t}(\cdot)$ denotes the average with respect to the measure $\pi_{\eta,\Delta t}$. Even when the function R, which describes the response of the system to the perturbation, is such that its average with respect to the unperturbed measure in the continuous

case is null, that is $\mathbb{E}_{\eta=0}(R) = 0$, this property is usually not conserved under discretization. It follows that

$$\alpha_{\Delta t} = \alpha_0 + \Delta t^p \int_{\mathcal{X}} R\, f_{\alpha,1}\, \mathrm{d}\pi + \mathcal{O}(\Delta t^{p+1}),$$

thus the error on the transport coefficient due to discretization is of order p.

1.5.2 Numerical schemes for Langevin dynamics

Many numerical schemes have been proposed for Langevin dynamics since the BBK scheme proposed by Brünger et al. (1984), among them splitting schemes; see Section 5.3.1.1 for an application of the BBK scheme and Lelièvre and Stoltz (2016) for references on more general numerical schemes. The strategy of the splitting techniques is that of decomposing the global dynamics in elementary dynamics that are analytically integrable and whose elementary generators possibly commute. To this aim, it is convenient to introduce the following elementary generators:

$$A = \frac{p}{m} \cdot \nabla_q, \qquad B = -\nabla U(q) \cdot \nabla_p, \qquad C = -\frac{p}{m} \cdot \nabla_p + \beta^{-1} \Delta_p,$$

defined in a space of smooth functions, so that the overall generator of the Langevin dynamics (1.10) can be written as

$$\mathcal{L}_0 = A + B + \xi C,$$

where the three operators A, B and C commute pairwise. Note that in this notation $\mathcal{L}_{\mathrm{ham}} = A + B$ and $C \equiv \mathcal{L}_{\mathrm{FD}}$ is the Ornstein-Uhlenbeck generator.

There are two main classes of splitting schemes: Lie-Trotter and Strang. A Lie-Trotter scheme is generated by transition operators such as

$$P_{\Delta t}^{Z,Y,X} = \mathrm{e}^{\Delta t Z}\, \mathrm{e}^{\Delta t Y}\, \mathrm{e}^{\Delta t X},$$

and are of weak order 1. Different versions can be obtained from $(A, B, \xi C)$ by all possible permutations[8] (Z, Y, X). There are six possible operators, whose invariant measures may have different properties. For instance, the Lie-Trotter scheme associated with the one-step transition operator

$$P_{\Delta t}^{B,A,\xi C} = \mathrm{e}^{\Delta t B}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\xi \Delta t C},$$

is

$$\begin{aligned} \tilde{p}^{n+1} &= p^n + \Delta t\, \nabla U(q^n), \\ q^{n+1} &= q^n + \Delta t\, \frac{\tilde{p}^{n+1}}{m}, \\ p^{n+1} &= \alpha_{\Delta t}\, \tilde{p}^{n+1} + \sqrt{\beta^{-1}(1 - \alpha_{\Delta t}^2)}\, G^n, \end{aligned} \tag{1.82}$$

[8] When two operators do not commute, one can resort to the Baker-Campbell-Hausdorff formula, which allows to express the exponential of a sum of generator as the product of the exponentials of the two operators at a cost of a first order error. In fact, suppose $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ with $[\mathcal{L}_1, \mathcal{L}_2] \neq 0$, then

$$\mathrm{e}^{\Delta t \mathcal{L}} = \mathrm{e}^{\Delta t \mathcal{L}_1} \mathrm{e}^{\Delta t \mathcal{L}_2} + \mathcal{O}(\Delta t).$$

where $\alpha_{\Delta t} = \exp(-\xi \Delta t/m)$ comes from the explicit analytic integration of the elementary Ornstein-Uhlenbeck process and G^n are independent and identically distributed Gaussian random vectors whose covariance matrix is the identity matrix[9].

Strang splitting schemes are obtained by composing the elementary transition operators in the following general form:

$$P_{\Delta t}^{Z,Y,X} = \mathrm{e}^{\Delta t Z/2}\, \mathrm{e}^{\Delta t Y/2}\, \mathrm{e}^{\Delta t X}\, \mathrm{e}^{\Delta t Y/2}\, \mathrm{e}^{\Delta t Z/2}.$$

They are symmetric and of weak order 2. There are six possible different schemes. We give here just an example of the Strang splitting scheme associated with

$$P_{\Delta t}^{A,B,\xi C,B,A} = \mathrm{e}^{\Delta t A/2}\, \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\xi \Delta t C}\, \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\Delta t A/2},$$

which is

$$\begin{aligned}
q^{n+1/2} &= q^n + \frac{\Delta t}{2}\frac{p^n}{m},\\
p^{n+1/2} &= p^n + \frac{\Delta t}{2}\nabla U(q^{n+1/2}),\\
\tilde{p}^{n+1/2} &= \alpha_{\Delta t}\, p^{n+1/2} + \sqrt{\beta^{-1}(1-\alpha_{\Delta t}^2)}\, G^n,\\
p^{n+1} &= \tilde{p}^{n+1/2} + \frac{\Delta t}{2}\nabla U(q^{n+1/2}),\\
q^{n+1} &= q^{n+1/2} + \frac{\Delta t}{2}\frac{p^{n+1}}{m},
\end{aligned} \tag{1.83}$$

where $\alpha_{\Delta t}$ and G^n have been defined after (1.82).

Second order accuracy on the invariant measure can be also obtained by the use of the so-called geometric Langevin algorithm (Hairer et al. (2003, 2006)), which consist in a first order splitting between the Hamiltonian and the fluctuation-dissipation parts and a second-order splitting scheme for the Hamiltonian part. We have

$$P_{\Delta t}^{B,A,B,\xi C} = \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\xi \Delta t C} \tag{1.84}$$

which is the composition of a Störmer-Verlet scheme $P_{\Delta t}^{\mathrm{Verlet}} = \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t B/2}$ (Verlet (1967)) followed by an update of the momenta by means of an analytic integration of the Ornstein-Uhlenbeck process. The Störmer-Verlet scheme is the standard second order integration scheme for Hamiltonian problems since it fulfills the fundamental requirement of energy preservation over long trajectories and also preserves all the geometric properties of the Hamiltonian flow, namely: symmetry, reversibility, phase-space volumes conservation and symplecticity (which is indeed ensured by the splitting strategy). Among all these splitting schemes, one chooses those that lead to smaller errors on the invariant measure and that have the correct behavior in the overdamped limit (see Leimkuhler et al. (2015)).

[9] The order of the operations performed on the configuration of the system is the inverse of the order of the operations mentioned in the superscript of the evolution operator when read from right to left. This inversion is known as *Vertauschungssatz* (see, for instance, the discussion in Hairer et al. (2006, Section III.5.1)).

In the nonequilibrium case, the splitting strategy has to be performed over the evolution generated by the perturbed operator $\mathcal{L}_\eta = \mathcal{L}_0 + \eta\widetilde{\mathcal{L}}$. Considering in particular the two cases discussed in Sections 1.3.1 and 1.3.2, a choice has to be made about whether to replace B by $B + \eta\widetilde{\mathcal{L}}$ or ξC by $\xi C + \eta\widetilde{\mathcal{L}}$. The choice is once again made in order to preserve the right behavior in the overdamped limit. Thus, in the mechanical forcing case, it is convenient to add the perturbation to the elementary operator B, see *e.g.* Lelièvre and Stoltz (2016). A first order splitting is thus

$$P_{\Delta t}^{A,B+\eta\widetilde{\mathcal{L}},\xi C} = \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t(B+\eta\widetilde{\mathcal{L}})}\, \mathrm{e}^{\xi \Delta t C} \tag{1.85}$$

and a second order splitting may be

$$P_{\Delta t} = \mathrm{e}^{\xi \Delta t C/2}\, \mathrm{e}^{\Delta t(B+\eta\widetilde{\mathcal{L}})/2}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t(B+\eta\widetilde{\mathcal{L}})/2}\, \mathrm{e}^{\xi \Delta t C/2}. \tag{1.86}$$

In the thermal forcing case, instead, it is convenient to add the perturbation to the elementary operator C. The first and second order schemes are analogous to (1.85) and (1.86) respectively.

The application of the geometric Langevin algorithm in these cases gives

$$P_{\Delta t}^{B+\eta\widetilde{\mathcal{L}},A,B+\eta\widetilde{\mathcal{L}},\xi C} = \mathrm{e}^{\Delta t(B+\eta\widetilde{\mathcal{L}})/2}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t(B+\eta\widetilde{\mathcal{L}})/2}\, \mathrm{e}^{\xi \Delta t C}$$

and

$$P_{\Delta t}^{B,A,B,\xi C+\eta\widetilde{\mathcal{L}}} = \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\Delta t A}\, \mathrm{e}^{\Delta t B/2}\, \mathrm{e}^{\Delta t(\xi C+\eta\widetilde{\mathcal{L}})}. \tag{1.87}$$

Of course, numerical schemes corresponding to the one-step elementary operators (1.84)-(1.87) are written following the same procedure (and the same inverse order!) as (1.83). An example of scheme for the integration of a nonequilibrium dynamics is given by (4.3) in Chapter 4, where we present the study of a one-dimensional chain of N atoms subject to both mechanical and thermal forcing. As we shall see, in that case, both perturbations are added to the dissipative part C of the generator.

1.6 Contributions

In this section I briefly introduce the works which are the subject of the subsequent chapters. I start by introducing the more theoretical results on the rotor model, even if this means completely inverting the chronological order. In fact, the two more recent articles, introduced in Sections 1.6.1.1 and 1.6.1.2 and thoroughly discussed in Chapters 2 and 3, are an attempt to answer some of the questions raised by the simulations results presented in a previous article, which is introduced in Section 1.6.2.1 and presented in Chapter 4. Finally, in Section 1.6.2.2, I introduce the work on the numerical simulations of the Toda model, presented in Chapter 5.

1.6.1 Theoretical contributions

We consider a d-dimensional Langevin dynamics in a compact position space $\mathcal{D} = (2\pi\mathbb{T})^d$. Physically, this dynamics can be viewed as the dynamics of a single

particle system in a d-dimensional space or as that of an assembly of n particles in a space of dimension d' such that $d = nd'$. The particles are subjected to a force τF in the direction F, $|F| = 1$ and the system is in thermal equilibrium with a Langevin thermostat at a given temperature β^{-1}. In absence of the external forcing ($\tau = 0$), the system is at equilibrium and has a stationary measure, which is given by the canonical Gibbs measure (1.3) corresponding to the temperature β^{-1}. When $\tau \neq 0$, it can be proved by the techniques outlined in Sections 1.1.5.1 and 1.2.3, that there exists a unique nonequilibrium stationary measure (whose explicit form is however unknown) and that the dynamics (1.49) converges exponentially fast to it.

1.6.1.1 Exponential convergence to the stationary state

With S. Olla and G. Stoltz (Iacobucci et al. (2017)), we study the exponential convergence to the stationary state for the nonequilibrium Langevin dynamics (1.49) through the analysis of the long-time behavior of the associated (stationary) Fokker-Planck equation solution. The system we consider is composed by one rotor in a d dimensional space. Our aim is that of obtaining an expression of the convergence rate that shows a more explicit dependence on the physical parameters (and in particular on the friction parameter) than that obtained by Lyapunov techniques (see Section 1.2.3). The results of this work and some complementary material are the subject of Chapter 2.

The main theoretical results of this work are obtained by two hypocoercive techniques and contained in three main theorems on the exponential convergence of the law of the process to the stationary solution of the related Fokker-Planck equation. In particular, we consider the two limiting regimes, the Hamiltonian and overdamped limits, corresponding respectively to the values of the friction ξ going to zero or infinity.

In the first approach, we apply the standard hypocoercive technique presented in Section 1.2.2.1. We choose the degenerate form (1.45) of the modified H^1 norm, since it allows the computation of more explicit bounds on the spectral gap of the generator as compared to the non-degenerate version. The obtained convergence result in $H^1(\mu)$ (Theorem 9) is "transferred" in $L^2(\mu)$ by hypoelliptic regularization (Theorem 10) following the procedure outlined in Hairer and Pavliotis (2008), which is based on a result presented in Hérau (2007). The modified $H^1(\mu)$ norm approach allows to treat nonequilibrium forcings of order $\tau = \mathcal{O}(\min(\xi, \xi^{-1}))$.

In the second approach, we apply the more direct $L^2(\mu)$ estimation technique introduced in Section 1.2.2.3, which makes it easier to quantify the convergence rates. This second method allows to better quantify the convergence rates in term of the physical parameters. Specifically, it gives an upper bound on the allowed values of τ of order $\tau = \mathcal{O}(\min(1, \xi))$ (see Theorem 11), in agreement with the upper bound on the series expansion of the invariant measure (see (2.9)).

We confirm our theoretical results by numerically computing the estimation of the spectral gap with a Galerkin discretization of the generator in the case of a single rotor in one dimension, with $U(q) = U_0(1 - \cos q)$ and for different values of the parameters τ, U_0 and ξ. We use an orthonormal basis of appropriately modified Fourier functions for the positions and a Hermite polynomial decomposition in the momenta.

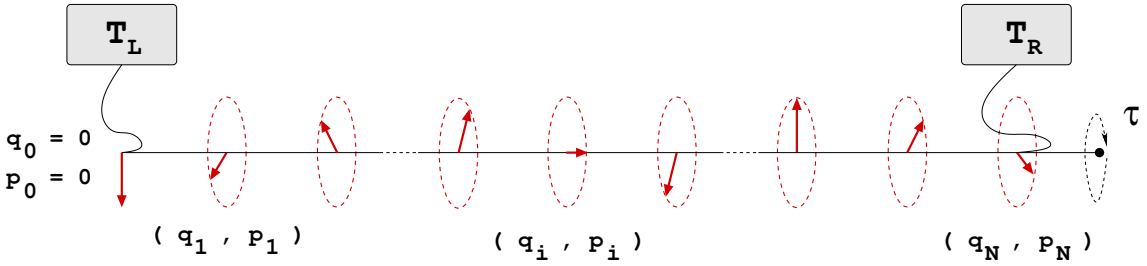


Figure 1.1 – The rotor chain model.

1.6.1.2 Perturbative construction of the nonequilibrium stationary measure

In Section 3.4, I present the results of the joint work with G. Gallavotti and S. Olla (Gallavotti et al. (2013)). The model we consider is composed of a single rotor in equilibrium with a heat bath at a given temperature and subjected to a constant torque. This work gives an example of the effort that may be necessary in actual constructions of stationary states in the apparently simple but surprisingly nontrivial case of a forced pendulum in the presence of noise.

We study the behavior of the system for small values of the potential energy U, controlled by the parameter g. Our goal is to obtain an explicit expression for the stationary measure, seeking to explicitly express the coefficients of the development in powers of g. To do this, we first assume that the solution $F(q,p;g)$ of the stationary Fokker-Planck equation for the adjoint in $L^2(\mathrm{d}q,\mathrm{d}p)$ of the generator of the dynamics can be expressed as the product of a Gaussian of zero mean and variance equal to the inverse of the temperature in the moment variable, and of a smooth density $f(q,p;g)$. Next, we assume that this density f admits an expansion in Hermite polynomials with coefficients ρ_n which depend on the position q and the parameter g. Finally, we assume that these coefficients are functions of class C^∞ in q and g, and that the derivatives in q, p and g of the solution F can be obtained by differentiating term by term the development of F, so as to obtain convergent series.

Under these assumptions, we obtain our main result: a formal expansion in powers of g of the density F with coefficients ρ_n such that their Fourier transforms can be determined by a constructive algorithm (see Section 3.4.4) and vanish for frequencies $|k| > R$. In addition, we estimate some upper bounds for these Fourier transforms, which explicitly depend on the physical parameters of the problem.

1.6.2 Numerical simulations

1.6.2.1 The rotor chain

In Iacobucci et al. (2011), we numerically study the far from equilibrium behavior of a one-dimensional chain of N interacting rotors. The results of this work are presented in Chapter 4.

The chain is subjected to a boundary temperature gradient $(T_L - T_R)/L$ and the effect of a constant torque τ acting on its right end, as shown in Figure 1.1. The leftmost rotor is attached to a wall and in contact with a Langevin thermostat at temperature T_L, while the rightmost rotor is subjected to the external force and in

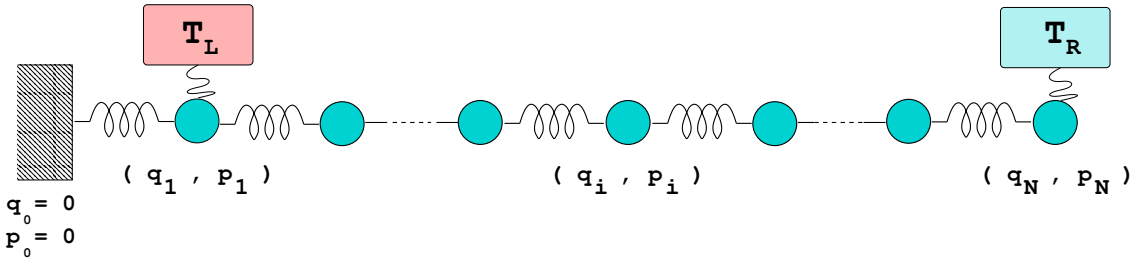


Figure 1.2 – The Toda chain model.

contact with the other Langevin thermostat at temperature T_R. The dynamics in the bulk is Hamiltonian with potential $U(q) = 1 - \cos q$. There are two conserved quantities, the total energy and angular momentum, that the system exchanges with the external thermostats. This situation therefore corresponds to that of coupled transport.

When $T_l \neq T_r$ and $\tau = 0$, the existence and uniqueness of the invariant measure has been rigorously proven only for very short chains (see Cuneo et al. (2015), Cuneo and Eckmann (2016) for the cases $N = 3$ and $N = 4$, and Cuneo and Poquet (2017) for the case $N = 2$ with one thermostat on one rotor). When $\tau \neq 0$ and even in the absence of a temperature difference, the existence of the invariant measure has not been proved. However, we numerically observe a stationary state for any N, and our simulations reveal that local equilibrium holds in the thermodynamic limit.

Moreover, the system shows some very surprising features: (i) temperature profiles are non-monotonic with a maximum observed inside the chain; (ii) momentum profiles are highly non-linear; and (iii) in the far from equilibrium case (*i.e.* of strong mechanical forcing), the thermal conductivity is a decreasing function of the temperature and, most surprisingly, in some cases, the average energy current can be increased by an opposed temperature gradient. This phenomenon can therefore be considered as "negative" conductivity. The last result shows that the two forcing mechanism (mechanical and thermal) are not simply additive and suggests that a straightforward extension of the definition of thermal conductivity to nonequilibrium settings may lead to some paradoxes.

As discussed in Iubini et al. (2016) (see also Iubini et al. (2014) and Lepri et al. (2016)), in order to understand to what extent the two forcing mechanisms are not additive, one should separately consider the currents of energy and momentum and their two related forces, a temperature and a pressure gradient, respectively. In the linear response approximation, this implies the study of a system of partial differential equations expressing each current as a function of both gradients via four non constant coefficients that form the Onsager matrix.

1.6.2.2 The Toda chain

In this work (Iacobucci et al. (2010)), which is the subject of Chapter 5, we present the results of simulations of nonequilibrium stationary states of a chain of nonlinear oscillators interacting via a Toda potential $U(r) = \frac{a}{b}e^{-br} + ar + c$. Analogously to the previous model, both ends of the chain are in contact with two thermostats at different temperatures (see Figure 1.2), modeled by Langevin dynamics. The system is perturbed by a stochastic dynamics which conserves both total energy and

momentum. Because of the form of the potential, the existence and uniqueness of the stationary measure can be proved by usual techniques (see *e.g.* Rey-Bellet (2006*b*), Carmona (2007)), although its explicit form is unknown.

We study the scaling $\kappa \sim N^{\alpha}$ of the thermal conductivity with respect to the chain length, for different values of the friction parameter ξ, the strength of the stochastic perturbation γ and the degree b of nonharmonicity of the potential at fixed values of the boundary temperatures. The results of our numerical experiments show that: (i) the ballistic transport ($\alpha = 1$) is broken as soon as $\gamma \neq 0$; (ii) $\alpha < 0.5$ in agreement with the analytic result of Basile et al. (2009); (iii) for a fixed parameter configuration, α seems to depend on the strength γ of the noise in a monotonically increasing way.

The last finding seems to challenge the universality of the scaling parameter supported by Spohn (2014). While such a phenomenon has already been observed by Basile et al. (2007), our result may be due to numerical biases and finite size effects, and would deserve some supplementary investigations.

Part 1

(Mostly) One rotor model

2

Perturbations of Langevin dynamics(*)

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(*) *This chapter contains a slightly extended version of the article "Convergence rates for nonequilibrium Langevin dynamics" (Iacobucci et al. (2017)), to appear in* Annales mathématiques du Québec. *I added an Appendix containing some computations related to the corresponding equilibrium model. In particular, entropy estimates for the equilibrium model are presented in Section 2.6.3.*

We study in this chapter the exponential convergence to the stationary state for nonequilibrium Langevin dynamics, by a perturbative approach based on hypocoercive techniques developed for equilibrium Langevin dynamics. The Hamiltonian and overdamped limits (corresponding respectively to frictions going to zero or infinity) are carefully investigated. In particular, the maximal magnitude of admissible perturbations are quantified as a function of the friction. Numerical results based on a Galerkin discretization of the generator of the dynamics confirm the theoretical lower bounds on the spectral gap.

2.1 Introduction

Langevin dynamics are a commonly used model to describe the evolution of systems at constant temperature, *i.e.* in contact with a heat bath at equilibrium at a given temperature. The interaction with the heat bath is modeled by a dissipative term and a random fluctuating term related by a fluctuation-dissipation relation. This dynamics is therefore a stochastic perturbation of the Hamiltonian dynamics. It can be used to sample configurations of a physical system at equilibrium, according to the canonical ensemble, which allows to numerically estimate average macroscopic properties; see for instance Leimkuhler and Matthews (2015) for a mathematically oriented introduction to molecular dynamics. The Langevin dynamics is by now well-understood, both for its theoretical properties and its discretization, see for instance the review article by Lelièvre and Stoltz (2016).

On the other hand, the properties of nonequilibrium Langevin dynamics, such as that obtained by the addition of a non-gradient drift term, have been less investigated. We consider in this work the following paradigmatic nonequilibrium Langevin dynamics in a compact position space with periodic boundary conditions (see Section 2.2 for a more precise description):

$$\begin{cases} \mathrm{d}q_t = \dfrac{p_t}{m}\,\mathrm{d}t, \\ \mathrm{d}p_t = (-\nabla U(q_t) + \tau F)\,\mathrm{d}t - \xi \dfrac{p_t}{m}\,\mathrm{d}t + \sqrt{\dfrac{2\xi}{\beta}}\,\mathrm{d}W_t, \end{cases} \tag{2.1}$$

where the position q belongs to $\mathcal{D} = (2\pi\mathbb{T})^d$ (with $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ the one-dimensional unit torus), the momentum p is in $\mathbb{R}^d$, W_t is a standard d-dimensional Brownian motion, and $U : \mathcal{D} \to \mathbb{R}$ is the potential energy function. We assume U to be smooth in all this work, and denote by $\mathscr{E} = \mathcal{D} \times \mathbb{R}$ the phase-space of the system. The dynamics (2.1) is parametrized by several constants: the mass $m > 0$ of the particles (for simplicity, we consider a single mass m, although our results can be extended to account for more general mass matrices), the inverse temperature $\beta > 0$, the friction $\xi > 0$ and the magnitude of the external force $\tau \in \mathbb{R}$, with given direction $F \in \mathbb{S}^{d-1}$ (*i.e.* $F \in \mathbb{R}^d$ with $|F| = 1$). Let us emphasize that the external forcing induced by τF is indeed non-gradient since τF is not the gradient of a smooth, periodic function. Let us also mention that our analysis could be extended to more general non-gradient forcings $F(q)$ genuinely depending on the position variable, as long as the function F is sufficiently smooth.

There are two interesting limiting regimes that can be considered: (i) the limit $\xi \to 0$, which corresponds to a Hamiltonian limit; (ii) the limit $m \to 0$ or $\xi \to +\infty$

(with, in the latter case, a time rescaling by a factor ξ), which corresponds to an overdamped limit. More precisely, fixing for instance $m = 1$ and setting $\tau = 0$, a simple proof shows that $q_{\xi t}$, the solution of (2.1) observed at time ξt, converges in law to the solution Q_t of the overdamped Langevin dynamics (see for instance Lelièvre et al. (2010, Proposition 2.14))

$$\mathrm{d}Q_t = -\nabla U(Q_t)\,\mathrm{d}t + \sqrt{\frac{2}{\beta}}\,\mathrm{d}\widetilde{W}_t. \tag{2.2}$$

In the absence of external forcing ($\tau = 0$), the system described by (2.1) has an *equilibrium* stationary measure given explicitly by the canonical Gibbs measure:

$$\mu(\mathrm{d}q\,\mathrm{d}p) = Z_\mu^{-1}\mathrm{e}^{-\beta H(q,p)}\,\mathrm{d}q\,\mathrm{d}p, \qquad H(q,p) = U(q) + \frac{p^2}{2m}, \qquad Z_\mu = \int_{\mathscr{E}} \mathrm{e}^{-\beta H}.$$

When $\tau \neq 0$, there exists a unique *nonequilibrium* stationary measure, but it cannot be computed explicitly.

Although the Langevin dynamics (2.1) is not elliptic (the noise acts only on the momenta and not directly on the positions), it can be shown to be hypoelliptic. The rate of the exponential convergence to the stationary state can be obtained by Lyapunov techniques, see for instance Mattingly et al. (2002), Rey-Bellet (2006*a*). The corresponding convergence rates are however usually not very explicit in terms of the parameters of the dynamics. In particular, it is difficult to make explicit their dependence on ξ. A more quantitative approach is based on estimates in $L^2(\mu)$, where exponential convergence rates for the law of the process towards μ can be obtained by a careful use of commutator identities, as pioneered in Talay (2002), Eckmann and Hairer (2003), Hérau and Nier (2004) and later abstracted in the theory of hypocoercivity by Villani (2009). The application of this theory to Langevin dynamics allows to quantify the convergence rates in terms of the parameters of the dynamics; see for instance Hairer and Pavliotis (2008) for the Hamiltonian limit $\xi \to 0$ and Leimkuhler et al. (2015), Lelièvre and Stoltz (2016) for partial results on the overdamped limit $\xi \to +\infty$. A more direct route to prove the convergence was subsequently proposed in Dolbeault et al. (2009, 2015), which makes it even easier to quantify convergence rates; see Dolbeault et al. (2013) for a complete study on the dependence of a parameter similar to ξ by this approach for a dynamics similar to an equilibrium Langevin dynamics, as well as Achleitner et al. (2015) for sharp estimates for equilibrium Langevin dynamics and a harmonic potential energy function. An extension to nonlinear potentials was also provided in the latter work, based on a non-symmetric Bakry–Emery condition; although further work is required to use this approach in our context because the results are stated for equilibrium dynamics with potentials U which are convex and such that $\sqrt{\max U''} - \sqrt{\min U''} \leqslant \xi$. Let us finally mention the recent work by Eberle et al. (2017) which provides the qualitative rates of convergence for Langevin dynamics by a coupling strategy.

Our aim in this work is to investigate the exponential convergence to the stationary state for nonequilibrium Langevin dynamics. The new contributions of this work are the following:

(1) we provide some technical variations/improvements on the theoretical side by

(a) giving explicit decay estimates for nonequilibrium Langevin dynamics, both in the Hamiltonian limit $\xi \to 0$ and in the overdamped limit $\xi \to +\infty$, thereby extending the results obtained at equilibrium. Similar convergence results were very recently stated for a different nonequilibrium model and a fixed friction in Bouin et al. (2016);

(b) deriving hypocoercive estimates in a degenerate $H^1(\mu)$ norm, which allows to obtain lower bounds on convergence rates which are more explicit than the ones obtained with a non-degenerate $H^1(\mu)$ norm. Such degenerate norms where already considered in Talay (2002), and were also recently used in Baudoin (2013), Olla and Letizia (2017), Baudoin (2016);

(c) comparing the results obtained by either the standard hypocoercive approach followed by hypoelliptic regularization, or the direct L^2 approach of Dolbeault et al. (2009, 2015).

(2) on the numerical side, we perform a study of the spectral gap of the generator of the dynamics (which is related to the exponential convergence of the law of the process to the invariant measure), as a function of the friction ξ and the magnitude τ of the external forcing, in order to assess the sharpness of the bounds provided by the theoretical results. Let us emphasize that we consider a situation where the invariant measure does not have an explicit expression, so that it is difficult to rely on Monte-Carlo techniques to estimate the convergence rate as in Dolbeault et al. (2013). We consider instead a Galerkin discretization of the generator of the dynamics.

This chapter is organized as follows. We first start by describing the stationary state of the nonequilibrium Langevin dynamics we consider in Section 2.2. We next state in Section 2.3 the exponential convergence to 0 of the evolution semigroup in various functional settings. Our emphasis is on carefully estimating the scaling of these rates with respect to the friction ξ and the magnitude τ of the external forcing. The estimates we obtain provide lower bounds on the spectral gap of the Fokker–Planck operator. The relevance/sharpness of these bounds is investigated from a numerical viewpoint in Section 2.4 by a Galerkin discretization. The longest proofs of the results presented in Section 2.3 are postponed to Section 2.5. Some supplementary material is contained in Section 2.6, namely: the calculation of the analytic spectral gap in the zero potential case, the estimation of Poincaré constants and a convergence result for the equilibrium model obtained by the hypocoercive entropic approach presented in Section 1.2.2.2.

2.2 Stationary states of nonequilibrium Langevin dynamics

We make precise in this section some properties of the nonequilibrium Langevin dynamics. We first state a result on the existence and uniqueness of the steady-state, as well as (non explicit) exponential convergence results (see Section 2.2.1). We next give some simple properties of the stationary state in Section 2.2.2. We conclude with a perturbative expansion of the steady-state in terms of the magnitude τ of the external forcing, making explicit the admissible magnitude of the perturbation τ in terms of the friction ξ (see Section 2.2.3).

2.2.1 Existence and uniqueness of the invariant measure

We recall in this section a result on the existence and uniqueness of the invariant measure for any value of τ, as well as exponential convergence rates in weighted L^∞ spaces (see Lelièvre and Stoltz (2016, Proposition 5.1)). To state this result, we denote by $\mathcal{L}_{\xi,\tau}$ the generator of the dynamics (2.1):

$$\mathcal{L}_{\xi,\tau} = \mathcal{L}_{\rm ham} + \xi \mathcal{L}_{\rm FD} + \tau \mathcal{L}_{\rm pert},$$

where the generator associated with the Hamiltonian part of the dynamics, the fluctuation/dissipation and the external perturbation respectively read

$$\mathcal{L}_{\rm ham} = \frac{p}{m} \cdot \nabla_q - \nabla U(q) \cdot \nabla_p, \qquad \mathcal{L}_{\rm FD} = -\frac{p}{m} \cdot \nabla_p + \frac{1}{\beta} \Delta_p, \qquad \mathcal{L}_{\rm pert} = F \cdot \nabla_p.$$

We also introduce the Lyapunov functions $W_n(q,p) = 1 + |p|^n$ for $n \geqslant 2$, and the functional spaces

$$L^\infty_{W_n} = \left\{ \varphi \text{ measurable}, \ \|\varphi\|_{L^\infty_{W_n}} = \left\| \frac{\varphi}{W_n} \right\|_{L^\infty} < +\infty \right\}.$$

Proposition 5. *Fix $\tau_* > 0$ and $\xi > 0$. For any $\tau \in [-\tau_*, \tau_*]$, the dynamics (2.1) admits a unique invariant probability measure which admits a C^∞ density $\psi_\tau(q,p)$ with respect to the Lebesgue measure. Moreover, for any $n \geqslant 2$, there exist $C_n, \lambda_n > 0$ (depending on τ_*) such that, for any $\tau \in [-\tau_*, \tau_*]$ and for any $\varphi \in L^\infty_{W_n}(\mathscr{E})$,*

$$\forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} \varphi - \int_{\mathscr{E}} \varphi \, \psi_\tau \right\|_{L^\infty_{W_n}} \leqslant C_n \mathrm{e}^{-\lambda_n t} \left\| \varphi - \int_{\mathscr{E}} \varphi \, \psi_\tau \right\|_{L^\infty_{W_n}}.$$

Let us however emphasize that it is difficult to quantify the above convergence rates in terms of the parameters of the dynamics (such as the friction ξ or the potential U) and the magnitude of the external forcing τ, since the proof relies on minorization conditions for which the dependence on the parameters is not very explicit.

In order to write more explicit convergence results, it will be convenient to work in (subspaces) of $L^2(\mu)$, see Section 2.3. In the sequel, we consider by default all operators as defined (by their extensions) on the Hilbert space $L^2(\mu)$, the adjoint A^* of a (closable) operator A being defined with respect to the associated canonical scalar product. Working in $L^2(\mu)$ however requires that the invariant measure itself admits a density h_τ with respect to μ which is in $L^2(\mu)$, *i.e.*

$$\psi_\tau = h_\tau \mu, \qquad h_\tau \in L^2(\mu). \tag{2.3}$$

Such a result is provided by perturbation results for linear operators, see Section 2.2.3. In this setting, the invariance of the measure ψ_τ can be translated into the following Fokker-Planck equation:

$$\mathcal{L}^*_{\xi,\tau} h_\tau = 0, \qquad \int_{\mathscr{E}} h_\tau \, \mathrm{d}\mu = 1, \tag{2.4}$$

with $h_\tau \geqslant 0$. More explicitly, the action of $\mathcal{L}^*_{\xi,\tau}$, the adjoint of $\mathcal{L}_{\xi,\tau}$ considered as an operator on $L^2(\mu)$, is given by

$$\mathcal{L}^*_{\xi,\tau} = -\mathcal{L}_{\rm ham} + \xi \mathcal{L}_{\rm FD} - \tau F \cdot \nabla_p + \frac{\tau\beta}{m} F \cdot p.$$

2.2.2 Qualitative properties of the steady-state

We provide here some simple properties of the stationary state. The first one is that, due to the constant force applied on the momenta, a non-zero velocity builds up in the system. More precisely, denoting by $\mathbb{E}_\tau$ the expectation with respect to ψ_τ, this average velocity v_τ satisfies

$$v_\tau = \mathbb{E}_\tau\left(\frac{p}{m}\right) = \frac{1}{\xi}\Big(\tau F - \mathbb{E}_\tau(\nabla U)\Big). \tag{2.5}$$

This relation follows from the following identities (the first equality arising from the invariance of ψ_τ through the nonequilibrium Langevin dynamics (2.1)):

$$\int_{\mathscr{E}} \Big(\mathcal{L}_{\xi,\tau} p\Big)\psi_\tau = 0 = -\xi \int_{\mathscr{E}} \frac{p}{m}\,\psi_\tau - \int_{\mathscr{E}} \nabla U\,\psi_\tau + \tau F.$$

Another relation is obtained by computing the average of $\mathcal{L}_{\xi,\tau}\mathcal{H}$ with respect to ψ_τ, where $\mathcal{H}$ is the Hamiltonian of the system:

$$\mathcal{H}(q,p) = \frac{p^2}{2m} + U(q).$$

Since

$$\mathcal{L}_{\xi,\tau}\mathcal{H}(q,p) = \xi\left(-\frac{p^2}{m^2} + \frac{d}{\beta m}\right) + \tau F \cdot \frac{p}{m},$$

it follows that

$$\tau F \cdot v_\tau = 2\frac{\xi}{m}\left(\mathbb{E}_\tau\left[\frac{p^2}{2m}\right] - \frac{d}{2\beta}\right).$$

This identity expresses the energy conservation of the system and its environment: the instantaneous work performed by the non-conservative force τF is equal to the energy (heat) exchanged with the thermal bath.

By the above discussion, the entropy production rate of the stationary state is proportional to $\tau F \cdot v_\tau$. To formally prove this latter statement, let us consider the entropy

$$\mathscr{H}(t) = \int_{\mathcal{E}} f_t \ln f_t \,\mathrm{d}\mu,$$

and its time derivative, which is equal to

$$\mathscr{H}'(t) = \int_{\mathcal{E}} f_t \mathcal{L}_{\xi,\tau}(\ln f_t)\,\mathrm{d}\mu$$

where $f_t = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f$ and we have considered the fact that $\int_{\mathcal{E}} f_t \,\mathrm{d}\mu = 1$, $\forall t$. If we set $f = f_{t=0} = h_\tau$ (where h_τ is introduced in (2.3)), by definition of the stationary state we have that $f_t = h_\tau$ at all times, thus $\mathscr{H}'(t) = 0$.

We next consider the quantity $h_\tau \mathcal{L}_{\xi,\tau}(\ln h_\tau)$. The following computations are formal but could be made rigorous upon obtaining appropriate estimates on $\nabla_p h_\tau$. Since

$$\int_{\mathcal{E}} h_\tau \mathcal{L}_{\xi,\tau}(\ln h_\tau)\,\mathrm{d}\mu = \int_{\mathcal{E}} \mathcal{L}_{0,\tau} h_\tau \,\mathrm{d}\mu - \frac{\xi}{\beta}\int_{\mathcal{E}} \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu,$$

and

$$\int_{\mathscr{E}} (\mathcal{L}_{0,\tau} h_\tau)\,\mathrm{d}\mu = \int_{\mathscr{E}} \left(\mathcal{L}_{0,\tau}^* \mathbf{1}\right) h_\tau \,\mathrm{d}\mu = \beta\tau F \cdot \int_{\mathscr{E}} \frac{p}{m} h_\tau \,\mathrm{d}\mu = \beta\tau F \cdot v_\tau,$$

it follows, after integration with respect to μ and in view of (2.4),

$$\int_{\mathscr{E}} h_\tau \mathcal{L}_{\xi,\tau}(\ln h_\tau)\,\mathrm{d}\mu = \int_{\mathscr{E}} \left(\mathcal{L}_{\xi,\tau}^* h_\tau\right) \ln h_\tau \,\mathrm{d}\mu = 0 = \beta\tau F \cdot v_\tau - \frac{\xi}{\beta} \int \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu.$$

The first term on the right hand side of the last equality is the entropy production rate, and this shows that

$$\beta\tau F \cdot v_\tau = \frac{\xi}{\beta} \int \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu,$$

therefore the entropy production rate is positive. Using (2.5), we also obtain the following bound on a degenerate Fisher information:

$$\int_{\mathscr{E}} \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu = \frac{\beta^2\tau}{\xi} F \cdot v_\tau = \left(\frac{\beta\tau}{\xi}\right)^2 - \frac{\beta^2\tau}{\xi^2} F \cdot \mathbb{E}_\tau(\nabla U) \leqslant \left(\frac{\beta\tau}{\xi}\right)^2 + \frac{\beta^2\tau}{\xi^2} \|\nabla U\|_\infty,$$

which provides some information on the distance of the stationary distribution of the momenta to the equilibrium Gaussian distribution with variance m/β.

A last information on the stationary state is provided by the Einstein relation, first proven in Rodenhausen (1989), which provides a linear response result on the average velocity v_τ:

$$\frac{d}{d\tau} v_\tau \Big|_{\tau=0} = \beta D F, \tag{2.6}$$

where $D \in \mathbb{R}^{d\times d}$ is the diffusivity of the system at $\tau = 0$ *i.e.* the asymptotic variance:

$$D := \lim_{t\to\infty} \frac{1}{2t} \mathbb{E}_0 \left[\left(\int_0^t \frac{p_s}{m}\, ds \right) \otimes \left(\int_0^t \frac{p_s}{m}\, ds \right) \right], \tag{2.7}$$

with $\mathbb{E}_0$ the expectation over all initial conditions $(q_0, p_0) \sim \mu$ and all realizations of the Brownian motion W_t. This relation also follows from the first order term in the expansion of h_τ recalled in Section 2.2.3.

2.2.3 Perturbative expansion of the invariant measure

We prove in this section that the decomposition (2.3) is well defined, and actually give a complete characterization of h_τ as some series expansion for τ sufficiently small. Define the subspace of $L^2(\mu)$ composed of functions with average 0 with respect to μ:

$$L_0^2(\mu) = \left\{ f \in L^2(\mu),\ \int_{\mathscr{E}} f \,\mathrm{d}\mu = 0 \right\}.$$

We also denote by $\mathscr{B}(X)$ the operator norm on a Banach space X.

The operator $\mathcal{L}_{\xi,0}$ is invertible on $L_0^2(\mu)$. This can be seen as a particular case of the convergence results provided in Section 2.3 (for $\tau = 0$). In fact, it can be proved that there exists $K > 0$ such that

$$\forall \xi \in (0, +\infty), \qquad \left\| \mathcal{L}_{\xi,0}^{-1} \right\|_{\mathscr{B}(L_0^2(\mu))} \leqslant \frac{K}{\min(\xi, \xi^{-1})}.$$

see also Hairer and Pavliotis (2008), Leimkuhler et al. (2015), Lelièvre and Stoltz (2016). In addition, recalling that $|F| = 1$, we obtain, for a smooth and compactly supported function $\varphi \in L^2_0(\mu)$,

$$\left\|\mathcal{L}_{\rm pert}\varphi\right\|^2_{L^2(\psi_0)} \leqslant \|\nabla_p \varphi\|^2_{L^2(\mu)} = -\frac{\beta}{\xi}\left\langle \varphi, \mathcal{L}_{\xi,0}\varphi\right\rangle_{L^2(\mu)} \leqslant \frac{\beta}{\xi}\|\mathcal{L}_{\xi,0}\varphi\|_{L^2(\psi_0)}\|\varphi\|_{L^2(\psi_0)}.$$

We next project $\mathcal{L}_{\rm pert}\varphi$ onto $L^2_0(\mu)$, replace φ by $\mathcal{L}^{-1}_{\xi,0}\phi$ and take the supremum over $\phi \in L^2_0(\mu)$ to obtain a bound on the operator $\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}$ considered as an operator on $L^2_0(\mu)$:

$$\left\|\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}\right\|_{\mathscr{B}(L^2_0(\mu))} \leqslant \sqrt{\frac{\beta}{\xi}\left\|\mathcal{L}^{-1}_{\xi,0}\right\|_{\mathscr{B}(L^2_0(\mu))}} \leqslant \frac{\sqrt{\beta K}}{\min(1,\xi)}.$$

Let us denote by r the spectral radius of the operator appearing in the left hand-side of the previous inequality, namely

$$r = \lim_{n\to+\infty}\left\|\left[\left(\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}\right)^*\right]^n\right\|^{1/n}_{\mathscr{B}(L^2_0(\mu))},$$

The following result (given by Lelièvre and Stoltz (2016, Theorem 5.2)) provides an expression of h_τ.

Proposition 6. *For $|\tau| < r^{-1}$, the unique invariant measure can be written as $\psi_\tau = h_\tau\mu$, where $h_\tau \in L^2(\mu)$ admits the following expansion in powers of τ:*

$$h_\tau = \left(1 + \tau\left(\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}\right)^*\right)^{-1}\mathbf{1} = \left(1 + \sum_{n=1}^{+\infty}(-\tau)^n\left[\left(\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}\right)^*\right]^n\right)\mathbf{1}. \tag{2.8}$$

Since $0 \leqslant r \leqslant \left\|\mathcal{L}_{\rm pert}\mathcal{L}^{-1}_{\xi,0}\right\|_{\mathscr{B}(L^2_0(\mu))}$, it holds

$$\frac{1}{r} \geqslant \frac{\min(1,\xi)}{\sqrt{\beta K}}. \tag{2.9}$$

This shows that the upper limit on τ for the validity of the expansion (2.8) should be of order $\min(1,\xi)$. This is consistent with physical intuition: when the fluctuation/dissipation is small, the external forcings which can be sustained by the system are at most of the same order of magnitude than the dissipation mechanism; while for large fluctuation/dissipation mechanisms, external forcings of the same order of magnitude as ∇U can be sustained. Let us mention that it is not clear whether the condition (2.9) really is a necessary one. For extremely large forcings τ, we expect that the invariant measure will be quite different from μ, so that it is not a surprise that the perturbative approach of Proposition 6 fails as such.

As an application of the power expansion provided in Proposition 6, let us recall one way to obtain (2.6)-(2.7). Note first that (2.7) can be rewritten as

$$D = \int_0^{+\infty}\mathbb{E}_0\left[\frac{p_t}{m}\otimes\frac{p_0}{m}\right]\mathrm{d}t.$$

Next, in view of (2.8) and using the following equality in the sense of bounded operators on $L^2_0(\mu)$ (relying for instance on the convergence results of Section 2.3 with $\tau = 0$, which ensure that the time integral is well defined):

$$-\mathcal{L}^{-1}_{\xi,0} = \int_0^{+\infty} \mathrm{e}^{t\mathcal{L}_{\xi,0}}\,\mathrm{d}t,$$

it follows that

$$\begin{aligned}\frac{d}{d\tau} v_\tau\Big|_{\tau=0} &= -\int_{\mathscr{E}} \frac{p}{m}\left(\mathcal{L}^*_{\xi,0}\right)^{-1} \mathcal{L}^*_{\mathrm{pert}}\mathbf{1}\,\mathrm{d}\mu \\ &= -\beta\int_{\mathscr{E}} \mathcal{L}^{-1}_{\xi,0}\left(\frac{p}{m}\right)\frac{p}{m}\cdot F\,\mathrm{d}\mu = \beta\int_0^{+\infty} \mathbb{E}_0\left[\frac{p_t}{m}\left(\frac{p_0}{m}\cdot F\right)\right]\mathrm{d}t.\end{aligned}$$

This is indeed (2.6).

2.3 Exponential convergence of the law

From the convergence result provided in Proposition 5 and the stationary Fokker-Planck equation (2.4), it is expected that $\mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f$ converges to h_τ for any initial density $f \in L^2(\mu)$ such that

$$\int_{\mathscr{E}} f\,\mathrm{d}\mu = 1, \qquad f \geqslant 0.$$

We state several such results in this section: the first two are based on the hypocoercive approach presented in Villani (2009) and used also in Hairer and Pavliotis (2008) for equilibrium Langevin dynamics (see Section 2.3.1 for a result in a degenerate $H^1(\mu)$ norm and the related convergence in $L^2(\mu)$ after hypoelliptic regularization), while the third one follows from the more direct approach of Dolbeault et al. (2009, 2015) (see Section 2.3.2). The main point is that the latter approach is the only one which allows to state exponential convergence results consistent with the upper bound (2.9) on the series expansion of the invariant measure, while the more traditional hypocoercive approach is limited to small forcings $\tau = \mathrm{O}(\xi^{-1})$ for large frictions.

Although the convergence results are stated here for probability densities, they can in fact be obtained for general elements of $L^2(\mu)$ (*i.e.* the functions under consideration need not be non-negative and be of integral 1 with respect to μ). We write them however for elements of $L^2(\mu)$ of mass 1, introducing to this end

$$L^2_1(\mu) = \left\{ f \in L^2(\mu),\ \int_{\mathscr{E}} f\,\mathrm{d}\mu = 1 \right\}.$$

Convergence results for arbitrary elements of $L^2(\mu)$ follow by an appropriate renormalization.

2.3.1 Standard hypocoercive approach

We start by stating a convergence result in a norm finer than the $L^2(\mu)$ norm, but coarser than the $H^1(\mu)$ norm usually considered in the theory of hypocoercivity. Instances of such degenerate norms can be found in Talay (2002), Baudoin (2013), Olla and Letizia (2017), Baudoin (2016). More precisely, we consider the Hilbert space

$$\mathcal{H} = \Big\{ f \in L^2(\mu),\ (\nabla_p + \nabla_q) f \in L^2(\mu) \Big\},$$

endowed with the scalar product (for $a > 0$)

$$\langle f, g \rangle_a = \langle f, g \rangle_{L^2(\mu)} + a \Big\langle (\nabla_p + \nabla_q) f, (\nabla_p + \nabla_q) g \Big\rangle_{L^2(\mu)}.$$

The associated scalar product is denoted by $\| \cdot \|_a$. The precise convergence result is the following.

Theorem 9. *There exist $\delta_* > 0$ and a continuous function $a : (0, +\infty) \to (0, +\infty)$ satisfying*

$$\lim_{\xi \to 0} \frac{a(\xi)}{\xi} = \overline{a}_0 > 0, \qquad \lim_{\xi \to +\infty} \xi a(\xi) = \overline{a}_\infty > 0,$$

such that, for any $\delta \in [0, \delta^*]$, there is $\overline{\lambda}_\delta > 0$ for which, for all $\xi \in (0, +\infty)$ and $\tau \in [-\delta \min(\xi, \xi^{-1}), \delta \min(\xi, \xi^{-1})]$,

$$\forall f \in \mathcal{H} \cap L^2_1(\mu),\ \forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t \mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{a(\xi)} \leqslant \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi, \xi^{-1}) t} \| f - h_\tau \|_{a(\xi)}. \quad (2.10)$$

Moreover, $\overline{\lambda}_\delta = \overline{\lambda}_0 + \mathrm{O}(\delta)$.

The proof of this result can be read in Section 2.5.1. A careful inspection of the final argument based on an asymptotic analysis of the key matrix inequality (2.27) would allow to give more precise expressions of $\overline{a}_0, \overline{a}_\infty$ and $\overline{\lambda}_\delta$ as a function of the parameters of the dynamics. Let us also emphasize that, in the degenerate norm we consider, there is no prefactor on the right-hand side of (2.10), contrarily to convergence theorems stated in $H^1(\mu)$ for which the prefactor degenerates in the limits $\xi \to 0$ or $\xi \to +\infty$. Let us finally mention that the way we formulate our result, by considering $\tau \in [-\delta \min(\xi, \xi^{-1}), \delta \min(\xi, \xi^{-1})]$ (rather than $\tau \in [-\delta_* \min(\xi, \xi^{-1}), \delta_* \min(\xi, \xi^{-1})]$), allows to emphasize that the convergence rate has some uniformity with respect to τ.

By hypoelliptic regularization, the convergence result of Theorem 9 can be transferred to $L^2(\mu)$ (see Section 2.5.2 for the proof).

Theorem 10. *There exist $C, \delta_* > 0$ such that, for any $\delta \in [0, \delta^*]$, there is $\overline{\lambda}_\delta > 0$ for which, for all $\xi \in (0, +\infty)$ and all $\tau \in [-\delta \min(\xi, \xi^{-1}), \delta \min(\xi, \xi^{-1})]$,*

$$\forall f \in L^2_1(\mu),\ \forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t \mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi, \xi^{-1}) t} \| f - h_\tau \|_{L^2(\mu)}.$$

The convergence rate $\overline{\lambda}_\delta$ is the same as in Theorem 9. Note also that the prefactor C is independent of δ since the regularization properties of the dynamics can be shown to be uniform with respect to τ (see Proposition 7 in Section 2.5.2).

We conclude by emphasizing an important restriction of the results in this section: in the large friction limit, only very small forcings τ, of order $1/\xi$ are allowed, whereas, in view of (2.9), the density h_τ is well defined for values of τ of order 1. This restriction can however be bypassed by the more direct approach from Dolbeault et al. (2009, 2015), as made precise in Section 2.3.2.

2.3.2 Direct L^2 estimates

We state a convergence result similar to Theorem 10, with the important difference that the too stringent restriction on the upper bound of τ is removed; see Section 2.5.3 for the proof.

Theorem 11. *There exist $C, \delta_* > 0$ such that, for any $\delta \in [0, \delta^*]$, there is $\overline{\lambda}_\delta > 0$ for which, for all $\xi \in (0, +\infty)$ and all $\tau \in [-\delta \min(\xi, 1), \delta \min(\xi, 1)]$,*

$$\forall f \in L^2_1(\mu),\ \forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi, \xi^{-1})t} \| f - h_\tau \|_{L^2(\mu)}. \quad (2.11)$$

Moreover, $\overline{\lambda}_\delta = \overline{\lambda}_0 + \mathrm{O}(\delta)$.

As in Section 2.3.1, the convergence rate $\overline{\lambda}_\delta$ can be quantified in terms of the various parameters of the dynamics by optimizing the smallest eigenvalue of a matrix (see (2.31) in the proof). It would also be possible to obtain a contraction result on $\| \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} g \|_{L^2(\mu)}$ for two elements $f, g \in L^2_1(\mu)$, from which the existence and uniqueness of an invariant measure characterized by h_τ can be deduced as in Bouin et al. (2016).

2.3.3 Entropy estimates

For equilibrium dynamics ($\tau = 0$), it is possible to state a convergence result similar to Theorem 9 using a functional involving the relative entropy with respect to μ and a degenerate Fisher information, instead of the degenerate H^1 norm $\| \cdot \|_a$. One of the main interests of entropic estimates is that they allow to consider more general initial densities, and, maybe more importantly, that they usually have a better scaling with respect to the dimension. Hypocoercive entropy estimates are already present in Villani (2009), but are made more explicit in Olla and Letizia (2017) (see also Lelièvre and Stoltz (2016) for an application to the dynamics (2.1)). It is possible to make precise the dependence of the prefactors and convergence rates with respect to the friction parameter, by following the same approach as for the proofs of Theorems 9 and 10, see Appendix 2.6.3.

The situation is more complicated for nonequilibrium dynamics, and, to our knowledge, no convergence result in the entropic sense has been obtained, even in a perturbative framework. We present formal computations here which motivate why this is a difficult problem, hoping to attract some interest on this issue. For an initial density f such that

$$\int_{\mathscr{E}} f \, \mathrm{d}\mu = 1, \qquad f \geqslant 0,$$

it seems relevant to consider the relative entropy of $\mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f$ with respect to the stationary solution h_τ, which corresponds to the following entropy functional:

$$\mathscr{F}(t) = \int_{\mathscr{E}} \ln\left(\frac{\mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f}{h_\tau}\right) \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f \, \mathrm{d}\mu.$$

Although there is no analytical expression of h_τ, the time-derivative of the entropy functional has a quite simple expression, given by a degenerate Fisher information.

Lemma 1. *Define*

$$\tilde{f}(t) = \frac{\mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f}{h_\tau}.$$

Then,

$$\mathscr{F}'(t) = -\frac{\xi}{\beta} \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \, \mathrm{d}\mu.$$

Let us again emphasize that this result is formal. More care is required in order to make the computations rigorous in the proof. In fact, similar results hold for general, degenerate, non-reversible diffusions, see Bolley and Gentil (2010) and Achleitner et al. (2015).

Proof. Define $A_\tau = \mathcal{L}_{\mathrm{ham}} + \tau \mathcal{L}_{\mathrm{pert}}$. Straightforward calculations give

$$A^*_\tau \tilde{f} = \frac{A^*_\tau f}{h_\tau} - \tilde{f} \frac{A^*_\tau h_\tau}{h_\tau} + \beta\tau F \cdot \frac{p}{m} \tilde{f},$$

and

$$\mathcal{L}_{\mathrm{FD}} \tilde{f} = \frac{\mathcal{L}_{\mathrm{FD}} f}{h_\tau} - \tilde{f} \frac{\mathcal{L}_{\mathrm{FD}} h_\tau}{h_\tau} - \frac{2}{\beta} \frac{\nabla_p h_\tau}{h_\tau} \cdot \nabla_p \tilde{f},$$

which, using (2.4), lead to

$$\mathcal{L}^*_\tau \tilde{f} = \frac{\mathcal{L}^*_\tau f}{h_\tau} - \frac{2\xi}{\beta} \frac{\nabla_p h_\tau}{h_\tau} \cdot \nabla_p \tilde{f} + \beta\tau F \cdot \frac{p}{m} \tilde{f} = \partial_t \tilde{f} - \frac{2\xi}{\beta} \frac{\nabla_p h_\tau}{h_\tau} \cdot \nabla_p \tilde{f} + \beta\tau F \cdot \frac{p}{m} \tilde{f}.$$

This shows that $\tilde{f}$ satisfies the following evolution equation:

$$\partial_t \tilde{f}(t) = (-A_\tau + \xi \mathcal{L}_{\mathrm{FD}}) \tilde{f}(t) + \frac{2\xi}{\beta} \frac{\nabla_p h_\tau}{h_\tau} \cdot \nabla_p \tilde{f}(t).$$

Since the relative entropy is given in terms of $\tilde{f}$ by

$$\mathscr{F}(t) = \int_{\mathscr{E}} \tilde{f}(t) \Big(\ln \tilde{f}(t)\Big) h_\tau \, \mathrm{d}\mu,$$

an explicit calculation of the time derivative leads to

$$\begin{aligned}
\mathscr{F}'(t) &= -\int_{\mathscr{E}} \left(A_\tau \tilde{f}\right)\left(\ln \tilde{f}\right) h_\tau \,\mathrm{d}\mu \\
&\qquad + \xi \int_{\mathscr{E}} \left(\mathcal{L}_{\mathrm{FD}} \tilde{f}\right)\left(\ln \tilde{f}\right) h_\tau \,\mathrm{d}\mu + \frac{2\xi}{\beta} \int_{\mathscr{E}} \nabla_p h_\tau \cdot \nabla_p \tilde{f} \left(\ln \tilde{f}\right) \mathrm{d}\mu \\
&= -\int_{\mathscr{E}} A_\tau \left(\tilde{f} \ln \tilde{f}\right) h_\tau \,\mathrm{d}\mu + \int_{\mathscr{E}} f A_\tau \left(\ln \tilde{f}\right) h_\tau \,\mathrm{d}\mu - \frac{\xi}{\beta} \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu \\
&\qquad + \frac{\xi}{\beta} \int_{\mathscr{E}} \nabla_p h_\tau \cdot \nabla_p \tilde{f} \left(\ln \tilde{f}\right) \mathrm{d}\mu \\
&= -\int_{\mathscr{E}} \tilde{f} \ln \tilde{f} \left(A_\tau^* h_\tau\right) \mathrm{d}\mu + \int_{\mathscr{E}} f A_\tau^* h_\tau \,\mathrm{d}\mu - \frac{\xi}{\beta} \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu \\
&\qquad + \frac{\xi}{\beta} \int_{\mathscr{E}} \nabla_p h_\tau \cdot \nabla_p \tilde{f} \left(\ln \tilde{f}\right) \mathrm{d}\mu \\
&= \xi \int_{\mathscr{E}} \tilde{f} \ln \tilde{f} \left(\mathcal{L}_{\mathrm{FD}} h_\tau\right) \mathrm{d}\mu - \xi \int_{\mathscr{E}} \tilde{f} \left(\mathcal{L}_{\mathrm{FD}} h_\tau\right) \mathrm{d}\mu - \frac{\xi}{\beta} \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu \\
&\qquad + \frac{\xi}{\beta} \int_{\mathscr{E}} \nabla_p h_\tau \cdot \nabla_p \tilde{f} \left(\ln \tilde{f}\right) \mathrm{d}\mu \\
&= -\frac{\xi}{\beta} \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu,
\end{aligned}$$

which concludes the proof. □

One consequence of Lemma 1 is the following bound on the time average

$$\frac{1}{T} \int_0^T \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu \,\mathrm{d}t \leqslant \frac{\beta}{\xi T} \mathscr{F}(0).$$

Moreover, considering the entropy functional

$$\mathscr{G}(t) = \mathscr{F}(t) + a(\xi) \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t) + \nabla_q \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu,$$

it should be possible to prove, by computations very similar to the ones performed in Olla and Letizia (2017) (see also Lelièvre and Stoltz (2016)), that there exists $\lambda > 0$ (which can be made explicit in terms of the parameters of the dynamics) for which

$$\mathscr{G}'(t) \leqslant -\lambda \int_{\mathscr{E}} \frac{\left|\nabla_p \tilde{f}(t) + \nabla_q \tilde{f}(t)\right|^2}{\tilde{f}(t)} h_\tau \,\mathrm{d}\mu.$$

To conclude to the exponential convergence of $\mathscr{G}(t)$ (and hence $\mathscr{F}(t)$), we would however need a log-Sobolev inequality for the stationary measure $h_\tau \,\mathrm{d}\mu$ in order to bound the right hand side of the above inequality by with $-C\lambda\mathscr{F}(t)$. Such a functional inequality is unfortunately not known since the analytical expression of h_τ is not available.

2.4 Numerical estimation of the spectral gap

Let us first relate the exponential decay of the semigroup $\mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}}$ with the spectral gap of $\mathcal{L}^*_{\xi,\tau}$ in $L^2(\mu)$; and in fact the spectral gap of $\mathcal{L}_{\xi,\tau}$. We fix $\xi \in (0,+\infty)$ and $\tau \in [-\delta \min(\xi,1), \delta_* \min(\xi,1)]$, where $0 \leqslant \delta \leqslant \delta_*$ is defined in Theorem 11. We first note that the decay estimate (2.11) implies that for all $f, g \in L^2(\mu)$,

$$\begin{aligned}
\left| \left\langle \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} g - \langle g, h_\tau \rangle_{L^2(\mu)}, f \right\rangle_{L^2(\mu)} \right| &= \left| \left\langle \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} g, f \right\rangle_{L^2(\mu)} - \langle g, h_\tau \rangle_{L^2(\mu)} \int_{\mathscr{E}} f \, \mathrm{d}\mu \right| \\
&= \left| \left\langle g, \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau \int_{\mathscr{E}} f \, \mathrm{d}\mu \right\rangle_{L^2(\mu)} \right| \\
&\leqslant \|g\|_{L^2(\mu)} \left\| \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau \int_{\mathscr{E}} f \, \mathrm{d}\mu \right\|_{L^2(\mu)} \\
&\leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi,\xi^{-1})t} \|g\|_{L^2(\mu)} \left\| f - h_\tau \int_{\mathscr{E}} f \, \mathrm{d}\mu \right\|_{L^2(\mu)} \\
&\leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi,\xi^{-1})t} \|g\|_{L^2(\mu)} \left(1 + \|h_\tau\|_{L^2(\mu)} \right) \|f\|_{L^2(\mu)},
\end{aligned}$$

using a Cauchy–Schwarz inequality for the bound $\|f\|_{L^1(\mu)} \leqslant \|f\|_{L^2(\mu)}$. By taking the supremum over $f \in L^2(\mu)$ with $\|f\|_{L^2(\mu)} = 1$, it follows that

$$\left\| \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} g - \langle g, h_\tau \rangle_{L^2(\mu)} \right\|_{L^2(\mu)} \leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\xi,\xi^{-1})t} \|g\|_{L^2(\mu)} \left(1 + \|h_\tau\|_{L^2(\mu)} \right). \tag{2.12}$$

Let us introduce the subspace of observables with average 0 with respect to the invariant measure of the nonequilibrium system:

$$L^2_{0,\tau}(\mu) = \left\{ g \in L^2(\mu) \,\middle|\, \langle g, h_\tau \rangle_{L^2(\mu)} = 0 \right\}.$$

A simple computation shows that this space is stable by $\mathrm{e}^{t\mathcal{L}_{\xi,\tau}}$. The decay estimate (2.12) then shows that the following equality holds in $L^2_{0,\tau}(\mu)$: for all $z \in \mathbb{C}$ such that $\mathrm{Re}(z) < \overline{\lambda}_\delta \min(\xi,\xi^{-1})$,

$$\left(z + \mathcal{L}_{\xi,\tau} \right)^{-1} = -\int_0^{+\infty} \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} \mathrm{e}^{zt} \, \mathrm{d}t,$$

with

$$\left\| \left(z + \mathcal{L}_{\xi,\tau} \right)^{-1} \right\|_{\mathscr{B}(L^2_{0,\tau}(\mu))} \leqslant \frac{C \left(1 + \|h_\tau\|_{L^2(\mu)} \right)}{\overline{\lambda}_\delta \min(\xi,\xi^{-1}) - \mathrm{Re}(z)}.$$

This means that the spectral gap $\gamma(\xi,\tau)$ of the generator $\mathcal{L}_{\xi,\tau}$ on $L^2_{0,\tau}(\mu)$, defined as

$$\gamma(\xi,\tau) = \min \left\{ \mathrm{Re}(z),\, z \in \sigma(-\mathcal{L}_{\xi,\tau}) \backslash \{0\} \right\},$$

is bounded from below as

$$\gamma(\xi,\tau) \geqslant \overline{\lambda}_\delta \min(\xi,\xi^{-1}). \tag{2.13}$$

We show in Section 2.4.1 how to approximate the spectral gap using a Galerkin discretization of the generator $\mathcal{L}_{\xi,\tau}$. We then study in Section 2.4.2 the relevance of the lower bound (2.13) from a numerical viewpoint, and check that it is in fact sharp.

2.4.1 Discretization by a Galerkin procedure

We consider $d = 1$ for simplicity, although the discretization procedure described below can be extended to any arbitrary dimension by a tensorization argument, with of course the caveat that the computational cost of the method explodes. The Galerkin discretization we use relies on a tensor product of Fourier modes in space and Hermite functions for the momenta, see for instance Latorre Biagini et al. (2013), Redon et al. (2016), Roussel and Stoltz (2017) for previous similar discretizations as well as Risken (1989) for a seminal presentation of such approaches. More precisely, we introduce the following discretization basis for $n \in \{0, \dots, N\}$ and $k \in \{-K, \dots, K\}$:

$$\psi_{nk}(q,p) = G_k(q) H_n(p), \qquad G_k(q) = \sqrt{\frac{Z_\nu}{2\pi}}\, \mathrm{e}^{\mathrm{i}kq + \beta U(q)/2},$$

where H_n is the Hermite polynomial of degree n:

$$H_n(p) = \frac{(-1)^n}{n!} \left(\sqrt{\frac{m}{\beta}}\right)^n \mathrm{e}^{\beta p^2/(2m)} \frac{\mathrm{d}^n}{\mathrm{d}p^n} \left(\mathrm{e}^{-\beta p^2/(2m)}\right),$$

and

$$Z_\nu = \int_0^{2\pi} \mathrm{e}^{-\beta U}$$

is the normalization constant of the marginal of μ in the position variable. Recall that the Hermite polynomials are orthonormal on $L^2(\kappa)$, where $\kappa(\mathrm{d}p)$ is the marginal of μ in the momentum variable:

$$\kappa(\mathrm{d}p) = \int_{\mathcal{D}} \mu(\mathrm{d}q\, \mathrm{d}p) = \sqrt{\frac{\beta}{2\pi m}} \mathrm{e}^{-\beta p^2/(2m)}\, \mathrm{d}p. \tag{2.14}$$

Note that the family $\{\psi_{nk}(q,p)\}_{0 \leqslant n \leqslant N, -K \leqslant k \leqslant K}$ is orthonormal in $L^2(\mu)$, and spans $L^2(\mu)$ in the limit $N \to +\infty$ and $K \to +\infty$.

The generator $\mathcal{L}_{\xi,\tau}$ is represented in this basis by a matrix with elements

$$\left[\hat{L}_{\xi,\tau}\right]_{n'k',nk} = \left\langle \psi_{n'k'}, \mathcal{L}_{\xi,\tau} \psi_{nk} \right\rangle_{L^2(\mu)}. \tag{2.15}$$

These matrix elements are easily computed using the following properties of Hermite functions:

$$\partial_p H_n(p) = \sqrt{\frac{\beta n}{m}} H_{n-1}(p),$$
$$\partial_p^* H_n(p) = \frac{\beta p}{m} H_n(p) - \partial_p H_{n-1}(p) = \sqrt{\frac{\beta(n+1)}{m}}\, H_{n+1}(p).$$

In particular, Hermite polynomials are a complete set of eigenfunctions for $\mathcal{L}_{\mathrm{FD}}$ on $L^2(\kappa)$, and $\mathcal{L}_{\mathrm{FD}} H_n = -n H_n/m$. In addition, the action of derivatives on the Fourier modes can be evaluated as

$$\left\langle G_{k'}, \partial_q G_k \right\rangle_{L^2(\nu)} = \mathrm{i}k\delta_{k,k'} + \frac{\beta}{2} u_{k-k'}, \qquad u_K = \frac{1}{2\pi} \int_0^{2\pi} U'(q)\, \mathrm{e}^{\mathrm{i}Kq}\, \mathrm{d}q.$$

Finally, note also that the Hamiltonian part of the generator can be rewritten as

$$\mathcal{L}_{\rm ham} = \frac{1}{\beta}\left(\partial_q \partial_p^* - \partial_p \partial_q^*\right).$$

Therefore,

$$\begin{aligned}\langle \psi_{n'k'}, \mathcal{L}_{\rm ham}\psi_{nk}\rangle_{L^2(\mu)} = \frac{1}{\beta}\Big(&\left\langle G_{k'}, \partial_q G_k\right\rangle_{L^2(\nu)}\left\langle H_{n'}, \partial_p^* H_n\right\rangle_{L^2(\kappa)} \\ &- \overline{\left\langle G_k, \partial_q G_{k'}\right\rangle_{L^2(\nu)}}\left\langle H_{n'}, \partial_p H_n\right\rangle_{L^2(\kappa)}\Big) \\ = &\sqrt{\frac{\beta(n+1)}{m}}\delta_{n',n+1}\left[\frac{\mathrm{i}k}{\beta}\delta_{k,k'} + \frac{1}{2}u_{k-k'}\right] \\ &+ \sqrt{\frac{\beta n}{m}}\delta_{n',n-1}\left[\frac{\mathrm{i}k}{\beta}\delta_{k,k'} - \frac{1}{2}u_{k-k'}\right].\end{aligned}$$

Moreover, with $F = 1$,

$$\left\langle \psi_{n'k'}, \mathcal{L}_{\rm pert}\psi_{nk}\right\rangle_{L^2(\mu)} = \sqrt{\frac{\beta n}{m}}\delta_{n',n-1}\delta_{k,k'}.$$

In conclusion,

$$\begin{aligned}\left\langle \psi_{n'k'}, \mathcal{L}_{\xi,\tau}\psi_{nk}\right\rangle_{L^2(\mu)} = &\sqrt{\frac{\beta(n+1)}{m}}\delta_{n',n+1}\left[\frac{\mathrm{i}k}{\beta}\delta_{k,k'} + \frac{1}{2}u_{k-k'}\right] \\ &+ \sqrt{\frac{\beta n}{m}}\delta_{n',n-1}\left[\left(\frac{\mathrm{i}k}{\beta} + \tau\right)\delta_{k,k'} - \frac{1}{2}u_{k-k'}\right] \\ &- \frac{\xi n}{m}\delta_{n,n'}\delta_{k,k'}.\end{aligned}$$

The spectral gap of $\mathcal{L}_{\xi,\tau}$ is approximated by the spectral gap of the matrix with elements (2.15). There are currently no error estimates on the spectral approximation provided by this procedure, while in contrast there is a large body of literature on the Galerkin approximation of operators defined by quadratic forms (see for instance Chatelin (2011) and references therein). Some preliminary steps in this direction are however provided in Roussel and Stoltz (2017) in the form of error estimates on the discretization of solutions of Poisson equations $-\mathcal{L}_{\xi,\tau}\Phi = f$.

Although the extension of the Galerkin procedure poses no difficulties from a conceptual viewpoint, it is strongly limited by the size of the matrices to be considered, which, for a standard tensorized basis, are of dimension $(N+1)^d(2K+1)^d$. The two-dimensional case is therefore already challenging. In order to make the method more efficient, it would be necessary to use the sparsity of the matrices under consideration (see (2.16)), devise better bases than tensorized ones by using tensor formats, see Hackbusch (2012), relying on preconditionning strategies, etc. This work is in progress.

2.4.2 Numerical results

We choose $U(q) = U_0(1 - \cos q)$, which corresponds to the so-called rotor model. The partition function Z_ν can be explicitly computed as

$$Z_\nu = 2\pi \mathrm{e}^{-\beta U_0} I_0(\beta U_0),$$

where $I_0(a) = (2\pi)^{-1} \int_0^{2\pi} \mathrm{e}^{a\cos(q)}\, \mathrm{d}q$ is the modified Bessel function of the first kind. In addition,

$$u_{k-k'} = -\frac{\mathrm{i}U_0}{2}(\delta_{k',k+1} - \delta_{k',k-1}).$$

We define as $\hat{0}$ the null squared matrix of order $2K+1$ and the following squared matrices of the same order:

$$\begin{aligned}
\hat{A}_m &\doteq \sqrt{\frac{\beta m}{m}}\, i \left[\frac{k}{\beta}\delta_{k'k} - \frac{U_0}{4}(\delta_{k'k+1} - \delta_{k'k-1})\right], \\
\hat{B}_m &\doteq \sqrt{\frac{\beta m}{m}} \left[\tau\,\delta_{k'k} + i\left(\frac{k}{\beta}\delta_{k'k} + \frac{U_0}{4}(\delta_{k'k+1} - \delta_{k'k-1})\right)\right], \\
\hat{C}_m &\doteq m\frac{\xi}{m}\delta_{k'k},
\end{aligned}$$

with $m \in [1, N]$. With this definitions, we can express the matrix $\hat{L}_{\xi,\tau}$ as

$$\hat{L} = \begin{pmatrix}
\hat{0} & \hat{A}_1 & \hat{0} & \cdots & \cdots & \cdots & \cdots & \cdots & \hat{0} \\
\hat{B}_1 & -\hat{C}_1 & \hat{A}_2 & \ddots & & & & & \vdots \\
\hat{0} & \hat{B}_2 & -\hat{C}_2 & \hat{A}_3 & \ddots & & & & \vdots \\
\vdots & \ddots & \hat{B}_3 & -\hat{C}_3 & \hat{A}_4 & \ddots & & & \vdots \\
\vdots & & \ddots & \hat{B}_4 & -\hat{C}_4 & \hat{A}_5 & \ddots & & \vdots \\
\vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & & & \ddots & \hat{B}_{N-2} & -\hat{C}_{N-2} & \hat{A}_{N-1} & \hat{0} \\
\vdots & & & & & \ddots & \hat{B}_{N-1} & -\hat{C}_{N-1} & \hat{A}_N \\
\hat{0} & \cdots & \cdots & \cdots & \cdots & \cdots & \hat{0} & \hat{B}_N & -\hat{C}_N
\end{pmatrix}. \tag{2.16}$$

We first show in Section 2.4.2.1 that the spectral gap can be estimated with the procedure described in Section 2.4.1, by comparing the computed spectral gap to known analytical values in the case when $U_0 = 0$ (see Kozlov (1989)) and studying the convergence of the spectral gap in the limit $N, K \to +\infty$. We next present in Section 2.4.2.2 plots of the spectral gap a function of the friction, for various values of the external forcing τ and magnitude U_0 of the potential energy.

2.4.2.1 Checking the convergence

We first study the convergence of the spectral gap with respect to the basis sizes N, K. We choose $N = 2K$ in all our simulations, as well as $m = \beta = 1$. As can be seen from the numerical results presented in Figure 2.1 and as confirmed by extensive simulations not reported here, the convergence is faster for larger values of the friction ξ. In the results reported below, we consider the spectral gap to be converged when the relative variation between the current estimation of the spectral gap for a given basis size $K = N/2$ and the average of the last three ones corresponding to values of $K-1, K-2, K-3$ is lower than 10^{-3}. Let us also emphasize that, when the values of τ are too large in the case of small frictions,

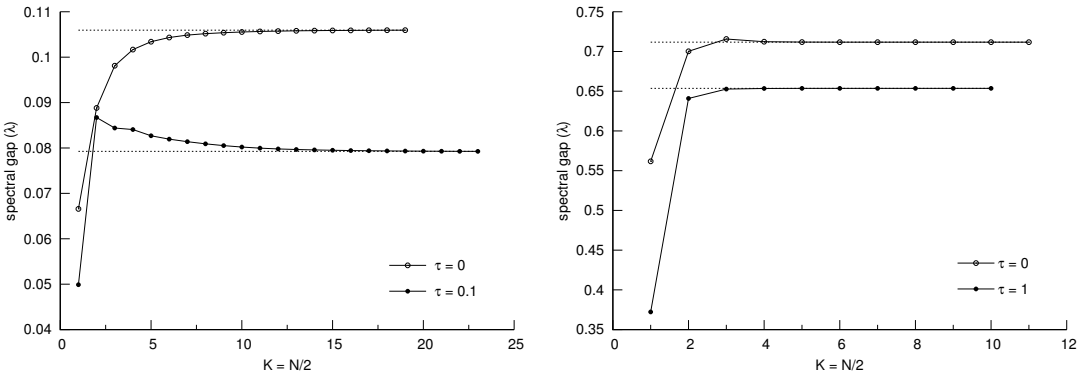


Figure 2.1 – Convergence of the estimated spectral gap as a function of the basis sizes $K = N/2$, for $U_0 = 1$. Left: $\xi = 0.1$. Right: $\xi = 1$.

we do not observe convergence for reasonable values of K (about 20). In fact, for too large forcings, we observe that the spectral gap is negative for the smallest values of K, but then becomes positive again for sufficiently large K; although this stabilization to a positive value may occur for prohibitely large values of K for small ξ.

As a consistency check, we next verify that the spectral gap predicted by the Galerkin method agrees with the one which can be analytically computed in the case when $U_0 = 0$. More precisely, the results of Kozlov (1989) show that the eigenvalues are

$$\lambda_{n,k} = -\frac{n\xi}{m} - \frac{k^2}{\beta\xi}, \tag{2.17}$$

so that the spectral gap is

$$\gamma(\xi, 0) = \min\left(\frac{\xi}{m}, \frac{1}{\beta\xi}\right). \tag{2.18}$$

We refer to Appendix 2.6.1 for the details of the computation leading to (2.17) and (2.18), and to Section 3.2 for another method to obtain the estimation (2.18). The crossover from one eigenvalue branch to the other occurs at $\xi = \sqrt{m/\beta}$. Figure 2.2 presents the eigenvalues which are numerically computed. They are in perfect agreement with the theoretical prediction (2.18).

2.4.2.2 Spectral gap as a function of the friction

We report in Figures 2.3 and 2.4 the spectral gap as a function of the friction ξ for various values of the forcing τ and the choice $U_0 = 1$ (with $m = 1$ and $\beta = 1$). The first point to mention is that the introduction of a potential smoothes out the sharp transition observed at $\xi = \sqrt{m/\beta} = 1$ when $U_0 = 0$ and $\tau = 0$ (recall Figure 2.2). As τ is increased, we were able to compute the spectral gap only for frictions above a certain treshold, roughly $\xi \geqslant |\tau|$. The spectral gap is increased with respect to the case $\tau = 0$ in a certain range of values of ξ (roughly, $1 \leqslant \xi \leqslant 4$), and decreased for other ones (in particular $\xi \leqslant 1$). Forcings however have to be sufficiently strong in order for the perturbation to have some non-negligible impact (when $\tau = 0.1$, the perturbation on the spectral gap is visible only around

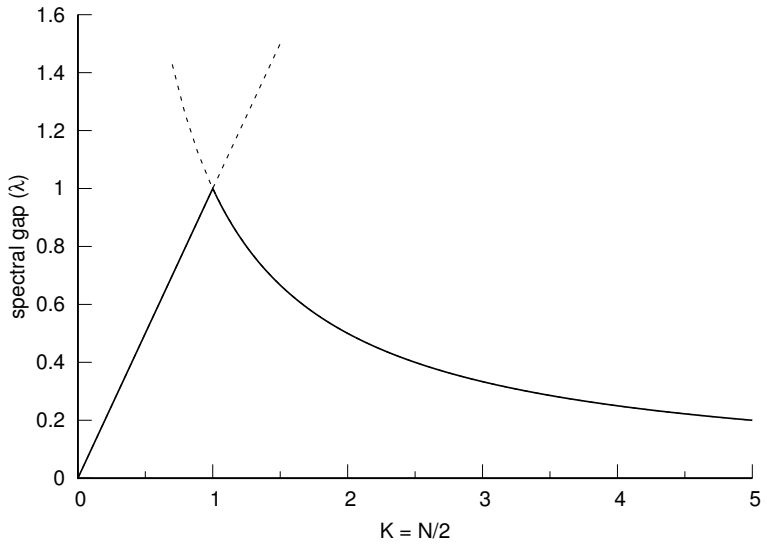


Figure 2.2 – Predicted spectral gap as a function of the friction ξ when $U_0 = 0$, $\beta = 1$ and $m = 1$ (solid line), and theoretical prediction (2.18) *(dashed lines; one of the lines represents ξ the other one $1/\xi$).*

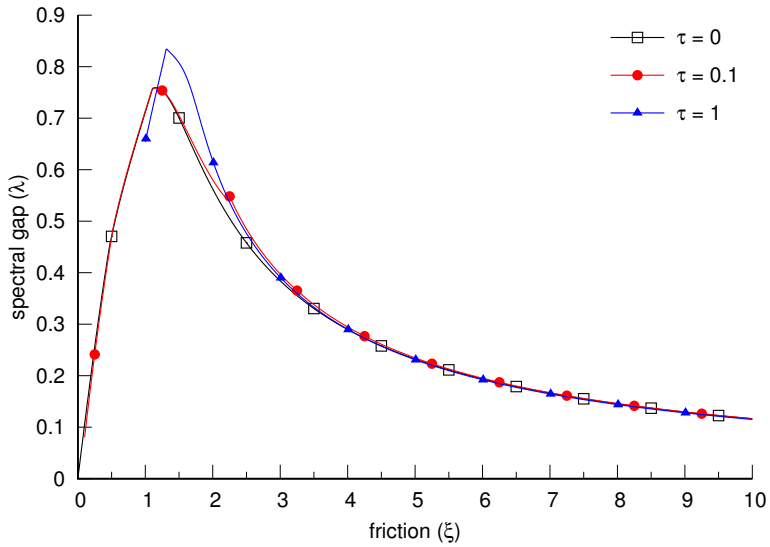


Figure 2.3 – Spectral gap as a function of ξ for $\tau = 0, 0.1, 1$ when $U(q) = 1 - \cos(q)$.

$\xi = 2$). Lastly, we observe that the spectral gap decreases as Γ_τ/ξ for large ξ (for some prefactor $\Gamma_\tau > 0$) whatever the value of τ we considered, with Γ_τ decreasing as τ increases.

We next study the influence of the potential by computing the spectral gap for various values of τ, ξ when the potential is $U(q) = U_0(1 - \cos(q))$. The results for $U_0 = 0.1$ and $U_0 = 10$ are reported in Figure 2.5. Note that the effect of the perturbation is less visible on these pictures: the spectral gaps are much closer to the ones corresponding to $\tau = 0$. For U_0 small, this is related to the fact that the spectral gap is independent of τ when $U_0 = 0$ (see Section 3.2), a feature which approximately persists for small but non-zero values of U_0. For large U_0, the perturbation τF is dominated by the gradient part of the force $U'(q)$; hence it has

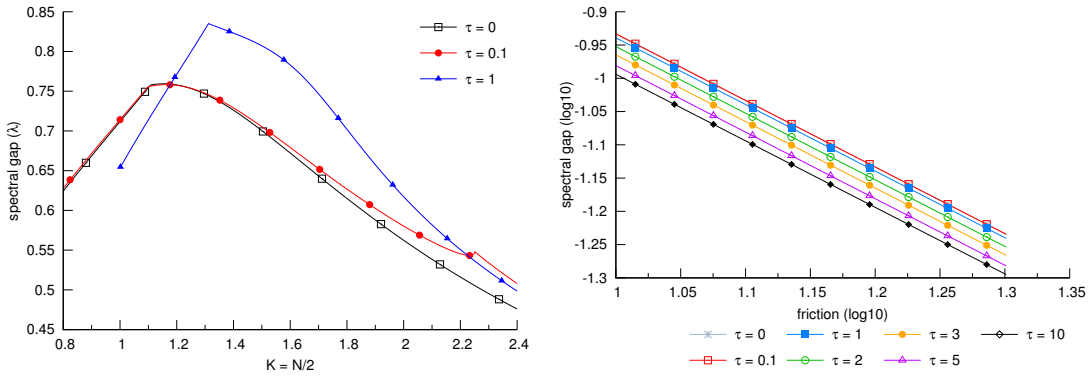


Figure 2.4 – Zoom of Figure 2.3 around $\xi = 1$ (Left) and large ξ (Right; logarithmic scale).

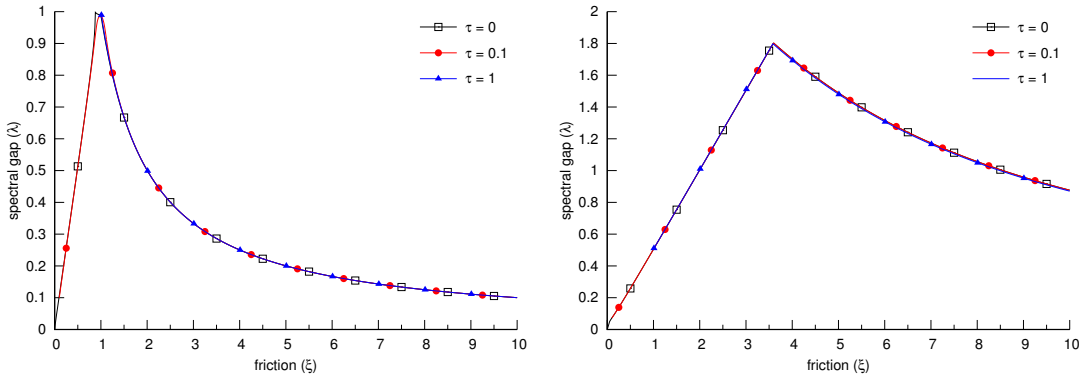


Figure 2.5 – Spectral gap as a function of ξ for $\tau = 0, 0.1, 1$ when $U(q) = U_0(1 - \cos(q))$. Left: $U_0 = 0.1$. Right: $U_0 = 10$.

less impact on the spectral gap.

2.5 Proofs of the results

We introduce the marginal measure in the position variable:

$$\nu(\mathrm{d}q) = \int_{\mathbb{R}^d} \mu(\mathrm{d}q\,\mathrm{d}p) = Z_\nu^{-1} \mathrm{e}^{-\beta U(q)}\,\mathrm{d}q.$$

Recall also the definition (2.14) for the marginal $\kappa(\mathrm{d}q)$ in the momentum variable. These measures satisfy the following Poincaré inequalities:

$$\forall \varphi \in H^1(\nu) \cap L^2_0(\nu), \qquad \|\varphi\|_{L^2(\nu)} \leqslant \frac{1}{K_\nu} \|\nabla_q \varphi\|_{L^2(\nu)}, \tag{2.19}$$

and

$$\forall \phi \in H^1(\kappa) \cap L^2_0(\kappa), \qquad \|\phi\|_{L^2(\kappa)} \leqslant \frac{1}{K_\kappa} \|\nabla_p \phi\|_{L^2(\kappa)}. \tag{2.20}$$

In fact, $K_\kappa = \sqrt{\beta/m}$. The measure μ therefore also satisfies a Poincaré inequality:

$$\forall g \in H^1(\mu) \cap L^2_0(\mu), \qquad \|g\|^2_{L^2(\mu)} \leqslant \frac{1}{K_\nu^2} \|\nabla_q g\|^2_{L^2(\mu)} + \frac{1}{K_\kappa^2} \|\nabla_p g\|^2_{L^2(\mu)}. \tag{2.21}$$

This also implies

$$\forall g \in H^1(\mu) \cap L^2_0(\mu), \qquad \|g\|_{L^2(\mu)} \leqslant \frac{1}{K_\nu}\|\nabla_q g\|_{L^2(\mu)} + \frac{1}{K_\kappa}\|\nabla_p g\|_{L^2(\mu)}. \tag{2.22}$$

We refer to Section 2.6.2 for further details and explicit estimations of K_ν and K_κ.

In all the proofs below, we start by fixing a function f in the Hilbert space under consideration, and define

$$f(t) = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau. \tag{2.23}$$

Note that, to simplify the notation, we omit the dependence of $f(t)$ on ξ, τ. We also consider that $\mathcal{L}_{\xi,\tau}$ is defined on $L^2(\mu)$, with domain

$$D(\mathcal{L}_{\xi,\tau}) = \{f \in L^2(\mu),\ \mathcal{L}_{\xi,\tau} f \in L^2(\mu)\}.$$

In all cases under consideration, $f(t)$ has average 0 with respect to μ for all times $t \geqslant 0$. We will also make use of the following remark: the smallest eigenvalue of the positive definite matrix

$$\mathcal{M} = \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix}$$

is

$$\Lambda_-(\mathcal{M}) = \frac{a+c}{2} - \frac{1}{2}\sqrt{(a-c)^2 + b^2} = \frac{4ac - b^2}{a + c + \sqrt{(a-c)^2 + b^2}}. \tag{2.24}$$

2.5.1 Proof of Theorem 9

Formally,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\|f(t)\|^2_{a(\xi)}\right) = \left\langle f(t), \mathcal{L}^*_{\xi,\tau} f(t)\right\rangle_{a(\xi)}.$$

The exponential decay therefore follows by a Gronwall inequality provided

$$\forall g \in D(\mathcal{L}^*_{\xi,\tau}) \cap L^2_0(\mu), \qquad \left\langle g, \mathcal{L}^*_{\xi,\tau} g\right\rangle_{a(\xi)} \leqslant -\lambda(\xi,\tau)\|g\|^2_{a(\xi)},$$

for some $\lambda(\xi,\tau) > 0$. Let us establish this inequality by considering a smooth and compactly supported function g with average 0 with respect to μ, and then conclude by density. By the computations recalled in Lelièvre and Stoltz (2016, Section 2.2.3) (which correspond to the equilibrium case $\tau = 0$),

$$\left\langle g, \mathcal{L}^*_{\xi,0} g\right\rangle_{a(\xi)} \leqslant -X^T S(\xi) X - \frac{\xi a(\xi)}{\beta}\|(\nabla_p + \nabla_q)\nabla_p g\|^2_{L^2(\mu)}, \tag{2.25}$$

with

$$X = \begin{pmatrix} \|\nabla_p g\|_{L^2(\mu)} \\ \|\nabla_q g\|_{L^2(\mu)} \end{pmatrix}, \quad S(\xi) = \begin{pmatrix} S_{pp}(\xi) 1_d & S_{qp}(\xi) 1_d/2 \\ S_{qp}(\xi) 1_d/2 & S_{qq}(\xi) 1_d \end{pmatrix},$$

the elements of the matrix S being

$$S_{pp}(\xi) = \xi\left(\frac{1}{\beta} + \frac{a(\xi)}{m}\right) - a(\xi)\|\nabla^2 U\|_{L^\infty}, \quad S_{qq}(\xi) = \frac{a(\xi)}{m},$$
$$S_{qp}(\xi) = -a(\xi)\left(\frac{1+\xi}{m} + \|\nabla^2 U\|_{L^\infty}\right).$$

In addition, the perturbation term can be bounded as

$$\left|\left\langle g, \mathcal{L}^*_{\mathrm{pert}} g\right\rangle_{a(\xi)}\right| \leqslant \left|\left\langle \mathcal{L}_{\mathrm{pert}} g, g\right\rangle_{L^2(\mu)}\right| + a(\xi)\left|\left\langle (\nabla_q + \nabla_p)g, (\nabla_q + \nabla_p)F \cdot \nabla_p^* g\right\rangle_{a(\xi)}\right|.$$

Since $(\partial_{q_i} + \partial_{p_i})\partial^*_{p_j} g = \partial^*_{p_j}(\partial_{q_i} + \partial_{p_i})g + \delta_{ij}\beta g/m$, it follows that

$$\begin{aligned}
\left|\left\langle g, \mathcal{L}^*_{\mathrm{pert}} g\right\rangle_{a(\xi)}\right| &\leqslant \|g\|_{L^2(\mu)}\|\nabla_p g\|_{L^2(\mu)} \\
&\quad + a(\xi)\|(\nabla_p + \nabla_q)g\|_{L^2(\mu)}\left(\|(\nabla_p + \nabla_q)\nabla_p g\|_{L^2(\mu)} + \frac{\beta}{m}\|g\|_{L^2(\mu)}\right) \\
&\leqslant \|g\|_{L^2(\mu)}\left[\left(1 + \frac{\beta a(\xi)}{m}\right)\|\nabla_p g\|_{L^2(\mu)} + \frac{\beta a(\xi)}{m}\|\nabla_q g\|_{L^2(\mu)}\right] \\
&\quad + \eta a(\xi)\left(\|\nabla_p g\|_{L^2(\mu)} + \|\nabla_q g\|_{L^2(\mu)}\right)^2 \\
&\quad + \frac{a(\xi)}{4\eta}\|(\nabla_p + \nabla_q)\nabla_p g\|^2_{L^2(\mu)},
\end{aligned}$$

for any $\eta > 0$ by Young's inequality. Therefore, using (2.22),

$$\left|\left\langle g, \mathcal{L}^*_{\mathrm{pert}} g\right\rangle_{a(\xi)}\right| \leqslant X^T T(\xi, \eta) X + \frac{a(\xi)}{4\eta}\|(\nabla_p + \nabla_q)\nabla_p g\|^2_{L^2(\mu)}, \tag{2.26}$$

where

$$T(\xi, \eta) = \begin{pmatrix} T_{pp}(\xi, \eta)1_d & T_{qp}(\xi, \eta)1_d/2 \\ T_{qp}(\xi, \eta)1_d/2 & T_{qq}(\xi, \eta)1_d \end{pmatrix},$$

the elements of the matrix T being

$$T_{pp}(\xi, \eta) = \frac{1}{K_\kappa}\left(1 + \frac{\beta a(\xi)}{m}\right) + \eta a(\xi), \quad T_{qq}(\xi, \eta) = \frac{\beta a(\xi)}{m K_\nu} + \eta a(\xi).$$

$$T_{qp}(\xi, \eta) = \frac{1}{K_\nu}\left(1 + \frac{\beta a(\xi)}{m}\right) + \frac{\beta a(\xi)}{m K_\kappa} + 2\eta a(\xi),$$

Finally, in view of the Poincaré inequality (2.21), the norm $\|\cdot\|_{a(\xi)}$ can be controlled by $|X|$ as

$$\|g\|^2_{a(\xi)} \leqslant X^T P(\xi) X, \qquad P(\xi) = \begin{pmatrix} a(\xi) + \dfrac{1}{K_\kappa^2} & a(\xi) \\ a(\xi) & a(\xi) + \dfrac{1}{K_\nu^2} \end{pmatrix}.$$

The comparison between (2.25) and (2.26) suggests choosing $\eta = \beta|\tau|/(4\xi)$. The constant $\lambda(\xi, \tau)$ can therefore be chosen as the largest real number such that

$$S(\xi) - |\tau| T\left(\xi, \frac{\beta|\tau|}{4\xi}\right) \geqslant \lambda(\xi, \tau) P(\xi). \tag{2.27}$$

Let us now make this condition more explicit by distinguishing the two limiting regimes $\xi \to 0$ and $\xi \to +\infty$.

(i) When $\xi \to 0$, the condition that S should be positive definite requires in particular that $S_{pp}(\xi) > 0$. This means that $a(\xi)$ should be sufficiently small, in fact at most of order ξ. We therefore consider $a(\xi) = \overline{a}_0\xi + \mathrm{O}(\xi^2)$. The condition (2.27) then reduces to

$$\begin{pmatrix} \xi\left(\frac{1}{\beta} - \overline{a}_0\|\nabla^2 U\|_{L^\infty}\right) - |\tau|\left(\frac{1}{K_\kappa} + \frac{\beta\overline{a}_0|\tau|}{4}\right) & -\frac{\overline{a}_0\xi}{2}\left(\frac{1}{m} + \|\nabla^2 U\|_{L^\infty}\right) - \frac{|\tau|}{2K_\nu} - \frac{\beta\overline{a}_0|\tau|^2}{4} \\ -\frac{\overline{a}_0\xi}{2}\left(\frac{1}{m} + \|\nabla^2 U\|_{L^\infty}\right) - \frac{|\tau|}{2K_\nu} - \frac{\beta\overline{a}_0|\tau|^2}{4} & \frac{\overline{a}_0\xi}{m} - \frac{\beta\overline{a}_0|\tau|^2}{4} \end{pmatrix}$$
$$+ \mathrm{O}\left(\xi^2, \xi|\tau|\right) \geqslant \lambda(\xi,\tau)\left[\begin{pmatrix} \frac{1}{K_\kappa^2} & 0 \\ 0 & \frac{1}{K_\nu^2} \end{pmatrix} + \mathrm{O}(\xi)\right].$$

It is then clear (by considering for instance the first element on the matrix on the left-hand side) that τ can be chosen to be at most of order ξ, which we write as $|\tau| = \delta\xi$. The above inequality then reduces to

$$\begin{pmatrix} \frac{1}{\beta} - \overline{a}_0\|\nabla^2 U\|_{L^\infty} - \frac{\delta}{K_\kappa} & -\frac{\overline{a}_0}{2}\left(\frac{1}{m} + \|\nabla^2 U\|_{L^\infty}\right) - \frac{\delta}{2K_\nu} \\ -\frac{\overline{a}_0}{2}\left(\frac{1}{m} + \|\nabla^2 U\|_{L^\infty}\right) - \frac{\delta}{2K_\nu} & \frac{\overline{a}_0}{m} \end{pmatrix} + \mathrm{O}(\xi)$$
$$\geqslant \frac{\lambda(\xi,\delta\xi)}{\xi}\left[\begin{pmatrix} \frac{1}{K_\kappa^2} & 0 \\ 0 & \frac{1}{K_\nu^2} \end{pmatrix} + \mathrm{O}(\xi)\right].$$

We next choose $\delta > 0$ sufficiently small and then $\overline{a}_0$ sufficiently small in order to satisfy the above inequality. In any case, $\lambda(\xi,\tau)$ is of order ξ. Moreover, from the above matrix expression, it is clear that $[\lambda(\xi,\delta\xi) - \lambda(\xi,0)]/\xi = \mathrm{O}(\delta)$.

(ii) When $\xi \to +\infty$, the limitation on $a(\xi)$ arises from the fact that the determinant of $S(\xi)$ should be positive, which requires $\xi a(\xi)$ to be bounded. We therefore consider $a(\xi) = \overline{a}_\infty/\xi + \mathrm{O}(\xi^{-2})$.The condition (2.27) then reduces to

$$\begin{pmatrix} \frac{\xi}{\beta} & -\frac{\overline{a}_\infty}{2m} \\ -\frac{\overline{a}_\infty}{2m} & \frac{\overline{a}_\infty}{m\xi} \end{pmatrix} - |\tau|\begin{pmatrix} \frac{1}{K_\kappa} & \frac{1}{2K_\nu} \\ \frac{1}{2K_\nu} & 0 \end{pmatrix} + \mathrm{O}\left(\frac{1}{\xi^2}, \frac{|\tau|}{\xi}\right) \geqslant \lambda(\xi,\tau)\left[\begin{pmatrix} \frac{1}{K_\kappa^2} & 0 \\ 0 & \frac{1}{K_\nu^2} \end{pmatrix} + \mathrm{O}\left(\frac{1}{\xi}\right)\right].$$

In view of (2.24), the smallest eigenvalue of the first matrix on the left-hand side is of order $1/\xi$, so that τ can be at most of order $1/\xi$, which we write as $\tau = \delta/\xi$. The above inequality then shows that $\lambda(\xi,\delta/\xi)$ is of order $1/\xi$, and that $\xi[\lambda(\xi,\delta\xi) - \lambda(\xi,0)] = \mathrm{O}(\delta)$.

2.5.2 Proof of Theorem 10

The key estimate for proving the result is the following hypoelliptic regularization result.

Proposition 7. *There exist $K, \delta_* > 0$ such that, for any $\xi > 0$ and $\tau \in [0, \delta_* \min(\xi, 1)]$,*

$$\forall g \in L^2(\mu),\ \forall 0 < t \leqslant 1, \qquad \left\|\nabla_p \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} g\right\|_{L^2(\mu)} + \left\|\nabla_q \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} g\right\|_{L^2(\mu)} \leqslant \frac{K \max\left(\xi, \xi^{-1}\right)}{t^{3/2}} \|g\|_{L^2(\mu)}.$$

Note that the hypoelliptic regularization is possible for values of τ of order 1 when ξ is large, and it is therefore not this step which limits the range of admissible forcings in Theorem 10.

As a corollary of Proposition 7, there exists a constant $\widetilde{K} > 0$ such that

$$\|f(t)\|_{a(\xi)}^2 \leqslant \widetilde{K} t^{-3/2} \|f\|_{L^2(\mu)}$$

for $0 < t \leqslant 1$ when the product $a(\xi)\max(\xi, \xi^{-1})$ is bounded, which is the case for the function $a(\xi)$ considered in Theorem 9. Combining this inequality and Theorem 9 with $t_0 = 1$, for instance, we can conclude that, for $t \geqslant 1$, and any $\xi \in (0, +\infty)$ and $\tau \in [-\delta \min(\xi, \xi^{-1}), \delta \min(\xi, \xi^{-1})]$

$$\|f(t)\|_{L^2(\mu)}^2 \leqslant \|f(t)\|_{a(\xi)}^2 \leqslant \mathrm{e}^{-2\overline{\lambda}_\delta \min(\xi,\xi^{-1})(t-t_0)} \|f(t_0)\|_{a(\xi)}^2 \leqslant \widetilde{K}\, \mathrm{e}^{-2\overline{\lambda}_\delta \min(\xi,\xi^{-1})(t-t_0)} \|f(0)\|_{L^2(\mu)}^2,$$

which gives the claimed exponential decay in $L^2(\mu)$.

Proof of Proposition 7. We denote $g(t) = \mathrm{e}^{t\mathcal{L}_{\xi,\tau}^*} g$, and introduce

$$N_g(t) = \frac{1}{2}\Big(\|g(t)\|_{L^2(\mu)}^2 + A(\xi) t \|\nabla_p g(t)\|_{L^2(\mu)}^2 + C(\xi) t^3 \|\nabla_q g(t)\|_{L^2(\mu)}^2 + 2B(\xi) t^2 \left\langle \nabla_p g(t), \nabla_q g(t) \right\rangle_{L^2(\mu)} \Big),$$

where $A(\xi), C(\xi)$ are positive and $A(\xi)C(\xi) - B(\xi)^2 > 0$. The result follows provided $N_g(t)$ has a controlled increase (in the sense that $N_g(1)$ can be controlled by $N_g(0)$ up to a multiplicative factor) and $A(\xi)C(\xi) - B(\xi)^2$ is of order $\min(\xi, \xi^{-1})$.

By computations similar to the ones leading to (2.25) (see for instance the proof of Lelièvre and Stoltz (2016, Theorem 2.18)), the following inequality holds when $B(\xi) > 3mC(\xi)/2$:

$$\begin{aligned}
\frac{\mathrm{d}N_g(t)}{\mathrm{d}t} \leqslant & -\left(\frac{\xi}{\beta} + A(\xi)\left(\frac{\xi t}{m} - \frac{1}{2} \right) - \|\nabla^2 U\|_{L^\infty} B(\xi) t^2 \right) \left\| \nabla_p g(t) \right\|_{L^2(\mu)}^2 \\
& - \left(\frac{B(\xi)}{m} - \frac{3C(\xi)}{2} \right) t^2 \left\| \nabla_q g(t) \right\|_{L^2(\mu)}^2 \\
& + t\left(2B(\xi) + \frac{A(\xi)}{m} + \frac{\xi B(\xi) t}{m} + C(\xi) \|\nabla^2 U\|_{L^\infty} t^2 \right) \left\| \nabla_p g(t) \right\|_{L^2(\mu)} \left\| \nabla_q g(t) \right\|_{L^2(\mu)} \\
& - \frac{\xi t}{\beta} \Big(A(\xi) \left\| \nabla_p^2 g(t) \right\|_{L^2(\mu)}^2 - 2B(\xi) t \|\nabla_p^2 g(t)\|_{L^2(\mu)} \|\nabla_{qp}^2 g(t)\|_{L^2(\mu)} \\
& \qquad + C(\xi) t^2 \left\| \nabla_{qp}^2 g(t) \right\|_{L^2(\mu)}^2 \Big) + \tau \widetilde{N}_g(t),
\end{aligned}$$

with

$$\begin{aligned}
\widetilde{N}_g(t) = & \left\langle g(t), \mathcal{L}_{\mathrm{pert}}^* g(t) \right\rangle_{L^2(\mu)} \\
& + A(\xi) t \left\langle \nabla_p g(t), \nabla_p \mathcal{L}_{\mathrm{pert}}^* g(t) \right\rangle_{L^2(\mu)} + C(\xi) t^3 \left\langle \nabla_q g(t), \nabla_q \mathcal{L}_{\mathrm{pert}}^* g(t) \right\rangle_{L^2(\mu)} \\
& + B(\xi) t^2 \left(\left\langle \nabla_q g(t), \nabla_p \mathcal{L}_{\mathrm{pert}}^* g(t) \right\rangle_{L^2(\mu)} + \left\langle \nabla_q \mathcal{L}_{\mathrm{pert}}^* g(t), \nabla_p g(t) \right\rangle_{L^2(\mu)} \right).
\end{aligned}$$

Note that, using $[\partial_{p_i}, \mathcal{L}^*_{\text{pert}}] = \beta F_i/m$,

$$\begin{aligned}\left|\widetilde{N}_g(t)\right| \leqslant{}& \|\nabla_p g(t)\|_{L^2(\mu)}\|g(t)\|_{L^2(\mu)} + A(\xi)t\|\nabla_p g(t)\|_{L^2(\mu)}\left(\frac{\beta}{m}\|g(t)\|_{L^2(\mu)} + \|\nabla_p^2 g(t)\|_{L^2(\mu)}\right)\\ &+ C(\xi)t^3\|\nabla_q g(t)\|_{L^2(\mu)}\|\nabla^2_{qp} g(t)\|_{L^2(\mu)}\\ &+ B(\xi)t^2\Big(\|\nabla_p g(t)\|_{L^2(\mu)}\|\nabla^2_{qp} g(t)\|_{L^2(\mu)}\\ &\qquad + \|\nabla_q g(t)\|_{L^2(\mu)}\left[\frac{\beta}{m}\|g(t)\|_{L^2(\mu)} + \|\nabla_p^2 g(t)\|_{L^2(\mu)}\right]\Big).\end{aligned}$$

We next recall that $\|g(t)\|^2_{L^2(\mu)} \leqslant 2N_g(t)$ and use Cauchy–Schwarz inequalities[(1)] such as

$$t^2\|\nabla_p g(t)\|_{L^2(\mu)}\|\nabla^2_{qp} g(t)\|_{L^2(\mu)} \leqslant \frac{t}{2}\Big(\|\nabla_p g(t)\|^2_{L^2(\mu)} + t^2\|\nabla^2_{qp} g(t)\|_{L^2(\mu)}\Big).$$

This allows the following bound on $\widetilde{N}_g(t)$

$$\begin{aligned}\left|\widetilde{N}_g(t)\right| \leqslant{}& \left(1 + \frac{\beta t(A(\xi)+B(\xi))}{m}\right)N_g(t)\\ &+ \frac{1}{2}\left(1 + A(\xi)t\left[1+\frac{\beta}{m}\right] + B(\xi)t\right)\|\nabla_p g(t)\|^2_{L^2(\mu)}\\ &+ \frac{1}{2}\left(C(\xi) + B(\xi)\left[1+\frac{\beta}{m}\right]\right)t^3\|\nabla_q g(t)\|^2_{L^2(\mu)}\\ &+ \frac{1}{2}\left(A(\xi)+B(\xi)\right)t\|\nabla_p^2 g(t)\|^2_{L^2(\mu)} + \frac{1}{2}\left(B(\xi)+C(\xi)\right)t^3\|\nabla^2_{qp} g(t)\|^2_{L^2(\mu)}.\end{aligned}$$

By combining the latter inequality and the above bound on $\mathrm{d}N_g/\mathrm{d}t$, it follows that, for any $t \in [0,1]$,

$$\begin{aligned}\frac{\mathrm{d}N_g(t)}{\mathrm{d}t} \leqslant{}& \left(1 + \frac{\beta(A(\xi)+B(\xi))}{m}\right)|\tau|N_g(t)\\ &- \left(\frac{\xi}{\beta} - \frac{A(\xi)}{2} - \|\nabla^2 U\|_{L^\infty}B(\xi) - \frac{|\tau|}{2}\left[1 + A(\xi)\left(1+\frac{\beta}{m}\right) + B(\xi)\right]\right)\left\|\nabla_p g(t)\right\|^2_{L^2(\mu)}\\ &- t^2\left(\frac{B(\xi)}{m} - \frac{3C(\xi)}{2} - \frac{|\tau|}{2}\left[C(\xi) + B(\xi)\left(1+\frac{\beta}{m}\right)\right]\right)\left\|\nabla_q g(t)\right\|^2_{L^2(\mu)}\\ &+ t\left(2B(\xi) + \frac{A(\xi)}{m} + \frac{\xi B(\xi)}{m} + C(\xi)\|\nabla^2 U\|_{L^\infty}\right)\left\|\nabla_p g(t)\right\|_{L^2(\mu)}\left\|\nabla_q g(t)\right\|_{L^2(\mu)}\\ &- \frac{\xi t}{\beta}\Big(A(\xi)\left\|\nabla_p^2 g(t)\right\|^2_{L^2(\mu)} + C(\xi)t^2\left\|\nabla^2_{qp} g(t)\right\|^2_{L^2(\mu)}\\ &\qquad - 2B(\xi)t\|\nabla_p^2 g(t)\|_{L^2(\mu)}\|\nabla^2_{qp} g(t)\|_{L^2(\mu)}\Big)\\ &+ \frac{|\tau|\left(A(\xi)+B(\xi)\right)t}{2}\|\nabla_p^2 g(t)\|^2_{L^2(\mu)} + \frac{|\tau|\left(B(\xi)+C(\xi)\right)t^3}{2}\|\nabla^2_{qp} g(t)\|^2_{L^2(\mu)}.\end{aligned}$$

(1) Although sharper results may be obtained with Young inequalities, the final scaling of admissible values of τ in terms of ξ is unaffected.

The discussion at this stage follows the same strategy as that at the end of Section 2.5.1, by rewriting the sum of the second to the fourth lines in matrix form as

$$-X^T S(\xi,\tau)X, \qquad X = \begin{pmatrix} \left\|\nabla_p g(t)\right\|_{L^2(\mu)} \\ \left\|\nabla_q g(t)\right\|_{L^2(\mu)} \end{pmatrix},$$

and the sum of the last two lines in matrix form as

$$-Y^T T(\xi,\tau)Y, \qquad Y = \begin{pmatrix} \left\|\nabla_p^2 g(t)\right\|_{L^2(\mu)} \\ \left\|\nabla_{qp}^2 g(t)\right\|_{L^2(\mu)} \end{pmatrix}.$$

We then distinguish the cases $\xi \to 0$ and $\xi \to +\infty$, and look for conditions ensuring that the matrices $S(\xi,\tau), T(\xi,\tau)$ are nonnegative. It is easily seen that the requirements translate into $A(\xi) = \overline{A}\min(\xi,\xi^{-1})$, $B(\xi) = \overline{B}\min(\xi,\xi^{-1})$, $C(\xi) = \overline{C}\min(\xi,\xi^{-1})$ for positive parameters $\overline{A},\overline{B},\overline{C}$ sufficiently small and such that $\overline{AC} - \overline{B}^2 > 0$; as well as $\tau \in [-\delta_* \min(\xi,1), \delta_* \min(\xi,1)]$ for $\delta_* > 0$ sufficiently small; and the further conditions that $\overline{C}$ and δ_* are sufficiently small compared to $\overline{B}$. There exists therefore $R > 0$ (independent of τ and ξ) such that

$$\frac{\mathrm{d}N_g(t)}{\mathrm{d}t} \leqslant R|\tau| N_g(t),$$

from which we deduce that $N_g(1) \leqslant \mathrm{e}^{R|\tau|} N_g(0) = 2\mathrm{e}^{R|\tau|}\|g\|^2_{L^2(\mu)}$. The latter inequality allows to conclude. □

2.5.3 Proof of Theorem 11

We closely follow the proof of Dolbeault et al. (2009, 2015), however specializing the operators under consideration to the case of Langevin dynamics, and considering all operators on $L^2(\mu)$. This allows to simplify several arguments in the proof.

Introduce the projection $\Pi : L^2(\mu) \to L^2(\nu)$ defined as

$$(\Pi g)(q) = \langle g(q,\cdot), \mathbf{1}\rangle_{L^2(\kappa)} = \int_{\mathbb{R}^d} g(q,p)\,\kappa(\mathrm{d}p).$$

A simple computation shows that $\Pi\mathcal{L}_{\mathrm{ham}}\Pi = 0$ since

$$(\mathcal{L}_{\mathrm{ham}}\Pi g)(q,p) = p^T \nabla_q (\Pi g)(q)/m$$

and $\Pi p = 0$. Consider also the following functional

$$\mathscr{E}(g) = \frac{1}{2}\|g\|^2_{L^2(\mu)} + a(\xi)\langle Ag, g\rangle_{L^2(\mu)},$$

for some parameter $a(\xi) \in (0,1)$ to be determined later on in terms of ξ, and with

$$A = -\left(1 - \Pi\mathcal{L}^2_{\mathrm{ham}}\Pi\right)^{-1} \Pi\mathcal{L}_{\mathrm{ham}}.$$

The latter operator can in fact be made somewhat more explicit, by computing the action of $\mathcal{L}_{\rm ham}^2\Pi$:

$$\mathcal{L}_{\rm ham}^2\Pi\varphi = \frac{1}{m^2}p^T(\nabla_q^2\Pi\varphi)p - \frac{1}{m}\nabla U\cdot\nabla_q\Pi\varphi. \tag{2.28}$$

A simple computation then shows that $\Pi\mathcal{L}_{\rm ham}^2\Pi$ is, up to a multiplicative factor $1/m$, the generator of the overdamped Langevin process (2.2):

$$\Pi\mathcal{L}_{\rm ham}^2\Pi\varphi = \frac{1}{m}\mathcal{L}_{\rm ovd}\Pi\varphi, \qquad \mathcal{L}_{\rm ovd} = -\nabla U\cdot\nabla_q + \frac{1}{\beta}\Delta_q\varphi.$$

The following result gathers some properties of the operator A (see Dolbeault et al. (2015, Lemma 1)).

Lemma 2. *It holds $\Pi A = A$. Moreover, for any function $g \in L^2(\mu)$,*

$$\|Ag\|_{L^2(\mu)} \leqslant \frac{1}{2}\|(1-\Pi)g\|_{L^2(\mu)}, \qquad \|\mathcal{L}_{\rm ham}Ag\|_{L^2(\mu)} \leqslant \|(1-\Pi)g\|_{L^2(\mu)}.$$

Proof. Consider $g \in L^2(\mu)$ and $u = Ag$. Then, $(1-\Pi\mathcal{L}_{\rm ham}^2\Pi)u = -\Pi\mathcal{L}_{\rm ham}g$, so that, taking the scalar product with respect to u,

$$\begin{aligned}\|u\|_{L^2(\mu)}^2 + \|\mathcal{L}_{\rm ham}\Pi u\|_{L^2(\mu)}^2 &= \langle\mathcal{L}_{\rm ham}\Pi u, (1-\Pi)g\rangle_{L^2(\mu)}\\ &\leqslant \|\mathcal{L}_{\rm ham}\Pi u\|_{L^2(\mu)}\|(1-\Pi)g\|_{L^2(\mu)}\\ &\leqslant \frac{1}{4}\|(1-\Pi)g\|_{L^2(\mu)}^2 + \|\mathcal{L}_{\rm ham}\Pi u\|_{L^2(\mu)}^2,\end{aligned}$$

which gives the claimed result. □

Denoting by $\mathscr{H}(t) = \mathscr{E}(f(t))$ with $f(t)$ defined in (2.23), a simple computation shows that

$$\begin{aligned}\mathscr{H}'(t) &= \langle f(t), \mathcal{L}_{\xi,\tau}f(t)\rangle_{L^2(\mu)} + a(\xi)\langle A\mathcal{L}_{\xi,\tau}^*f(t), f(t)\rangle_{L^2(\mu)} + a(\xi)\langle\mathcal{L}_{\xi,\tau}Af(t), f(t)\rangle_{L^2(\mu)}\\ &= \xi\langle f(t), \mathcal{L}_{\rm FD}f(t)\rangle_{L^2(\mu)} + \tau\langle f(t), \mathcal{L}_{\rm pert}f(t)\rangle_{L^2(\mu)}\\ &\quad - a(\xi)\langle A\mathcal{L}_{\rm ham}f(t), f(t)\rangle_{L^2(\mu)} + \xi a(\xi)\langle A\mathcal{L}_{\rm FD}f(t), f(t)\rangle_{L^2(\mu)}\\ &\quad + \tau a(\xi)\langle A\mathcal{L}_{\rm pert}^*f(t), f(t)\rangle_{L^2(\mu)} + a(\xi)\langle\mathcal{L}_{\rm ham}Af(t), f(t)\rangle_{L^2(\mu)},\end{aligned}$$

where we used in the last line that $\mathcal{L}_{\rm FD}A = \mathcal{L}_{\rm FD}\Pi A = 0$ and $\mathcal{L}_{\rm pert}A = \mathcal{L}_{\rm pert}\Pi A = 0$. Therefore,

$$\begin{aligned}\mathscr{H}'(t) &\leqslant \xi\langle f(t), \mathcal{L}_{\rm FD}f(t)\rangle_{L^2(\mu)} + \tau\langle f(t), \mathcal{L}_{\rm pert}f(t)\rangle_{L^2(\mu)}\\ &\quad - a(\xi)\langle A\mathcal{L}_{\rm ham}f(t), f(t)\rangle_{L^2(\mu)} + \xi a(\xi)\langle A\mathcal{L}_{\rm FD}f(t), f(t)\rangle_{L^2(\mu)}\\ &\quad + |\tau|a(\xi)\|A\mathcal{L}_{\rm pert}^*\|\|f(t)\|_{L^2(\mu)}\|\Pi f(t)\|_{L^2(\mu)} + a(\xi)\|(1-\Pi)f(t)\|_{L^2(\mu)}^2,\end{aligned} \tag{2.29}$$

where we used Lemma 2 to write $\mathcal{L}_{\rm ham}A = \mathcal{L}_{\rm ham}\Pi A = (1-\Pi)\mathcal{L}_{\rm ham}A$, so that

$$\left|\langle\mathcal{L}_{\rm ham}Ah, h\rangle_{L^2(\mu)}\right| = \left|\langle\mathcal{L}_{\rm ham}Ah, (1-\Pi)h\rangle_{L^2(\mu)}\right| \leqslant \|(1-\Pi)h\|_{L^2(\mu)}^2.$$

Let us now consider successively the various terms in (2.29):

- The sum first two terms on the right-hand side of (2.29) can be bounded as

$$\begin{aligned}\xi\langle f(t),\mathcal{L}_{\mathrm{FD}}f(t)\rangle_{L^2(\mu)}+\tau\langle f(t),\mathcal{L}_{\mathrm{pert}}f(t)\rangle_{L^2(\mu)}&\\ \leqslant -\frac{\xi}{\beta}\|\nabla_p f(t)\|^2_{L^2(\mu)}+|\tau|\|f(t)\|_{L^2(\mu)}\|\nabla_p f(t)\|_{L^2(\mu)}&\\ \leqslant -\left(\frac{\xi}{\beta}-\frac{|\tau|}{2\eta}\right)\|\nabla_p f(t)\|^2_{L^2(\mu)}+\frac{\eta|\tau|}{2}\|f(t)\|^2_{L^2(\mu)},&\\ \leqslant -K_\kappa^2\left(\frac{\xi}{\beta}-\frac{|\tau|}{2\eta}\right)\|(1-\Pi)f(t)\|^2_{L^2(\mu)}+\frac{\eta|\tau|}{2}\|f(t)\|^2_{L^2(\mu)},&\end{aligned}$$

  where $\eta > \beta|\tau|/(2\xi)$, and where we used $\nabla_p\Pi = 0$ and a Poincaré inequality to obtain the last inequality (since $(1-\Pi)g(t,q,\cdot) \in L^2_0(\kappa)$ for almost all q).

- We rewrite the first term of the second line of (2.29) as

$$\langle A\mathcal{L}_{\mathrm{ham}}f(t),f(t)\rangle_{L^2(\mu)} = \langle A\mathcal{L}_{\mathrm{ham}}\Pi f(t),f(t)\rangle_{L^2(\mu)}+\langle A\mathcal{L}_{\mathrm{ham}}(1-\Pi)f(t),f(t)\rangle_{L^2(\mu)}. \tag{2.30}$$

  We start with the first term on the right-hand side of the above equality. Denoting by $B = \mathcal{L}_{\mathrm{ham}}\Pi$, it holds $(Bh)(q,p) = p^T\nabla_q(\Pi h)(q)/m$. When $h \in L^2_0(\mu)$, and since ν satisfies the Poincaré inequality (2.19), it holds

$$\|Bh\|_{L^2(\mu)} = \sqrt{\frac{d}{m\beta}}\|\nabla_q(\Pi h)\|_{L^2(\nu)} \geqslant K_\nu\sqrt{\frac{d}{m\beta}}\|\Pi h\|_{L^2(\nu)}.$$

  This can be rephrased as

$$B^*B \geqslant \frac{dK_\nu^2}{m\beta}\Pi$$

  in the sense of symmetric operators on $L^2_0(\mu)$. Since

$$A\mathcal{L}_{\mathrm{ham}}\Pi = (1+B^*B)^{-1}B^*B = 1-(1+B^*B)^{-1},$$

  we can conclude that

$$-\langle A\mathcal{L}_{\mathrm{ham}}\Pi f(t),f(t)\rangle_{L^2(\mu)} \leqslant -\frac{dK_\nu^2/(m\beta)}{1+dK_\nu^2/(m\beta)}\|\Pi f(t)\|^2_{L^2(\mu)}.$$

  For the second term on the right-hand side of (2.30), we write (using $\Pi A = A$)

$$\langle A\mathcal{L}_{\mathrm{ham}}(1-\Pi)f(t),f(t)\rangle_{L^2(\mu)} = -\langle(1-\Pi)f(t),\mathcal{L}_{\mathrm{ham}}A^*\Pi f(t)\rangle_{L^2(\mu)}.$$

  By Lemma 3 below, the operator $\mathcal{L}_{\mathrm{ham}}A^*$ is bounded, so that the absolute value of the right-hand side of the above equality is bounded by

$$\|\mathcal{L}_{\mathrm{ham}}A^*\|\|(1-\Pi)f(t)\|_{L^2(\mu)}\|\Pi f(t)\|_{L^2(\mu)}.$$

- In order to treat the second term in the second line of (2.29), we compute the action of $A\mathcal{L}_{\mathrm{FD}}$. Now,

$$A\mathcal{L}_{\mathrm{FD}} = -(1-\Pi\mathcal{L}_{\mathrm{ham}}^2\Pi)^{-1}\Pi\mathcal{L}_{\mathrm{ham}}\mathcal{L}_{\mathrm{FD}} = -(1-\Pi\mathcal{L}_{\mathrm{ham}}^2\Pi)^{-1}\Pi[\mathcal{L}_{\mathrm{ham}},\mathcal{L}_{\mathrm{FD}}]$$

since $\Pi\mathcal{L}_{\mathrm{FD}} = 0$. In order to evaluate the commutator, we compute

$$[\mathcal{L}_{\mathrm{ham}},\mathcal{L}_{\mathrm{FD}}]h = \frac{1}{m}\nabla U\cdot\nabla_p h + \frac{p}{m^2}\cdot\nabla_q h - \frac{2}{m\beta}\sum_{i=1}^{d}\partial^2_{q_ip_i}h.$$

Upon applying Π to the various terms and noting that

$$\int_{\mathbb{R}^d}\partial^2_{q_ip_i}h\,d\kappa = \frac{\beta}{m}\int_{\mathbb{R}^d}p_i\partial_{q_i}h\,d\kappa,$$

it follows that $\Pi[\mathcal{L}_{\mathrm{ham}},\mathcal{L}_{\mathrm{FD}}] = -\Pi\mathcal{L}_{\mathrm{ham}}/m$ and therefore, $A\mathcal{L}_{\mathrm{FD}} = -A/m$ is bounded by Lemma 2. More precisely,

$$\left|\langle A\mathcal{L}_{\mathrm{FD}}f(t), f(t)\rangle_{L^2(\mu)}\right| \leqslant \frac{1}{2m}\|(1-\Pi)f(t)\|_{L^2(\mu)}\|\Pi f(t)\|_{L^2(\mu)}.$$

- Finally, $A\mathcal{L}^*_{\mathrm{pert}}$ is bounded by Lemma 3 below, with $\|A\mathcal{L}^*_{\mathrm{pert}}\| \leqslant \sqrt{\beta/(4m)}$.

Gathering all estimates, we obtain

$$\mathscr{H}'(t) \leqslant -X(t)^T\Big(S(\xi) - |\tau|T(\xi)\Big)X(t),$$

with

$$X = \begin{pmatrix}\|\Pi f(t)\|_{L^2(\mu)}\\ \|(1-\Pi)f(t)\|_{L^2(\mu)}\end{pmatrix},$$

$$S(\xi) = \begin{pmatrix}S_{--}(\xi) & S_{-+}(\xi)/2\\ S_{-+}(\xi)/2 & S_{++}(\xi)\end{pmatrix}, \qquad T(\xi) = \begin{pmatrix}T_{--}(\xi) & T_{-+}(\xi)/2\\ T_{-+}(\xi)/2 & T_{++}(\xi)\end{pmatrix},$$

where

$$\begin{cases} S_{--}(\xi) = a(\xi)\dfrac{dK_v^2/(m\beta)}{1+dK_v^2/(m\beta)},\\ S_{-+}(\xi) = -a(\xi)\left(\|\mathcal{L}_{\mathrm{ham}}A^*\| + \dfrac{\xi}{2m}\right),\\ S_{++}(\xi) = \dfrac{\xi K_\kappa^2}{\beta} - a(\xi), \end{cases} \qquad \begin{cases} T_{--}(\xi) = \dfrac{1}{2}\left(a(\xi)\sqrt{\dfrac{\beta}{m}} + \eta\right),\\ T_{-+}(\xi) = \dfrac{a(\xi)}{2}\sqrt{\dfrac{\beta}{m}},\\ T_{++}(\xi) = \dfrac{1}{2}\left(\eta + \dfrac{K_\kappa^2}{\eta}\right). \end{cases}.$$

Therefore, since $2\mathscr{H}(t) \leqslant (1+a(\xi))\|f(t)\|^2_{L^2(\mu)}$ by Lemma 2,

$$\mathscr{H}'(t) \leqslant -\Lambda_-\Big(S(\xi) - |\tau|T(\xi)\Big)\|f(t)\|^2_{L^2(\mu)} \leqslant -\frac{2\Lambda_-\Big(S(\xi)-|\tau|T(\xi)\Big)}{1+a(\xi)}\mathscr{H}(t), \qquad (2.31)$$

where Λ_- is defined in (2.24). We next follow a discussion similar to the one performed at the end of Section 2.5.1. When $\tau = 0$, the requirement that $S(\xi)$ is positive definite shows that $a(\xi)$ should be chosen of order $\min(\xi, \xi^{-1})$. Next, in order for $S(\xi) - |\tau| T(\xi)$ to be positive definite for $\tau \neq 0$, we see that τ should be of order ξ when $\xi \to 0$ (choosing $\eta = \beta\tau/(4\xi)$ for instance), but can be taken to be of order 1 as $\xi \to +\infty$ by setting $\eta = 1/\xi$. Indeed, this choice leads to

$$S(\xi) - |\tau| T(\xi) \simeq \begin{pmatrix} \dfrac{\overline{a}_\infty}{\xi} \dfrac{dK_\nu^2/(m\beta)}{1 + dK_\nu^2/(m\beta)} & -\dfrac{\overline{a}_\infty}{4m} \\ -\dfrac{\overline{a}_\infty}{4m} & \dfrac{\xi K_\kappa^2}{\beta} \end{pmatrix} - \frac{|\tau|}{2} \begin{pmatrix} \dfrac{1 + \overline{a}_\infty \sqrt{\beta/m}}{\xi} & 0 \\ 0 & \dfrac{\xi K_\kappa^2}{2} \end{pmatrix},$$

where $\overline{a}_\infty$, the limit of $\xi a(\xi)$ as $\xi \to +\infty$, should be sufficiently small. In conclusion, it is possible to set $\tau = \delta \min(\xi, 1)$ for $|\delta|$ sufficiently small, and, for such a choice, there exists $\overline{\lambda}_\delta > 0$ for which, for any $\xi \in (0, +\infty)$,

$$\mathscr{H}'(t) \leqslant -\overline{\lambda}_\delta \min(\xi, \xi^{-1}) \|f(t)\|^2_{L^2(\mu)}.$$

Moreover, $\overline{\lambda}_\delta = \overline{\lambda}_0 + \mathrm{O}(\delta)$.

The final result is obtained by noting that, in view of Lemma 2, and considering functions a with values in a compact subset of $(0, 1)$,

$$\|f(t)\|^2_{L^2(\mu)} \leqslant \frac{2}{1 - a(\xi)} \mathscr{H}(t), \qquad \mathscr{H}(0) \leqslant \frac{1 + a(\xi)}{2} \|f(0)\|^2_{L^2(\mu)}.$$

This shows that the constant C in (2.11) can be chosen as (by restricting $a(\xi)$ to remain lower than $1/2$ for instance)

$$C = \sup_{\xi > 0} \sqrt{\frac{1 + a(\xi)}{1 - a(\xi)}}.$$

It remains to prove the following technical result.

Lemma 3. *The operators $\mathcal{L}_{\mathrm{ham}} A^* = \mathcal{L}^2_{\mathrm{ham}} \Pi (1 - \Pi \mathcal{L}^2_{\mathrm{ham}} \Pi)^{-1}$ and $\mathcal{L}_{\mathrm{pert}} A^*$ are bounded. Moreover, $\|\mathcal{L}_{\mathrm{pert}} A^*\| \leqslant \sqrt{\beta/(4m)}$.*

Proof. In view of (2.28), the action of $\mathcal{L}_{\mathrm{ham}} A^* = \mathcal{L}_{\mathrm{ham}} A^* \Pi$ is

$$\mathcal{L}_{\mathrm{ham}} A^* \Pi \varphi(q, p) = \frac{1}{m^2} p^T (\nabla_q^2 \Pi \psi)(q) p - \frac{1}{m} \nabla U(q) \cdot \nabla_q \Pi \psi(q),$$

with

$$\psi = \left(1 - \frac{1}{m} \mathcal{L}_{\mathrm{ovd}}\right)^{-1} \Pi \varphi.$$

The operator $\mathcal{L}_{\mathrm{ham}} A^* \Pi$ is then bounded since $1 - \mathcal{L}_{\mathrm{ovd}}/m$ is a bounded operator from $L^2(\nu)$ to $H^2(\nu)$.

We next consider $\mathcal{L}_{\mathrm{pert}} A^* = \mathcal{L}_{\mathrm{pert}} \mathcal{L}_{\mathrm{ham}} \Pi \left(1 - \mathcal{L}_{\mathrm{ovd}}/m\right)^{-1} \Pi$. Since

$$\mathcal{L}_{\mathrm{pert}} \mathcal{L}_{\mathrm{ham}} \Pi h = \frac{1}{m} \mathcal{L}_{\mathrm{pert}} \left(p \cdot \nabla_q \Pi h\right) = \frac{1}{m} F \cdot \nabla_q \Pi h,$$

the operator $\mathcal{L}_{\text{pert}}A^*$ is also bounded since $1-\mathcal{L}_{\text{ovd}}/m$ is a bounded operator from $L^2(\nu)$ to $H^1(\nu)$. Moreover, for $\varphi \in L^2(\mu)$,

$$\begin{aligned}\|\mathcal{L}_{\text{pert}}A^*\varphi\|^2 &= \langle \varphi, A\mathcal{L}^*_{\text{pert}}\mathcal{L}_{\text{pert}}A^*\varphi\rangle_{L^2(\mu)} \\ &= \frac{1}{m^2}\Big\langle \varphi, \Pi(1-\mathcal{L}_{\text{ovd}}/m)^{-1}(F\cdot\nabla_q)^*F\cdot\nabla_q(1-\mathcal{L}_{\text{ovd}}/m)^{-1}\Pi\varphi\Big\rangle_{L^2(\mu)}.\end{aligned}$$

Since $0 \leqslant (F\cdot\nabla_q)^*F\cdot\nabla_q \leqslant \nabla_q^*\nabla_q = -\beta\mathcal{L}_{\text{ovd}}$ in the sense of symmetric operators, it follows that, by spectral calculus,

$$\|\mathcal{L}_{\text{pert}}A^*\|^2 \leqslant \sup_{x\geqslant 0}\frac{\beta x}{m^2(1+x/m)^2} = \frac{\beta}{m}\sup_{y\geqslant 0}\frac{y}{(1+y)^2} = \frac{\beta}{4m},$$

which gives the claimed bound. □

2.6 Appendix

To simplify the notations, the results contained in this appendix have all been obtained in the one-dimensional case. However, their d-dimensional generalization is straightforward.

2.6.1 Explicit solution of the eigenvalue problem for the non-interacting particle system

I recall here the result by Kozlov (1989) which is used in (2.18). Let us set

$$\mu \doteq \frac{\xi}{\beta}m, \qquad \alpha \doteq \xi,$$

and perform the following change of variables

$$p = \sqrt{\frac{\mu}{\alpha}}p', \qquad q = \sqrt{\frac{\mu}{\alpha^3}}q',$$

so as to rewrite $\mathcal{L}_{\xi,0}$ as

$$\mathcal{L}_{\xi,0} = \frac{\xi}{m}\mathcal{L}'_0 = \frac{\xi}{m}\left(p'\partial_{q'} + \partial^2_{p'} - p'\partial_{p'}\right).$$

Introducing the operators

$$\begin{aligned} S_1 &: (q,p)\to(q,p), \quad S_1u(q,p) \doteq \mathrm{e}^{p^2/4}u(q,p),\\ S_2 &: (q,\gamma)\to(q,p), \quad S_2u(q,\gamma) \doteq (2\pi)^{-1}\int_{\mathbb{R}}\mathrm{e}^{ip\gamma}u(q,p)\,\mathrm{d}\gamma,\\ S_3 &: (q,\gamma)\to(q,\gamma), \quad S_3u(q,\gamma) \doteq u(q-2i\gamma,\gamma),\end{aligned}$$

we find, after some calculations, that

$$H_0 : (q,\gamma) \to (q,\gamma), \quad H_0 \doteq S_3^{-1} S_2^{-1} S_1^{-1} \mathcal{L}_0' S_1 S_2 S_3 = \frac{1}{4}\partial_\gamma^2 - \gamma^2 + \partial_q^2 + \frac{1}{2}.$$

The spectral gap λ is the smallest eigenvalue of this new operator. Let us consider $\widetilde{H}_0 = H_0 - \frac{1}{2}$. Since $\widetilde{H}_0$ is separable in q and γ, its eigenfunctions are of the form $\psi_{n,k}(q,\gamma) = \psi_k^{(1)}(q)\psi_n^{(2)}(\gamma)$. Concerning the q term, $\psi_k^{(1)}(q) = \mathrm{e}^{ikq}$ so that

$$\frac{\mu}{\alpha^3}\partial_q^2 \psi_k^{(1)}(q) = -\frac{\mu}{\alpha^3} k^2 \psi_k^{(1)}(q).$$

As for the γ term, the equation is basically a Schrödinger equation of a particle in a harmonic potential, so that

$$\begin{aligned}
&\left(-\frac{\hbar^2}{2m}\partial_\gamma^2 + m\omega^2\gamma^2\right)\psi_n^{(2)}(\gamma) = E_n\,\psi_n^{(2)}(\gamma),\\
&\psi_n^{(2)}(\gamma) = \frac{(-1)^n}{\sqrt{2^{n-1/2}n!\sqrt{\pi}}}\,\partial_\gamma^n \mathrm{e}^{-\gamma^2},\\
&E_n = \hbar\omega\left(n+\frac{1}{2}\right),
\end{aligned}$$

with $\hbar = \omega = 1$, $m = 2$. Gathering the results,

$$\begin{aligned}
&H_0\,\psi_{n,k}(q,\gamma) = -\lambda_{n,k}\,\psi_{n,k}(q,\gamma),\\
&\psi_{n,k}(q,\gamma) = \frac{(-1)^n\, e^{ikq}}{\sqrt{2^{n-1/2}n!\sqrt{\pi}}}\\
&\lambda_{n,k} = \frac{\mu}{\alpha^3}k^2 + \left(n+\frac{1}{2}\right) - \frac{1}{2} = \frac{\mu}{\alpha^3}k^2 + n.
\end{aligned}$$

Getting back to the (q,p) coordinates

$$\frac{\xi}{m}\mathcal{L}_0' S_1 S_2 S_3\,\psi_{n,k}(q,\gamma) = -\frac{\xi}{m}\,\lambda_{n,k}\,S_1\,S_2\,S_3\,\psi_{n,k}(q,\gamma).$$

Therefore the spectral gap is the smallest non-zero eigenvalue

$$\lambda_{\mathrm{Koz}} = \frac{\xi}{m}\min_{n,k\geq 0,\lambda_{n,k}\neq 0}\lambda_{n,k} = \min\left(\frac{1}{\beta\xi}, \frac{\xi}{m}\right). \tag{2.32}$$

2.6.2 Poincaré inequalities

In this section, we first give a more explicit statement of the tensorization property of the Poincaré inequality (see Proposition 3 in Section 1.2.1.1), which is useful for the proofs in Section 2.5. Then we estimate the Poincaré constants for both $U(q) = 0$ and $U(q) \neq 0$ cases. Note the different notation with respect to the definitions (2.19) and (2.20). In fact, in this section we have $K_q = K_v^{-2}$ and $K_p = K_\kappa^{-2}$.

Proposition 8. *Given a product probability measure $\mu = \nu \times \kappa$ defined on $2\pi\mathbb{T}\times\mathbb{R}$ and two constants K_q and K_p such that*

$$\begin{aligned} \|f\|^2_{L^2(\nu)} &\leqslant K_q \|f'\|^2_{L^2(\nu)}, \\ \|g\|^2_{L^2(\kappa)} &\leqslant K_p \|g'\|^2_{L^2(\kappa)}, \end{aligned} \tag{2.33}$$

for every $f(q) \in H^1(\nu) \cap L^2_0(\nu)$ and $g(p) \in H^1(\kappa) \cap L^2_0(\kappa)$, then

$$\|\varphi\|^2_{L^2(\mu)} \leqslant K_q \|\partial_q \varphi\|^2_{L^2(\mu)} + K_p \|\partial_p \varphi\|^2_{L^2(\mu)}$$

for every function $\varphi(p,q) \in H^1(\mu) \cap L^2_0(\mu)$.

Proof. Defining $\bar\varphi(q) = \int_{\mathbb{R}} \varphi(p,q)\kappa(\mathrm{d}p)$, we write

$$\varphi(p,q) = \widetilde\varphi(p,q) + \bar\varphi(q).$$

For each q we have $\int_{\mathbb{R}} \widetilde\varphi(p,q)\,\kappa(\mathrm{d}p) = 0$, so

$$\int_{\mathbb{R}} \widetilde\varphi(p,q)^2\,\kappa(\mathrm{d}p) \leqslant K_p \int_{\mathbb{R}} (\partial_p \widetilde\varphi)^2\,\kappa(\mathrm{d}p) = K_p \int_{\mathbb{R}} (\partial_p \varphi)^2\,\kappa(\mathrm{d}p).$$

Integrating both terms with respect to ν, we get

$$\|\widetilde\varphi\|^2_{L^2(\mu)} \leqslant K_p \int_{\mathbb{R}\times 2\pi\mathbb{T}} (\partial_p \varphi)^2\,\mu(\mathrm{d}p,\mathrm{d}q). \tag{2.34}$$

On the other hand, since $\int_{2\pi\mathbb{T}} \bar\varphi(q)\nu(\mathrm{d}q) = 0$, we also have

$$\int_{2\pi\mathbb{T}} \bar\varphi(q)^2\,\nu(\mathrm{d}q) \leqslant K_q \int_{2\pi\mathbb{T}} (\bar\varphi'(q))^2\,\nu(\mathrm{d}q). \tag{2.35}$$

Finally, by (2.34), (2.35) and Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} \|\varphi\|^2_{L^2(\mu)} &= \|\widetilde\varphi\|^2_{L^2(\mu)} + \|\bar\varphi\|^2_{L^2(\mu)} \\ &\leqslant K_p \|\partial_p \varphi\|^2_{L^2(\mu)} + K_q \|\partial_q \bar\varphi\|^2_{L^2(\mu)} \\ &\leqslant K_p \|\partial_p \varphi\|^2_{L^2(\mu)} + K_q \|\partial_q \varphi\|^2_{L^2(\mu)}, \end{aligned}$$

which concludes the proof. □

Estimation of K_p and K_p. Let us know focus on the Poincaré inequalities (2.33). The optimal value of K_q and K_p are the reciprocal of the first nonzero eigenvalues of

$$\mathcal{D}_q \phi_k(q) \doteq \partial_q^* \partial_q \phi_k(q) = \eta_k \phi_k(q)$$

and

$$\mathcal{D}_p \psi_n(p) \doteq \partial_p^* \partial_p \psi_n(p) = \left(-\partial_p^2 + \frac{\beta}{m} p\right) \psi_n(p) = \zeta_n \psi_n(p)$$

respectively.

We first consider the p case. It is easy to see that the eigenfunctions of $\mathcal{D}_q$ are $\psi_n(p) = h_n(p)$, where $h_n(p)$ is the Hermite polynomial of degree n and weight $\exp(-\beta p^2/2m)/\sqrt{2\pi\beta^{-1}m}$, while $\zeta_n = n\beta/m$. This means that the optimal value is $K_p = m\beta^{-1}$. Note that this result holds for both $U(q) = 0$ and $U(q) \neq 0$.

Concerning the eigenvalue problem in q, it can only be solved analitically in the case of zero potential. In fact, in this case, $\mathcal{D}_q = -\partial_q^2$, thus $\phi_k(q) = \sqrt{2}\cos(kq)$ and $\eta_k = k^2$, with $k \in \mathbb{N}$, implying that $K_q = 1$ is the optimal value.

In presence of the potential, one has $\mathcal{D}_q = -\partial_q^2 + \beta U'(q)$ and it is not possible in general to find the explicit form of $\phi_k(q)$, although we know these eigenfunctions exist because of the compactness of the resolvant $\mathcal{D}_q^{-1}$. Nevertheless, we are able to provide an upper bound, namely

$$\|f - \mathbb{E}_\nu(f)\|^2_{L^2(\nu)} \leqslant K_q \|f'\|^2_{L^2(\nu)},$$

where $f(q)$ is a generic test function. Of course this result holds for functions $f(q)$ such that $\mathbb{E}_\nu(f) = 0$. We start from

$$\mathbb{E}_\nu\left([f - \mathbb{E}_\nu(f)]^2\right) = \frac{1}{2}\int_0^{2\pi}\int_0^{2\pi} (f(q) - f(q'))^2 \, \nu(\mathrm{d}q)\, \nu(\mathrm{d}q'),$$

and consider

$$f(q) - f(q') = \int_0^1 (q - q')\, f'(tq + (1-t)q')\, \mathrm{d}t,$$

thus

$$\begin{aligned}
&\mathbb{E}_\nu\left([f - \mathbb{E}_\nu(f)]^2\right) \\
&\quad = \frac{1}{2}\int_0^{2\pi}\int_0^{2\pi}\left[\int_0^1 (q - q')\, f'(tq + (1-t)q')\, \mathrm{d}t\right]^2 \nu(\mathrm{d}q)\, \nu(\mathrm{d}q'). \qquad (2.36)
\end{aligned}$$

By Cauchy-Schwarz inequality,

$$\begin{aligned}
&\left[\int_0^1 t^{-1/4} t^{1/4} (q - q')\, f'(tq + (1-t)q')\, \mathrm{d}t\right]^2 \\
&\qquad \leqslant \int_0^1 t^{-1/2}\, \mathrm{d}t \int_0^1 t^{1/2} (q - q')^2 (f'(tq + (1-t)q'))^2\, \mathrm{d}t \\
&\qquad \leqslant 2(2\pi)^2 \int_0^1 t^{1/2} (f'(tq + (1-t)q'))^2\, \mathrm{d}t,
\end{aligned}$$

so that, plugging back into (2.36),

$$\begin{aligned}
&\mathbb{E}_\nu\left([f - \mathbb{E}_\nu(f)]^2\right) \\
&\quad \leqslant (2\pi)^2 \int_0^{2\pi}\int_0^{2\pi}\left(\int_0^1 t^{1/2} (f'(tq + (1-t)q'))^2\, \mathrm{d}t\right)\nu(\mathrm{d}q)\, \nu(\mathrm{d}q') \\
&\quad = (2\pi)^2 \int_0^1 t^{-1/2}\left(\int_0^{2\pi} \frac{e^{-\beta U(w)}}{Z_\nu} \int_{(1-t)w}^{2\pi t + (1-t)w} \frac{e^{-\beta U(t^{-1}(z + (t-1)w))}}{Z_\nu} (f'(z))^2\, dz\, dw\right)\mathrm{d}t,
\end{aligned}$$

where we have set $z = tq + (1-t)q'$ and $w = q'$ in the last step. Considering that:

(i) for $0 \leqslant t \leqslant 1$ and $0 \leqslant w \leqslant 1$ we have $[(1-t)w, 2\pi t(1-t)w] \subseteq [0, 2\pi]$ and the integrand in z is positive;

(ii) $U(t^{-1}(z+(t-1)w)) \geq U(z) + C$ with $C = -(U_{\max} - U_{\min})$,

it follows

$$\begin{aligned}
&\mathbb{E}_\nu\left([f - \mathbb{E}_\nu(f)]^2\right) \leqslant \\
&\leqslant (2\pi)^2 \mathrm{e}^{\beta(U_{\max}-U_{\min})} \int_0^1 t^{-1/2} \left(\int_0^{2\pi} \frac{e^{-\beta U(w)}}{Z_\nu} \,\mathrm{d}w \int_0^{2\pi} \frac{e^{-\beta U(z)}}{Z_\nu} (f'(z))^2 \,\mathrm{d}z \right) \mathrm{d}t \\
&= 2\,(2\pi)^2 \mathrm{e}^{\beta(U_{\max}-U_{\min})} \|f'\|^2_{L(\nu)},
\end{aligned}$$

thus

$$K_q = 2\,(2\pi)^2 \mathrm{e}^{\beta(U_{\max}-U_{\min})}.$$

Note that this estimation of the Poincaré constant is non-optimal, as we should get $K_q = 1$ for $U = 0$.

2.6.3 Hypocoercive entropic approach

We recall in this section a convergence result in the entropic sense for equilibrium Langevin dynamics. We operate in a degenerate setting, reminiscent of the one introduced in the $H^1(\mu)$ context in Section 2.3.1. We consider the probability density $f(t)$ with respect to the invariant measure μ of the process at time t . This function is the solution of the Fokker-Planck equation

$$\partial_t f(t) = \mathcal{L}^*_{\xi,0} f(t), \tag{2.37}$$

with

$$\mathcal{L}^*_{\xi,0} = \mathcal{L}^*_{\mathrm{ham}} + \xi \mathcal{L}^*_{\mathrm{FD}} = -\left(\frac{p}{m}\partial_q - U'\partial_p\right) + \xi\left(\beta^{-1}\partial_p^2 - \frac{p}{m}\partial_p\right),$$

and initial condition $f(0) = f \geq 0$. We introduce the entropy functional

$$\mathscr{E}_{a(\xi)}(f) \doteq \mathrm{Ent}(f) + \mathcal{I}_\xi(f) = \int_\Omega f \ln f \,\mathrm{d}\mu + a(\xi) \int_\Omega \frac{\left(\partial_q f + \partial_p f\right)^2}{f} \,\mathrm{d}\mu, \tag{2.38}$$

which is the sum of the relative entropy $\mathrm{Ent}(f)$ and a generalization of the Fisher information

$$\mathcal{I}_\xi(f) \doteq \int_\Omega \frac{(\nabla f)^T \hat{S}_\xi (\nabla f)}{f} \mathrm{d}\mu, \quad \text{with} \quad \nabla \doteq \begin{pmatrix} \partial_p \\ \partial_q \end{pmatrix}, \quad \text{and} \quad \hat{S}_\xi \doteq a(\xi) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{2.39}$$

Note that both $\mathrm{Ent}(f)$ and $\mathcal{I}_\xi(f)$ are non-negative. We introduce the space $\mathcal{M} = \left\{ h \in H^1(\mu) \middle| \int_\Omega h \,\mathrm{d}\mu = 1 \right\}$ and recall that μ satisfies a log-Sobolev inequality (see Gross (1975)).

Theorem 12. *The probability measure $\mu(\mathrm{d}q, \mathrm{d}p)$ satisfies an LSI(R)*

$$\int_\Omega f \ln f \,\mathrm{d}\mu \leqslant \frac{1}{R} \int_\Omega \frac{(\partial_p f)^2 + (\partial_q f)^2}{f} \,\mathrm{d}\mu,$$

with $R = \min\left(m\beta^{-1}, \mathrm{e}^{-\beta(U_{\max}-U_{\min})}\right)$, for every $f \in \mathcal{M}$.

Proof. This is easily done by noticing once again that $\mu = \nu \times \kappa$ is a product of measures: κ is a gaussian measure of variance $\sigma^2 = m\beta^{-1}$, which satisfies a log-Sobolev inequality with constant σ^2, while, by Theorem 3, ν satisfies a log-Sobolev inequality with constant $\widetilde{R} = \mathrm{e}^{-\beta(U_{\max}-U_{\min})}$, since the measure ν of the theorem is in this case a uniform measure which satisfies a LSI(R) with $R = 1$. The result is then obtained by tensorization (see Gross (1975)). □

We next prove the following result.

Theorem 13. *There exist a positive continuous function $a(\xi)$ such that*

$$\lim_{\xi\to 0} \quad \frac{a(\xi)}{\xi} = a_- > 0,$$

$$\lim_{\xi\to\infty} \quad \xi\, a(\xi) = a_+ > 0,$$

and a constant $\alpha(a(\xi))$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(f(t)) = -\alpha \int_\Omega \frac{(\partial_p f)^2 + (\partial_q f)^2}{f(t)}\,\mathrm{d}\mu.$$

Furthermore, if μ satisfies a logarithmic Sobolev inequality, then there exist a positive constant $\bar\kappa$ such that

$$\mathscr{E}_{a(\xi)}(e^{t\mathcal{L}^*_{\xi,0}} f) \leqslant \mathrm{e}^{-\bar\kappa \min(\xi,\xi^{-1})\, t}\, \mathscr{E}_{a(\xi)}(f),$$

for all $t \geq 0$ and $f \in \mathcal{M}$.

Proof. Setting $g(t) = \sqrt{f(t)}$, equation (2.37) becomes

$$\partial_t g(t) = \mathcal{L}^*_{\xi,0} g(t) + \xi\beta^{-1} \frac{(\partial_p g(t))^2}{g(t)}.$$

Let us now compute the time derivative of $\mathcal{E}(f(t))$. We denote $\mathcal{L}^*_{\xi,0}$ by $\mathcal{L}^*_0$ throughout the proof for simplicity. We start with the relative entropy term:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_\Omega f(t)\ln f(t)\,\mathrm{d}\mu\right) &= \int_\Omega (\ln f(t) + 1)\mathcal{L}^*_0 f(t)\,\mathrm{d}\mu \\
&= \int_\Omega \mathcal{L}_{\mathrm{ham}}(\ln f(t) + 1) f(t)\,\mathrm{d}\mu + \xi \int_\Omega \mathcal{L}_{\mathrm{FD}}(\ln f(t) + 1) f(t)\,\mathrm{d}\mu \\
&= \int_\Omega \mathcal{L}_{\mathrm{ham}} f(t)\,\mathrm{d}\mu - \xi\beta^{-1} \int_\Omega \frac{(\partial_p f(t))^2}{f(t)}\,\mathrm{d}\mu \\
&= -\xi\beta^{-1} \int_\Omega \frac{(\partial_p f(t))^2}{f(t)}\,\mathrm{d}\mu = -4\xi\beta^{-1} \int_\Omega (\partial_p g(t))^2\,\mathrm{d}\mu.
\end{aligned}$$

The Fisher information term in (2.38) becomes

$$\mathcal{I}(g(t)) = 4a(\xi) \int_\Omega (\partial_p g + \partial_q g)^2\,\mathrm{d}\mu,$$

so its time derivative is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(g(t)) = 8a(\xi)\Bigg[&\int_\Omega \partial_q g\,\partial_q(\partial_t g)\,\mathrm{d}\mu + \int_\Omega \partial_q(\partial_t g)\,\partial_p g\,\mathrm{d}\mu \\ &+ \int_\Omega \partial_q g\,\partial_p(\partial_t g)\,\mathrm{d}\mu + \int_\Omega \partial_p g\,\partial_p(\partial_t g)\,\mathrm{d}\mu\Bigg].\end{aligned} \tag{2.40}$$

We use the following commutator identities:

$$\begin{aligned}\left[\partial_q, \mathcal{L}^*_{\mathrm{ham}}\right] &= U''\partial_p & \left[\partial_p, \mathcal{L}^*_{\mathrm{ham}}\right] &= -m^{-1}\partial_q, \\ \left[\partial_q, \mathcal{L}^*_{\mathrm{FD}}\right] &= 0 & \left[\partial_p, \mathcal{L}^*_{\mathrm{FD}}\right] &= -m^{-1}\partial_p.\end{aligned}$$

The first term in (2.40) gives

$$\int_\Omega \partial_q g\,\partial_q(\partial_t g)\,\mathrm{d}\mu = \int_\Omega U''(q)\,\partial_q g\,\partial_p g\,\mathrm{d}\mu - \xi\beta^{-1}\int_\Omega \left(\frac{\partial_q g\,\partial_p g}{q} - \partial_p\partial_q g\right)^2 \mathrm{d}\mu.$$

The sum of the second and third terms gives

$$\begin{aligned}&\int_\Omega \partial_q(\partial_t g)\,\partial_p g\,\mathrm{d}\mu + \int_\Omega \partial_q g\,\partial_p(\partial_t g)\,\mathrm{d}\mu \\ &= \int_\Omega U''(q)(\partial_p g)^2\,\mathrm{d}\mu - m^{-1}\int_\Omega (\partial_q g)^2\,\mathrm{d}\mu - \frac{\xi}{m}\int_\Omega \partial_q g\,\partial_p g\,\mathrm{d}\mu + \\ &\quad + 2\xi\beta^{-1}\int_\Omega \left(\frac{(\partial_p g)^2}{g} - \partial_p^2 g\right)\left(\partial_p\partial_q g - \frac{\partial_p g\,\partial_q g}{g}\right)\mathrm{d}\mu.\end{aligned}$$

Finally the fourth term reads

$$\begin{aligned}\int_\Omega \partial_p g\,\partial_p(\partial_t g)\,\mathrm{d}\mu = -m^{-1}\int_\Omega \partial_p g\,\partial_q g\,\mathrm{d}\mu - \xi m^{-1}\int_\Omega (\partial_p g)^2\,\mathrm{d}\mu \\ -\xi\beta^{-1}\int_\Omega \left(\partial_p^2 g - \frac{(\partial_p g)^2}{g}\right)\mathrm{d}\mu.\end{aligned}$$

The time derivative of $\mathcal{I}(g(t))$ is then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(g(t)) = 8a(\xi)\Bigg[&\int_\Omega U''(q)\,\partial_q g\,\partial_p g\,\mathrm{d}\mu - \xi\beta^{-1}\int_\Omega\left(\frac{\partial_q g\,\partial_p g}{q} - \partial_p\partial_q g\right)^2\mathrm{d}\mu\\ &+\int_\Omega U''(q)(\partial_p g)^2\,\mathrm{d}\mu - m^{-1}\int_\Omega(\partial_q g)^2\,\mathrm{d}\mu - \frac{\xi}{m}\int_\Omega\partial_q g\,\partial_p g\,\mathrm{d}\mu\\ &+2\xi\beta^{-1}\int_\Omega\left(\frac{(\partial_p g)^2}{g} - \partial_p^2 g\right)\left(\partial_p\partial_q g - \frac{\partial_p g\,\partial_q g}{g}\right)\mathrm{d}\mu\\ &-m^{-1}\int_\Omega\partial_p g\,\partial_q g\,\mathrm{d}\mu - \xi m^{-1}\int_\Omega(\partial_p g)^2\,\mathrm{d}\mu\\ &-\xi\beta^{-1}\int_\Omega\left(\partial_p^2 g - \frac{(\partial_p g)^2}{g}\right)\mathrm{d}\mu\Bigg]\\ = 8a(\xi)\Bigg[&\int_\Omega U''(q)\,\partial_q g\,\partial_p g\,\mathrm{d}\mu + \int_\Omega U''(q)(\partial_p g)^2\,\mathrm{d}\mu\\ &-m^{-1}\int_\Omega(\partial_q g)^2\,\mathrm{d}\mu - m^{-1}\int_\Omega\partial_p g\,\partial_q g\,\mathrm{d}\mu\\ &-\xi m^{-1}\int_\Omega\partial_q g\,\partial_p g\,\mathrm{d}\mu - \xi m^{-1}\int_\Omega(\partial_p g)^2\,\mathrm{d}\mu\\ &-\xi\beta^{-1}\int_\Omega\left(\frac{\partial_q g\,\partial_p g}{q} - \partial_p\partial_q g + \frac{(\partial_p g)^2}{g} - \partial_p^2 g\right)^2\mathrm{d}\mu\Bigg].\end{aligned}$$

Ultimately

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(g(t)) \leqslant 8a(\xi)\Bigg[&\int_\Omega U''(q)\,\partial_q g\,\partial_p g\,\mathrm{d}\mu + \int_\Omega U''(q)(\partial_p g)^2\,\mathrm{d}\mu\\ &-m^{-1}\int_\Omega(\partial_q g)^2\,\mathrm{d}\mu - m^{-1}\int_\Omega\partial_p g\,\partial_q g\,\mathrm{d}\mu\\ &-\xi m^{-1}\int_\Omega\partial_q g\,\partial_p g\,\mathrm{d}\mu - \xi m^{-1}\int_\Omega(\partial_p g)^2\,\mathrm{d}\mu\Bigg]\end{aligned}$$

which by Cauchy-Schwarz gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(g(t)) \leqslant -8a(\xi)\left[\left(\frac{\xi}{m} - U_0\right)\|\partial_p g\|^2 + \frac{1}{m}\|\partial_q g\|^2 + \left(\frac{\xi+1}{m} - U_0\right)\|\partial_p g\|\,\|\partial_q g\|\right],$$

where we considered $U(q) = U_0(1-\cos q)$. Gathering all the terms

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(g(t)) \leqslant -4\Bigg[&\left(\xi\beta^{-1} + 2\left(\frac{\xi}{m} - U_0\right)a(\xi)\right)\|\partial_p g\|^2 + \frac{2a(\xi)}{m}\|\partial_q g\|^2\\ &+2\,a(\xi)\left(\frac{\xi+1}{m} - U_0\right)\|\partial_p g\|\,\|\partial_q g\|\Bigg].\end{aligned}\tag{2.41}$$

We define

$$X \doteq \begin{pmatrix}\|\partial_p g\|\\ \|\partial_q g\|\end{pmatrix}, \quad \hat{A} \doteq \begin{pmatrix}\xi\beta^{-1} + 2a(\xi)\left(\frac{\xi}{m} - U_0\right) & 2\,a(\xi)\left(\frac{\xi+1}{m} - U_0\right)\\ 2\,a(\xi)\left(\frac{\xi+1}{m} - U_0\right) & \frac{2a(\xi)}{m}\end{pmatrix},$$

and we rewrite (2.41) in matrix form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(g(t)) \leqslant -4X^T\hat{A}X \leqslant -4\lambda_- X^T X,$$

by computations similar to those performed in Section 2.5, where λ_- is the smallest eigenvalue of $\hat{A}$. Thus, in terms of f, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(f(t)) \leqslant -\alpha \int_\Omega \frac{(\partial_p f)^2 + (\partial_q f)^2}{f}\,\mathrm{d}\mu_U,$$

which proves the first part of the Theorem 13, with $\alpha = \lambda_-$.

Let us now find the explicit dependence of λ_- from the physical parameters of the problem. As already seen in the case of $L^2(\mu)$ or $H^1(\mu)$ hypocoercivity, we consider the asymptotic regimes $\xi \to 0$ and $\xi \to \infty$, to find an explicit dependence of these quantities from the physical parameters of the problem.

Case $\xi \ll 1$ In this case, considering $a(\xi) = \bar{a}\xi + \mathcal{O}(\xi^2)$, we have

$$\hat{A} \simeq \xi \begin{pmatrix} \beta^{-1} - 2\bar{a}U_0 & \left(\frac{1}{m} - U_0\right)\bar{a} \\ \left(\frac{1}{m} - U_0\right)\bar{a} & 2\frac{\bar{a}}{m} \end{pmatrix} + \mathcal{O}(\xi^2),$$

whose smallest eigenvalues is $\lambda_- = \lambda_{\xi\ll 1} + \mathcal{O}(\xi^2)$ with

$$\lambda_{\xi\ll 1} = \frac{\xi}{2}\left(\beta^{-1} + 2\bar{a}\left(\frac{1}{m} - U_0\right) - \sqrt{\left[\beta^{-1} + 2\bar{a}\left(U_0 + \frac{1}{m}\right)\right]^2 + 4\left[\left(\frac{1}{m} - U_0\right)\bar{a}\right]^2}\right). \quad (2.42)$$

The value of a_- is the value of $\bar{a}$ that maximises $\lim_{\xi\to 0}\frac{\lambda_{\xi\ll 1}}{\xi}$, that is

$$a_- = \frac{\beta^{-1}}{2\left(\frac{1}{m} + U_0\right)}.$$

Substituting a_- in (2.42) we get

$$\bar{\lambda} = \frac{\beta^{-1}}{2}.$$

Case $\xi \gg 1$ In this case, considering $a(\xi) = \bar{a}\xi^{-1} + \mathcal{O}(\xi^{-2})$, we have

$$\hat{A} \simeq \begin{pmatrix} \xi\beta^{-1} & \frac{\bar{a}}{m} \\ \frac{\bar{a}}{m} & \frac{2\bar{a}}{\xi m} \end{pmatrix} + \mathcal{O}(\xi^{-2}),$$

whose smallest eigenvalue is

$$\begin{aligned}
\lambda_- &= \frac{1}{2}\left(\xi\beta^{-1} + \frac{2\bar{a}}{\xi m} - \sqrt{\left(\xi\beta^{-1} - \frac{2\bar{a}}{\xi m}\right)^2 + 4\,\frac{\bar{a}^2}{m^2}}\right) + \mathcal{O}(\xi^{-2}) \\
&= \frac{1}{2}\,\frac{\left(\xi\beta^{-1} + \frac{2\bar{a}}{\xi m}\right)^2 - \left[\left(\xi\beta^{-1} - \frac{2\bar{a}}{\xi m}\right)^2 + 4\,\frac{\bar{a}^2}{m^2}\right]}{\xi\beta^{-1} + \frac{2\bar{a}}{\xi m} + \sqrt{\left(\xi\beta^{-1} - \frac{2\bar{a}}{\xi m}\right)^2 + 4\,\frac{\bar{a}^2}{m^2}}} + \mathcal{O}(\xi^{-2}) \\
&= \frac{2\bar{a}}{\xi m\beta^{-1}}\left(2\beta^{-1} - \frac{\bar{a}}{m}\right) + \mathcal{O}(\xi^{-2}) \\
&\doteq \lambda_{\xi\gg 1} + \mathcal{O}(\xi^{-2})
\end{aligned} \tag{2.43}$$

The value of a_+ is the value of $\bar{a}$ that maximises $\lim_{\xi\to+\infty}\xi\,\lambda_{\xi\gg 1}$, namely

$$a_+ = m\beta^{-1}.$$

Substituting in (2.43), we get

$$\bar{\lambda} = 2\beta^{-1}.$$

By (2.39) and the result of Theorem 12, which ensures that μ satisfies a logarithmic Sobolev inequality with constant $R = \min(m(2\beta)^{-1}, \mathrm{e}^{2\beta U_0})$, we find that

$$\mathscr{E}(f(t)) = \int_\Omega f(t)\ln f(t)\,\mathrm{d}\mu + \mathcal{I}(f(t)) \leqslant \left[(2R)^{-1} + \lambda_S\right]\int_\Omega \frac{(\partial_p f)^2 + (\partial_q f)^2}{f}\,\mathrm{d}\mu$$

where $\lambda_S = 2a(\xi)$ is the maximum eigenvalue of S in (2.39). Finally,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(f(t)) \leqslant -\alpha\int_\Omega \frac{(\partial_p f)^2 + (\partial_q f)^2}{f}\,\mathrm{d}\mu \leqslant -\frac{\lambda_-}{\lambda_S + \frac{1}{2R}}\mathscr{E}(f(t)) \doteq -\kappa\,\mathscr{E}(f(t)),$$

from which the result follows. □

3

Nonequilibrium Langevin dynamics with a weak potential

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We consider the one-dimensional version of the rotor model studied in the previous chapter for small values of the potential energy U. We thus rename the generator of the dynamics $\mathcal{L}_{\xi,\tau}$ in order to highlight the relevant parameters as

$$\begin{aligned}\mathcal{L}_{\tau,\eta} &= \frac{p}{m}\partial_q + \xi\left(\beta^{-1}\partial_p^2 - \left(\frac{p}{m}-\tau\right)\partial_p\right) + \eta\, U'(q)\,\partial_p \\ &\doteq \mathcal{A}_0 + \xi\mathcal{S}_\tau + \eta\mathcal{L}_{\text{pert}} \\ &\doteq \mathcal{L}_{\tau,0} + \eta\mathcal{L}_{\text{pert}},\end{aligned}$$

with $q \in \mathcal{D} \doteq 2\pi\mathbb{T}$ and $U(q) = U_0(1-\cos q)$.

We start by computing, in Section 3.1, the explicit expression of the transition kernel of the Markov process generated by $\mathcal{L}_{\tau,0}$. This transition probability is employed in Section 3.2 to estimate the spectral gap of $\mathcal{L}_{\tau,0}$ and the result is compared with the one analytically computed in Kozlov (1989) and reported in Section 2.6.1. A perturbative expansion result in $L^2(\mu)$ is then presented in Section 3.3, while Section 3.4 contains the technical work by Gallavotti et al. (2013), where we present a formal perturbative expansion in the potential of the invariant measure.

3.1 Transition probability for $U = 0$

We start from the dynamics

$$\begin{aligned}\mathrm{d}Q_t &= \frac{P_t}{m}\,\mathrm{d}t, \\ \mathrm{d}P_t &= -\frac{\xi}{m}P_t\,\mathrm{d}t + \sqrt{2\xi\beta^{-1}}\,\mathrm{d}w_t + \tau\,\mathrm{d}t,\end{aligned}$$

$Q_t \in \mathbb{R}$, $P_t \in \mathbb{R}$, which can be reduced to

$$\mathrm{d}Q_t = \frac{p_t + \bar{p}_\tau}{m}\,\mathrm{d}t, \tag{3.1}$$

$$\mathrm{d}p_t = -\frac{\xi}{m}p_t\,\mathrm{d}t + \sqrt{2\xi\beta^{-1}}\,\mathrm{d}w_t, \tag{3.2}$$

where $p_t = P_t - \bar{p}_\tau$ and $\bar{p}_\tau = m\tau/\xi$. Consequently we define the shifted (in p) generator

$$\mathcal{L}_{\tau,0} \doteq -\xi\beta^{-1}\,\partial_p^*\partial_p + \frac{p+\bar{p}_\tau}{m}\partial_Q.$$

Equation (3.2) is a standard Ornstein–Uhlenbeck process whose solution is

$$p_t = p_0\,\mathrm{e}^{-\frac{\xi}{m}t} + \sqrt{2\xi\beta^{-1}}\int_0^t \mathrm{e}^{-\frac{\xi}{m}(t-s)}\,\mathrm{d}w_s.$$

Concerning the position, from (3.1) we obtain

$$Q_t = Q_0 + \frac{\tau}{\xi}t + \frac{p_0}{\xi}\left(1-\mathrm{e}^{-\frac{\xi}{m}t}\right) + \sqrt{\frac{2\beta^{-1}}{\xi}}\int_0^t\left(1-\mathrm{e}^{-\frac{\xi}{m}(t-s)}\right)\mathrm{d}w_s.$$

The expectations, variances and covariance of Q_t and p_t are

$$\begin{aligned}
\mu_Q(t) \doteq \mathbb{E}[Q] &= Q_0 + \frac{\tau}{\xi}t + \frac{p_0}{\xi}\left(1 - \mathrm{e}^{-\frac{\xi}{m}t}\right), \\
\mu_p(t) \doteq \mathbb{E}[p] &= p_0\,\mathrm{e}^{-\frac{\xi}{m}t}, \\
\sigma_Q^2(t) \doteq \mathbb{E}[(Q_t - \mu_Q)^2] &= \frac{2\beta^{-1}}{\xi}\left(t + \frac{m}{2\xi}\right) - \frac{\beta^{-1}}{\xi}\frac{m}{\xi}\left(2 - \mathrm{e}^{-\frac{\xi}{m}t}\right)^2, \\
\sigma_p^2(t) \doteq \mathbb{E}[(p_t - \mu_p)^2] &= \beta^{-1} m\left(1 - \mathrm{e}^{-2\frac{\xi}{m}t}\right), \\
\kappa_{Q_t,p_t}(t) \doteq \mathrm{Cov}[Q_t, p_t] &= \beta^{-1}\frac{m}{\xi}\left(1 - \mathrm{e}^{-\frac{\xi}{m}t}\right)^2.
\end{aligned}$$

The variables Q_t and p_t are two correlated Gaussian random variables with variance-covariance matrix

$$\Sigma(t) = \begin{pmatrix} \sigma_Q^2(t) & \kappa_{Q,p}(t) \\ \kappa_{Q,p}(t) & \sigma_p^2(t) \end{pmatrix},$$

and joint probability density

$$\widetilde{\Phi}_t(Q_0, p_0; Q, p) = \frac{1}{2\pi\sqrt{\Delta(t)}} \exp\left[-\frac{1}{2(1-\rho(t)^2)}\left(\frac{\mathcal{Q}(t)^2}{\sigma_q^2(t)} - 2\rho(t)\frac{\mathcal{Q}(t)}{\sigma_q(t)}\frac{\mathcal{P}(t)}{\sigma_p(t)} + \frac{\mathcal{P}(t)^2}{\sigma_p^2(t)}\right)\right],$$

where

$$\begin{aligned}
\mathcal{Q}(t) &= Q - \mu_q(t), \qquad \mathcal{P}(t) = p - \mu_p(t), \\
\Delta(t) &= \det\Sigma(t), \qquad \rho(t) = \frac{\kappa_{Q,p}(t)}{\sigma_Q(t)\,\sigma_p(t)}.
\end{aligned}$$

Since the space variable Q is actually an angle, $\widetilde{\Phi}_t(Q_0, p_0; Q, p)$ can be wrapped around the circle $q \in [0, 2\pi)$, which implies that the wrapped density is

$$\Phi_t(q_0, p_0; q, p) = \sum_{m\in\mathcal{Z}} \widetilde{\Phi}_t(q_0, p_0; q + 2\pi m, p), \qquad q_0 = Q_0 \bmod 2\pi.$$

To perform this wrapping, we compute (*i*) the Fourier Transform (FT) in Q of $\widetilde{\Phi}_t(Q_0, p_0; Q, p)$ and then (*ii*) a discrete inverse Fourier Transform (DIFT) on integer values of the frequencies. To rigorously prove this procedure, one should work with functions in the Schwarz space $\mathcal{S}(\mathbb{R})$ and consider Fourier transforms as tempered distributions, see Schwartz (1997). One can formally show the validity of such a procedure on a function $f(Q)$, $Q \in \mathbb{R}$: given its FT

$$\hat{f}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-ikQ'} f(Q')\,\mathrm{d}Q',$$

and its DIFT

$$\widetilde{f}(q) = \sum_{n\in\mathcal{Z}} \mathrm{e}^{inq}\hat{f}(n),$$

with $q \in [0, 2\pi)$, we have

$$\begin{aligned}\widetilde{f}(q) &= \sum_{n\in\mathcal{Z}} \mathrm{e}^{inq}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-inQ'} f(Q')\,\mathrm{d}Q'\right)\\ &= \int_{-\infty}^{\infty}\left(\frac{1}{2\pi}\sum_{n\in\mathcal{Z}} \mathrm{e}^{-in(Q'-q)}\right) f(Q')\,\mathrm{d}Q'\\ &= \int_{-\infty}^{\infty} \Delta_{2\pi}(q-Q')\, f(Q')\,\mathrm{d}Q' = \sum_{m\in\mathcal{Z}} f(q+2\pi m),\end{aligned}$$

where $\Delta_{2\pi}(q) = \sum_{m\in\mathcal{Z}} \delta(Q+2\pi m) = \frac{1}{2\pi}\sum_{n\in\mathcal{Z}} \mathrm{e}^{-inQ}$ is the Dirac comb, expressed as a sum of complex exponentials.

Let us now apply the procedure to $\widetilde{\Phi}_t(Q_0, p_0; Q, p)$. We first compute the FT with respect to the Q variable as follows

$$\begin{aligned}\widehat{\Phi}_t(q_0, p_0; k, p) &= \frac{1}{2\pi}\int_{\mathbb{R}} \Phi_t(q_0, p_0; Q, p)\,\mathrm{e}^{-ikQ}\,\mathrm{d}Q\\ &= \frac{\mathrm{e}^{-\frac{\mathcal{P}(t)^2}{2\sigma_p^2(t)}}}{\sigma_p(t)(2\pi)^{3/2}}\,\exp\left(-\frac{[1-\rho(t)^2]\,\sigma_q^2(t)}{2}k^2 - i\left[\rho(t)\sigma_q(t)\frac{\mathcal{P}(t)}{\sigma_p} + \mu_q(t)\right]k\right).\end{aligned}$$

Then we compute its discrete inverse Fourier transform:

$$\Phi_t(q_0, p_0; q, p) = \sum_{n=-\infty}^{+\infty} \widehat{\Phi}_t(q_0, p_0; n, p)\,\mathrm{e}^{inq},$$

where $q \in [0, 2\pi)$ and $n \in \mathbb{Z}$. Note that $\sigma_Q^2 = \sigma_q^2$. The resulting transition probability density is

$$\begin{aligned}\Phi_t(q_0, p_0; q, p) &= \frac{1}{2\pi}\Lambda_t(\mathcal{P})\sum_{n=-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}\left[1-\rho(t)^2\right]\sigma_q^2(t)\,n^2}\,\mathrm{e}^{-i\,n\left[\rho(t)\,\sigma_q(t)\,\frac{\mathcal{P}(t)}{\sigma_p(t)} - \mathcal{Q}(t)\right]}\\ &= \frac{1}{2\pi}\Lambda_t(\mathcal{P})\left[1 + 2\sum_{n=-\infty}^{\infty} \mathrm{e}^{-G(t)\,n^2}\cos\left(n\,M_t(\mathcal{Q},\mathcal{P})\right)\right]\end{aligned}$$

where $\mathcal{Q}(t) = q - \mu_q(t)$ and

$$\begin{aligned}\Lambda_t(\mathcal{P}) &\doteq \frac{1}{\sigma_p(t)\sqrt{2\pi}}\,\mathrm{e}^{-\frac{\mathcal{P}(t)^2}{2\sigma_p^2(t)}},\\ G(t) &\doteq \frac{1}{2}\left[1-\rho(t)^2\right]\sigma_q^2(t) = \frac{2m}{\beta\xi^2}\left[\frac{\xi}{2m}t - \tanh\left(\frac{\xi}{2m}t\right)\right],\\ M_t(\mathcal{Q},\mathcal{P}) &\doteq \rho(t)\,\sigma_q(t)\,\frac{\mathcal{P}(t)}{\sigma_p(t)} - \mathcal{Q}(t)\\ &= \xi^{-1}\,\frac{1-\mathrm{e}^{-\frac{\xi}{m}t}}{1+\mathrm{e}^{-\frac{\xi}{m}t}}\,(p+p_0) - q + q_0 + \frac{\tau}{\xi}t.\end{aligned}$$

Note that $G(t) > 0$ for all $t > 0$. Also, for small values of t,

$$\Lambda_t(\mathcal{P}) \xrightarrow{t\to 0} \delta(\mathcal{P}),$$
$$G(t) \xrightarrow{t\to 0} 0, \quad \sum_{n=-\infty}^{\infty} \mathrm{e}^{-i\,n\,M_t(\mathcal{Q},\mathcal{P})} \xrightarrow{t\to 0} \sum_{n=-\infty}^{\infty} \delta(\mathcal{Q}-2\pi n),$$

thus

$$\Phi_t(q_0,p_0;q,p) \xrightarrow{t\to 0} \delta(\mathcal{P}) \sum_{n=-\infty}^{\infty} \delta(\mathcal{Q}-2\pi n).$$

3.2 The spectral gap of $\mathcal{L}_{\tau,0}$

When $U = 0$, the non-reversible dynamics has an explicit invariant measure on $\mathcal{E} = \mathcal{D}\times\mathbb{R}$, with $\mathcal{D} = 2\pi\mathbb{T}$ given by

$$\mathrm{d}\mu_\tau = \frac{\mathrm{e}^{-\frac{\beta}{2m}p^2}}{2\pi\sqrt{2\pi m\beta^{-1}}}\,\mathrm{d}p\,\mathrm{d}q \doteq \frac{g(p)}{2\pi}\,\mathrm{d}q\,\mathrm{d}p, \tag{3.3}$$

where $g(p)$ is the Gaussian distribution of zero mean and variance $m\beta^{-1}$. We point out that in this section, the subscript τ acts only as a reminder of the fact that $p = P - m\tau/\xi$ is the shifted momentum. Indeed, the results are independent of τ, as we shall see. The adjoint of ∂_p with respect to μ_τ is $\partial_p^* = -\partial_p + \frac{\beta}{m}p$ and the generator of the unperturbed ($U = 0$) dynamics as

$$\mathcal{L}_{\tau,0} = -\xi\beta^{-1}\partial_p^*\partial_p + m^{-1}p\partial_q \doteq \mathcal{S}_\tau + \mathcal{A}_{\tau,0},$$

where $\mathcal{S}_\tau$ and $\mathcal{A}_{\tau,0}$ are respectively symmetric and antisymmetric with respect to μ_τ.

Theorem 14. *There exists $C > 0$ (depending on β, m and ξ), such that*

$$\forall t \geq 0, \quad \forall f \in L^2(\mu_\tau), \qquad \left\|\mathrm{e}^{t\mathcal{L}_{\tau,0}}f - \mathbb{E}_{\mu_\tau}(f)\right\|_{L^2(\mu_\tau)} \leqslant C\,\mathrm{e}^{-\lambda t}\|f\|_{L^2(\mu_\tau)}, \tag{3.4}$$

where the spectral gap,

$$\lambda = \min\left(\frac{1}{\beta\xi}, \frac{\xi}{m}\right), \tag{3.5}$$

is independent from τ.

As a consequence, introducing the space

$$L^2_0(\mu_\tau) = \left\{ f \in L^2(\mu_\tau) \;\middle|\; \int_{\mathcal{D}\times\mathbb{R}} f\,\mathrm{d}\mu_\tau = 0 \right\},$$

one can define the inverse of the generator $\mathcal{L}_{\tau,0}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}_{\tau,0}}\,\mathrm{d}t$, and it holds

$$\forall f \in L^2_0(\mu_\tau), \qquad \left\|(-\mathcal{L}_{\tau,0}^{-1})f\right\|_{L^2(\mu_\tau)} \leqslant \frac{C}{\lambda}\,\|f\|_{L^2(\mu_\tau)}. \tag{3.6}$$

Proof. The following proof is based on a direct estimation of λ from the explicit expression of the transition probability. As we shall see, the exponential bound is obtained for a value of t not too small, but the result holds for all $t \geq 0$, possibly upon increasing the value of the prefactor C before the exponential in (3.4).

Given a fixed initial condition (q_0, p_0), we consider

$$\begin{aligned}
\left|\mathrm{e}^{t\mathcal{L}_{\tau,0}} f - \mathbb{E}_{\mu_\tau}(f)\right|^2 &= \left[\int_0^{2\pi} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p f(q,p)\left(\Phi_t(q_0,p_0;q,p) - \frac{g(p)}{2\pi}\right)\right]^2 \\
&\leqslant \left(\int_0^{2\pi} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \, \frac{g(p)}{2\pi} f^2(q,p)\right)\left[\int_0^{2\pi} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \left(\frac{2\pi\Phi_t(q_0,p_0;q,p)}{g(p)} - 1\right)^2 \frac{g(p)}{2\pi}\right] \\
&= \left[\int_0^{2\pi} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \left(\frac{2\pi\Phi_t(q_0,p_0;q,p)}{g(p)} - 1\right)^2 \frac{g(p)}{2\pi}\right] \|f\|^2_{L^2(\mu_\tau)} \qquad (3.7) \\
&\doteq \left[\int_0^{2\pi} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \, (\Psi_t(q,p))^2 \, \frac{g(p)}{2\pi}\right] \|f\|^2_{L^2(\mu_\tau)},
\end{aligned}$$

where we have defined $\Psi_t \doteq \left|\frac{2\pi\Phi_t(q_0,p_0;q,p)}{g(p)} - 1\right|$. By (3.1), we have

$$\Psi_t = \left|\alpha_t \mathrm{e}^{-h_t(p,p_0)}\left(1 + 2\sum_{n\geq 1} \mathrm{e}^{-G(t)n^2} \cos\left(nM_t(q_0,p_0;q,p)\right)\right) - 1\right|,$$

with

$$\alpha_t \doteq \frac{1}{\sqrt{1-\mathrm{e}^{-2\frac{\xi}{m}t}}}, \qquad h_t(p,p_0) \doteq \frac{(p_0^2+p^2)\mathrm{e}^{-2\frac{\xi}{m}t} - 2pp_0\mathrm{e}^{-\frac{\xi}{m}t}}{2m\beta^{-1}(1-\mathrm{e}^{-2\frac{\xi}{m}t})}.$$

It holds

$$\begin{aligned}
\Psi_t &= \left|\alpha_t \mathrm{e}^{-h_t} - 1 + 2\alpha_t \mathrm{e}^{-h_t} \sum_{n\geq 1} \mathrm{e}^{-G(t)n^2} \cos\left(nM_t(q_0,p_0;q,p)\right)\right| \\
&\leqslant (\alpha_t - 1)\mathrm{e}^{-h_t} + \left|\mathrm{e}^{-h_t} - 1\right| + 2\alpha_t \mathrm{e}^{-h_t} \sum_{n\geq 1} \mathrm{e}^{-G(t)n^2} \\
&\leqslant (\alpha_t - 1)\mathrm{e}^{-h_t} + |h_t| + 2\alpha_t \mathrm{e}^{-h_t}\mathrm{e}^{-G(t)}.
\end{aligned}$$

Fixing t_* such that $\left(1 - \mathrm{e}^{-\frac{\xi}{m}t_*}\right) = 1/2$ and considering values of $t \geq t_*$, we obtain the following bounds

$$\begin{aligned}
h_t(p,p_0) &\leqslant \frac{(p^2+p_0^2)\mathrm{e}^{-\frac{\xi}{m}t}}{2m\beta^{-1}\left(1-\mathrm{e}^{-\frac{\xi}{m}t}\right)} \leqslant \frac{(p^2+p_0^2)\,\mathrm{e}^{-\frac{\xi}{m}t}}{m\beta^{-1}}, \\
\alpha_t &\leqslant 2/\sqrt{3}, \qquad |\alpha_t - 1| \leqslant C\,\mathrm{e}^{-2\frac{\xi}{m}t}, \\
\mathrm{e}^{-h_t} &\leqslant \exp\left(\frac{pp_0}{m\beta^{-1}} \frac{\mathrm{e}^{-\frac{\xi}{m}t}}{1-\mathrm{e}^{-2\frac{\xi}{m}t}}\right) \leqslant \mathrm{e}^{\frac{2}{3}\frac{pp_0}{m\beta^{-1}}},
\end{aligned}$$

which lead to

$$\Psi_t \leqslant \widetilde{C}\left[(p^2+p_0^2)\,\mathrm{e}^{-\frac{\xi}{m}t} \;+\; \mathrm{e}^{\frac{2}{3}\frac{pp_0}{m\beta^{-1}}}\left(\mathrm{e}^{-\frac{t}{\beta\xi}}+\mathrm{e}^{-2\frac{\xi}{m}t}\right)\right],$$

We substitute this expression in (3.7), integrate both over (q,p) and all possible initial conditions (q_0,p_0) and, after some lengthy algebra, we finally obtain

$$\left\|\left(\mathrm{e}^{t\mathcal{L}_{\tau,0}}f\right)(q_0,p_0) - \mathbb{E}_{\mu_\tau}(f)\right\|_{L^2(\mu_\tau)} \leqslant C\,\mathrm{e}^{-\lambda t}\,\|f\|_{L^2(\mu_\tau)},$$

with $C>0$ depending on β and m and

$$\lambda = \min\left(\frac{1}{\beta\xi}, \frac{\xi}{m}\right),$$

which concludes the proof.

□

Remark. The spectral gap λ in (3.5) obtained by a pointwise estimation is equal to the spectral gap (2.32) computed in Section 2.6.1 following Kozlov (1989).

3.3 Perturbative result in $L^2(\mu)$

We consider in this section a perturbative expansion in the potential of the non-equilibrium stationary measure, which we denote by ψ_η. In presence of the perturbation $U \neq 0$, the analytical form of the invariant measure is not explicit anymore, but has a non-negative density $f_\eta(q,p)$ with respect to the measure μ_τ defined in (3.3). This density satisfies the equation

$$\mathcal{L}^*_{\tau,\eta} f_\eta = \left(\mathcal{L}^*_{\tau,0} + \eta U(q)\,\partial_p^*\right) f_\eta \;=\; 0\,.$$

The result in Theorem 15 is proved in the particular case of case of $U(q) = U_0(1-\cos q)$. However, the structure of the proof remains unchanged if one considers a generic periodic potential $U(q)$. In what follows, $\mathcal{L}_{\tau,0}$ is called $\mathcal{L}_0$ for simplicity.

Theorem 15. *There exists $\overline{\eta}_U(\beta,\xi,m,U_0) > 0$, independent from τ, such that the expansion*

$$f_\eta(q,p) = \sum_{k\geq 0} u_k(q,p)\,\eta^k \;=\; 1 + \sum_{k\geq 1} u_k(q,p)\,\eta^k \tag{3.8}$$

holds in $L^2(\mu_\tau)$ for any $|\eta| < \overline{\eta}_U$, with $u_0(q,p) = 1$.

Remark. The dependence of the constant $\overline{\eta}_U$ on the parameters can be made explicit, see (3.16) below.

Proof. It is a standard perturbative argument. The density $f_\eta(q,p)$ is solution of the equation

$$\left[\mathcal{L}_0^* - \eta\,(U_0 \sin q)\partial_p^*\right] f_\eta = 0\,.$$

Note that $\mathcal{L}_0^*$ has the same properties as $\mathcal{L}_0$, in particular it satisfies Theorem 14 with the same exponential rate λ and the same constant C.

Consider now the solution to the sequence of equations

$$\begin{aligned}\mathcal{L}_0^* u_{k+1} &= U_0(\sin q)\partial_p^* u_k \\ &= U_0(\sin q)\Big(\frac{\beta}{m}p - \partial_p\Big)u_k, \qquad k>0, \\ \mathcal{L}_0^* u_1 &= U_0(\sin q)\frac{\beta}{m}p.\end{aligned} \tag{3.9}$$

From the second equation in (3.9), by (3.6), we get

$$\|u_1\|^2_{L^2(\mu_\tau)} \leqslant \bar{C}_\lambda\, U_0^2 \frac{\beta}{m}. \tag{3.10}$$

For $k>1$, applying (3.6) to the first equation in (3.9), we get

$$\|u_{k+1}\|^2_{L^2(\mu_\tau)} = \|(-\mathcal{L}_0^*)^{-1}(U_0\sin q)\,(-\partial_p^*)u_k\|^2_{L^2(\mu_\tau)} \leqslant \bar{C}_\lambda\, U_0^2\, \|\partial_p^* u_k\|^2_{L^2(\mu_\tau)},$$

where

$$\|\partial_p^* u_k\|^2_{L^2(\mu_\tau)} = \|\partial_p u_k\|^2_{L^2(\mu_\tau)} + \frac{\beta}{m}\|u_k\|^2_{L^2(\mu_\tau)}, \tag{3.11}$$

which is easy to check by simple substitution. In fact,

$$\|\partial_p^* u_k\|^2_{L^2(\mu_\tau)} = \|\partial_p u_k\|^2_{L^2(\mu_\tau)} - 2\frac{\beta}{m}\langle \partial_p u_k, p u_k\rangle_{L^2(\mu_\tau)} + \frac{\beta^2}{m^2}\|p u_k\|^2_{L^2(\mu_\tau)}, \tag{3.12}$$

and since

$$\langle \partial_p u_k, p u_k\rangle_{L^2(\mu_\tau)} = -\langle \partial_p u_k, p u_k\rangle_{L^2(\mu_\tau)} - \|u_k\|^2_{L^2(\mu_\tau)} + \frac{\beta}{m}\|p u_k\|^2_{L^2(\mu_\tau)},$$

we obtain

$$\langle \partial_p u_k, p u_k\rangle_{L^2(\mu_\tau)} = \frac{1}{2}\Big(\frac{\beta}{m}\|p u_k\|^2_{L^2(\mu_\tau)} - \|u_k\|^2_{L^2(\mu_\tau)}\Big).$$

Substituting in (3.12), one obtains (3.11).

From the first equation in (3.9),

$$\begin{aligned}\langle u_{k+1}, \mathcal{L}_0^* u_{k+1}\rangle_{L^2(\mu_\tau)} &= \langle u_{k+1}, S_\tau u_{k+1}\rangle_{L^2(\mu_\tau)} = \\ -\frac{\xi}{\beta}\|\partial_p u_{k+1}\|^2_{L^2(\mu_\tau)} &= \langle (\partial_p u_{k+1}), U_0(\sin q)u_k\rangle_{L^2(\mu_\tau)},\end{aligned}$$

which, by Cauchy-Schwarz inequality and taking the square of both members, gives

$$\|\partial_p u_{k+1}\|^2_{L^2(\mu_\tau)} \leqslant \frac{1}{2}\Big(\frac{U_0\beta}{\xi}\Big)^2 \|u_k\|^2_{L^2(\mu_\tau)}.$$

Therefore

$$\|u_{k+1}\|^2_{L^2(\mu_\tau)} \leqslant \bar{C}_\lambda\, U_0^2\left[\frac{1}{2}\Big(\frac{U_0\beta}{\xi}\Big)^2 \|u_{k-1}\|^2_{L^2(\mu_\tau)} + \frac{\beta}{m}\|u_k\|^2_{L^2(\mu_\tau)}\right], \quad k>0. \tag{3.13}$$

Since $u_0 = 1$ and u_1 satisfies the bound (3.10), all the u_k's are bounded in $L^2(\mu_\tau)$.

Introducing the two positive constants a and b defined hereafter, we can rewrite the inequlity (3.13) as

$$\begin{aligned} &a \doteq \bar{C}_\lambda U_0^2 \frac{\beta}{m}, \quad b \doteq \frac{1}{2}\bar{C}_\lambda U_0^2 \left(\frac{U_0\beta}{\xi}\right)^2, \\ &\|u_{k+2}\|^2_{L^2(\mu_\tau)} - a\|u_{k+1}\|^2_{L^2(\mu_\tau)} - b\|u_k\|^2_{L^2(\mu_\tau)} \leqslant 0, \qquad k > 0, \\ &\quad \|u_0\|^2_{L^2(\mu_\tau)} = 1, \quad \|u_1\|^2_{L^2(\mu_\tau)} \leqslant a. \end{aligned} \tag{3.14}$$

Solving the second-order difference equation associated with (3.14) we get

$$\|u_k\|^2_{L^2(\mu_\tau)} \leqslant 2\left(\frac{a}{2}\right)^k \left(1 + \sqrt{1 + \frac{4b}{a^2}}\right)^k = 2\left[\frac{U_0^2\bar{C}_\lambda\beta}{2m}\left(1 + \sqrt{1 + \frac{2m^2}{\bar{C}_\lambda\xi^2}}\right)\right]^k. \tag{3.15}$$

We must now study the convergence of the expansion (3.8). Since $\mathbb{E}_{\mu_\tau}(u_k) = 0$ for each $k \geq 1$, applying the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} \|f_\eta\|^2_{L^2(\mu_\tau)} &= \left\|1 + \sum_{k\geq 1} u_k \eta^k\right\|^2_{L^2(\mu_\tau)} \leqslant 1 + \left\|\sum_{k\geq 1} u_k \eta^k\right\|^2_{L^2(\mu_\tau)} \\ &\leqslant 1 + \frac{\pi^2}{6}\sum_{k\geq 1} k^2 \|u_k\|^2_{L^2(\mu_\tau)} \eta^{2k} \leqslant 1 + \frac{\pi^2}{3}\sum_{k\geq 1} k^2 \left[\frac{a}{2}\left(1 + \sqrt{1 + \frac{4b}{a^2}}\right)\eta^2\right]^k, \end{aligned}$$

which converges for $\eta < \overline{\eta}_U = \left[\frac{a}{2}\left(1 + \sqrt{1 + \frac{4b}{a^2}}\right)\right]^{-1/2}$ that is

$$\overline{\eta}_U = \left[\frac{U_0^2\bar{C}_\lambda\beta}{2m}\left(1 + \sqrt{1 + \frac{2m^2}{\bar{C}_\lambda\xi^2}}\right)\right]^{-1/2}. \tag{3.16}$$

This concludes the proof. □

3.4 Perturbative expansion of the invariant measure(*)

When the torque $\tau = 0$, the stationary probability is simply given by the equilibrium Gibbs state proportional to $\mathrm{e}^{-\beta H(p,q)}\,\mathrm{d}q\,\mathrm{d}p$, where $H(p,q) = \frac{1}{2m}p^2 + U(q)$ is the Hamiltonian of the system. The torque τ is a non-conservative (or non-gradient) force and drives the system out of equilibrium. The thermostatting action of the noise acting on the rotator is essential, as it may take energy out, allowing reaching a steady state.

(*) *This section contains a modified version of our article "Nonequilibrium stationary state for a damped rotator" (Gallavotti et al. (2013)).*

The overdamped case corresponds to the limit equation obtained rescaling time $t' = \lambda t$ and $\xi' = \lambda\xi$ and taking the limit $\lambda \to +\infty$: $q'_\xi(t')$ converges in law to the solution $\bar{q}(t)$ of the stochastic differential equation on T^1

$$\dot{\bar{q}} = -\frac{1}{\xi}(\partial U + \tau) + \sqrt{\frac{2}{\beta\xi}}\,\dot{\bar{w}}. \tag{3.17}$$

The generator for a distribution $F(q)\frac{\mathrm{d}q}{2\pi}$ of such evolution is $\mathcal{L}^*_{od}F$ defined by $\mathcal{L}^*_{od}F = \xi^{-1}\Big(\partial_q\Big((\tau + \partial_q U)F\Big) + \partial_q^2 F\Big)$. The process therefore has an explicit stationary state given by

$$F_{od}(q) = \mathrm{e}^{-\beta U(q)} \int_0^{2\pi} \mathrm{e}^{\beta(\tau y + U(q+y))}\,\mathrm{d}y/Z\,,$$

where Z is the normalization (to 1), see Reimann (2002), Faggionato and Gabrielli (2012). In fact defining $B(y) = \tau y + U(y)$, it is $F_{od}(q) = Z^{-1}\int_q^{q+2\pi} \mathrm{e}^{\beta(B(y)-B(q))}\,dy$ and $\partial F_{od}(q) = -\beta(\tau + \partial U(q))F_{od}(q)$, so that $\mathcal{L}^*_{od}F_{od} = 0$.

The study of the overdamped Langevin equation on the circle T^1 is surprisingly involved, see Faggionato and Gabrielli (2012). There is indeed a remarkable lack of smoothness of some properties (large deviation functions) of the above stationary distribution in some region of the model parameters.

Going beyond the overdamped motion assumption is the aim of the present work: hence the particle state will be described by a pair of coordinates $(q,p) \in \mathbb{T} \times R$.

The physical dimensions are $[m] = [time \times action]$, $[p] = [action]$, $q = [angle]$, $[V] = [U] = [\tau] = [energy] = [action/time]$, $[\xi] = [action]$, $[\beta] = [energy^{-1}]$ and $\dot{w}$ has dimension $[\dot{w}] = [action/\sqrt{time}]$: the "unusual" dimensions arise because q is dimensionless (an angle) rather than with dimension of a length.

The generator for the evolution of a distribution $F(q,p)\frac{\mathrm{d}q\,\mathrm{d}p}{2\pi}$ is

$$\begin{aligned}\mathcal{L}^*F = -\Big\{&\Big(\frac{p}{m}\partial_q F(q,p) - (\partial_q U(q) + \tau)\partial_p F(q,p)\Big)\\ &-\xi\Big(\beta^{-1}\partial_p^2 F(q,p) + \frac{1}{m}\partial_p(p\,F(q,p))\Big)\Big\}.\end{aligned} \tag{3.18}$$

The solution of $\mathcal{L}^*F = 0$ will be searched within the class of probability distributions satisfying the following hypotheses:

(H1) The function $F(p,q)$ is smooth and admits an expansion in Hermite polynomials (or "Wick monomials") H_n of the form

$$\begin{aligned}F(q,p) =& G_\beta(p)\sum_a \rho_a(q) : p^a :, \qquad G_\beta(p) = \frac{\mathrm{e}^{-\frac{\beta}{2}p^2}}{\sqrt{2\pi\beta^{-1}}},\\ : p^n : \stackrel{def}{=}& \Big(\frac{m\beta^{-1}}{2}\Big)^{\frac{n}{2}} H_n\Big(\frac{p}{\sqrt{2m\beta^{-1}}}\Big),\end{aligned} \tag{3.19}$$

where $a \geq 0$ are integers; so that $\int :p^n::p^m: G_\beta(p)\,\mathrm{d}p = \delta_{nm} n!\,(m\beta^{-1})^n$.
(H2) The coefficients $\rho_n(q)$ are C^∞-differentiable in q, g and the p, q, g-derivatives of F can be computed by term by term differentiation, obtaining convergent series.

It is known (Mattingly and Stuart (2002)) that the equation $\mathcal{L}^* F(p,q) = 0$ admits a unique smooth and positive solution in $L_2(G_\beta(\mathrm{d}p)\,\mathrm{d}q)$, hence in $L_1(\mathrm{d}q\,\mathrm{d}p) \cap L_2(\mathrm{d}q\,\mathrm{d}p)$, with $\int F\,\mathrm{d}p\,\mathrm{d}q = 1$.

In this paper [1] we show that

Theorem 16 (Power expansion of the stationary measure)**.** *There is a formal power series expansion in g for a solution of the equation $\mathcal{L}^* F = 0$ with coefficients $\rho_n^{[r]}(q)$; their Fourier's transforms $\rho_{n,k}^{[r]}$ can be determined by a constructive algorithm, vanish for $|k| > r$ and satisfy the bounds*

$$\xi^n |\rho_{n,k}^{[r]}| \leqslant A_r \frac{(B_r)^n}{n!} \delta_{|k| \leqslant r}, \qquad \forall r, k, \tag{3.20}$$

for A_r, B_r suitably chosen, depending also on the dimensionless parameters of the problem $\beta V, \beta\tau, \eta = \frac{\beta\xi^2}{2m} > 0$.

The properties (H1), (H2) allow us to perform the algebra needed to turn the stationarity condition $\mathcal{L}^* F = 0$ into a hierarchy of equations for the coefficients $\rho_n(q)$, $\forall n \geq 0$

$$\begin{aligned} &n\beta^{-1}\partial\rho_n(q) + \Big[\frac{1}{m}\partial\rho_{n-2}(q) + \frac{\beta}{m}(\partial U(q) + \tau)\rho_{n-2}(q) \\ &+ (n-1)\frac{\xi}{m}\rho_{n-1}(q)\Big] = 0, \end{aligned} \tag{3.21}$$

where ρ_{-1}, ρ_{-2} are to be set equal to zero.

Remarks: (1) Adapting the procedure by Mattingly and Stuart (2002), it can be seen that $\mathcal{L}^* F(p,q) = 0$ admits a unique solution smooth in p, q. However its analyticity in g and the properties of its representation in the form in Eq.(3.19), are not proven by the above Theorem, as it only deals with the Taylor coefficients of a formal expansion in powers of g.
(2) Identities follow immediately by normalization or by integration.
Let $\overline{\rho}_n \stackrel{def}{=} \int \rho_n(q)\frac{\mathrm{d}q}{2\pi}$ and $\widetilde{\rho}_n(q) \stackrel{def}{=} \rho_n(q) - \overline{\rho}_n$; then for $n = 1$

$$\int \rho_0(q)\frac{\mathrm{d}q}{2\pi} = 1, \quad \widetilde{\rho}_1 = 0. \tag{3.22}$$

(3) The bound in Eq.(3.20) yields a convergent expression for the $\rho_n^{[r]}(q)$ or for $F^{[r]}(q,p)$ or, for bounded f, of $\int F^{[r]}(q,p)\cdot f(p)\,\mathrm{d}p$. Such expressions can possibly be compared with results of numerical simulations.

[1] Note that, throughout the remainder of this chapter, the parameter g takes the role of η to denote the intensity of the perturbation.

3.4.1 Dimensionless equations

It is convenient to introduce the dimensionless quantities

$$\sigma_n(q) \stackrel{def}{=} \rho_n(q)\xi^n n!, \qquad \eta \stackrel{def}{=} \beta\xi^2/m, \qquad \beta\tau, \qquad \beta V,$$

which will be relevant in the following.

Let a tilde over a function $f(q)$ mean $f - \overline{f}$, with $\overline{f} \stackrel{def}{=} \int_0^{2\pi} f(q)\frac{\mathrm{d}q}{2\pi} \stackrel{def}{=} \langle f \rangle$. If $\sigma_n(q) \stackrel{def}{=} \widetilde{\sigma}_n(q) + \overline{\sigma}_n$ with $\langle \widetilde{\sigma}_n \rangle = 0$, consider the sequence of functions

$$\sigma(q) = (\widetilde{\sigma}_n(q), \overline{\sigma}_n)_{n\geq 1}\,.$$

The stationarity Eq.(3.21), for $n \geq 1$ and using the Hermite polynomials properties $p : p^n := p^{n+1} : + \frac{m}{\beta} : p^{n-1}:$, $\partial_p : p^n := n : p^{n-1}:$ and $\partial_p G(p) = -\frac{\beta}{m}\, p\, G(p)$, becomes, after dividing both sides by n

$$\begin{aligned}
\partial\widetilde{\sigma}_n =& -\eta\Big((n-1)\Big(\partial\widetilde{\sigma}_{n-2} + \beta\widetilde{\partial U\widetilde{\sigma}_{n-2}} + \beta\partial U\overline{\sigma}_{n-2} \\
&+ \beta\tau\widetilde{\sigma}_{n-2} + \widetilde{\sigma}_{n-1}\Big)\Big), \\
\overline{\sigma}_n =& -\Big(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau\,\overline{\sigma}_{n-1}\Big),
\end{aligned} \tag{3.23}$$

where $\sigma_j = 0$ for $j < 0$. For $n = 0$, Eq.(3.21) is an identity, thus Eq.(3.23) holds only for $n \geq 1$. By normalization $\overline{\sigma}_0 \equiv 1$, as also implied by the second of Eqs.(3.23).

The Fourier transform of Eqs.(3.23) for $n \geq 1$ is

$$\begin{aligned}
\widetilde{\sigma}_{n,k} =& -\frac{\eta(n-1)}{ik}\widetilde{\sigma}_{n-1,k} - \eta(n-1)(1+\frac{\beta\tau}{ik})\widetilde{\sigma}_{n-2,k} \\
&- \eta(n-1)\Big(\frac{\beta g V}{ik}\sum_{k'=\pm 1} ik'\widetilde{\sigma}_{n-2,k-k'} + \beta g V\overline{\sigma}_{n-2}\delta_{k,\pm 1}\Big), \\
\overline{\sigma}_n =& -\Big(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau\overline{\sigma}_{n-1}\Big) \\
\equiv& (-\beta\tau)^n + \sum_{j=0}^{n-1}(-\beta\tau)^j\overline{(-\beta\partial U)\widetilde{\sigma}_{n-1-j}}\,.
\end{aligned} \tag{3.24}$$

After defining $\mathbf{S}_{n,k} \stackrel{def}{=} \begin{pmatrix} \widetilde{\sigma}_{n,k} \\ \widetilde{\sigma}_{n-1,k} \end{pmatrix}$, it is natural to introduce the g–independent 2×2 matrices $M_{n,k}$

$$M_{n+1,k} \stackrel{def}{=} \begin{pmatrix} -\frac{n}{ik}\eta & ina_k\eta \\ 1 & 0 \end{pmatrix}, \qquad a_k \stackrel{def}{=} \Big(i + \frac{\beta\tau}{k}\Big),$$

so that Eqs.(3.24) can be written more concisely, for $n \geq 0$,

$$\begin{aligned}
\mathbf{S}_{n+1,k} =& M_{n+1,k}\Big(\mathbf{S}_{n,k} + \mathbf{X}_{n+1,k}\Big), \quad \mathbf{X}_{n+1,k} \stackrel{def}{=} \begin{pmatrix} 0 \\ x_{n+1,k} \end{pmatrix}, \\
x_{n+1,k} \stackrel{def}{=}& -\frac{\beta g V}{i a_k}\Big(\delta_{|k|=1}\overline{\sigma}_{n-1} + \sum_{k'=\pm 1}\frac{k'}{k}\widetilde{\sigma}_{n-1,k-k'}\Big), \\
\overline{\sigma}_{n+1} =& -(\overline{\beta\partial U\widetilde{\sigma}_n} + \beta\tau\overline{\sigma}_n).
\end{aligned} \tag{3.25}$$

Note that $M_{n,k}$ is defined for $n \geq 1$, while $M^{-1}_{n,k}$ is defined for $n \geq 2$.

Remarks: (1) The case $g = 0$ is an exercise: $\sigma_n(q)$ must be constant simply by symmetry, and $\sigma_0 = 1$. It follows, from Eqs.(3.23) and (3.18) $\sigma_n \equiv \overline{\sigma}_n = (-\beta\tau)^n$ and the series in Eq.(3.18) becomes

$$\begin{aligned}
\sigma_n \equiv \overline{\sigma}_n &= (-\beta\tau)^n, \\
F(p,q) =& G_\beta(p)\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Big(\frac{\beta\tau}{\xi}\Big)^n\Big(\frac{m\beta^{-1}}{2}\Big)^{\frac{n}{2}}H_n\Big(\frac{p}{\sqrt{(2\beta^{-1}m)}}\Big),
\end{aligned}$$

which, by the definition of the Hermite polynomials via their generating function (Gradshtein and Ryzhik (1965, 8.957)), is

$$F(p,q) = G_\beta(p - v), \qquad v = -\frac{m\tau}{\xi}.$$

(2) Eqs.(3.25) implies for $n = 0, 1$ (*i.e.* for $n = 1, 2$ in Eq.(3.24)) that

$$\mathbf{S}_1 = \begin{pmatrix} 0 \\ \widetilde{\sigma}_0 \end{pmatrix}, \quad \mathbf{S}_2 = \begin{pmatrix} \widetilde{\sigma}_2 \\ 0 \end{pmatrix}. \tag{3.26}$$

It is important to note that Eq.(3.22) (hence also (3.24)) implies $\widetilde{\sigma}_1 \equiv 0$.

If $\widetilde{\sigma}_2$ is known, $\widetilde{\sigma}_0$ can be derived by solving, if possible, the equation (see the first of Eqs.(3.24) or (3.25))

$$\widetilde{\sigma}_{2,k} = i\eta a_k\widetilde{\sigma}_{0,k} - \eta\frac{\beta g V}{ik}\sum_{k'=\pm 1} ik'\widetilde{\sigma}_{0,k-k'} - \eta\beta g V\delta_{|k|=1}. \tag{3.27}$$

(3) Eqs.(3.25) can be regarded as equations for $\mathbf{S}_n, n \geq 1$: if $\mathbf{S}_1 \equiv \binom{0}{\widetilde{\sigma}_0}$ (*i.e.* if $\widetilde{\sigma}_0$) is known, then all $\mathbf{S}_n$, $n \geq 3$, can be immediately computed. To this end, $\mathbf{S}_1$ and $\overline{\sigma}_1$ are computed from Eqs.(3.25) ($\overline{\sigma}_0 = 1$), together with $x_{2,k}$; then, from the pair $(\mathbf{S}_1, \overline{\sigma}_1)$ and $x_{2,k}$, we compute $\mathbf{S}_2, \overline{\sigma}_2$ and x_3, by Eq.(3.25), hence $\mathbf{S}_3, \overline{\sigma}_3$ and x_4 follow &tc.

(4) Eqs.(3.23) and its Fourier transform (3.24) will be considered as equations for $\mathbf{S}_{n,k}$ for $n \geq 2$ to be solved under the condition that $\mathbf{S}_2 = \binom{\widetilde{\sigma}_2}{0}$. The condition that the second component of $\mathbf{S}_2$ be 0 is the only condition to impose *a priori* and to use in the construction.

3.4.2 Perturbation expansion

Consider the expansion in g by writing

$$\begin{aligned}\widetilde{\sigma}_n(q) =& g\widetilde{\sigma}_n^{[1]}(q) + g^2\widetilde{\sigma}_n^{[2]}(q) + \dots,\\ \overline{\sigma}_n =& \overline{\sigma}_n^{[0]} + g\overline{\sigma}_n^{[1]} + g^2\overline{\sigma}_n^{[2]} + \dots,\end{aligned}$$

and, correspondingly, $F = F^{[0]} + gF^{[1]} + \dots$.

Eqs.(3.25) become a recursive relation for the the real constants $\overline{\sigma}_n^{[r]}$ and for the vectors $\mathbf{S}_{n,k}^{[r]} \stackrel{def}{=} \begin{pmatrix}\widetilde{\sigma}_{n,k}^{[r]}\\ \widetilde{\sigma}_{n-1,k}^{[r]}\end{pmatrix}$, $k > 0$, keeping in mind the c.c. symmetry $\widetilde{\sigma}_{n,k}^{[r]} = \overline{\widetilde{\sigma}_{n,-k}^{[r]}}$. The order $r = 0$ is simply $\widetilde{\sigma}_n^{[0]} = 0$, $\overline{\sigma}_0 = 1$ and for $r \geq 0$ the recursion will be conveniently written in matrix form for $n \geq 0$

$$\begin{aligned}\mathbf{S}_{n+1,k}^{[r]} =& M_{n+1,k}\left(\mathbf{S}_{n,k}^{[r]} + x_{n+1,k}^{[r]}\begin{pmatrix}0\\1\end{pmatrix}\right), \quad \mathbf{S}_{0,k}^{[r]} = y_{0,k}^{[r]}\begin{pmatrix}1\\0\end{pmatrix} \stackrel{def}{=} \mathbf{Y}_k^{[r]},\\ \overline{\sigma}_{n+1}^{[r]} =& -\beta\tau\overline{\sigma}_n^{[r]} + v_{n+1}^{[r]}, \quad \overline{\sigma}_n^{[0]} = (-\beta\tau)^n,\end{aligned} \tag{3.28}$$

where $y_{0,k}^{[r]} \equiv \widetilde{\sigma}_{0,k}^{[r]}$ (so that, by Eq.(3.22),(3.26), $\mathbf{S}_{1,k}^{[r]} = \begin{pmatrix}0\\ y_{0,k}^{[r]}\end{pmatrix}$) and $v_n^{[r]}, x_{n,k}^{[r]}$ are given by

$$\begin{aligned}x_{n+1,k}^{[r]} \stackrel{def}{=}& -\frac{\beta V}{ia_k}\left(\overline{\sigma}_{n-1}^{[r-1]}\delta_{|k|=1} + \sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}_{n-1,k-k'}^{[r-1]}\right), \quad n \geq 0,\\ v_{n+1}^{[r]} \stackrel{def}{=}& -\sum_{k'=\pm1}\beta V\, ik'\widetilde{\sigma}_{n,-k'}^{[r-1]}, \quad n \geq 0, \qquad \mathbf{S}_{1,k}^{[r]} = \begin{pmatrix}0\\ y_{0,k}^{[r]}\end{pmatrix},\\ x_{2,k}^{[r]} =& \frac{-\beta V}{ia_k}(\delta_{|k|=1}\delta_{r=1} + \sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}_{0,k-k'}^{[r-1]}),\end{aligned} \tag{3.29}$$

and depend on quantities of order lower than r. Here, quantities of order lower than 0 are interpreted as 0.

Therefore, at order r, all coefficients are determined in terms of the constants $\widetilde{\sigma}_{0,k}^{[r]} \equiv y_{0,k}^{[r]}$ and of the $\mathbf{S}_{n,k'}^{[r']}$ with $r' < r$; since the only harmonics in $U(q)$ are $k = \pm1$, it can be supposed that $\widetilde{\mathbf{S}}_{n,k}^{[r]} \equiv 0$ for $|k| > r$ and all n.

Furthermore, the harmonics $\widetilde{\sigma}_{0,k}^{[r]}$ and $\widetilde{\sigma}_{0,-k}^{[r]}$ are complex conjugate, so it is possible to always suppose $k > 0$ and to interpret harmonics with negative values of k as complex conjugate of the corresponding harmonics with $k > 0$.

3.4.3 The expansion coefficients

The recursion can be reduced to an iterative determination of $x_{n,k}^{[r]}$ and $\overline{\sigma}_n^{[r]}$ starting from $r = 1$, as the case $r = 0$ has been already evaluated at the end of Sec. 3.4.1, namely $x_{n,k}^{[0]} = 0$, $\overline{\sigma}_n^{[0]} = (-\beta\tau)^n$ and $\mathbf{S}_n^{[0]} = 0$, since $\widetilde{\sigma}_n^{[0]} \equiv 0$.

For $r \geq 1$ it is, see Eqs.(3.27) and (3.29),

$$\mathbf{S}_0^{[r]} \stackrel{def}{=} \mathbf{Y}^{[r]} = \begin{pmatrix} y^{[r]} \\ 0 \end{pmatrix}, \quad \mathbf{S}_1^{[r]} \stackrel{def}{=} \begin{pmatrix} 0 \\ y^{[r]} \end{pmatrix},$$
$$\mathbf{S}_2^{[r]} \stackrel{def}{=} \begin{pmatrix} i\, a_k\, \eta\, (y^{[r]} + x_2^{[r]}) \\ 0 \end{pmatrix}, \qquad \overline{\sigma}_0^{[r]} = 0\,,$$
$$r \geq 1\,. \tag{3.30}$$

Eqs.(3.28), for $r \geq 1$, are related to the general r-independent equations for $n \geq 2$, conveniently written by means of the inverse matrix $M_{n+1,k}^{-1}$ as

$$M_{n+1,k}^{-1} \stackrel{def}{=} \begin{pmatrix} 0 & 1 \\ \frac{1}{i\, n\, a_k\, \eta} & -\frac{1}{k\, a_k} \end{pmatrix},$$
$$\mathbf{S}_n = M_{n+1,k}^{-1} \mathbf{S}_{n+1} - \mathbf{X}_{n+1}, \qquad \mathbf{S}_2 = y' \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$
$$\overline{\sigma}_n = (-\beta\tau)\overline{\sigma}_{n-1} + v_n, \quad \overline{\sigma}_0 = w, \quad \mathbf{X}_n = x_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \; x_0 = x_1 = 0\,. \tag{3.31}$$

This is inhomogeneous in the unknowns $(\mathbf{S}_n, \overline{\sigma}_n)_{n\geq 2}$, imagining $\mathbf{S}_2, \mathbf{X}_n$, v_n, w (*i.e.* y, x_n, v_n, w) as known inhomogeneous quantities depending on the orders r and k, as prescribed by Eqs.(3.29). In the following, Eqs.(3.31) will be considered for different orders r. Moreover, $w = 0$ if $r \geq 1$ and $w = (-\beta\tau)^n$ if $r = 0$.

A few properties of products of matrices $M_{n,k}$ will be needed.

Let $(M_p^{-1})^{*s} \stackrel{def}{=} M_p^{-1} \cdots M_{p+s-1}^{-1}$ for $s \geq 1$, $(M_p^{-1})^{*0} \stackrel{def}{=} 1$ and define

$$\boldsymbol{\xi}_n \stackrel{def}{=} -\sum_{h=n}^{\infty} (M_{n+1}^{-1})^{*(h-n)} \mathbf{X}_{h+1}\,,$$
$$\overline{\sigma}_n \stackrel{def}{=} \sum_{s\geq 1}^{n} (-\beta\tau)^{n-s} v_s + w, \qquad n \geq 2\,, \tag{3.32}$$

then $M_{n+1}^{-1} \boldsymbol{\xi}_{n+1} = \boldsymbol{\xi}_n + \mathbf{X}_{n+1}$, if the series converges and if y' is left free. Eq.(3.32) is thus a special solution of the recursion (3.31) ($n \geq 2$).

To proceed, we introduce some notation; given k, let

$$|\uparrow\rangle \stackrel{def}{=} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |1\rangle, \qquad |\downarrow\rangle \stackrel{def}{=} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |0\rangle,$$
$$\mathcal{L}_{\nu,\nu'}(n,h) \stackrel{def}{=} \langle \nu | (M_{n+1}^{-1})^{*(h-n)} | \nu' \rangle, \qquad \nu, \nu' = 0, 1\,,$$
$$\mathcal{L}(n,h) \stackrel{def}{=} \mathcal{L}_{0,0}(n,h), \qquad \mathcal{L}(n,n) = 1 \equiv \langle \downarrow | \downarrow \rangle,$$
$$\zeta(n,h) \stackrel{def}{=} \frac{\langle \uparrow | (M_{n+1}^{-1})^{*(h-n)} | \downarrow \rangle}{\mathcal{L}(n,h)}, \qquad \zeta(n,n) = 0 \equiv \langle 1 | 0 \rangle.$$

Note that, by explicitly computing the vectors $\langle \nu | M_{n+1}^{-1}$ and $M_h^{-1} | \nu' \rangle$, the general relation (due to the special form, Eq.(3.31), of M_j^{-1}) is

$$\langle \nu | (M_{n+1}^{-1})^{*(h-n)} | \nu' \rangle = \frac{\mathcal{L}(n+\nu, h-\nu')}{(i\eta a_k (h-1))^{\nu'}}, \quad \nu, \nu' = 0, 1\,, \tag{3.33}$$

which, provided $\mathcal{L}(n,h) \neq 0$, implies the identities

$$\begin{aligned}
&\zeta(n,h) \stackrel{def}{=} \begin{pmatrix} \zeta(n,h) \\ 1 \end{pmatrix},\ \zeta(n,h) = \frac{\mathcal{L}(n+1,h)}{\mathcal{L}(n,h)}, \qquad 2 \leqslant n \leqslant h, \\
&(M^{-1}_{n'+1})^{*(n-n')}\zeta(n,n') = \frac{\mathcal{L}(n',N)}{\mathcal{L}(n,N)}\zeta(n',N), \quad n+1 > n'.
\end{aligned} \tag{3.34}$$

with $\zeta(n,n) = 0$. Here, the second relation will be called the *eigenvector property* of the $\zeta(n,h)$. Eq.(3.33) also implies the recurrence

$$\begin{aligned}
\varphi(n,h) &\stackrel{def}{=} -\frac{\zeta(n,h)}{ka_k} = \frac{1}{1+\frac{z}{n}\varphi(n+1,h)} \\
&= \frac{1}{1+\frac{z}{n}\frac{1}{1+\frac{z}{n+1}}\cdots\frac{1}{1+\frac{z}{h-2}}}, \qquad h-2 \geq n, \qquad z \stackrel{def}{=} \frac{a_k k^2}{i\eta}
\end{aligned} \tag{3.35}$$

and $\varphi(n-1,n) = 1, \varphi(n,n) = 0$, representing the ζ's as continued fractions and showing that $\zeta(n,h)$ and the limit $\zeta(n,\infty)$ are analytic in z for $|z| < \frac{1}{4}$ (Cuyt et al. (2004, p.45)).

The continued fraction for $\varphi(n,\infty)$ is the S-fraction $\frac{n-1}{z}\mathbf{K}^{\infty}_{m=n-1}(\frac{z/m}{1})$, following Cuyt et al. (2004, p.35), and defines an holomorphic function of z in the complex plane cut along the negative real axis (see Cuyt et al. (2004, p.47,(A))). The $\varphi(n,h)$ is also a (truncated) S-fraction obtained by setting $m = \infty$ for $m \geq h-1$ in the previous continued fraction. Hence, by Cuyt et al. (2004, p.47,(B)), $\varphi(n,h)$ has the same holomorphy properties as $\varphi(n,\infty)$. Furhermore, $\varphi(n,h)$ is holomorphic for $|z| < \frac{1}{4}$, continuous and bounded by $\frac{1}{2}$ in $|z| \leqslant \frac{1}{4}$ (Cuyt et al. (2004, p.45)).

Relevant inequalities can be derived from the inequality in Cuyt et al. (2004, p.138), see Sec.3.4.5.

The definitions imply $\xi_n \equiv -\sum_{h=n}^{\infty} x_{h+1}\mathcal{L}(n,h)\zeta(n,h)$ (see Eq.(3.32)). Furthermore, if the limits $\lim_{N\to\infty}\frac{\mathcal{L}(2,N)^{-1}}{\mathcal{L}(n,N)^{-1}}$ exist, and are symbolically denoted $\frac{\mathcal{L}(2,\infty)^{-1}}{\mathcal{L}(n,\infty)^{-1}}$, then

$$\mathbf{T}^0_n = \frac{\mathcal{L}(2,\infty)^{-1}}{\mathcal{L}(n,\infty)^{-1}}\zeta(n), \qquad \zeta(n) \stackrel{def}{=} \zeta(n,\infty)$$

is a solution of Eq.(3.31) with $\mathbf{X} = 0$ and some initial data for $n = 2$.

A solution to the r-th order equations will thus have the form

$$\mathbf{S}_n = \xi_n + \lambda\mathbf{T}^0_n, \tag{3.36}$$

where the constant λ will be fixed to match the data at $n = 2$, *i.e.* null $\mathbf{S}_2$ second component, see Eqs.(3.26),(3.28). Concerning the r-th order equation, the initial data of interest are $\overline{\sigma}^{[r]}_1$ and $y^{[r]}_{2,k}$ and $\mathbf{X}^{[r]}_{n,k}, v^{[r]}_n$ are given by Eq.(3.29), in terms of quantities of order $r-1$.

Therefore there seems to be no freedom, because we expect that the condition that $\mathbf{Y}$ is proportional to $|\uparrow\rangle$, *i.e.* that its second component is 0, fixes the free constant λ. Thus the (unique) solution to the recursion with initial data $\mathbf{S}^{[r]}_2 =$

$y|\uparrow\rangle$ has necessarily the form

$$\mathbf{S}^{[r]}_{2,k} = -\sum_{h=2}^{\infty} x^{[r]}_{h+1,k}\mathcal{L}(2,h)(\zeta(2,h)-\zeta(2)) \tag{3.37}$$

which is proportional to $|\uparrow\rangle$, because the second components of $\zeta(2,h)$ and $\zeta(2)$ are 1; hence in Eq.(3.36)

$$\lambda = \sum_{h=2}^{\infty} x^{[r]}_{h+1,k}\mathcal{L}(2,h).$$

Proceeding formally, for $n > 2$,$\mathbf{S}^{[r-1]}_n$ will be given by applying the recursion. Since ξ_n is a formal solution and $\zeta(n)$ has the eigenvector property Eq.(3.34), it is

$$\begin{aligned}\mathbf{S}^{[r]}_{n,k} =& \sum_{h=2}^{n-1} x^{[r]}_{h+1,k}\frac{\mathcal{L}(2,h)\mathcal{L}(n,\infty)}{\mathcal{L}(2,\infty)}\zeta(n)\\ &-\sum_{h=n}^{\infty} x^{[r]}_{h+1,k}\Big(\mathcal{L}(n,h)\zeta(n,h)-\frac{\mathcal{L}(2,h)\mathcal{L}(n,\infty)}{\mathcal{L}(2,\infty)}\zeta(n)\Big).\end{aligned} \tag{3.38}$$

It should be stressed that the series in Eq.(3.32) might diverge; nevertheless, cancellations may (and will) occur in Eq.(3.38), so that Eq.(3.32) would still be a solution, if the series in Eq.(3.38) converges (as can be checked by inserting it in the equation Eq.(3.31)).

To compute the first component of $\mathbf{S}^{[r]}_{n,k}$, we left multiply Eq.(3.38) by $\langle\uparrow|$, considering that $\zeta_k(n,m) = \frac{\mathcal{L}(n+1,m)}{\mathcal{L}(n,m)}$ by the first of the (3.34) and that $\mathcal{L}(n+1,n) = \zeta_k(n,n)\mathcal{L}(n,n) \equiv 0$. Setting $\mathcal{L}(n,m) = 0\,, \forall\, m < n$, we obtain

$$\begin{aligned}\widetilde{\sigma}^{[r]}_{n,k} =& \sum_{m=2}^{n} x^{[r]}_{m+1,k}\mathcal{L}(2,m)\frac{\mathcal{L}(n,\infty)}{\mathcal{L}(2,\infty)}\zeta(n)\\ &-\sum_{m=n+1}^{\infty} x^{[r]}_{m+1,k}\Big(\mathcal{L}(n,m)\zeta(n,m)-\mathcal{L}(2,m)\frac{\mathcal{L}(n,\infty)}{\mathcal{L}(2,\infty)}\zeta(n)\Big)\\ \equiv& \sum_{m=2}^{n} x^{[r]}_{m+1,k}\Big(\prod_{j=2}^{m-1}\frac{\zeta(j,\infty)}{\zeta(j,m)}\Big)\Big(\prod_{j=m}^{n}\zeta(j,\infty)\Big)\\ &-\sum_{m=n+1}^{\infty} x^{[r]}_{m+1,k}\Big(\prod_{j=n+1}^{m-1}\frac{1}{\zeta(j,m)}\Big)\Big(1-\prod_{j=2}^{n}\frac{\zeta(j,\infty)}{\zeta(j,m)}\Big),\end{aligned} \tag{3.39}$$

for $n \geq 2$. From $\widetilde{\sigma}^{[r]}_{2,k}$ and $x^{[r]}_{2,k}$ (derived from Eq.(3.29)) and using $\widetilde{\sigma}^{[r]}_{1,k} = 0$ (see Eq.(3.30)) the "main unknown" $y^{[r]}_{0,k}$, *i.e.* $\sigma^{[r]}_{0,k}$, is computed.

As stressed above, Eqs.(3.37),(3.39) are acceptable if the series converge. When $r = 1$, they do for $\beta\tau$ small enough using $x^{[1]}_{n,k} = -\frac{\beta V}{ia_k}(-\beta\tau)^{n-1}\ \delta_{|k|=1}$, since (i) the

squared norm of $M_{n+1,k}$ in C^2 is equal to

$$\frac{1}{2}(1+\frac{1}{\eta^2 n^2|a_k|^2}+\frac{1}{k^2|a_k|^2})\Big(1+\Big(1-\frac{4\frac{1}{\eta^2|a_k|^2 n^2}\frac{1}{k^2|a_k|^2}}{(1+\frac{1}{\eta^2 n^2|a_k|^2}+\frac{1}{k^2|a_k|^2})^2}\Big)^{\frac{1}{2}}\Big),$$

i.e. to the square root of the maximum eigenvalue of $M^{-1\,*}_{n+1,k}M^{-1}_{n+1,k}$ and (ii) the convergence condition of the first of Eqs.(3.32) is $\beta\tau\|M^{-1}_{2,1}\|<1$, meaning that $\beta\tau$ should be small enough. As it will be seen from the estimates of Sec.3.4.5, this restriction on $\beta\tau$ can be removed, because of the cancellations that occur between the two addends in Eq.(3.37)). Therefore, it will be possible to try an iterative construction, $\forall\,\eta,\beta\tau,r>0$.

3.4.4 A constructive algorithm

If $x^{[r]}_{n,k},\overline{\sigma}^{[r]}_n$ are known, it is possible to compute $\widetilde{\sigma}^{[r]}_{n,k}$ from Eqs.(3.29),(3.39) for all $n\geq 0$. In particular,

$$\begin{aligned}
\widetilde{\sigma}^{[r]}_{2,k} =& x^{[r]}_{3,k}\zeta(2,\infty)-\sum_{m=3}^{\infty}x^{[r]}_{m+1,k}\mathcal{L}(3,m)\Big(1-\frac{\mathcal{L}(2,m)\mathcal{L}(3,\infty)}{\mathcal{L}(2,\infty)\mathcal{L}(3,m)}\Big),\\
\widetilde{\sigma}^{[r]}_{0,k} =& \frac{1}{i\eta a_k}\widetilde{\sigma}^{[r]}_{2,k}+\frac{\beta V}{ia_k}\Big(\delta_{|k|=1}\delta_{r=1}+\sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}^{[r-1]}_{0,k-k'}\Big)\Big), \qquad \widetilde{\sigma}_1\equiv 0
\end{aligned} \tag{3.40}$$

The order $r=1$ is therefore known because $x^{[1]}_{m+1,k}=\frac{-\beta V}{ia_k}(-\beta\tau)^{m+1}\delta_{k,1}$, provided the series in Eqs.(3.40),(3.39) converge. It is convenient to introduce the kernels $\vartheta_k(n;m)$ to abridge the Eqs.(3.39),(3.40) into the form:

$$\begin{aligned}
\widetilde{\sigma}^{[r]}_{n,k} =& \sum_{m=0}^{\infty}\vartheta_k(n;m)\,x^{[r]}_{m+1,k}, \quad n\neq 1, \quad \vartheta_k(n;0)=0, \quad \forall n\geq 2,\\
\vartheta_k(n;m) =& \Big(\prod_{j=2}^{m-1}\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}\Big)\Big(\prod_{j=m}^{n}\zeta_k(j,\infty)\Big), \quad 2\leqslant m\leqslant n,\\
\vartheta_k(n;m) =& \Big(\prod_{j=n+1}^{m-1}\frac{1}{\zeta_k(j,m)}\Big)\Big(\prod_{j=2}^{n}\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}-1\Big), \quad 2\leqslant n<m,\\
\vartheta_k(0,m) \overset{def}{=}& \frac{\vartheta_k(2,m)}{i\eta a_k}\delta_{m\geq 2}-\delta_{m,1}, \qquad \vartheta_k(1;m)\equiv 0,
\end{aligned} \tag{3.41}$$

where products over an empty set of labels are interpreted as 1.

Consider the sequences $\mathbf{Z}=\binom{\widetilde{\sigma}_{n,k}}{\widetilde{\sigma}'_{n,k}}$, $n=0,1,\ldots$, $k=\pm1,\pm2,\ldots$, in the particular cases $\mathbf{Z}^{[r]}=\binom{\widetilde{\sigma}^{[r]}_{n,k}}{\widetilde{\sigma}^{[r-1]}_{n,k}}$, $n=0,1,\ldots$, $k=\pm1,\pm2,\ldots$. Remark that $\mathbf{Z}^{[1]}_{n,k}=\begin{bmatrix}\widetilde{\sigma}^{[1]}_{n,k}\\0\end{bmatrix}$ and $\widetilde{\sigma}^{[1]}_{n,k}$ is known (see comment after Eq.(3.40) and remark that $\widetilde{\sigma}^{[0]}=0$), if the series

defining it converges. Then Eqs.(3.39),(3.41) can be rewritten as

$$\mathbf{Z}^{[r]} = \mathcal{B}\mathbf{Z}^{[r-1]}, \qquad r \geq 2, \qquad \mathbf{Z}^{[1]}_{n,k} = \begin{bmatrix} \widetilde{\sigma}^{[1]}_{n,k} \\ 0 \end{bmatrix},$$

with the map $\mathcal{B}$ defined by taking into account the above relations and also Eqs.(3.29),(3.31), which yield

$$\begin{aligned}
\overline{\sigma}^{[r]}_n &= \Big((-\beta\tau)^n \delta_{r,0} - \beta V \sum_{k'=\pm 1} ik' \sum_{h=0}^{n-1} (-\beta\tau)^h \widetilde{\sigma}^{[r-1]}_{n-1-h,-k'} \Big), \quad n \geq 1, \\
x^{[r]}_{n,k} &= -\frac{\beta V}{ia_k} \Big(\overline{\sigma}^{[r-1]}_{n-2} \delta_{|k|=1} + \sum_{k'=\pm 1} \frac{k'}{k} \widetilde{\sigma}^{[r-1]}_{n-2,k-k'} \Big), \qquad n \geq 2, \\
x^{[r]}_{2,k} &= -\frac{\beta V}{ika_k} (\delta_{|k|=1}\delta_{r=1} + \sum_{k'=\pm 1} k' \widetilde{\sigma}^{[r-1]}_{0,k-k'}),
\end{aligned}$$

$\forall n \neq 1, |k| \leqslant r$. Therefore, if $\widetilde{\vartheta}_k(n;m) \stackrel{def}{=} \sum_{h=0}^{\infty} (-\beta\tau)^h \vartheta_k(n, m+h+1)\,\delta_{m\geq 1}$ and the kernels $t_k(n;m), \widetilde{t}_k(n;m)$ are defined as

$$\begin{aligned}
t_k(n,m) &\stackrel{def}{=} \frac{-\beta V}{ika_k}\, \vartheta_k(n;m)\,\delta_{m\geq 2}, \quad n \geq 2 \\
\widetilde{t}_k(n,m) &\stackrel{def}{=} \frac{(\beta V)^2}{a_k}\, \widetilde{\vartheta}_k(n;m), \quad n \geq 2 \\
t_k(0,m) &= \frac{t_k(2,m)}{i\eta a_k}\delta_{m\geq 2} + \delta_{m,1}\frac{\beta V}{ika_k}, \quad \widetilde{t}_k(0,m) = \frac{\widetilde{t}_k(2,m)}{i\eta a_k}\delta_{m\geq 1}, \\
t_k(1,m) &= \widetilde{t}_k(1,m) = 0,
\end{aligned}$$

the map $\mathcal{B}$ acquires the form $\binom{y'_{n,k}}{z'_{n,k}} = \mathcal{B}\binom{y_{n,k}}{z_{n,k}}$, with

$$\begin{aligned}
y'_{n,k} &= \sum_{m=1}^{\infty} \sum_{k'=\pm 1} k' \Big(t_k(n,m) y_{m-1,k-k'} + \delta_{|k|=1} \widetilde{t}_k(n,m) z_{m-1,-k'} \Big), \\
z'_{n,k} &= y_{n,k},
\end{aligned} \tag{3.42}$$

In conclusion, if
(i) $\mathbf{Z}^{[1]}$ is given,
(ii) the series over m converge,
the map $\mathcal{B}$ determines $\mathbf{Z}^{[r]}$ for $r \geq 2$. Convergence will be studied in Sec.3.4.5.

Remark: an interesting check is that, if $\tau = 0$, the recursion gives $\overline{\sigma}^{[r]}_n \equiv 0, \forall n \geq 1, r \geq 0$ and $\widetilde{\sigma}^{[r]}_{2,k} = 0, \forall r > 0$ and this leads, as expected, to $\sigma_n \equiv 0, \forall n > 0$ and $\sigma_0(q) = Z^{-1} \mathrm{e}^{-\beta\, 2g\, V \cos q}$, after some algebra and after summation of the series in g.

3.4.5 Bounds and theorem proof

Let $z = \frac{k^2 a_k}{i\eta} \equiv (1 + \frac{\beta\tau}{ik})\frac{k^2}{\eta}$. If $z = |z|e^{2i\alpha}$, $|\alpha| < \frac{1}{2}\mathrm{arctg}\frac{\beta\tau}{|k|} < \frac{\pi}{4}$ (so that $|\cos\alpha| > \frac{1}{\sqrt{2}}$), let $\lambda^{\alpha}_{\ell,\pm} \stackrel{def}{=} \sqrt{1 + \frac{4|z|}{(\ell-1)\cos^2\alpha}} \pm 1$; then from the inequality in Cuyt et al. (2004, p.138) we derive that

$$|\varphi(j,\infty) - \varphi(j,h)| \leqslant 2\sqrt{2}\prod_{\ell=j}^{h-2}\frac{\lambda^{\alpha}_{\ell,-}}{\lambda^{\alpha}_{\ell,+}} \stackrel{def}{=} \mathcal{D}(j,h),$$

for $h \geq j+1$ and $\varphi(j,j+1) = 1, \varphi(j,j) = 0$. Furthermore, the recursion for $\varphi(j,h)$ implies $|\arg(\frac{z\varphi(j+1,h)}{j})| \leqslant |\arg(\frac{z}{j})| \leqslant 2\alpha$, and

$$\begin{aligned}
&\Big|\varphi(j,h) - 1\Big| \equiv |\frac{z\varphi(j+1,h)}{j + z\varphi(j+1,h)}| \leqslant 1\,,\\
&\Big|\varphi(j,h)^{-1} - 1\Big| \equiv |\frac{z}{j}\varphi(j+1,h)| \leqslant 2\frac{|z|}{j}, \qquad h \geq j+2\,,
\end{aligned}$$

therefore

$$\Big|\frac{\varphi(j,\infty)}{\varphi(j,h)} - 1\Big| \leqslant \Big(1 + 2\frac{|z|}{j}\Big)\mathcal{D}(j,h), \qquad h \geq j+2\,.$$

The above inequalities are useful to estimate the kernels $t_k(n;m)$ and $\widetilde{t_k}(n;m)$ appearing in Eq.(3.41).

Lemma 4. *There exist a constant C_k, B_k, depending from all parameters of the dynamics, such that for any $n, m \geq 0$:*

$$\max\Big\{t_k(n;m+1), \widetilde{t_k}(n;m+1)\Big\} \leqslant C_k|2ka_k|\Big(\frac{B_k^{m-n}}{(m-n)!}\Big)^{\delta_{m\geq n}}$$

Proof. Recalling that $\varphi(j,h) = -\frac{\zeta_k(j,h)}{ka_k}$,

$$\frac{1}{1 + 2\frac{|z|}{j}} \leqslant \Big|\frac{\zeta_k(j,\infty)}{ka_k}\Big| \leqslant 2$$

By using $\frac{\sqrt{1+x}-1}{\sqrt{1+x}+1} \leqslant \frac{x}{1+x}$, and that $\cos^2\alpha > 1/2$, we obtain

$$\begin{aligned}
\Big|\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)} - 1\Big| &\leqslant \Big(1 + 2\frac{|z|}{j}\Big)2\sqrt{2}\prod_{\ell=j}^{m-2}\frac{\sqrt{1 + \frac{4|z|}{(\ell-1)\cos^2\alpha}} - 1}{\sqrt{1 + \frac{4|z|}{(\ell-1)\cos^2\alpha}} + 1}\\
&\leqslant 8\Big(1 + \frac{|z|}{j}\Big)\prod_{\ell=j}^{m-2}\frac{8|z|}{\ell - 1 + 8|z|}, \qquad m \geq j+1\,.
\end{aligned}$$

Hence, for $n \geq 2$ (as $|1 - X| = |e^{\log X} - 1| \leqslant e^{|\log X|} - 1$ and $\log(1+X) \leqslant X$)

$$\Big|1 - \prod_{j=2}^{n}\frac{\zeta_k(j,\infty)_1}{\zeta_k(j,m)_1}\Big| \leqslant \Big[e^{\sum_{j=2}^{n}\log\Big(1+8\Big(1+\frac{|z|}{j}\Big)\prod_{\ell=j}^{m-2}\frac{8|z|}{\ell-1+8|z|}\Big)}\Big] - 1$$

and consequently

$$\left|\prod_{j=2}^{m-1}\frac{\zeta(j,\infty)}{\zeta(j,m)}\right| \leqslant \mathrm{e}^{\sum_{j=2}^{m-1} 8(1+|z|)\frac{(8|z|)^{-(m-1-j)}}{(m-1-j)!}} \leqslant \mathrm{e}^{8\mathrm{e}^{9|z|}}$$

Then for $n \geq 2$; sacrificing better bounds for simpler ones, for $m \leqslant n$,

$$|\prod_{j=m}^{n}\zeta(j,\infty)| \leqslant (2|ka_k|)^{n-m+1}$$

and in particular

$$|\vartheta_k(n;m)| \leqslant |2\,k\,a_k|^{n-m+1}\mathrm{e}^{8\mathrm{e}^{9|z|}} \qquad m \leqslant n.$$

About the case $m > n$, using $\mathrm{e}^X - 1 \leqslant \mathrm{e}^X X$, $\forall X \geq 0$:

$$\begin{aligned}\frac{|\vartheta_k(n;m)|}{|ka_k|^{n-m+1}} &\leqslant \left[\prod_{j=n+1}^{m-1}1+\frac{2|z|}{j})\right]\left(\mathrm{e}^{\sum_{j=2}^{n}\left(1+\frac{8|z|}{j}\right)\prod_{\ell=j}^{m-2}\frac{8|z|}{\ell-1+8|z|}}-1\right)\\ &\leqslant \mathrm{e}^{2|z|(m-n-1)}\left(\mathrm{e}^{(1+8|z|)\frac{(8|z|)^{m-n-1}}{(m-n-1)!}\sum_{j=2}^{n}\frac{(8|z|)^{n-j}}{(n-j)!}}-1\right)\\ &\leqslant \mathrm{e}^{2|z|(m-n-1)}\left(\mathrm{e}^{8\mathrm{e}^{9|z|}\frac{(8|z|)^{m-n-1}}{(m-n-1)!}}-1\right) \leqslant 8\mathrm{e}^{9|z|}\mathrm{e}^{8\mathrm{e}^{9|z|+8|z|}}\frac{(8|z|\mathrm{e}^{2|z|})^{m-n-1}}{(m-n-1)!}\end{aligned}$$

Therefore, $\forall z$:

$$\frac{|\vartheta_k(n;m)|}{|2\,k\,a_k|^{n-m+1}} \leqslant C(z)\left(\frac{(2^4\mathrm{e}^{2|z|})^{m-n-1}}{(m-n-1)!}\right)^{\delta_{m>n}}, \quad C(z) \leqslant 8\mathrm{e}^{9|z|}\mathrm{e}^{8\mathrm{e}^{17|z|}}$$

This implies, if $\widetilde{\vartheta}_k(n;m) \stackrel{def}{=} \sum_{h=0}^{\infty}(-\beta\tau)^h\,\vartheta_k(n,m+h+1)$,

$$|\widetilde{\vartheta}_k(n;m)| \leqslant C(z)\sum_{h=0}^{\infty}|\beta\tau|^h|2ka_k|^{n-m-h}\left(\frac{|B(z)|^{m+h-n}}{(m+h-n)!}\right)^{\delta_{h>n-m-1}}$$

In particular for $n \geq m$

$$|\widetilde{\vartheta}_k(n;m)| \leqslant C(z)|2ka_k|^{n-m}\left(\frac{1}{1-\beta\tau|2ka_k|^{-1}}+\mathrm{e}^{\beta\tau B(z)|2ka_k|^{-1}}\right)$$

and similarly for $m > n$ we have

$$\begin{aligned}|\widetilde{\vartheta}_k(n;m)| &\leqslant C(z)|2ka_k|^{n-m}\frac{|B(z)|^{m-n}}{(m-n)!}\sum_{h\geq 0}\frac{(\beta\tau B(z)|2ka_k|^{-1})^h}{h!}\\ &\leqslant C'|2ka_k|^{n-m}\frac{|B(z)|^{m-n}}{(m-n)!}\end{aligned}$$

□

Proof of main Theorem: We first estimate, for $k = \pm 1$, $\sigma^{[1]}_{n,k} = \sum_{m\geq 0} t_k(n, m+1)(-\beta\tau)^m$ by

$$\begin{aligned}\left|\widetilde{\sigma}^{[1]}_{n,k}\right| &\leqslant C_1 \sum_{m=0}^{n-1} (2|a_1|)^{n-m}|\beta\tau|^m + |\beta\tau|^n C_1 \sum_{m=n}^{\infty} \frac{(\beta\tau B_1 |2a_1|^{-1})^{m-n}}{(m-n)!} \\ &\leqslant C_1|2a_1|^n \left(\sum_{m=0}^{n-1} (2|a_1|)^{-m}|\beta\tau|^m + \mathrm{e}^{\beta\tau B_1|2a_1|^{-1}} \right) \\ &\leqslant C_1|2a_1|^n \left(2 + \mathrm{e}^{\beta\tau B_1|2a_1|^{-1}}\right) \equiv A_1|2a_1|^n\end{aligned}$$

Assume now that $\left|\widetilde{\sigma}^{[r]}_{n,k}\right| \leqslant A_r|2ra_r|^n$, then,

$$\begin{aligned}\left|\widetilde{\sigma}^{[r+1]}_{n,k}\right| &\leqslant \sum_{m\geq 0} |t_k(n, m+1)| \left(\left|\widetilde{\sigma}^{[r]}_{m,k+1}\right| + \left|\widetilde{\sigma}^{[r]}_{m,k-1}\right| \right) \\ &+ \delta_{|k|=1} \sum_{m\geq 0} |\widetilde{t}_k(n, m+1)| \left(\left|\widetilde{\sigma}^{[r-1]}_{m,1}\right| + \left|\widetilde{\sigma}^{[r-1]}_{m,-1}\right| \right)\end{aligned}$$

The four terms are similar, we just estimate the first one:

$$\begin{aligned}\sum_{m\geq 0} |t_k(n, m+1)| \left|\widetilde{\sigma}^{[r]}_{m,k+1}\right| &\leqslant C_k \sum_{m=0}^{n-1} |2ka_k|^{n-m} A_r |2ra_r|^m \\ &+ C_k \sum_{m=n}^{\infty} |2ka_k|^{n-m} A_r |2ra_r|^m \frac{B_k^{m-n}}{(m-n)!} \\ &\leqslant C_k A_r |2ka_k|^n \sum_{m=0}^{n-1} \left| \frac{(r+1)a_{r+1}}{ka_k} \right|^m \\ &+ C_k A_r |2ra_r|^n \mathrm{e}^{2ra_r B_k |2ka_k|^{-1}} \\ &\leqslant C_k A_r |2ka_k|^n \left| \frac{2(r+1)a_{r+1}}{2ka_k} \right|^n \left(\left| \frac{2(r+1)a_{r+1}}{2ka_k} \right| - 1 \right)^{-1} \\ &+ C_k A_r |2(r+1)a_{r+1}|^n \mathrm{e}^{2ra_r B_k |2ka_k|^{-1}} \\ &\leqslant A_{I,r+1} |2(r+1)a_{r+1}|^n\end{aligned}$$

The bounds on the other three terms are similar with constant $A_{II,r+1}$, $A_{III,r+1}$, $A_{IV,r+1}$, and the final A_{r+1} is obtained by their sum. □

3.4.6 Weak small scale dissipation. Conclusions

The bounds on $|\rho^{[r]}_{n,k}|$ hold with a suitable choice of the constants A_r, B_r which are positive if $\eta, \beta\tau > 0$. Therefore a formal asymptotic series at $g = 0$ is $\forall R \geq 0$:

$$\rho^{[\leqslant R]}(q,p) = \sum_{r=0}^{R} g^r \sum_{k=-R}^{R} \sum_{n=0}^{\infty} \mathrm{e}^{iqk} \rho^{[r]}_{n,k} : p^n :$$

is bounded by (using the bound on Hermite functions, see Gradshtein and Ryzhik (1965, 8.954.2))

$$|\rho^{[\leqslant R]}(p,q)| \leqslant \sum_{r=0}^{R}\sum_{k=-R}^{R}\sum_{n=0}^{\infty} \overline{A}_r g^r B_r^n \frac{1}{n!}\frac{\sqrt{n!}2^{1-n/2}}{\xi\sqrt{\eta^n}} \mathrm{e}^{\frac{\beta}{4m}p^2}$$
$$|F^{[\leqslant R]}(p,q)| \leqslant \mathrm{e}^{-\frac{\beta}{4m}p^2} B'_R$$

with a suitably chosen B'_R. A natural question is whether having obtained non convergent bounds is due to a poor estimate or to a singularity at $g = 0$.

The mechanical system has two qualitatively different motion regimes: if $\tau > 0$ is fixed then for g small ($\tau \gg gV$) the pendulum will in the average rotate on a time scale of order $\frac{m\tau}{\xi}$; if, instead, g is fixed and τ small ($\beta\tau \ll g\beta V$), the pendulum will oscillate, very rarely performing full rotations.

Our theory, however, gives a formal power series with estimates uniform in $\beta\tau$, for $|\beta\tau|$ in a bounded interval, thus the power series would be the same for g in an interval where motions with $\tau \gg gV$ or $\tau \ll gV$ take place. Therefore we think that our series is really only formal and resummations have to be devised that would treat differently the large τ and large g regimes.

Remarks: (1) If the series for F could be shown to converge (in "any" sense) it could be concluded that the coefficients that have been formally computed are indeed the coefficients of the Hermite expansion for F, as even the positivity of F could be derived by the following simple argument. Adapting the proof in Mattingly and Stuart (2002) , any $0 \leqslant f \in L_1 \cap L_\infty$ function with $\int f \,\mathrm{d}p\,\mathrm{d}q = 1$ has the property that $\lim_{t\to+\infty} \mathrm{e}^{\mathcal{L}^* t} f = F_\infty > 0$ with $\mathcal{L}^* F_\infty = 0$ and F_∞ is the unique smooth, positive, integrable, normalized solution of $\mathcal{L}^* F_\infty = 0$. Hence if f_+, f_- denote the positive and negative parts of F it will be

$$F \equiv \mathrm{e}^{\mathcal{L}^* t} F \equiv \mathrm{e}^{\mathcal{L}^* t} f_+ - \mathrm{e}^{\mathcal{L}^* t} f_- \xrightarrow[t\to+\infty]{} (a - a')F_\infty$$

if $\int f_+ = a, \int f_- = a'$. Therefore $a - a' = 1, F = F_\infty, a = 1, a' = 0$ and this would prove that $F > 0$ and that it is the unique stationary probability density in $L_1 \cap L_2$ for the process with generator $\mathcal{L}^*$.

(2) The algorithm in Sec.3.4.3 can be implemented numerically, by computing with prefixed precision a prefixed number of coefficients $\rho_n^{[r]}(q)$, and programming the recursion in Eq.(3.42).

(3) The overdamped case (3.17) can be treated in the same way: in this case $\rho_n \equiv 0$ for $n \neq 0$ and $\rho_0(q)$ is analytic in g for g small: it is possible to study the distribution ρ_0 in great detail and for all g, obtaining interesting results on large fluctuations of several observables, see Faggionato and Gabrielli (2012).

(4) The continued fractions in (3.35) are really remarkable and a natural question is whether they are related to known special functions or, alternatively, which are their properties near the negative real axis.

Part 2

Chains

4

Rotors(*)

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(*) *This chapter contains the article "Negative thermal conductivity of chains of rotors with mechanical forcing" (Iacobucci et al. (2011)).*

We consider chains of rotors subjected to both thermal and mechanical forcing, in a nonequilibrium steady-state. Unusual nonlinear profiles of temperature and velocities are observed in the system. In particular, the temperature is maximal in the center of the chain, which is an indication of the nonlocal behavior of the system. Despite this uncommon behavior, local equilibrium holds for long enough chains. Our numerical results also show that, when the mechanical forcing is strong enough, the energy current can be increased by an inverse temperature gradient. This counterintuitive result again reveals the complexity of nonequilibrium states.

4.1 Introduction

Thermodynamic properties of non-equilibrium stationary states are poorly understood. They are usually characterized by currents of conserved quantities, such as energy, flowing through the system. When stationary states are *close* to equilibrium states, linear response theory is effective and explains common macroscopic phenomena like Fourier's law: in a system in contact with two thermostats at different temperatures, the heat flux is proportional to the temperature gradient (as long as the relative difference between the two temperatures is small).

In contrast, there is no general theory to describe systems in a stationary state *far* from equilibrium, and the corresponding macroscopic properties seem to depend on the specific details of the dynamics.

In this chapter, we numerically investigate the energy transport properties of a simple one-dimensional system, a chain of N rotors, in a stationary state far from equilibrium. Many studies considered one-dimensional chains of oscillators subjected to a temperature gradient, see Lepri et al. (2003), Dhar (2008) for a review. Here we consider both thermal and mechanical forcings, obtained as follows: the leftmost rotor is attached to a wall and put in contact with a Langevin thermostat at temperature T_{L}, while the rightmost rotor is subjected to a constant external force F and put in contact with another Langevin thermostat at temperature T_{R}.

What we observe in our numerical experiments is that *the combined effect of these two generalized forces can reduce the current instead of increasing it*. This counterintuitive effect is observed for large mechanical forcings F, when T_{R} is increased while T_{L} remains fixed (see Figure 4.4 below). Since the mechanical forcing always induces a negative current (from the right to the left), when T_{R} is increased while T_{L} remains fixed one would naively expect that the (negative) thermal forcing would also be larger, and thus that the negative current would be (in absolute value) larger. In contrast to this expectation, we observe that, in this case, the current is *reduced*. This strange effect does not appear if, instead, T_{L} is lowered and T_{R} is kept fixed (see Figure 4.3, top panels, below), in which case the current indeed becomes larger in absolute value.

We are unable to provide explanations to the above described phenomena. We believe that such behaviors show the complexity of non-equilibrium stationary states far from equilibrium, and also suggest that Fourier's law is only valid close to equilibrium. A naive extension of the definition of thermal conductivity to genuinely non-equilibrium settings can give negative values to this quantity

(whence the somehow provocative title of the article).

In the sequel of this chapter, we first describe the system we work with, and the numerical integrator we have used (see Sec. 4.2). We next turn to studying various properties of the system. In particular, we numerically check that local equilibrium holds for systems large enough, despite the fact that, globally, the system is out of equilibrium (see Sec. 4.3.2). In Sec. 4.3.3, we study how the current depends on the magnitude of the mechanical force and on the temperatures that are imposed on both ends of the chain. All these numerical studies are performed for chains of increasing lengths.

4.2 Description of the system

The configuration of the system is described by the positions $q = (q_1, \dots, q_N)$ (angles) of the rotors, which belong to the one-dimensional torus $2\pi\mathbb{T}$, as well as their associated (angular) momenta $p = (p_1, \dots, p_N)$. The masses of the particles are set to 1 for simplicity. The Hamiltonian of the system is

$$H(q,p) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + (1 - \cos r_i) \right], \tag{4.1}$$

where we have set $r_i = q_i - q_{i-1}$ for $i \geqslant 2$ and $r_1 = q_1$.

We consider a system with free boundary conditions on the right end, whose evolution equations read:

$$\begin{cases} \mathrm{d}q_i = p_i \, \mathrm{d}t, \\ \mathrm{d}p_i = \Big(\sin(q_{i+1} - q_i) - \sin(q_i - q_{i-1}) \Big) \mathrm{d}t, \ i \neq 1, N, \\ \mathrm{d}p_1 = \Big(\sin(q_2 - q_1) - \sin(q_1) \Big) \mathrm{d}t \\ \qquad\qquad - \xi p_1 \, \mathrm{d}t + \sqrt{2\xi T_{\mathrm{L}}} \, \mathrm{d}W_t^1, \\ \mathrm{d}p_N = \Big(F - \sin(q_N - q_{N-1}) \Big) \mathrm{d}t \\ \qquad\qquad - \xi p_N \, \mathrm{d}t + \sqrt{2\xi T_{\mathrm{R}}} \, \mathrm{d}W_t^N, \end{cases} \tag{4.2}$$

where W_t^1 and W_t^N are independent standard Wiener processes, and $\xi > 0$ determines the strength of the coupling to the thermostat. In the sequel, we consider $\xi = 1$. Note that the external constant force F is non-gradient since it does not derive from a periodic potential.

We checked the robustness of the results we describe below with respect to the choice of boundary conditions. Indeed, we also considered fixed boundary conditions on the right end (this amounts to adding an extra force $-\sin(q_N)$ to the last atom). In particular, we checked that our counterintuitive results on the behavior of the thermal current as a function of the strength of the nongradient force are still observed with these boundary conditions.

4.2.1 Equilibrium and nonequilibrium states

If $F = 0$ and $T_{\mathrm{L}} = T_{\mathrm{R}} = T$, the system is in *equilibrium*, and the unique stationary measure is given by the Gibbs measure at temperature T associated with the Hamiltonian (4.1). When $T_{\mathrm{L}} \neq T_{\mathrm{R}}$ with $F = 0$, the properties of the nonequilibrium stationary state have been studied numerically by various authors, see *e.g.* Giardiná et al. (2000), Gendelman and Savin (2000), Yang and Hu (2005), Gendelman and Savin (2005). The thermal conductivity of the system, defined as the stationary energy current multiplied by the size of the system and divided by the temperature difference (Bonetto et al. (2000)), has a finite limit for large system sizes, even though the rotor chain is a momentum conserving one-dimensional system (Basile et al. (2006, 2009)). Besides, it is shown by Giardiná et al. (2000), that the thermal conductivity decreases dramatically as the average temperature T increases above the value 0.5.

If $F \neq 0$, the system is out-of-equilibrium even if $T_{\mathrm{L}} = T_{\mathrm{R}}$ (recall indeed that F is non-gradient). In the stationary state, the force induces an energy current towards the left. The stationary state cannot be computed explicitly and, if F is large, linear response theory cannot be used to obtain information about the conductivity of the system.

If $T_{\mathrm{L}} < T_{\mathrm{R}}$, there are two mechanisms that *separately* generate an energy current towards the left of the system: the mechanical force F and the thermal force given by the temperature gradient. It seems however difficult to separate the contributions of each mechanism. The numerical experiments reported below show that these two mechanisms are not necessarily additive, and that one mechanism may reduce the effect of the other one, leading to counterintuitive results.

4.2.2 Numerical integration

The numerical integration of (4.2) is performed using a splitting strategy where the Hamiltonian part of the evolution is integrated with the Verlet scheme (Verlet (1967)). The fluctuation-dissipation parts, with the additional non-gradient force, are Ornstein-Uhlenbeck processes and can thus be integrated analytically. We have thus used the following algorithm:

$$\begin{aligned}
\widetilde{p}_1^n &= \alpha p_1^n + \sigma_{\mathrm{L}} G_1^n, \\
\widetilde{p}_N^n &= F + \alpha(p_N^n - F) + \sigma_{\mathrm{R}} G_N^n, \\
\widetilde{p}_i^n &= p_i^n, \quad i \neq 1, N, \\
p_i^{n+1/2} &= \widetilde{p}_i^n - \frac{\Delta t}{2} \frac{\partial H}{\partial q_i}(q^n, \widetilde{p}^n), \\
q_i^{n+1} &= q_i^n + \Delta t \, p_i^{n+1/2}, \\
p_i^{n+1} &= p_i^{n+1/2} - \frac{\Delta t}{2} \frac{\partial H}{\partial q_i}(q^{n+1}, p^{n+1/2}),
\end{aligned} \tag{4.3}$$

where $\alpha = \exp(-\xi \Delta t)$, $\sigma_{\mathrm{L}} = \sqrt{(1-\alpha^2) T_{\mathrm{L}}}$, $\sigma_{\mathrm{R}} = \sqrt{(1-\alpha^2) T_{\mathrm{R}}}$, and H is given by (4.1). In turn, G_1^n and G_N^n are independent normal Gaussian random variables. Recall also that the friction parameter ξ is set to 1. The three first lines of the above algorithm consist in exactly integrating the Ornstein-Uhlenbeck processes on p_1 and p_N, whereas the remaining lines are based on the standard Verlet algorithm.

The time-step $\Delta t = 0.05$ ensures that the energy conservation in the Verlet scheme is accurate enough. While there might be some time-step bias in the value of the currents, the qualitative conclusions are robust with respect to the choice of the time-step.

4.3 Properties of the nonequilibrium system

This section is organized as follows. First, we discuss the existence of a stationary measure for the dynamics (4.2). Under the assumption that such a stationary measure exists, we establish some relations that are consistent with physical intuition. We next point out that this system shows some very surprising features. For instance, the temperature profile is non-monotonic and a maximum is observed in the center of the system, while the velocity profiles are very nonlinear. Despite these nonlocal features, we show that local equilibrium holds. We finally turn to investigating the dependence of the stationary energy current on F, T_{L} and T_{R}.

4.3.1 Stationary measure

We believe that there exists a unique smooth stationary measure for the dynamics (4.2). However, as far as we know, there is no rigorous result in this direction for rotor chains, even in the case $F = 0$. Indeed, the standard techniques (see for instance Rey-Bellet (2006*b*), Carmona (2007)) used to prove existence and uniqueness of an invariant measure for chains of oscillators under thermal forcing do not apply here.

A possible pathology for rotor chains is that the (internal) energy concentrates locally on one or more rotors, which rotate faster and faster. Since the interaction forces are bounded, it may not be possible to prevent this fast rotation. In practice, we have not observed such catastrophes in the parameter regime we considered, but the kinetic temperature profiles presented in Figure 4.1 (top left panel, obtained from the variance of the momenta, with the previously mentioned caveat on the interpretation of this quantity) are quite unexpected and show that the internal energy tends to be larger in the middle of the chain[(1)]. The results presented in Figure 4.1 also allow to understand what happens when the imposed temperatures at the right and left ends change: the maximal temperature in the chain is almost unchanged, but the position of the maximum is displaced (see top left panel). This shows that the linear response correction to the stationary measure is necessarily *nonlocal*. Such nonlocal effects were already observed in nonequilibrium exclusion processes by Derrida et al. (2002*a*,*b*).

Figure 4.1 shows also that the momentum profile (bottom left panel) is not linear, and that its derivative is maximal where the temperature (top left panel) is maximal. We also observe (see right panel) that the profile seems to become steeper in the thermodynamic limit.

Some interesting relations can nonetheless be obtained under the assumption that the stationary state exists. We denote by $\langle \cdot \rangle$ the expectation with respect to

[(1)] This result may be connected to the behavior of the solution of the corresponding diffusive problem, see Komorowski et al. (2016).

the stationary measure. First, a constant profile of force settles down in the bulk. Taking expectations in (4.2) indeed gives

$$\begin{aligned} \langle \sin r_{i+1} \rangle &= \langle \sin r_i \rangle, && i \neq 1, N, \\ \langle \sin r_2 \rangle &= \langle \sin r_1 \rangle + \xi \langle p_1 \rangle, \\ \langle \sin r_N \rangle &= F - \xi \langle p_N \rangle. \end{aligned}$$

This leads to the following profile: $F_i := \langle \sin r_i \rangle = F - \xi \langle p_N \rangle$ for all $i \geq 2$, while $F_1 := \langle \sin r_1 \rangle = F - \xi(\langle p_N \rangle + \langle p_1 \rangle)$.

The balance between the average work done by the force and the energy dissipated by the thermostats is given by

$$0 = F\langle p_N \rangle + \xi(T_{\mathrm{L}} - \langle p_1^2 \rangle) + \xi(T_{\mathrm{R}} - \langle p_N^2 \rangle), \tag{4.4}$$

as can be seen by noticing that the average variation of the total energy H is zero.

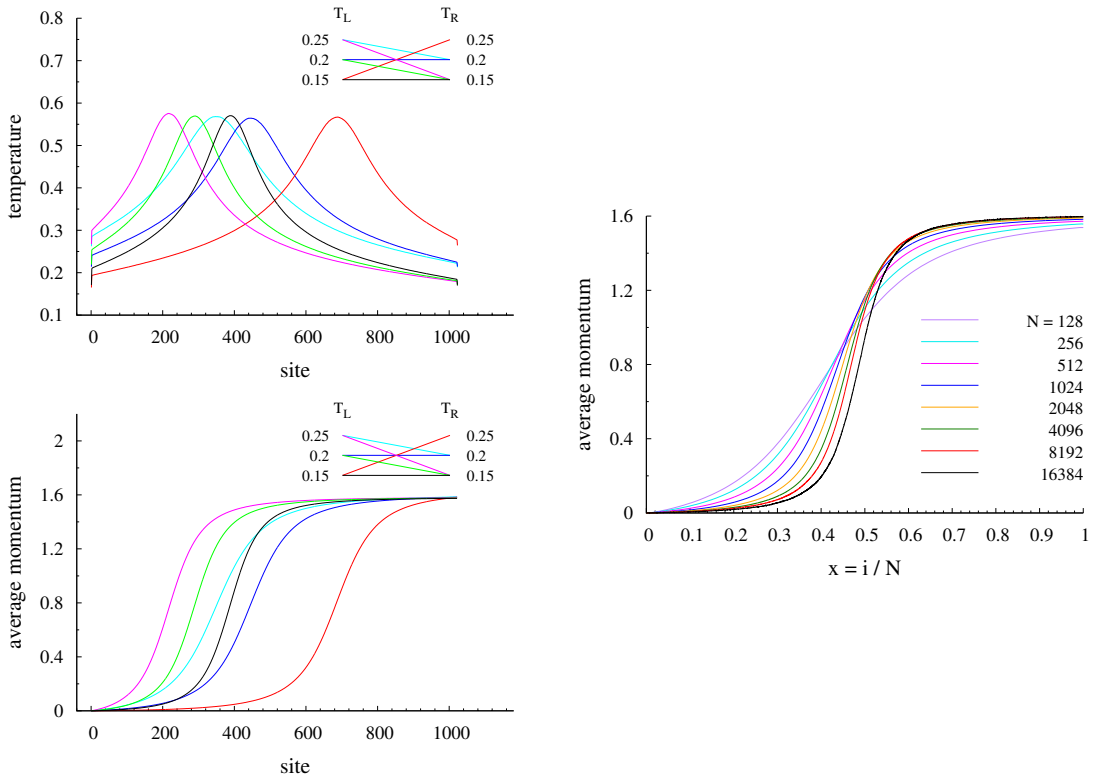


Figure 4.1 – Left: profiles for chains of length $N = 1024$, with $F = 1.6$ and different temperature gradients. Top left: kinetic temperature profiles. Bottom left: momentum profiles. Right: rescaled momentum profiles for system of increasing size $N = 2^k$ with $k = 7, \ldots, 14$: the x variable is the site index i divided by N. The value of the nongradient force is $F = 1.6$ and $T_{\mathrm{L}} = T_{\mathrm{R}} = 0.2$.

Moreover, the entropy production inequality (obtained by computing the variations of the relative entropy with respect to the invariant measure, see e.g. Bernardin and Olla (2011)) gives

$$T_{\mathrm{L}}^{-1}(T_{\mathrm{L}} - \langle p_1^2 \rangle) + T_{\mathrm{R}}^{-1}(T_{\mathrm{R}} - \langle p_N^2 \rangle) \leqslant 0.$$

In the case $T_L = T_R = T$, this relation, combined with (4.4), yields $F\langle p_N \rangle \geq 0$. Therefore the stationary momentum on the right end has the same sign as the driving force, as expected.

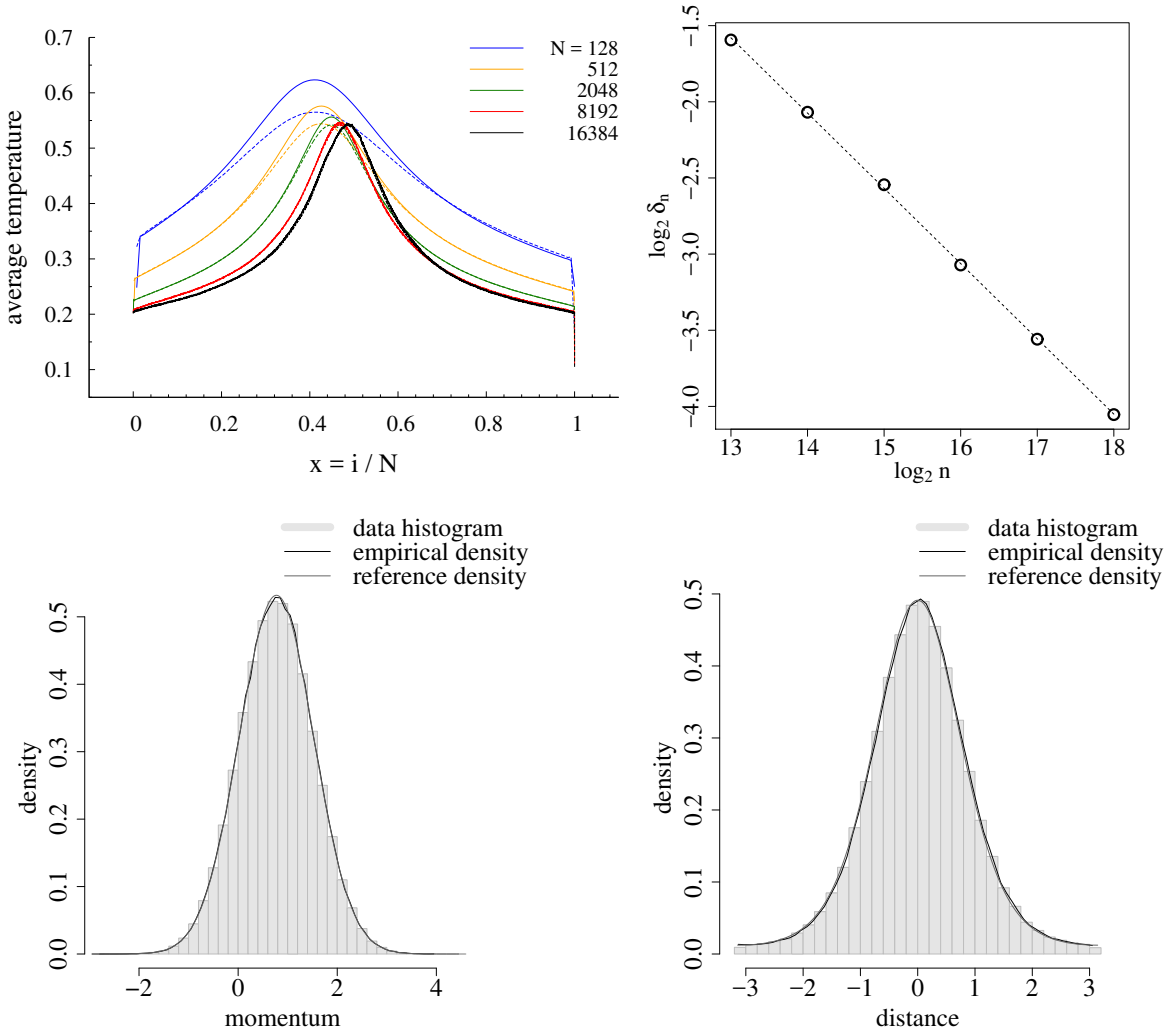


Figure 4.2 – (Color online) Top left: empirical distribution of momenta at the site $i_{\max}$ (where the temperature is maximal), and comparison with the local Gibbs equilibrium with the same average and variance. Tob right: empirical distribution of the distances at bond $i_{\max}$ and comparison with the local Gibbs equilibrium with the same average energy. Both plots correspond to a chain of length $N = 1024$, with $F = 1.6$ and $T_L = T_R = 0.2$. Bottom: decrease of the error δ_n defined by (4.5) as a function of the number of sample points n. Estimated rate of decrease: $\delta_n \simeq 28.7 \times n^{-0.494}$.

4.3.2 Local equilibrium and thermodynamic limit

A very interesting question is whether nonequilibrium systems are *locally* close to equilibrium. This issue was considered in Mai et al. (2007) for systems subjected to thermal forcings only. We check in three steps the local equilibrium assumption in presence of the mechanical forcing only.

(i) We study the agreement between the local kinetic temperature (defined as

the variance of the velocities) and the local potential temperature. The latter is obtained as follows. First, we numerically precompute the function

$$g : T \mapsto \frac{\displaystyle\int_0^{2\pi} V(r)\exp(-V(r)/T)\,\mathrm{d}r}{\displaystyle\int_0^{2\pi} \exp(-V(r)/T)\,\mathrm{d}r}$$

which associates the canonical average of the potential energy $V(r) = 1-\cos r$ of one bond to a given temperature. The local potential temperature at bond i is then defined as the value T_i such that $g(T_i)$ is equal to the time average of the potential energy of the bond r_i along the trajectory defined by (4.2). The results presented in Figure 4.2 (top left panel) show that the two local temperatures are quite different for small systems, but are identical for larger ones. Besides, as the length of the system increases, the profiles become more symmetric.

(ii) We check that the individual distributions of p and r are in accordance with a local Gibbs equilibrium. To this end, we build the histograms of the momenta and distances at the site $i_{\max}$ where the local temperature is maximal (since this is the location where the disagreement between the local kinetic and potential temperatures is the strongest). The results presented in Figure 4.2 (bottom panels) show that the empirical distributions of p and r at the site $i_{\max}$ are in excellent agreement with the Gibbs distributions with the same parameters (average velocity $\overline{p}_i$, temperature T_i), namely

$$Z_{\mathrm{kin}}^{-1} \exp\left[-(p-\overline{p}_i)^2/(2T_i)\right] \mathrm{d}p$$

and

$$Z_{\mathrm{pot}}^{-1} \exp\left[-V(r)/T_i\right] \mathrm{d}r,$$

except for the smallest systems (say, $N \leqslant 512$).

(iii) We check that momenta and distances are independent. To this end, we compare the joint law $\psi = \psi(r_{i_{\max}}, p_{i_{\max}})$ of $(r_{i_{\max}}, p_{i_{\max}})$ and the product law obtained from the tensor product of the individual distributions of these two variables (denoted respectively by $\overline{\psi}_r(r_{i_{\max}})$ and $\overline{\psi}_p(p_{i_{\max}})$). More precisely, for a given number n of sample points (obtained by subsampling a long trajectory every 10^4 steps), we check that the distance

$$\delta_n = \int_{[0,2\pi]\times\mathbb{R}} \left|\psi^n(r,p) - \overline{\psi}_r^n(r)\overline{\psi}_p^n(p)\right| \mathrm{d}r\,\mathrm{d}p \tag{4.5}$$

between these two distributions indeed decreases as the inverse square-root of the number of configurations used to build the histograms. Again, this is true for systems large enough. Figure 4.2 (top right panel) shows that $\delta_n \sim n^{-1/2}$.

4.3.3 Behavior of the energy current

We consider the following situations:

(i) same temperatures on the left and on the right:
$(T_L, T_R) = (0.20, 0.20)$ or $(0.15, 0.15)$;

(ii) hot left end and cold right end:
$(T_L, T_R) = (0.25, 0.15)$, $(0.20, 0.15)$ or $(0.25, 0.20)$;

(iii) cold left end and hot right end:
$(T_L, T_R) = (0.15, 0.25)$.

Currents are computed as functions of the magnitude F of the non-gradient forcing term for systems of different lengths: $N = 128, 256, 512, 1024, 2048$. Recall that local equilibrium holds at the leading order, so that the energy current is induced by the first order corrections in $1/N$.

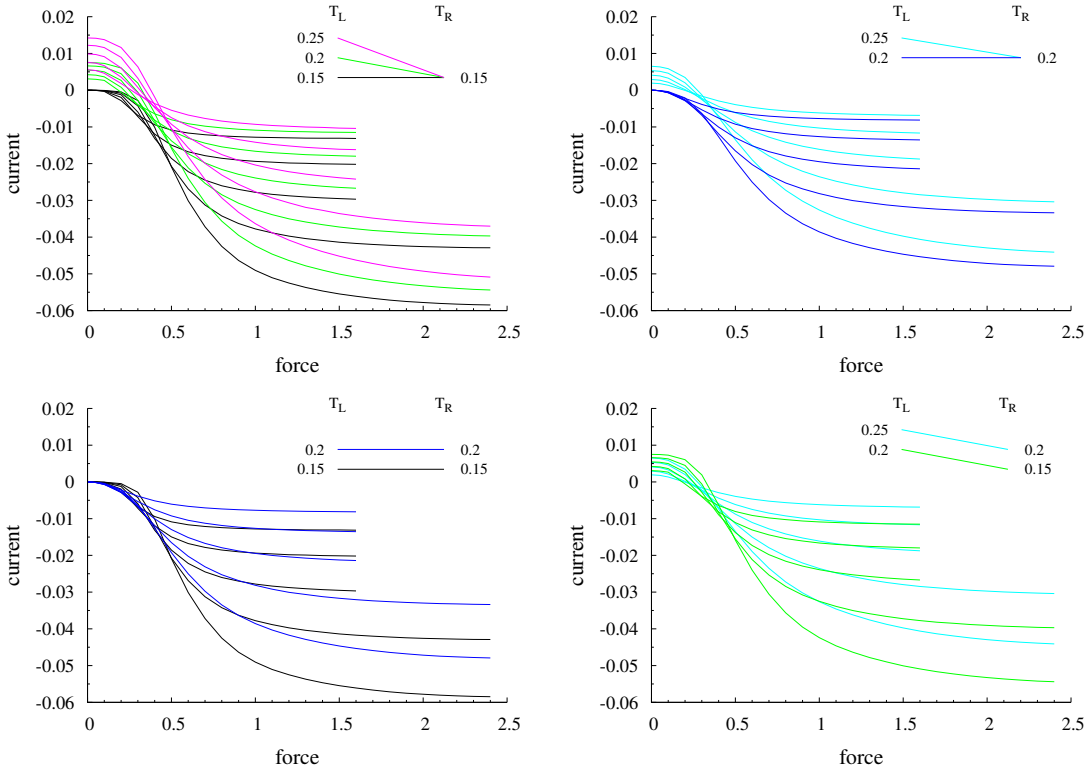


Figure 4.3 – (Color online) Comparison of the currents with: (a) fixed temperature on the right end and increasing temperatures on the left end (top panels); (b) fixed temperature at the left end and various temperature differences (bottom panels). From top to bottom: decreasing system sizes $N = 2048, 1024, 512, 256, 128$ (the ordering is the same for all situations considered; for the longest systems, we have considered forces $0 \leqslant F \leqslant 1.6$; for the shortest ones, we have considered the range $F \in [0; 2.4]$).

We first compare the currents when the temperature on the right end is fixed (see Figure 4.3, top panels). As expected, the negative current induced by the mechanical forcing is reduced by the opposite, positive thermal current.

We next compare the currents at fixed temperature difference $T_R - T_L$, for different average temperatures (see Figure 4.3, bottom panels). In this case, we observe that, for strong mechanical forcings, the current is enhanced when the average temperature decreases, while the opposite happens when the mechanical forcing is small.

We finally turn to the most interesting situation. The temperature on the left end is fixed and the temperature on the right end varies (see Figure 4.4). In this case, counterintuitive results are observed for large mechanical forcings: the total current is enhanced as T_R decreases, even though, in such a situation, the thermal gradient is in the opposite direction. The mechanical forcing induces a negative current, while the thermal gradient induces a positive current, in the absence of any mechanical forcing. The combined effect of both mechanical and thermal forcings induces a negative current *larger* (in absolute value) than the one in the absence of any thermal gradient!

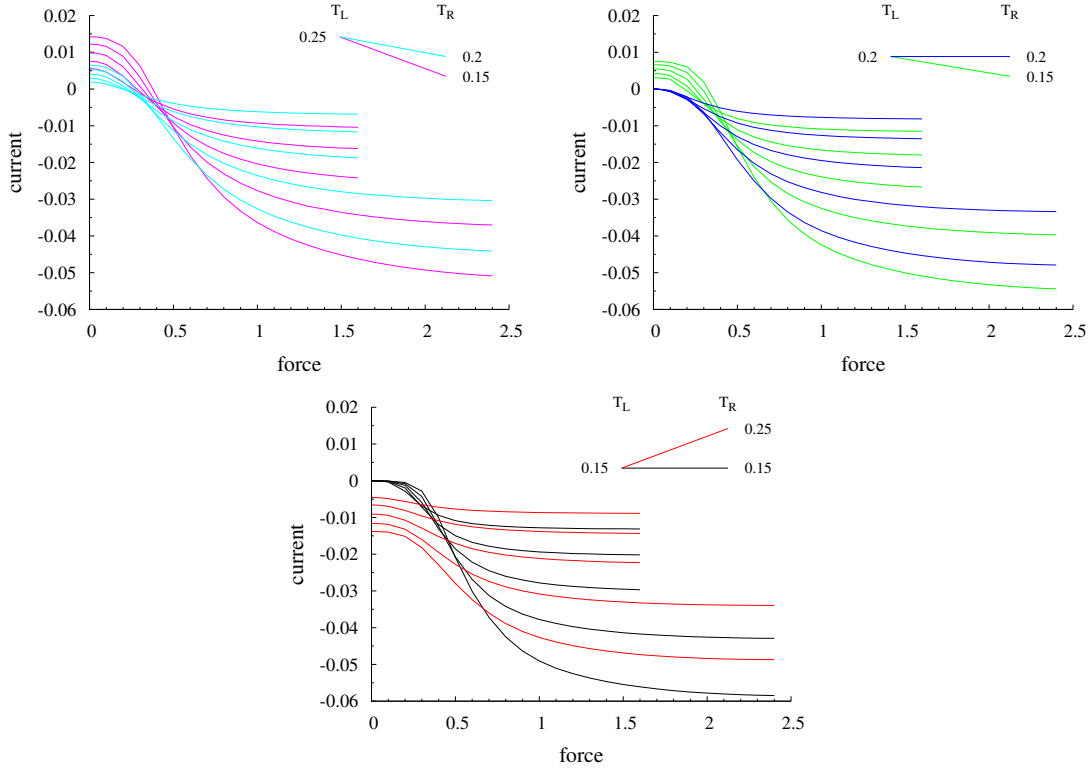


Figure 4.4 – (Color online) Comparison of the currents for a fixed temperature at the left end and various temperature differences. From top to bottom: decreasing system sizes $N = 2048, 1024, 512, 256, 128$ *(the ordering is the same for all situations considered).*

4.4 Discussion of the results

In conclusion, for large mechanical forcings F, we observe that

(a) when T_R is fixed, the current varies qualitatively as when there is no mechanical forcing: the absolute value of the current increases when T_L decreases, which means that the current induced by the thermal forcing and the current induced by the mechanical forcing are somehow additive. In this case, a positive thermal conductivity is observed (for a fixed value F of the mechanical forcing, considering only the response in the limit when $T_R - T_L \to 0$).

(b) when T_L is fixed, the current has a surprising behavior: its absolute value increases when T_R decreases. This means that the thermal forcing, which is

naively expected to reduce the current induced by the mechanical forcing, actually enhances it. In this case, a negative thermal conductivity is observed (again, for a fixed value F of the mechanical forcing).

A possible interpretation is based on the fact that, for such a system, the thermal conductivity is a decreasing function of the temperature when F is large (see Figure 4.3, bottom panels). It is possible that, by lowering T_R and thus increasing the conductivity at the right end, one makes the system more sensitive to the mechanical forcing. The increased mechanical current may hence counterbalance the increased opposite thermal current.

An interesting question which we did not discuss here is the scaling of the energy current as a function of the system size when $F \neq 0$. Some preliminary results suggest that the thermal conductivity is finite, as when $F = 0$, but this question definitely calls for additional studies.

5

The Toda lattice(*)

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(*) *This chapter contains the article "Thermal Conductivity of the Toda Lattice with Conservative Noise" (Iacobucci et al. (2010)).*

We study the thermal conductivity of the one dimensional Toda lattice perturbed by a stochastic dynamics preserving energy and momentum. The strength of the stochastic noise is controlled by a parameter γ. We show that heat transport is anomalous, and that the thermal conductivity diverges with the length n of the chain according to $\kappa(n) \sim n^\alpha$, with $0 < \alpha \leqslant 1/2$. In particular, the ballistic heat conduction of the unperturbed Toda chain is destroyed. Besides, the exponent α of the divergence depends on γ.

5.1 Introduction

For a one dimensional system of length L, the thermal conductivity can be defined through the stationary flux of energy induced by connecting the system to two thermostats at different temperatures T_l and T_r. This flux of energy J_L is proportional to the difference of temperature $\Delta T = T_l - T_r$, and we define the thermal conductivity κ_L as

$$J_L = \kappa_L \frac{\Delta T}{L}. \tag{5.1}$$

If $\lim_{L\to\infty} \lim_{\Delta T\to 0} \kappa_L = \kappa$ exists and is finite, then the conductivity is normal and the system is said to satisfy Fourier's law (Bonetto et al. (2000)). The limit κ is the thermal conductivity of the system.

It is well known, by numerical experiments and certain analytical considerations, that the thermal conductivity diverges for one dimensional systems of oscillators with a momentum conserving dynamics (Lepri et al. (2003, 1997)). This is also consistent with some experimental results on the length dependence of the thermal conductance of carbon nanotubes (Wang et al. (2007), Chang et al. (2008)). In the case of a chain of harmonic oscillators, J_L can be computed explicitly (Rieder et al. (1967)) and does not decrease when the size L of the system increases. This is due to the ballistic transport of energy carried by the non-interacting phonons, and it happens also for *optical* (pinned) harmonic chains, where momentum is not conserved. Ballistic transport of energy is expected for all systems whose dynamics is completely integrable (Zotos (2002)), as for the Toda chain (Toda (1979), Hatano (1999)).

Numerical evidence shows that *non-integrability* (whatever the definition of this concept one considers) is not a sufficient condition for normal conductivity, in particular for anharmonic chains of unpinned oscillators like the FPU model (Lepri et al. (1997)). An energy superdiffusion is expected in these momentum conserving systems, and the thermal conductivity diverges as $\kappa_L \sim L^\alpha$, for some $\alpha \in (0,1)$. There exists a wide debate in the physical literature about the existence or non-existence of one (or more) universal value of α, see *e.g.* Narayan and Ramaswamy (2002), Lepri et al. (2003).

Stochastic perturbations of the dynamics have been introduced in order to understand these phenomena. A model where Langevin thermostats are attached to each oscillator in a harmonic chain was first introduced by Bolsterli et al. (1970). This noise destroys all types of conservation laws, including energy, and the corresponding conductivity is finite (see Bonetto et al. (2004) and Bonetto et al. (2009) for the anharmonic case). Also, stochastic perturbations that preserve only the energy of the system give finite thermal conductivity (Bernardin and Olla (2005)).

The situation changes dramatically if the stochastic perturbation conserves both the energy *and* the momentum, as observed by Basile et al. (2006). Such stochastic conservative perturbations model the chaotic effect of nonlinearities. These systems may then be seen as *completely non-integrable*, since the only conserved quantities left are the energy and the momentum. In this case, at least for harmonic interactions, the thermal conductivity can be explicitly computed by the Green-Kubo formula. For unpinned models, it remains finite only in dimension $d \geq 3$, while it diverges when $d = 1$ or 2. More precisely $\kappa_L \sim \sqrt{L}$ when $d = 1$, and $\kappa_L \sim \log L$ when $d = 2$ (Basile et al. (2006, 2009)). Analytical considerations for the same harmonic stochastic systems in a nonequilibrium setting give the same results for the thermal conductivity computed according to (5.1), see Lepri et al. (2009). For anharmonic interactions, rigorous upper bounds can be established, again by the Green-Kubo formula. In the one dimensional case, this leads to $\kappa_L \leqslant C\sqrt{L}$, as established by Basile et al. (2009).

These rigorous results motivated us to analyze the effect of stochastic perturbations on another completely integrable system, the Toda chain. The thermal conductivity of Toda lattices was already studied in Hatano (1999), where it was shown that the ballistic energy transport is destroyed for a diatomic system. In contrast with the harmonic case where many computations can be performed analytically, the nonlinear dynamics considered here has to be solved numerically. We considered a chain in the nonequilibrium steady state setting, with two Langevin thermostats at different temperatures attached to its boundaries. We chose the simplest possible stochastic perturbation conserving both momentum and energy: each couple of nearest neighbor particles exchange their momentum at random times distributed according to an exponential law of parameter $\gamma > 0$.

Our main results are the following:

A) As soon as some noise is present, *i.e.* $\gamma > 0$, the ballistic transport is immediately destroyed (as in the harmonic case) and energy superdiffuses, with $\kappa_L \sim L^\alpha$ for $0 < \alpha \leqslant 1/2$;

B) The exponent α seems to depend on the noise strength γ, in a monotonically increasing way.

If the first results was somehow expected, the second one is quite surprising. It may be explained by the fact that the noise destroys some diffusive phenomena due to nonlinearities, like localized breathers, with the result that current-current correlation decays slower when more noise is present (see also Basile et al. (2007) where such a phenomenon has already been observed). Besides, result B suggests that any theory claiming the existence of a universal parameter α has to be properly circumstanced.

This paper is organized as follows. The dynamics we consider is presented in Section 5.2. The numerical simulations we performed are described in details in Section 5.3, whereas the obtained results are discussed in Section 5.4.

5.2 The stochastic dynamics

5.2.1 Description of the system

Hamiltonian. The configuration of the system is given by $\{q_i, p_i, i = 1, \dots, n\} \in \mathbb{R}^{2n}$, where q_i is the displacement with respect to the equilibrium position of the i-th particle, and p_i is its momentum. All masses are set equal to 1, and we fix the particle 0 to a wall ($q_0 = 0$). The Hamiltonian is given by

$$\mathcal{H} = \sum_{i=1}^{n} \frac{p_i^2}{2} + \sum_{i=1}^{n} V(q_i - q_{i-1}),$$

where the interaction potential is defined by

$$V(r) = \frac{a}{b} \mathrm{e}^{-br} + ar + c,$$

and a, b, c are constants, $a > 0$, $b > 0$. Observe that if the product ab is kept constant, the harmonic chain is obtained in the limit $b \to 0$, while the hard sphere system is recovered as $b \to \infty$. In our simulations, we chose $a = 1/b$ and $c = -1/b^2$ in order for V to be non-negative and minimal at $r = 0$, along with the normalization condition $V''(0) = 1$. The potential is therefore determined by a single parameter b, which determines the strength of the anharmonicity.

Boundary conditions. We set $q_0 = 0$, which amounts to removing the center-of-mass motion by attaching the particle at the left end of the system to a wall. However, we do not fix the total length q_n, and consider free boundary conditions on the right end. We checked that our numerical results are robust with respect to the boundary conditions. In particular, the same kind of scalings are obtained for fixed boundary conditions.

5.2.2 Description of the dynamics

The stochastic dynamics we consider has the following generator:

$$L = A + \xi(B_1 + B_n) + \gamma S + \tau \partial_{p_n}, \tag{5.2}$$

where ξ and γ are two positive constants. In (5.2), A is the Hamiltonian vector field:

$$A = \sum_{i=1}^{n} \left(p_i \, \partial_{q_i} - \partial_{q_i} \mathcal{H} \, \partial_{p_i} \right), \tag{5.3}$$

B_j are the generators of the Langevin thermostats attached at atom $j = 1$ and $j = n$:

$$B_j = T_j \partial_{p_j}^2 - p_j \partial_{p_j}, \tag{5.4}$$

and S is the generator of the random exchanges of momenta between nearest neighbor atoms. For any smooth function f defined on $\mathbb{R}^n \times \mathbb{R}^n$,

$$Sf(q,p) = \sum_{i=1}^{n-1} \Big(f(q, p^{i,i+1}) - f(q,p) \Big),$$

where $p^{i,i+1} \in \mathbb{R}^n$ is defined from $p \in \mathbb{R}^n$ by

$$p_i^{i,i+1} = p_{i+1}\,, \qquad p_{i+1}^{i,i+1} = p_i\,,$$

and $p_j^{i,i+1} = p_j$ if $j \neq i, i+1$. Finally τ is the strength of a constant external force applied to the last particle n. In (5.4), we choose the temperatures $T_1 = T_l$ and $T_n = T_r$.

5.2.3 Energy currents

We define the energy of the oscillator i for $1 \leqslant i \leqslant n-1$ as

$$\mathcal{E}_i = \frac{p_i^2}{2} + \frac{1}{2}\Big(V(q_i - q_{i-1}) + V(q_{i+1} - q_i)\Big).$$

Locally the energy conservation is expressed by the stochastic differential equation

$$d\mathcal{E}_i(t) = dJ_{i-1,i}(t) - dJ_{i,i+1}(t).$$

The energy currents $J_{i,i+1}(t)$ are the sum of contributions from the Hamiltonian and the stochastic mechanisms. For $i = 1, \ldots, n-1$, the currents are

$$J_{i,i+1}(t) = \int_0^t \left(\mathbf{J}^a_{i,i+1} + \gamma\, \mathbf{J}^s_{i,i+1}\right) ds + M^\gamma_{i,i+1}(t),$$

where $M^\gamma_{i,i+1}(t)$ is a martingale,

$$\mathbf{J}^a_{i,i+1} = -\frac{1}{2}(p_i + p_{i+1})V'(q_{i+1} - q_i) \tag{5.5}$$

is the instantaneous Hamiltonian current, while

$$\mathbf{J}^s_{i,i+1} = \frac{1}{2}\left(p_i^2 - p_{i+1}^2\right)$$

is the instantaneous stochastic current (the intrinsic transport of energy due to the stochastic exchange). The martingale term $M^\gamma_{i,i+1}(t)$ can be characterized in the following way: Let $\{N_{i,i+1}(t)\}_{i=1}^{n-2}$ be independent Poisson processes of intensity γ. Then

$$M^\gamma_{i,i+1}(t) = \int_0^t \frac{1}{2}\Big(p_i^2(s^-) - p_{i+1}^2(s^-)\Big)\Big(dN_{i,i+1}(s) - \gamma\, ds\Big),$$

where $p_i^2(s^-) = \lim_{t \to s,\ t<s} p_i^2(t)$. At the boundaries of the system, the energy currents are

$$\begin{aligned} J_{0,1}(t) &= \int_0^t \frac{\xi}{2}\left(T_l - p_1^2(s)\right) ds + \sqrt{\xi T_l} \int_0^t p_1(s)\, dw_1(s), \\ J_{n,n+1}(t) &= \int_0^t \left[\frac{\xi}{2}\left(p_n^2(s) - T_r\right) + \tau p_n(s)\right] ds + \sqrt{\xi T_r} \int_0^t p_n(s)\, dw_n(s), \end{aligned}$$

where $w_1(t)$ and $w_n(t)$ are independent standard Wiener processes, and the last integrals on the right hand side of the previous formulas are Itô stochastic integrals.

5.2.4 The stationary state

If $T_l = T_r = T$, we know explicitly the stationary probability measure of the dynamics, given by the Gibbs measure

$$\frac{\mathrm{e}^{(-\mathcal{H}+\tau q_n)/T}}{Z_n(T,\tau)} \prod_{i=1}^{n} \mathrm{d}r_i \, \mathrm{d}p_i = \frac{\mathrm{e}^{-\mathcal{B}/T}}{Z_n(T,\tau)} \prod_{i=1}^{n-1} \left(\mathrm{e}^{(-\mathcal{E}_i+\tau r_i)/T} \, \mathrm{d}r_i \, \mathrm{d}p_i \right) \mathrm{d}r_n \, \mathrm{d}p_n, \tag{5.6}$$

where $r_i = q_i - q_{i-1}$ is the relative displacement, $Z_n(T,\tau)$ is a normalization constant, and $\mathcal{B} = p_n^2/2 + V(r_1)/2 + V(r_n)/2 - \tau r_n$ is a boundary term.

If $T_l \neq T_r$, there is no explicit expression of the stationary measure for anharmonic potentials. For certain classes of anharmonic potentials, the results of Rey-Bellet (2006*b*), Carmona (2007) show that there exists a unique stationary probability measure. The assumptions on the potential made in Carmona (2007) or similar works are not satisfied by the Toda potential (in particular, the growth at infinity is too slow in the limit $r \to +\infty$), but we believe that the techniques from Rey-Bellet (2006*b*), Carmona (2007) can be extended to treat the case under consideration here.

We denote by $\langle \cdot \rangle$ the expectation with respect to this stationary measure, as well as the expectation on the path space of the dynamics in the stationary state. By stationarity we have

$$\left\langle J_{i,i+1}(t) \right\rangle = t \left\langle \mathbf{J}^a_{i,i+1} + \gamma \, \mathbf{J}^s_{i,i+1} \right\rangle =: t J_n^i.$$

Because of energy conservation, J_n^i does not depend on i, but only of the size n of the system. It will be denoted by J_n in the sequel. Therefore,

$$J_n = \frac{1}{n-1} \sum_{i=1}^{n-1} \left\langle \mathbf{J}^a_{i,i+1} \right\rangle + \frac{\gamma}{2} \, \frac{\left\langle p_1^2 \right\rangle - \left\langle p_n^2 \right\rangle}{n-1}. \tag{5.7}$$

In view of (5.1), the thermal conductivity can be defined by

$$\kappa_n(T,\tau) = \lim_{\substack{T_l - T_r \to 0 \\ T_r \to T}} \frac{n J_n}{T_l - T_r}. \tag{5.8}$$

It is clear from (5.7)-(5.8) that the direct contribution of the stochastic current to the conductivity is close to γ and remains bounded in n. Hence only the first term of (5.7), namely the Hamiltonian current

$$J_n^{\mathrm{ham}} = \frac{1}{n-1} \sum_{i=1}^{n-1} \left\langle \mathbf{J}^a_{i,i+1} \right\rangle, \tag{5.9}$$

can be responsible for a possible divergence of the conductivity. In the sequel, we therefore consider the conductivity

$$\kappa_n^{\mathrm{ham}}(T,\tau) = \lim_{\substack{T_l - T_r \to 0 \\ T_r \to T}} \frac{n J_n^{\mathrm{ham}}}{T_l - T_r}$$

rather than (5.8). We are also motivated by the following numerical considerations. As reported below, we numerically observe that $\kappa_n^{\mathrm{ham}} \sim n^\alpha$ for some $\alpha \in (0,1)$, hence $J_n^{\mathrm{ham}} \sim n^\nu$ for $\nu = \alpha - 1 \in (-1,0)$. As a consequence, the second term of (5.7) is indeed negligible with respect to the first term, in the limit $n \to \infty$. The hope is however that the asymptotic regime for the Hamiltonian part of the current is attained faster than the asymptotic regime for the total current. The regime of large n where the stochastic current contribution in (5.7) is negligible compared with (5.9) may indeed be difficult to reach numerically.

By a linear response theory argument, the thermal conductivity of the finite system is also given by a Green-Kubo formula (Rey-Bellet (2006*b*)):

$$\kappa_n(T,\tau) = \frac{1}{T^2} \int_0^\infty \sum_{i=1}^{n-1} \left\langle \left(\mathbf{J}^a_{i,i+1}(t) + \tau p_i(t) \right) \mathbf{J}^a_{1,2}(0) \right\rangle_{T,\tau} \mathrm{d}t + \frac{\gamma}{2}, \tag{5.10}$$

where here the expectation $\langle \cdot \rangle_{T,\tau}$ is with respect to the dynamics starting with the equilibrium Gibbs measure given by (5.6) (we assume here that the integral (5.10) indeed exists).

5.3 Numerical simulations

5.3.1 Implementation

All the simulations were done with $T_l = 1.05$ and $T_r = 0.95$. This temperature difference is small enough so that the thermal conductivity around $T = 1$ should be approximated correctly. We also set the external force to $\tau = 0$.

5.3.1.1 Integration of the dynamics

We denote by q_i^m, p_i^m the approximation of $q_i(t_m), p_i(t_m)$ at time $t_m = m\Delta t$. The time-discretization of the dynamics with generator (5.2) is done with a standard splitting strategy, decomposing the generator as the sum of $A + \xi(B_1 + B_n)$ and γS.

The Hamiltonian part of the dynamics and the action of the thermostats on both ends of the chain are taken care of by the so-called BBK discretization from

Brünger et al. (1984) of the Langevin dynamics:

$$\left\{\begin{array}{rcl} p_i^{m+1/2} &=& p_i^m - \dfrac{\Delta t}{2}\nabla_{q_i}\mathcal{H}(q^m) \\ && +\delta_{i,1}\left(-\dfrac{\Delta t}{2}\xi p_1^m + \sqrt{\dfrac{\xi\Delta t}{2}\,T_l}\;G_1^m\right) \\ && +\delta_{i,n}\left(-\dfrac{\Delta t}{2}\xi p_n^m + \sqrt{\dfrac{\xi\Delta t}{2}\,T_r}\;G_n^m\right), \\ q_i^{m+1} &=& q_i^m + \Delta t\, p_i^{m+1/2}, \\ p_i^{m+1} &=& p_i^{m+1/2} - \dfrac{\Delta t}{2}\nabla_{q_i}\mathcal{H}(q^{m+1}) \\ && +\delta_{i,1}\left(-\dfrac{\Delta t}{2}\xi p_1^{m+1} + \sqrt{\dfrac{\xi\Delta t}{2}\,T_l}\;G_1^m\right) \\ && +\delta_{i,n}\left(-\dfrac{\Delta t}{2}\xi p_n^{m+1} + \sqrt{\dfrac{\xi\Delta t}{2}\,T_r}\;G_n^m\right), \end{array}\right. \tag{5.11}$$

where $\delta_{i,1}$ and $\delta_{i,n}$ are Kronecker symbols and G_1^m, G_n^m are independent and identically distributed random Gaussian variables of mean 0 and variance 1. Notice that the last step in the algorithm, written as an implicit update of the momenta, can in fact be rewritten in an explicit manner. Alternatively, one can first integrate the Hamiltonian part of the dynamics with the scheme by Verlet (1967) using a time-step Δt, and next analytically integrate the Ornstein-Uhlenbeck processes on the momenta at both ends of the chain, associated with the generator $\xi(B_1 + B_n)$. In this work, we rather considered algorithm (5.11). We tested two different friction parameters, $\xi = 1$ and $\xi = 0.1$, to study how the results depend on the boundary conditions.

The noise term with generator γS is simulated by exchanging p_i and p_{i+1} at exponentially distributed random times, with an average time γ^{-1} between two such exchanges. More precisely, we attach to each spring a random time τ_i^m, with τ_i^0 drawn from an exponential law with parameter γ. This time is updated as follows: If $\tau_i^m \geqslant \Delta t$, then $\tau_i^{m+1} = \tau_i^m - \Delta t$, otherwise p_i and p_{i+1} are exchanged and τ_i^{m+1} is resampled from an exponential law of parameter γ.

5.3.1.2 Initial conditions and thermalization

The initial conditions are chosen by imposing a linear temperature profile. We used to this end the Langevin dynamics of generator $L_{\mathrm{IC}} = A + \xi\widetilde{B}$, where A is given by (5.3), and

$$\widetilde{B} = \sum_{i=1}^{n} T_i\,\partial_{p_i}^2 - p_i\,\partial_{p_i}, \qquad T_i = \frac{n-i}{n-1}T_l + \frac{i-1}{n-1}T_r.$$

Once a linear temperature profile, obtained from the time-average of the local kinetic energy, is indeed obtained, the term $\xi\widetilde{B}$ is switched off, and replaced by $\xi(B_1 + B_n) + \gamma S$. The dynamics with generator (5.2) is then integrated using the

numerical scheme described in Section 5.3.1.1, and the spatially averaged instantaneous Hamiltonian current is monitored. At time $t_m = m\Delta t$, this current is defined as

$$\mathbf{J}^m = \frac{1}{n-2} \sum_{i=1}^{n-2} \mathbf{J}_{i,i+1}^{a,m}, \tag{5.12}$$

where the instantaneous Hamiltonian current $\mathbf{J}_{i,i+1}^{a,m}$ is defined as in (5.5), upon replacing $q_i(t)$ and $p_i(t)$ by their approximations q_i^m and p_i^m. The thermalization time is somehow loosely defined as the time after which the variations of the instantaneous current stabilize (see Figure 5.1 for an illustration). This time could be determined more carefully by estimating some local-in-time variance of the current, and requiring that this variance stabilizes.

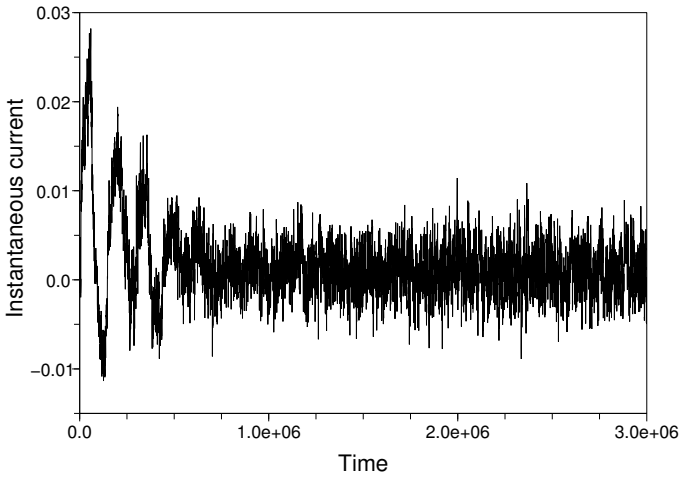


Figure 5.1 – Instantaneous Hamiltonian current (5.12) *as a function of time, in the case* $b = 1$, $\gamma = 10^{-3}$, $\xi = 0.1$, $\Delta t = 0.05$, $n = 2^{16} = 65536$. *The thermalization time is* $T_{\text{thm}} \simeq 2 \times 10^6$.

5.3.1.3 Computation of the energy currents

Once some steady state has been reached, the instantaneous Hamiltonian current (5.12) is computed at each time-step, and an approximation of the Hamiltonian current (5.9) is obtained as a time average:

$$\widehat{J}_n^M = \frac{1}{M} \sum_{m=1}^{M} \mathbf{J}^m. \tag{5.13}$$

In the limit of a large number of time-steps M and for a small time-step Δt, we have $\widehat{J}_n^M \simeq J_n^{\text{ham}}$. Using the current (5.13), we define the conductivity $\widehat{\kappa}_n^M$ and the exponent α by

$$\widehat{\kappa}_n^M = \frac{n\widehat{J}_n^M}{T_l - T_r} \sim n^\alpha. \tag{5.14}$$

A priori, the exponent α depends on all the parameters of the model: the anharmonicity parameter b, the magnitude ξ of the coupling to the end thermostats, the noise strength γ, and the temperatures T_l and T_r. In our simulations, we

have explored how the numerical results (and in particular the exponent α) depend on the first three parameters, and we have kept T_l and T_r fixed. We wish to point out that the results reported here already required an extremely large CPU time. Indeed, for the largest system considered ($n = 2^{17}$), several months were needed to integrate the dynamics with a time-step small enough to ensure accuracy ($\Delta t = 0.05$ here), on a time $T = 10^7$ long enough such that convergence of the time average (5.13) is reached (see Section 5.3.2.2 for more details).

5.3.2 Error estimates

There are two types of errors in the numerical estimation of the currents: a systematic error (bias) due to the time-step error ($\Delta t > 0$), and a statistical error due to the finiteness of the sampling ($M < +\infty$). We consider successively these two issues.

5.3.2.1 Choice of time-step

The time-step should be small enough in order for the dynamics to be numerically stable. When the size n of the system, the noise strength γ, the anharmonicity b or the Langevin friction ξ are increased, the time-step should be reduced. Indeed, in all these cases, the energy of the system increases (at least locally). Due to nonlinearities, this energy may concentrate on a few sites, and hence trigger numerical instabilities. Such issues are not encountered with harmonic potentials, where some uniform stability condition is valid.

In the case $b = 1$ and $\xi = 0.1$, most of our computations have been done with $\Delta t = 0.05$. However, for the largest systems, and for the largest values of γ, we had to use the smaller value $\Delta t = 0.025$ (otherwise, the simulation blows up due to numerical instabilities, as for $n = 2^{14}$ and $\gamma = 1$). For $b = 1$ and $\xi = 1$, that is a stronger noise at the boundaries thermostats, we also observe that we have to reduce the time-step. We worked with $\Delta t = 0.025$ for all values of n. When b is increased from $b = 1$ to $b = 10$ (with $\xi = 0.1$), the potential energy becomes stiffer, and we again need to use a smaller time-step. In the case $b = 10$ and $\xi = 0.1$, we worked with $\Delta t = 0.01$ for all values of n and γ, except for the large values of γ and when $n \geqslant 2^{13}$, for which we used $\Delta t = 0.005$.

Let us now describe two artifacts of the numerical results that occur when the time-step is too large. Observing them in practice is an indication that the time-step is too large and should be reduced. In Figure 5.2, we plot the Hamiltonian current as a function of the chain length n, for $b = 1$, $\xi = 1$ and $\gamma = 1$, for two different time-steps. These currents have been computed as the time averages (5.13) on simulations long enough. For $\Delta t = 0.05$, the current is not monotically decreasing with n, which is clearly a numerical artifact. The simulation blows up for $n = 2^{14}$ and is stable for $n = 2^{13}$, but it is clear that the latter point cannot be trusted.

On Figure 5.3, we plot the temperature profile, at the end of the simulation ($T = M\Delta t = 4.24 \times 10^7$), in the case of a chain of length $n = 2^{13}$ (with $b = 1$, $\xi = 1$ and $\gamma = 1$). When we use $\Delta t = 0.025$, we obtain a decreasing temperature from the left end to the right end, which is in agreement with what is expected. When $\Delta t = 0.05$, the results are completely different, and physically unreasonable. This

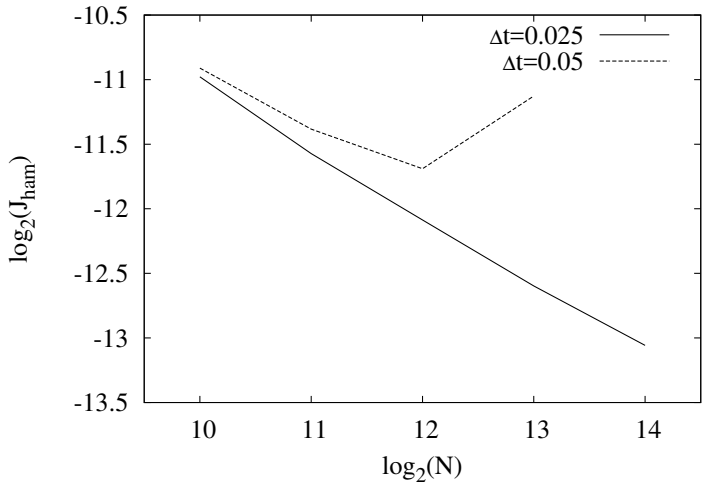


Figure 5.2 – Hamiltonian current (5.13) *as a function of the chain length n, for* $\Delta t = 0.05$ *and* $\Delta t = 0.025$ *(with* $b = 1$, $\xi = 1$ *and* $\gamma = 1$*).*

again shows that these results cannot be trusted.

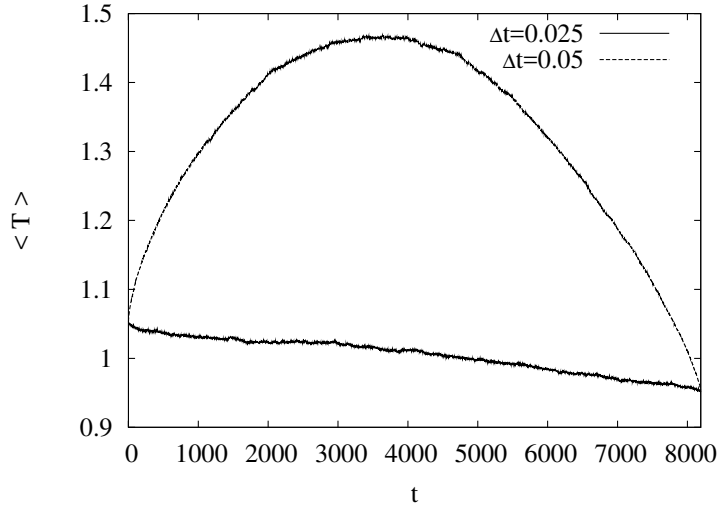


Figure 5.3 – Averaged temperature profiles along the chain of length $n = 2^{13} = 8192$*, for* $\Delta t = 0.05$ *and* $\Delta t = 0.025$ *(with* $b = 1$, $\xi = 1$ *and* $\gamma = 1$*) at the end of the simulation.*

On the other hand, we also checked that the results do not change significantly when the time-step is divided by 2, *i.e.* for $\Delta t = 0.0125$. It therefore seems to us that choosing $\Delta t = 0.025$ is a good trade-off between obtaining converged results (minimizing variances of the estimates at a given computational cost), and reducing time-step related biases (which are usually dominated by variance related statistical errors anyway).

5.3.2.2 Variability of the results

We mentioned earlier than we needed extremely long simulations to obtain a good accuracy. The reason for that can be well understood from Figure 5.4, on which we plot the instantaneous Hamiltonian current $\mathbf{J}^m$ (defined by (5.12)) and

its time average (5.13) as a function of time, for a chain of length $n = 2^{14}$ (for the parameters $b = 1$, $\xi = 1$ and $\gamma = 1$). We observe that $\mathbf{J}^m$ roughly oscillates between -0.02 and 0.02, whereas its time average is close to 10^{-4}. Hence the variability of $\mathbf{J}^m$ is extremely large in comparison with its expectation. We hence need to run a very long simulation to be able to average out most of the fluctuation and obtain $\langle \mathbf{J}^m \rangle$ with a good accuracy.

These heuristic considerations can be quantified by a simple computation. The standard deviation of the instantaneous current in Figure 5.4 is of the order of $\sigma \sim 0.02$, while the average value of the current is $\mu \sim 10^{-4}$. In addition, it is possible to estimate the typical correlation time τ_{corr} using block averaging (also called batch means in the statistics literature), see Flyvbjerg and Petersen (1989), Geyer (1992). Here, we obtain $\tau_{\text{corr}} \sim 10^3$. The time t_{req} required to obtain a 1% relative accuracy on the average current is such that

$$\frac{\sigma}{\sqrt{t_{\text{req}}/\tau_{\text{corr}}}} = 0.01\,\mu.$$

This yields $t_{\text{req}} \sim 4 \times 10^{11}$. Since the time-step is $\Delta t \simeq 0.05$, this means that a huge number of time-steps should be used to reach convergence.

For large values of n and large values of γ, we observe that $\langle \mathbf{J}^m \rangle$ is very small (see the numerical results below). Its accurate computation hence needs an even longer simulation time. In addition, the cost of the simulation of a chain, on a given time range, linearly increases with the size of the chain. This explains why computing the average currents for the longest chains is an extremely computationally demanding task.

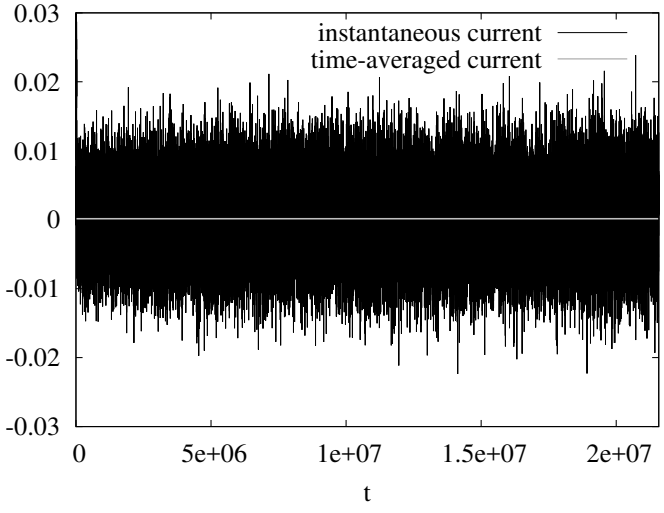


Figure 5.4 – Instantaneous Hamiltonian current (5.12) *and its time average* (5.13) *as a function of time, for a chain of length $n = 2^{14}$ (for the parameters $b = 1$, $\xi = 1$ and $\gamma = 1$).*

5.3.3 Numerical results

We present the conductivity (5.14) as a function of the system length in Figure 5.5. We considered the choices $b = 1$ and $b = 10$ for $\xi = 0.1$ to study the influence of the potential energy anharmonicity. We also simulated the system

γ	α $(b = 1, \xi = 1)$	α $(b = 1, \xi = 0.1)$	α $(b = 10, \xi = 0.1)$
0.001	0.10	–	–
0.01	0.11	0.17	0.25
0.1	0.32	0.30	0.32
1	0.44	0.44	0.43

Table 5.1 – Conductivity exponent α, estimated from (5.14)*, for different values of γ and ξ, and different potential energies.*

with $b = 1$ and $\xi = 1$ to study how the results depend on ξ. The total simulation time for each point ranges from $T = M\Delta t = 10^6$ to $T = 5 \times 10^7$, depending on the size n of the system.

The slope α, defined by (5.14), is estimated using a least square fit in a log-log diagram. This estimate is quite sensitive to the choice of the number of points entering the fitting procedure, and only the very first digits of the estimated slope are reliable. Theoretical results (see Basile et al. (2009)) show that the exponent α is expected to be lower than 0.5. Our numerical results, gathered in Table 5.1, are in accordance with this theoretical upper bound.

We also observe that, for $\gamma = 1$, the value of α is close to 0.5. Now recall that, in the harmonic case $V(r) = ar^2$, the value of α is always equal to 0.5, independently of γ. This seems consistent with the fact that, for large values of γ, the precise details of the potential V do not matter (the dynamics is mostly governed by the stochastic terms), and the behavior of the system is close to the harmonic behavior.

5.4 Discussion of the numerical results

Several conclusions can be drawn from the numerical results given in the previous section:

(i) The ballistic transport, observed in the deterministic Toda lattice, which is due to the complete integrability of the system (Zotos (2002)), is broken by the presence of noise in the dynamics in the cases we considered ($\gamma \geqslant 10^{-3}$). Energy transport becomes superdiffusive, *i.e.* $\kappa_n \sim n^\alpha$, with $\alpha \in (0, 0.5)$. For a low level of noise (γ small), this superdiffusive regime may be seen only for systems large enough ($n \geqslant 2^{12}$ or more, depending on the stiffness parameter b of the system and the coupling ξ to the boundaries thermostats). The asymptotic regime in n for the conductivity is attained for smaller values of n when γ or ξ is larger, or when b is smaller. Studying the limit $\gamma \to 0$ is very challenging since the asymptotic regime in n for which an exponent can be estimated is attained for extremely large system sizes.

(ii) The value of α seems to depend on the noise strength γ in a monotonically increasing way. If κ_n^{GK} had the same behavior, this would suggest that increasing the noise induces a slower time decay of the current-current correlations, in contradiction with the naive intuition that a stronger noise en-

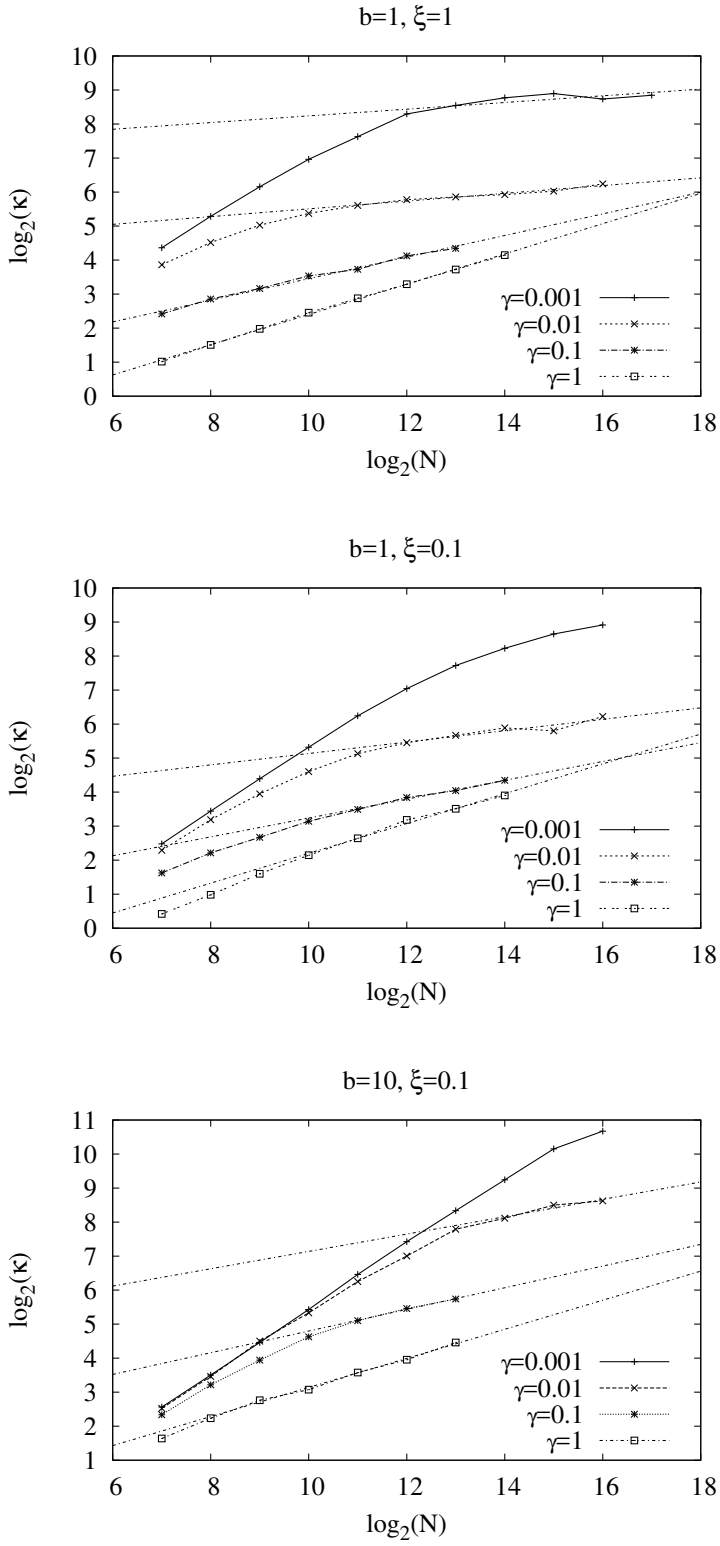


Figure 5.5 – Conductivity $\widehat{\kappa}_n^M$, defined by (5.14)*, as a function of the system size n.*

hances the decay of time correlations. See also Basile et al. (2007) where such a phenomenon has already been observed. We believe that noise tends to suppress scattering effects due to the nonlinearity of the interaction. Observe that, in the harmonic case $V(r) = ar^2$, the value of α is always equal to 0.5 and in particular does not depend on γ (Basile et al. (2006, 2009), Lepri et al. (2009)). The dependence of the exponent α on the noise strength γ in the Toda case also contradicts general theories about the universality of α (see for instance Narayan and Ramaswamy (2002)). These theories need then to be restricted to more specific dynamics.

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Résumé

Nous étudions les propriétés des états stationnaires de dynamiques hors-équilibre, d'un point de vue théorique et numérique. Ces dynamiques sont obtenues en perturbant la dynamique d'équilibre par forçage mécanique et/ou thermique.

Dans l'approche théorique, le système considéré évolue selon une dynamique de Langevin à laquelle on ajoute une force extérieure. Nous étudions la convergence de la loi de la dynamique vers la mesure stationnaire, en donnant des estimations quantitatives du taux exponentiel dans les régimes Hamiltonien et suramorties.

Dans l'approche numérique, nous considérons une chaine de rotateurs soumise aux deux forçages et une chaine d'oscillateurs de Toda soumise à un forçage thermique et à une perturbation stochastique. Nous étudions les caractéristiques de l'état stationnaire et les propriétés de transport. Dans le cas de la chaine de rotateurs, nous observons en particulier que le courant d'énergie moyen est, dans certains cas, accru par un gradient de température opposé.

Abstract

We study the properties of stationary states associated with nonequilibrium dynamics from a theoretical and a numerical point of view. These dynamics are obtained by perturbing equilibrium dynamics with mechanical and/or thermal forcings.

In the theoretical approach, the considered system evolves according to a Langevin dynamics perturbed by a torque. In this framework, we study the convergence of the law of the dynamics to the stationary measure, giving quantitative estimates of the exponential rate, both in the Hamiltonian and "overdamped" regimes.

In the numerical approach, we consider a chain of rotors subjected to both forcings and a chain of Toda oscillators subject to a thermal forcing and a stochastic perturbation. We study the features of the stationary state and analyze its transport properties. In particular, in the case of the rotor chain, we observe that the average energy current is in some cases increased by an opposite temperature gradient, contrary to what is naively expected.

Mots Clés

Dynamiques hors-équilibre, dynamique de Langevin, mésure invariante, hypocoércivité, trou spéctral, transport anormal.

Keywords

Nonequilibrium dynamics, Langevin dynamics, invariant measure, hypocoercivity, spectral gap, anomalous transport.