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Mathematical analysis of quantum mechanics with non-self-adjoint operators

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Abstracts

Abstract in English

The importance of non-self-adjoint operators in modern physics increases every day as they start to play more prominent role in quantum mechanics. However, the significance of their examination is much more recent than the interest in the examination of their self-adjoint counterparts. Thus, since many self-adjoint techniques fail to be generalized to this context, there are not many well-developed methods for examining their properties. This thesis aims to contribute to filling this gap and demonstrates several non-self-adjoint models and the means of their study. The topics include pseudospectrum as a suitable analogue of the spectrum, a model of a quantum layer with balanced gain and loss at the boundary, and the Kramers-Fokker-Planck equation with a short-range potential.

Keywords: quantum mechanics, non-self-adjoint operator, quantum waveguide, pseudospectrum, Kramers-Fokker-Planck equation

Abstrakt v češtině

Důležitost nesamosdružených operátorů v moderní fyzice se zvyšuje každým dnem jak začínají hrát stále podstatnější roli v kvantové mechanice. Avšak důležitost jejich zkoumání je mnohem více čerstá než zájem o zkoumání jejich samosdružených protějšků. Jelikož mnoho samosdružených technik nelze být zobecněno do tohoto kontextu, není zde mnoho dobře vypracovaných metod pro vyšetřování jejich vlastností. Tato teze se snaží trochu zaplnit tuto mezeru a prezentuje několik nesamosdružených modelů a způsoby jejich studia. Témata zahrnují pseudospektrum jako vhodný analog spektra, model kvantové vrstvy s vyváženou ztrátou a ziskem na hranici, a Kramers-Fokker-Planckovu rovnici s krátkodosahovým potenciálem.

Klíčová slova: kvantová mechanika, nesamosdružený operátor, kvantový vlnovod, pseudospektrum, Kramers-Fokker-Planck rovnice

Résumé en français

La mécanique quantique est sans conteste l'une des parties les plus établies de la physique moderne avec des milliers d'expériences à l'appui de ses revendications et des applications allant des transistors à l'imagerie par résonance magnétique. L'une des équations fondamentales de la théorie est l'équation de Schrödinger [31],

$$H\psi = \mathrm{i}\,\frac{\partial \psi}{\partial t}.$$

Il décrit l'état de la particule quantique comme un vecteur ψ dans un espace de Hilbert et donne sa dépendance à l'énergie totale du système exprimée via un opérateur auto-adjoint linéaire H, le Hamiltonien. Un outil fondamental pour l'étude des points λ de son spectre (les énergies admissibles de la particule) est l'opérateur résolvante $(H - \lambda)^{-1}$ et la solution de l'équation est alors donnée par le propagateur $\mathrm{e}^{-\mathrm{i}tH}$ appliqué à un état initial. Aucun de ces deux opérateurs n'est nécessairement auto-adjoint, en fait, la résolvante est non auto-adjointe pour λ avec une partie complexe non nulle et le propagateur forme un groupe unitaire. On peut trouver des opérateurs non auto-adjoints aussi bien dans d'autres outils techniques - mentionnons l'utilisation de la méthode de mise à l'échelle complexe pour l'analyse des résonances ou l'utilisation d'opérateurs de création et d'annihilation pour l'étude des oscillateurs harmoniques. Tous ces exemples ont une chose en commun: les opérateurs non auto-adjoints n'apparaissent qu'en fonction de l'opérateur auto-adjoint ou en tant qu'instrument mathématique pour son étude, ils n'apparaissent jamais comme observables.

En effet, outre les différents modèles phénoménologiques et efficaces, la mécanique quantique exige toujours que son opérateur central soit auto-adjoint. Ce n'est qu'alors que la réalité du spectre (c'est-à-dire les valeurs observables des grandeurs physiques) et l'évolution unitaire des solutions de Schrödinger sont garanties. Clairement, toute ≪extension≫ de la mécanique quantique doit traiter de ces questions et cette thèse vise à fournir un bref résumé de la recherche dans ce sens et présente les contributions de l'auteur au sujet.

L'une des difficultés fondamentales que l'on rencontre lorsqu'on traite avec des opérateurs non auto-adjoints en mécanique quantique est le manque de techniques mathématiques rigoureuses pour leur étude. Bien que les premières mentions des problèmes de valeurs limites non auto-adjoints dans le contexte de la mécanique quantique se soient produites il y a plus de cent ans dans les travaux de G. D. Birkhoff [2], les problèmes n'ont pas suscité un intérêt suffisant de la communauté. En effet, il a fallu plus de quarante ans pour que les premiers résultats abstraits apparaissent dans les travaux de Keldyš [16] en 1951. À cette époque, la théorie des opérateurs auto-adjoints était bien établie et fournissait des résultats solides. s'aventurer en dehors de son cadre et essayer de contester ses

fondamentaux. A ce jour, l'étude des opérateurs auto-adjoints peut bénéficier de divers outils puissants tels que le théorème spectral ou le principe variationnel, alors que ces outils ne sont pas applicables aux opérateurs non auto-adjoints. De plus, les opérateurs non auto-adjoints sont plus divers que leurs homologues auto-adjoints, un scientifique habitué au cadre auto-adjoint typique peut rencontrer des phénomènes étranges et inattendus. Il est difficile de trouver un théorème suffisamment général pour les englober et l'étude d'exemples spécifiques et la recherche d'attributs communs semblent être une approche fructueuse.

La notion d'observateurs non auto-adjoints a été suggérée en 1992 dans le domaine de la physique nucléaire par F. G. Scholtz, H. B. Geyer et F. J. W. Hahne [30]. Ils ont observé que l'un peut construire une théorie quantique cohérente avec un opérateur non auto-adjoint H, à condition qu'il s'agisse d'un quasi-hermitien (quasi-auto-adjoint), c'est-à-dire

$$H^* = \Theta H \Theta^{-1}.$$

Ici, Θ est un opérateur positif, borné avec un inverse borné, également appelé métrique. (La quasi-Hermicité semble apparaître pour la première fois en 1962 dans les travaux de J. Dieudonné [9].) Tous les principes fondamentaux de la mécanique quantique sont valables si l'on considère un changement du produit intérieur de l'espace Hilbert – on prend $\langle \cdot, \Theta \rangle$ au lieu de $\langle \cdot, \cdot \rangle$. Ceci peut sembler à première vue une extension de la mécanique quantique standard (car elle suit dans le cas particulier $\Theta = I$) mais on peut voir que la notion de quasi-auto-adjointe est équivalente à l'opérateur H similaire à un opérateur auto-adjoint h, c.-à-d.

$$h = \Omega H \Omega^{-1}$$

avec un opérateur borné Ω avec un inverse borné, nous avons $\Omega = \Theta^{1/2}$. Ainsi, la propriété de quasi-auto-adjointe représente simplement une reformulation de la mécanique quantique avec des opérateurs auto-adjoints. Notez qu'il peut encore apporter des avantages en tant que représentation potentiellement plus simple des problèmes auto-adjoints. Cependant, la morale ici est que la quasi-auto-adjonction constitue un critère fondamental pour déterminer si un opérateur non auto-adjoint peut produire une dynamique quantique cohérente.

L'ère de l'intérêt pour les opérateurs non-autoadjoints a commencé en 1998, lorsque C. M. Bender et P. N. Boettcher ont remarqué qu'une grande classe de l'opérateur non-autoadjoints possède spectres réel [1]. Cette propriété a été attribuée à une symétrie espace-temps physique du système, appelée symétrie $\mathcal{PT}$. Bien que leur première observation ait été uniquement numérique, une preuve rigoureuse a été faite plusieurs années plus tard par P. Dorey, C. Dunning et R. Tateo [10]. La connexion entre quasi-auto-adjointe et symétrie $\mathcal{PT}$ a été observée dans la série d'articles de A. Mostafazadeh

[21, 22, 23] et aujourd'hui On pense généralement que la quasi-auto-adjonction est une propriété nécessaire pour qu'un opérateur $\mathcal{PT}$-symétrique soit une observable physique.

Cette thèse présente trois thèmes distincts concernant les problèmes non auto-adjoints: pseudospectre, guides d'ondes quantiques et équation de Kramers-Fokker-Planck.

Pseudospectre Pour un système dynamique décrit via un opérateur auto-adjoint, le minimum de son spectre nous donne une estimation simple de la norme du semi-groupe d'évolution. Cependant, pour un opérateur non auto-adjoint, il n'y a pas de résultat analogue et de plus, il y a des contre-exemples. De même, une petite perturbation de l'opérateur ne provoque pas de changement important dans la localisation des valeurs propres d'un opérateur auto-adjoint, cependant, un contraire peut être vrai pour un opérateur non auto-adjoint. Ainsi, il semble que le spectre ne soit pas la chose la plus appropriée à étudier dans le cas non auto-adjoint. Heureusement, il y a une généralisation appropriée de la notion de spectre, le pseudo-spectre. Nous arrivons à la définition du ε-pseudospectre

$$\sigma_\varepsilon(H) = \sigma(H) \cup \{\lambda \in \mathbb{C} \mid (H-\lambda)^{-1} > \varepsilon^{-1}\}$$

pour un parameter ε positive. La propriété évidente de cette notion est que le ε-voisinage du spectre de H est toujours contenu dans le ε-pseudospectre, comme il ressort de l'inégalité de résolvante. Puisque l'égalité vaut pour un H auto-adjoint, la notion de pseudospectre est triviale et il suffit d'étudier le spectre.

Le pseudospectre peut servir d'indicateur d'une non-stabilité du spectre par rapport à une petite perturbation depuis

$$\sigma_\varepsilon(H) = \bigcup_{\|V\|<\varepsilon} \sigma(H+V). \tag{1}$$

De plus, si un opérateur non auto-adjoint H est similaire à un opérateur auto-adjoint $\widetilde{H}$ via une transformation bornée avec un inverse borné, alors le ε -pseudospectre de H a se situer dans un voisinage tubulaire du ε -pseudospectre de $\widetilde{H}$.

Pour l'étude du pseudospectre, nous introduisons une technique applicable à une classe d'opérateurs semi-classiques. Nous démontrons son applicabilité sur un modèle simple non auto-adjoint. Nous considérons un oscillateur harmonique à une dimension avec un potentiel cubique imaginaire ajouté,

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \mathrm{i}x^3$$

sur son domaine maximal. Ses fonctions propres forment un ensemble complet dans $L^2(\mathbb{R})$ mais elles ne forment pas une base de Schauder. Ceci est une conséquence des propriétés pseudospectrales sauvages - le pseudospectre peut contenir des points arbitrairement loin du spectre même pour de petites valeurs de ε. Cela est particulièrement frappant si l'on considère que chaque point du pseudospectre peut être converti en point de spectre en ajoutant une petite perturbation à l'opérateur. Ainsi, il est impossible à l'opérateur étudié d'être similaire à un opérateur auto-adjoint (dans le sens ci-dessus) et il ne peut pas générer un semigroupe à évolution limitée.

Guides d'ondes quantiques Un autre domaine, où les opérateurs non auto-adjoints peuvent trouver une application, sont les guides d'ondes quantiques. L'étude des guides d'ondes quantiques vise à fournir une description mathématique rigoureuse des tubes ou couches semi-conducteurs longs et fins produits à partir de matériaux très purs et cristallins. Typiquement, cette description est obtenue en considérant l'équation de Schrödinger dans une région tubulaire sans limite Ω avec des conditions aux limites imposées de Dirichlet, Neumann ou Robin sur $\partial\Omega$ [13, 12]. Ces conditions reflètent le confinement de la particule à l'intérieur du guide d'ondes. Une caractéristique commune des modèles étudiés était l'auto-adjonction de l'opérateur de soulignement. Un modèle non auto-adjoint d 'un guide d' onde quantique a d 'abord été étudié dans [4], où les auteurs imposaient des conditions de limites de Robin complexes et représentaient ainsi la perméabilité de la limite. Nous visons à fournir une approche différente pour obtenir leurs résultats et les généraliser à des dimensions plus élevées.

Nous étudions les propriétés d'un laplacien dans un voisinage tubulaire d'un hyperplan. Considérons une région $\Omega := \mathbb{R}^n \times I$ embarqué dans $\mathbb{R}^{n+1}$, où $I = (0, d)$ est un intervalle fini. Pour $n = 1$ il se réduit à une bande plane, pour $n = 2$ à un calque en trois dimensions. Nous nous intéressons à l'action de le Hamiltonien d'une particule libre dans cette région soumise à la condition de limite de Robin $\mathcal{PT}$ symétrique sur $\partial\Omega$ agissant dans l'espace de Hilbert $L^2(\Omega)$. Étant donné une fonction à valeur réelle $\alpha \in W^{1,\infty}(\mathbb{R}^n)$, nous définissons le Hamiltonien comme

$$\begin{aligned} H_\alpha \Psi &:= -\Delta\Psi, \\ \mathrm{Dom}(H_\alpha) &:= \left\{ \Psi \in W^{2,2}(\Omega) \,|\, \partial_u \Psi + \mathrm{i}\alpha\Psi = 0 \quad \text{on} \quad \partial\Omega \right\}, \end{aligned} \tag{2}$$

où ∂_u signifie différenciation par rapport à u (la variable á I), de même Δ représente la somme de toutes les dérivées secondes. L'effet de H_α doit être compris dans un sens distributionnel et les conditions aux limites au sens de traces.

À partir des propriétés de symétrie de l'opérateur, on en déduit que son spectre résiduel est toujours vide. Nous considérons alors un cas simple des conditions aux limites où la fonction $\alpha(x) = \alpha_0$ est identique le long de la limite. Dans ce cas, il n'y a pas de valeurs propres isolées et le spectre est purement essentiel et égal à l'intervalle $[\mu_0^2, +\infty)$, où μ_0^2 est la plus basse valeur du laplacien agissant sur I avec les conditions aux limites de Robin. Notre dernière étape est d'introduire une petite perturbation des conditions aux limites, $\alpha(x) = \alpha_0 + \varepsilon\beta(x)$ et d'étudier son effet sur l'apparition d'états liés (= valeurs propres isolées de multiplicité finie) pour une bande dans le plan et une couche en trois dimensions. Dans certaines conditions de régularité et de décroissance asymptotique de la fonction β, nous démontrons l'existence d'une valeur propre unique, simple et réelle si $\alpha_0 \int_{\mathbb{R}^n} \beta(x)\,\mathrm{d}x < 0$ pour $n = 1, 2$. La série asymptotique de premier ordre pour cette valeur propre est calculée.

Équation de Kramers-Fokker-Planck De nombreux systèmes physiques du monde réel sont soumis à de petites forces et à des influences complexes à décrire et sont généralement appelées bruit ou fluctuations. (Les applications vont de la physique des solides à la théorie des circuits). Celles-ci sont impossibles à décrire en raison du grand nombre de variables inconnues et ne peuvent être incluses dans l'équation que sous l'influence d'une force extérieure aléatoire. Un des exemples les plus simples de ce phénomène est le mouvement brownien - la position des particules macroscopiques immergées dans un fluide se déplace de manière aléatoire à la suite de collisions avec des molécules du fluide. Nous pouvons localiser la particule dans une certaine région avec une certaine probabilité - ceci est donné par l'équation de Fokker-Planck [14, 28].

L'équation de Kramers est une équation spéciale de Fokker-Planck décrivant le mouvement brownien dans un champ externe. Cette équation a été dérivée et utilisée par H. Kramers [17] pour décrire la cinétique de la réaction chimique. Plus tard, il s'est avéré qu'il s'appliquait plus généralement à différents domaines tels que les conducteurs supersoniques, la jonction tunnel Josephson et la relaxation des dipôles [29]. L'analyse mathématique de l'équation de Kramers-Fokker-Planck (KFP, en bref) est initialement motivée par la tendance à l'équilibre des potentiels de confinement [8]. Les problèmes spectraux de l'opérateur KFP se révèlent très intéressants, car cet opérateur n'est ni elliptique ni auto-adjoint. Après avoir défini correctement les constantes physiques et les modifications des inconnues, l'équation de KFP en fonction du temps peut être écrite dans la forme.

$$\partial_t u(t; x, v) + Pu(t; x, v) = 0, \tag{3}$$

oú $(x, v) \in \mathbb{R}^n \times \mathbb{R}^n$, $t > 0$, avec les données initiales $u(0; x, v) = u_0(x, v)$. Ici x et v représentent respectivement la position et la vitesse de la particule, P est l'opérateur KFP donné par

$$P = -\Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2} + v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v, \tag{4}$$

où le potentiel $V(x)$ est supposé être une fonction réelle $C^1(\mathbb{R}^n)$.

La situation qui nous intéresse ici est une équation KFP à une dimension avec un potentiel rapidement décroissant. Notre objectif est d'obtenir un comportement asymptotique à long terme de ses solutions. Du point de vue de l'analyse spectrale, ceci est

étroitement lié aux propriétés spectrales de faible énergie de P. On sait que pour les opérateurs de Schr ”odinger, l'analyse spectrale à basse énergie dans les cas à une et deux dimensions est plus difficile que dans les dimensions supérieures et nécessite des méthodes spécifiques ([3]) car le seuil zéro est déjà une résonance du laplacien en dimension un et deux: pour l'opérateur KFP aux potentiels décroissants, les notions de seuils et de résonances de seuil sont discutées dans [36], pour $n \geq 3$, zéro n'est pas une résonance de P alors que pour $n = 1, 2$, zéro est une résonance de P. C'est la principale différence entre le travail actuel et [36]. Nous calculons le terme principal de l'opérateur d'évolution et nous pouvons encore observer sa dépendance sur le état de résonance.

Mots clés: Mécanique quantique, opérateur non-auto-adjoint, guide d'onde quantique, pseudo-spectre, équation de Kramers-Fokker-Planck

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Contents

CHAPTER I

Introduction

Quantum mechanics is indisputably one of the most established parts of modern physics with thousands of experiments supporting its claims and with applications ranging from transistors to magnetic resonance imaging and lasers. One of the fundamental equations of the theory is the Schrödinger equation [31],

$$H\psi = \mathrm{i}\,\frac{\partial \psi}{\partial t}. \tag{I.1}$$

It describes the state of the quantum particle as a vector ψ in a Hilbert space and gives its dependence on the total energy of the system expressed via a linear self-adjoint operator H, the Hamiltonian. A fundamental tool for the study of the points λ of its spectrum (the admissible energies of the particle) is the resolvent operator $(H-\lambda)^{-1}$ and the solutions of the equation are then given by the propagator $\mathrm{e}^{-\mathrm{i}tH}$ applied to an initial state. Neither of these two operators is necessarily self-adjoint, in fact, the resolvent is non-self-adjoint for λ with non-zero imaginary part and the propagator forms a unitary group. One can find non-self-adjoint operators as well in other technical tools – let us mention the use of the method of complex scaling for analysis of resonances or use of creation and annihilation operators for the study of harmonic oscillator. All these examples have one thing in common – the non-self-adjoint operators appear only as functions of the underlying self-adjoint operator or as a mathematical instrument for its study, they never appear as the observables.

Indeed, besides various phenomenological and effective models, the quantum mechanics always demands operators corresponding to variables to be self-adjoint. Only then is the reality of the spectrum (i.e. the observable values of physical quantities) and the unitary evolution of the solutions of (I.1) guaranteed. Clearly, any "extension" of quantum mechanics has to deal with the lack of these properties and this thesis aims to provide a short summary of the research in this direction and presents author's contributions to the subject.

I.1 Non-self-adjoint operators in quantum mechanics

One of the basic difficulties one encounters when dealing with non-self-adjoint operators in quantum mechanic is the lack of rigorous mathematical techniques for their study. Although the first mentions of non-self-adjoint boundary value problems in context of quantum mechanics occur more than one hundred years ago in works of G. D. Birkhoff [2], the problems did not attract sufficient interest of the community. Indeed, it took more than forty years for the first abstract results to appear in Keldyš' work [16] in 1951. By this time, the theory of self-adjoint operators were well established and providing solid results, there was no need need to venture outside of its framework and try to challenge its fundamentals. At this day, study of self-adjoint operators can benefit from various potent tools such as the spectral theorem or the variational principle, whereas these tools are non-applicable on the non-self-adjoint operators. Moreover, the non-self-adjoint operators are more diverse than their self-adjoint counterparts, a scientist used to the standard self-adjoint framework may encounter strange and unexpected phenomena. It is a challenging task to find theorems general enough to encompass them all, the study of specific examples and search for a common attributes seems to be a fruitful approach.

The notion of non-self-adjoint operators as observables was suggested in 1992 in the field of nuclear physics by F. G. Scholtz, H. B. Geyer and F. J. W. Hahne [30]. They observed that the one can build a consistent quantum theory with a non-self-adjoint operator H, provided it is quasi-Hermitian (quasi-self-adjoint), i.e.

$$H^* = \Theta H \Theta^{-1}. \tag{I.2}$$

Here Θ is some positive, bounded and boundedly invertible operator called metric. (The quasi-Hermicity seems to first appear in 1962 in work of J. Dieudonné [9].) All the fundamentals of quantum mechanics then hold if one considers a change of the inner product of the Hilbert space – one takes $\langle \cdot, \Theta \rangle$ instead of $\langle \cdot, \cdot \rangle$. This can seem at first glance an extension of standard quantum mechanics (since it follows in the special case $\Theta = I$) but it can be seen that the notion (I.2) is equivalent to operator H being similar to a self-adjoint operator h, i.e.

$$h = \Omega H \Omega^{-1} \tag{I.3}$$

with a bounded and boundedly invertible operator Ω and we have $\Omega = \Theta^{1/2}$. Thus the property of quasi-self-adjointness represents just a reformulation of the quantum mechanics with self-adjoint operators. Note that it can still bring benefits as a potentially simpler representation of self-adjoint problems. However, the moral here is that quasi-self-adjointness stands as a fundamental criterion to determine whether a non-self-adjoint operator can produce a consistent quantum dynamics.

The era of interest in non-self-adjoint operators began in 1998 when C. M. Bender and P. N. Boettcher noticed that a large class of non-self-adjoint operator possesses real spectra [1]. This property was attributed to a physical space-time symmetry of the system, the so-called $\mathcal{PT}$-symmetry. Although their first observation was only numerical, a rigorous proof was done several years later by P. Dorey, C. Dunning and R. Tateo [10]. The connection between quasi-self-adjointness and $\mathcal{PT}$-symmetry was observed in the series of papers of A. Mostafazadeh [21, 22, 23] and today it is widely believed that quasi-self-adjointness is a necessary property for a $\mathcal{PT}$-symmetric operator as a physical observable.

This thesis presents three distinct topics concerning non-self-adjoint problems. We briefly describe the studied problems and refer the reader to Chapter II to a more detailed summary of our results.

Pseudospectrum For a dynamical system described via a self-adjoint operator, the infimum of its spectrum gives us a simple estimate on the norm of the evolution semigroup. However, for a non-self-adjoint operator, there is no analogues result and furthermore, there are counterexamples to it. Similarly, a small perturbation of the operator does not cause a large change in the location of the eigenvalues of a self-adjoint operator, however, an opposite can be true for a non-self-adjoint operator. Thus, it seems that the spectrum may not be the most appropriate thing to study in the non-self-adjoint case. Luckily it turns out there is a suitable generalization of the notion of the spectrum, the pseudospectrum. In Section II.1, we aim to elaborate this notion further and apply the results to a simple $\mathcal{PT}$-symmetric model. As mentioned earlier, the $\mathcal{PT}$-symmetric models can be physically relevant only when they are also quasi-self-adjoint. We can directly test whether this property can hold with the study of the pseudospectrum alone. This is demonstrated on the harmonic oscillater with an added imaginary cubic potential. This system has wild pseudospectral behaviour and as a consequence we argue the impossibility of its relevance as an observable.

Quantum waveguides Another area, where non-self-adjoint operators can find application, are quantum waveguides. Customarily, these miniature semiconductor tubes or layers are described by a self-adjoint operator. However, all these models describe only the situation when the particle is perfectly contained inside the waveguide. There is a natural question what happens in the case of a permeable boundary. It turns out for a strip in two dimensions and a layer in three dimensions, there is an interesting interplay between reality of the eigenvalues of the underlining operator and the probability gain and loss at the boundary. Section II.2 is devoted to describing this interaction in more detail.

Kramers-Fokker-Planck equation Unlike the previous model, the operator appearing in the Kramers-Fokker-Planck equation is inherently non-self-adjoint due to the convection term and furthermore, it is even non-elliptic. This operator is well-studied in the case of a confining potential where it is shown that for large times the system converges to an equilibrium. However, no such result was known for a long time in the case of a potential acting near the origin. The first result in this direction dealt only with the case of dimensions higher than three. We explore the situation in dimension one and two in Section II.3.

CHAPTER II

Results

II.1 Pseudospectrum

Among properties of the self-ajoint systems one may wish to study, spectrum takes a prominent role, as it gives information, among other things, about evolution semigroup, resonances or helps to diagonalize the operator. For a closed operator H it is defined as

$$\sigma(H) = \{\lambda \in \mathbb{C} \mid H - \lambda \text{ is not bijective as an operator } \mathrm{Dom}(H) \to \mathscr{H}\},$$

where $\mathscr{H}$ is the Hilbert space where H acts. The complement set of the spectrum, the resolvent set, thus contains complex points λ where the norm $\|(H-\lambda)^{-1}\|$ is finite. The natural extension of the notion of the spectrum is to include points λ where the aforementioned norm is large. We arrive at the definition of the ε-pseudospectrum

$$\sigma_\varepsilon(H) = \sigma(H) \cup \{\lambda \in \mathbb{C} \mid (H-\lambda)^{-1} > \varepsilon^{-1}\}.$$

The evident property of this notion is that the ε-neighborhood of the spectrum of H is always contained in the ε-pseudospectrum, as follows from the resolvent inequality $\|(H-\lambda)^{-1}\| \geq \mathrm{dist}(\lambda, \sigma(H))$. Since equality holds for a self-adjoint H, the notion of pseudospectrum is trivial and it suffices to study the spectrum. However, for a non-self-adjoint operator the situation can be far from trivial.

One of the most useful properties of the pseudospectrum is its relation to the spectrum of the perturbed operator:

$$\sigma_\varepsilon(H) = \bigcup_{\|V\|<\varepsilon} \sigma(H+V). \tag{II.1}$$

Thus, pseudospectrum can serve as an indicator of a non-stability of the spectrum with respect to a small perturbation. If it contains points far from the spectrum, small perturbation of the operator can cause huge changes in its spectrum.

Another equivalent definition of pseudospectrum can be stated in terms of the so-called pseudomodes:

$$\sigma_\varepsilon(H) = \{\lambda \in \mathbb{C} \mid \lambda \in \sigma(H) \vee (\exists \psi \in \mathrm{Dom}(H))\,(\|(H-\lambda)\psi\| < \varepsilon\|\psi\|)\}\,. \tag{II.2}$$

Numbers λ in this definition are called pseudoeigenvalues and the functions ψ pseudoeigenvectors of pseudomodes. In view of the property (II.1) we see that for an operator with a wild pseudospectral behaviour, there can be points far from the spectrum, which can be turned into true eigenvalues by a small perturbation.

One last property to mention is the relation between pseudospectra of an operator and pseudospectra of a similar operator. To specify this, we say that operators H and $\widetilde{H}$ are similar if there is a bounded and boundedly invertible operator Ω such that

$$\widetilde{H} = \Theta H \Theta^{-1}. \tag{II.3}$$

It is well known that the spectra of H and $\widetilde{H}$ then coincide. However, their pseudospectra can still be very different. Given the condition number $\kappa := \|\Omega\|\|\Omega^{-1}\|$, only the relation

$$\sigma_{\varepsilon/\kappa}(H) \subseteq \sigma_\varepsilon(\widetilde{H}) \subseteq \sigma_{\varepsilon\kappa}(H) \tag{II.4}$$

can be established. This property is particularly striking when we consider the situation where $\widetilde{H}$ is self-adjoint. The spectrum of any operator similar to $\widetilde{H}$ would have to lie in a tubular neighborhood of the spectrum of $\widetilde{H}$. Compare this also to the property (II.1) – pseudospectrum of an operator similar to a self-adjoint operator via a bounded and boundedly invertible transformation should be well-behaved, otherwise we may observe a serious spectral instability. We refer the reader to classical monographs [35] and [7] for more information on this topic and references on stated results.

This notion of similarity of non-self-adjoint operator to self-adjoint ones found application in the so-called $\mathcal{PT}$-symmetric quantum mechanics. The property of $\mathcal{PT}$-symmetry of an operator H should be understood in this work as the invariance of H with respect to the space inversion and the time reversal on the Hilbert space $L^2(\mathbb{R})$, i.e.

$$[H, \mathcal{PT}] = 0 \tag{II.5}$$

in the operator sense, where $(\mathcal{P}\psi)(x) := \psi(-x)$ stands for spatial reflection and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$ stands for time reversal in quantum mechanics. As mentioned earlier, the quantum-physical interpretation of these models was based on the quasi-self-adjointness of the considered operator. However, this does not automatically hold for every $\mathcal{PT}$-symmetric operator. There are several ways how to prove or disprove this property and in the following we suggest one of the latter.

We state general theorem for a study of the pseudospectrum of a class of semiclassical operators and then we apply it to one of the operators first studied in [5]. The authors studied the class of operators $-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \beta x^{2n+1}$ on $L^2(\mathbb{R})$ for a general complex β and noticed that the spectrum is real provided $\arg(\beta) = \pi/2$ and β is sufficiently small. This property was later attributed to the $\mathcal{PT}$-symmetry of the considered operator. We restrict ourselves to studying the case $\beta = \mathrm{i}$ and $n = 1$, generalizations can be obtained using the same approach.

These results can also be considered as a continuation of [33], where authors studied the operator $-\mathrm{d}^2/\mathrm{d}x^2 + \mathrm{i}x^3$ (so-called imaginary cubic oscillator, first appearing in [1]) and derived completeness of its eigenfunctions, found the bounded metric operator Θ and proved that it can not have a bounded inverse. These results were further supplemented in [19] where the existence of points in the pseudospectrum far from the spectrum was established.

The use of semiclassical techniques in the study of non-self-adjoint operators was first suggested in [6], and the idea was further developed e.g. in [37]. Let H_h be an operator acting in $L^2(\mathbb{R})$ of the form

$$H_h := -h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_h(x). \tag{II.6}$$

Here V_h are analytic potentials in x for all $h > 0$ small enough which take the form $V_h(x) = V_0(x) + \widetilde{V}(x,h)$, where $\widetilde{V}(x,h) \to 0$ locally uniformly as $h \to 0$. This operator should be understood as some closed extension of an operator originally defined on $C_c^\infty(\mathbb{R})$. The main result is an analogue of [6, Thm. 1] for a potential depending on h and its proof relies on approach of the proof of [19, Thm. 1].

Theorem II.1.1 ([25, Thm. 2])**.**
Let H_h be defined as above and let λ be from the set

$$\Lambda := \left\{ \xi^2 + V_h(x) \;\middle|\; (x,\xi) \in \mathbb{R}^2, \xi \operatorname{Im} V_h'(x) < 0 \right\}, \tag{II.7}$$

where the dash denotes standard differentiation with respect to x in $\mathbb{R}$. Then there exists some $C = C(\lambda) > 1$, some $h_0 = h_0(\lambda) > 0$, and an h-dependent family of $C_c^\infty(\mathbb{R})$ functions $\{\psi_h\}_{0<h\le h_0}$ with the property that, for all $0 < h \le h_0$,

$$\|(H_h - \lambda)\psi_h\| < C^{-1/h}\|\psi_h\|. \tag{II.8}$$

The function $f(x,\xi) := \xi^2 + V_h(x)$ is called the symbol associated with H_h. Note that relation (II.2) gives us that $\lambda \in \sigma_\varepsilon(H_h)$ for all $\varepsilon \ge C(\lambda)^{-1/h}$. Here ε can get arbitrarily close to 0, provided h is sufficiently small. Application of Theorem II.1.1 to non-semiclassical operators is sometimes possible by using scaling techniques and sending the spectral parameter to infinity. This is based on a more general principle that the semiclassical limit is equivalent to the high-energy limit after a change of variables.

Let us now define the operator H acting on its maximal domain:

$$\begin{aligned} H &:= -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \mathrm{i}x^3, \\ \mathrm{Dom}(H) &:= \left\{ \psi \in W^{2,2}(\mathbb{R}) \;\middle|\; -\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + x^2\psi + \mathrm{i}x^3\psi \in L^2(\mathbb{R}) \right\}. \end{aligned} \tag{II.9}$$

It was shown in [5] that $\mathrm{Dom}(H)$ coincides with $\{\psi \in W^{2,2}(\mathbb{R}) \mid x^3\psi \in L^2(\mathbb{R})\}$ and that H is closed. Furthermore, it is an operator with compact resolvent and therefore its spectrum is discrete (i.e. consists of isolated eigenvalues of finite algebraic multiplicity). The reality and the simplicity of the eigenvalues was established in [32]. Using standard methods one can show that H coincides with the closure of (II.9) defined on smooth functions with compact support and that it is an m-accretive operator. Recall that this means that H is closed and that $\{\lambda \in \mathbb{C} \mid \mathrm{Re}\,\lambda < 0\} \subset \rho(H)$ and $\|(H-\lambda)^{-1}\| \leq 1/|\mathrm{Re}\,\lambda|$ for $\mathrm{Re}\,\lambda < 0$. The main new results for this operator are summarized in the following theorem.

Theorem II.1.2 ([25, Thm. 1])**.**
Let H be the operator defined in (II.9)*. Then:*

1. *The eigenfunctions of H form a complete set in $L^2(\mathbb{R})$.*
2. *The eigenfunctions of H do not form a (Schauder) basis in $L^2(\mathbb{R})$.*
3. *For any $\delta > 0$ there exist constants $A, B > 0$ such that for all $\varepsilon > 0$ small,*

$$\left\{ \lambda \in \mathbb{C} \;\middle|\; |\lambda| > A,\ |\mathrm{arg}\lambda| < \arctan \mathrm{Re}\,\lambda - \delta,\ |\lambda| \geq B\left(\log\frac{1}{\varepsilon}\right)^{6/5} \right\} \subset \sigma_\varepsilon(H). \tag{II.10}$$

4. *H is not similar to a self-adjoint operator via bounded and boundedly invertible transformation*
5. *H is not quasi-self-adjoint with a bounded and boundedly invertible metric.*
6. *$-\mathrm{i}H$ is not a generator of a bounded semigroup.*

The key step in the proof of this theorem is the bottom estimate on this pseudospectrum (II.10) achieved using II.1.1. All the other negative properties then follow from the exponential growth of the resolvent at infinity. We can see that for any ε the pseudospectrum contains complex points with positive real part, non-negative imaginary part and large magnitude. This result is in particular important in view of the characterisation of pseudospectrum (II.1) – it implies the existence of pseudomodes very far from the spectrum. This non-trivial behaviour of the pseudospectrum was without details announced in [33]. A numerical computation of several of the pseudospectral lines of H can be seen in Figure II.1. As a consequence of the last point in Theorem II.1.2, the time-dependent Schrödinger equation with H does not admit a bounded time-evolution.

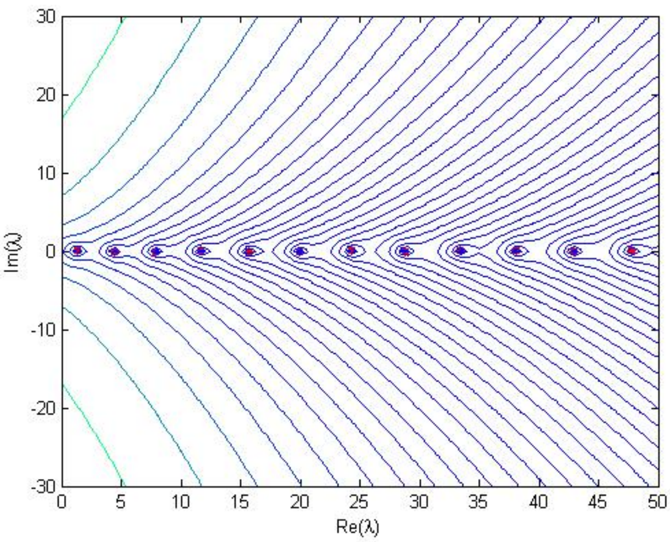

Figure II.1 – Spectrum (red dots) and ε-pseudospectra (enclosed by blue-green contour lines) of harmonic oscillator with imaginary cubic potential. The border of the ε-pseudospectrum is plotted for the values $\varepsilon = 10^{-7}, 10^{-6.75}, 10^{-6.5}, \ldots, 10^{1}$*, the green contour lines correspond to large values of* ε*, the blue ones correspond to smaller values of* ε*. We notice that for each* ε *from the selected range the contour lines quickly diverge and therefore the corresponding ε-pseudospectrum contains points very far from the real axes. More details about the used computational method can be found in [34].*

II.2 Quantum waveguides

The study of quantum waveguides aims to provide a rigorous mathematical description of long and thin semiconductor tubes or layers produced of very pure and crystalline materials. Typically this description is achieved by considering Schrödinger equation in an unbounded tubular region Ω with imposed Dirichlet, Neumann or Robin boundary conditions on $\partial\Omega$ [13, 12]. These conditions reflect confinement of the particle to the interior of the waveguide. One common feature of the studied models was the self-adjointness of the underlining operator. A non-self-adjoint model of a quantum waveguide was first considered in [4], where authors imposed complex Robin boundary conditions and so represented permeability of the boundary. We aim to provide a different approach to obtaining their results and generalizing them to higher dimensions.

In this section we are going to discuss properties of a Laplacian in a tubular neighbourhood of a hyperplane. Let us consider a region $\Omega := \mathbb{R}^n \times I$ embedded into $\mathbb{R}^{n+1}$, where $I = (0, d)$ is a finite interval. For $n = 1$ it reduces to a planar strip, for $n = 2$ to a layer in three dimensions. We are interested in the action of the Hamiltonian of a free particle in this region subjected to $\mathcal{PT}$-symmetric Robin boundary condition on $\partial\Omega$ acting in the Hilbert space $L^2(\Omega)$. Elements of this Hilbert space are going to be consistently denoted with capital Greek letters (usually Ψ or Φ). The variables are going to be split as (x,u), where $x \in \mathbb{R}^n$ and $u \in (0,d)$. Given a real-valued function $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ we define the Hamiltonian as

$$\begin{aligned} H_\alpha \Psi &:= -\Delta\Psi, \\ \mathrm{Dom}(H_\alpha) &:= \left\{ \Psi \in W^{2,2}(\Omega) \,|\, \partial_u \Psi + \mathrm{i}\alpha\Psi = 0 \quad \text{on} \quad \partial\Omega \right\}, \end{aligned} \tag{II.11}$$

where ∂_u stands for differentiation with respect to u, similarly Δ stands for sum of all second derivatives. The effect of H_α should be understood in a distributional sense and the boundary conditions in the sense of traces.

Note that these imposed boundary conditions involve complex numbers and therefore the operator H_α cannot be self-adjoint (for non-trivial α). Furthermore, with these condition we indeed see that the probability current in $\mathbb{R}^{n+1}$ of the wavefunction from the operator domain in the point (x,u) of $\partial\Omega$ is

$$\vec{j}(x,u) = \frac{1}{\mathrm{i}} \left(\overline{\Psi}\partial_u\Psi - \Psi\partial_u\overline{\Psi} \right)(x,u)\,\vec{e}_{n+1} = -2\alpha(x)|\Psi(x,u)|^2\,\vec{e}_{n+1}, \tag{II.12}$$

where $\vec{e}_{n+1}$ stands for $(n+1)$-th vector of the standard basis in $\mathbb{R}^{n+1}$. Clearly, the current is non-zero for non-trivial Robin boundary conditions and the particles are allowed to enter and exit the waveguide.

Another reason for choosing complex Robin boundary conditions arises from the context of the $\mathcal{PT}$-symmetric quantum mechanics. We understand the $\mathcal{PT}$-symmetry property of the operator H in this case in the sense of relation II.5, however, the relevant operators now stand for $(\mathcal{P}\Psi)(x,u) := \Psi(x, d-u)$ and $(\mathcal{T}\Psi)(x,u) := \overline{\Psi(x,u)}$. One can easily check that the Laplace term is $\mathcal{PT}$-symmetric and the same holds for the boundary conditions as well. This symmetry is also reflected in the balance in the gain and loss at the boundary – the probability current II.12 does not depend on whether we are at $u = 0$ or $u = d$.

In the paper [4] the authors focused on the case of the planar waveguide, $n = 1$. The spectrum of the waveguide with constant boundary conditions (i.e. $\alpha(x) = \alpha_0$ along the boundary) was found to be purely essential and equal to the half-line $[\mu_0^2, +\infty)$, where $\mu_0^2 := \min\left\{\alpha_0^2, \left(\frac{\pi}{d}\right)^2\right\}$. Furthermore, it is stable under sufficiently smooth compact perturbation β of the function α. In the case of a weakly coupled perturbation $\varepsilon\beta$ the existence and uniqueness of an isolated eigenvalue was established under the condition that $\alpha_0 \int_{\mathbb{R}} \beta(x)\,\mathrm{d}x < 0$ holds and its asymptotic expansion up to the order ε^3 was calculated. The borderline case $\alpha_0 \int_{\mathbb{R}} \beta(x)\,\mathrm{d}x = 0$ was studied as well. This paper aims to generalize some of the above mentioned results to higher dimensions and to more general perturbations without compact support. In [4] method of matched asymptotic expansions was used, we choose a different approach to the problem based on the Birman-Schwinger principle.

Using the quadratic form approach and the First representation theorem, it follows that H_α is an m-sectorial operator if $\alpha \in W^{1,\infty}(\mathbb{R}^n)$. This yields that the operator is closed, therefore its spectrum is well defined and contained in a sector. Furthermore, the spectrum of H_α is localized inside a parabola, more precisely,

$$\sigma(H_\alpha) \subset \left\{ z \in \mathbb{C} \,\middle|\, \operatorname{Re} z \geq 0, |\operatorname{Im} z| \leq 2\|\alpha\|_{L^\infty(\mathbb{R}^n)} \sqrt{\operatorname{Re} z} \right\}. \tag{II.13}$$

Using the quadratic forms it can be shown for its adjoint operator that $H_\alpha^* = H_{-\alpha}$. Another important property of H_α is $\mathcal{T}$-selfadjointness, i.e $\mathcal{T} H_\alpha \mathcal{T} = H_\alpha^*$. A major consequence of this is that the residual spectrum of H_α is empty [4, Cor. 2.1], i.e

$$\sigma_{\mathrm{r}}(H_\alpha) = \varnothing. \tag{II.14}$$

We emphasize that in our non-self-adjoint case it was impossible to a priori say anything about the residual spectrum, compared to the self-adjoint case, in which it is always empty.

First of all we present a simple case of the boundary conditions $\alpha(x) = \alpha_0$ for all $x \in \mathbb{R}^n$, where α_0 is a real constant. Using the decomposition of the resolvent into the transversal basis, it is possible to show that the Hamiltonian H_{α_0} can be written as a sum

$$H_{\alpha_0} = -\Delta' \otimes 1^I + 1^{\mathbb{R}^n} \otimes -\Delta_{\alpha_0}^I, \tag{II.15}$$

where $1^{\mathbb{R}^n}$ and 1^I are identity operators on $L^2(\mathbb{R}^n)$ and $L^2(I)$ respectively, $-\Delta'$ is a self-adjoint Laplacian in $L^2(\mathbb{R}^n)$ and $-\Delta_{\alpha_0}^I$ is a Laplacian in $L^2(I)$ with complex Robin-type boundary conditions

$$\begin{aligned} -\Delta_{\alpha_0}^I \psi &:= -\psi'', \\ \operatorname{Dom}(-\Delta_{\alpha_0}^I) &:= \left\{ \psi \in W^{2,2}(I) \,\middle|\, \psi' + \mathrm{i}\alpha_0 \psi = 0 \quad \text{at} \quad \partial I \right\}. \end{aligned} \tag{II.16}$$

The latter operator has been extensively studied in [18]. It was shown that it is an m-sectorial and quasi-self-adjoint operator. It has purely discrete spectrum, its lowest lying point we denote as μ_0^2. It holds that $\mu_0^2 := \min\left\{\alpha_0^2, \left(\frac{\pi}{d}\right)^2\right\}$. Our main conclusion about the spectrum of H_{α_0} is the following:

Proposition II.2.1 ([26, Prop. 2.1])**.**
Let $\alpha_0 \in \mathbb{R}$. Then

$$\sigma(H_{\alpha_0}) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = [\mu_0^2, +\infty). \tag{II.17}$$

There are several different definitions of the essential spectra in the literature. For the self-adjoint operators they coincide, however, this needs not to be true when the operator is non-self-adjoint and the various essential spectra can differ significantly. We employ the definition via so-called singular sequences – for a closed operator A we say that $\lambda \in \mathbb{C}$ belongs to the essential spectrum of A (denoted $\sigma_{\mathrm{ess}}(A)$) if there exists a sequence $(\psi_n)_{n=1}^{+\infty}$ (called a singular sequence), $\|\psi_n\|_{\mathscr{H}} = 1$ for all n, such that it does not contain any convergent subsequence and $\lim_{n\to+\infty}(T-\lambda)\psi_n = 0$. Other definitions are based e.g. on the violation of the Fredholm property (i.e. range of the studied operator is not closed or its kernel or cokernel are not finite-dimensional). However, many of these different essential spectra coincide, provided the resolvent set is connected, as it is in our case.

Further on we study the perturbed waveguide, where the function α from the boundary conditions takes the form

$$\alpha(x) = \alpha_0 + \varepsilon\beta(x). \tag{II.18}$$

Here $\beta \in W^{2,\infty}(\mathbb{R}^n)$ and $\varepsilon > 0$. The stability of the essential spectrum is ensured when the boundary conditions approach uniform boundary conditions in infinity.

Theorem II.2.2 ([26, Thm. 2.3])**.**
Let $\alpha - \alpha_0 \in W^{1,\infty}(\mathbb{R})$ with $\alpha_0 \in \mathbb{R}$ such that

$$\lim_{|x|\to+\infty}(\alpha-\alpha_0)(x) = 0 \tag{II.19}$$

Then

$$\sigma_{\mathrm{ess}}(H_\alpha) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = [\mu_0^2, +\infty). \tag{II.20}$$

In the rest of the paper we search for conditions under which a small perturbation allows the existence of a bound state, i.e. of an isolated eigenvalue with finite geometric multiplicity. Due to the singularity of the resolvent this effect can be expected when the effective infinite dimension of the problem is 1 or 2. (We expand on this in the end of the section.) Our method of ensuring its existence works under the assumtion of a sufficiently fast decay of β in infinity, which is summarized in technical conditions

$$\begin{aligned} \lim_{|x|\to+\infty} |x|^{5+\delta}\,\beta(x) &= 0,\\ \lim_{|x|\to+\infty} |x|^{5+\delta}\,\partial_{x_1}\beta(x) &= 0,\\ \lim_{|x|\to+\infty} |x|^{5+\delta}\,\partial_{x_1}^2\beta(x) &= 0, \end{aligned} \tag{II.21}$$

for $n = 1$ and

$$\begin{aligned} \lim_{|x|\to+\infty} |x|^{4+\delta}\,\beta(x) &= 0,\\ \lim_{|x|\to+\infty} |x|^{4+\delta}\,\partial_{x_j}\beta(x) &= 0,\\ \lim_{|x|\to+\infty} |x|^{4+\delta}\,\partial_{x_j}^2\beta(x) &= 0, \end{aligned} \tag{II.22}$$

for $n = 2$ with $j = 1, 2$ for some $\delta > 0$. Using different estimates in the proofs they could be possibly improved. In further text the mean value of β is denoted as $\langle\beta\rangle := \int_{\mathbb{R}^n}\beta(x)\,\mathrm{d}x$.

Theorem II.2.3 ([26, Thm. 2.4]).
Let (II.21) *if* $n = 1$ *or* (II.22) *if* $n = 2$ *with* $\beta \in W^{2,\infty}(\mathbb{R}^n)$. *If* $\varepsilon > 0$ *is sufficiently small and* $|\alpha_0| < \pi/d$, *then* H_α *possesses a unique, simple and real eigenvalue* $\lambda = \lambda(\varepsilon) \in \mathbb{C} \setminus [0, +\infty)$ *if* $\alpha_0 \langle \beta \rangle < 0$. *The asymptotic expansion*

$$\lambda(\varepsilon) = \begin{cases} \mu_0^2 - \varepsilon^2 \alpha_0^2 \langle \beta \rangle^2 + \mathcal{O}(\varepsilon^3), \\ \mu_0^2 - \mathrm{e}^{2/w(\varepsilon)}, \end{cases} \tag{II.23}$$

where $w(\varepsilon) = \frac{\varepsilon}{\pi} \alpha_0 \langle \beta \rangle + \mathcal{O}(\varepsilon^2)$, *holds as* $\varepsilon \to 0$. *If* $\alpha_0 \langle \beta \rangle > 0$, H_α *has no eigenvalues.*

The proof is based on Birman-Schwinger principle. As a first step, we unitarily transform H_α to $H_{\alpha_0} + W_\varepsilon$, where W_ε is a differential operator which can be decomposed as $W_\varepsilon = \varepsilon C_\varepsilon^* D$. Then we first prove that $\lambda \in \sigma_p(H_\alpha)$ if and only if $-1 \in \sigma_p(K_\varepsilon^\lambda)$, where $K_\varepsilon^\lambda := \varepsilon D (H_{\alpha_0} - \lambda)^{-1} C_\varepsilon^*$. From the integral representation of this Green function we deduce the eigenvalue asymptotics.

When $\alpha_0 > \pi/d$, we are unable to say anything about the eigenvalue. To do so it would be necessary to take higher terms in the expansion of λ, which turns out to be computationally challenging by the present method. We would encounter similar difficulties when trying to obtain more than just the leading term in the asymptotic expansion(II.23) to check the equality situation $\alpha_0 \langle \beta \rangle = 0$.

We have just seen that the existence of the weakly coupled bound state is conditioned by fulfilment of $\alpha_0 \langle \beta \rangle < 0$. Both α_0 and β play equivalent role in the boundary conditions – they cause a non-zero probability current over each component of the boundary. However, the negative sign of their product means, that they generate the probability current against each other. We may conclude that the weakening of the probability current through the waveguide due to the small perturbation is responsible for the existence of the bound state.

Note the important role of the singularity of the resolvent function on the existence of the bound state. For this purpose it was necessary for K_ε^λ to have an eigenvalue -1, a necessity for this is $\|K_\varepsilon^\lambda\| \geq 1$. It would not be possible in the limit $\varepsilon \to 0$ if the resolvent function inside K_ε^λ had not a singularity in the limit $\lambda \to \mu_0^2$. Since the resolvent function in dimension $n \geq 3$ does not possess a singularity, it can not be expected that a weak perturbation of the boundary would yield a bound state. More likely there would be a critical value of the parameter ε, giving a lower bound on ε enabling a bound state.

II.3 Kramers-Fokker-Planck equation

Many real-world physical systems are subjected to small forces and influences which are complicated to describe and are usually referred to as noise or fluctuations. (Applications range from solid-state physics to circuit theory.) These are impossible to describe due to huge amount of unknown variables and can only be included in the equation as an influence of a random outside force. One of the simplest examples of this phenomenon is Brownian motion – the position of a macroscopic particles submerged in fluid randomly moves as a consequence of collisions with molecules of the fluid. We can locate the particle in a certain region only with some probability. With Fokker-Planck equation [14, 28] we are able to determine this probability.

The Kramers equation is a special Fokker-Planck equation describing the Brownian motion in an external field. This equation was derived and used by H. A. Kramers [17] to describe kinetics of chemical reaction. Later on it turned out that it has more general applicability to different fields such as supersonic conductors, Josephson tunneling junction and relaxation of dipoles ([29]). Mathematical analysis of the Kramers-Fokker-Planck (KFP, in short) equation is initially motivated by trend to equilibrium for confining potentials ([8]). Spectral problems of the KFP operator reveal to be quite interesting, because this operator is neither elliptic nor self-adjoint. After appropriate setting of physical constants and a change of unknowns, the time-dependent KFP equation can be written into the form

$$\partial_t u(t;x,v) + Pu(t;x,v) = 0, \tag{II.24}$$

where $(x,v) \in \mathbb{R}^n \times \mathbb{R}^n$, $t > 0$, with initial data

$$u(0;x,v) = u_0(x,v). \tag{II.25}$$

Here x and v represent respectively position and velocity of the particle, P is the KFP operator given by

$$P = -\Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2} + v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v, \tag{II.26}$$

where the potential $V(x)$ is supposed to be a real-valued $C^1(\mathbb{R}^n)$ function.

In literature one can find many different types of studied potential. If $V(x) \geq C|x|$ for some constant $C > 0$ outside some compact set, then it is known (see e.g. [8, 15]) that the state of the particle approaches exponentially fast the equilibrium state $\mathfrak{m}$:

$$u(t) - \langle u_0, \mathfrak{m} \rangle\, \mathfrak{m} = O(e^{-\sigma t}) \tag{II.27}$$

as $t \to +\infty$ in $L^2(\mathbb{R}^{2n})$, where $\sigma > 0$ can by evaluated in terms of spectral gap between zero eigenvalue and the real part of the other eigenvalues of P. Here $\mathfrak{m}$ is an eigenfunction corresponding to a discrete eigenvalue zero which is defined as

$$\mathfrak{m}(x,v) = \frac{1}{(2\pi)^{\frac{n}{4}}} e^{-\frac{1}{2}(\frac{v^2}{4}+V(x))}. \tag{II.28}$$

If we assume that and $V(x)$ is normalized by $\int_{\mathbb{R}^n} e^{-V(x)}\,\mathrm{d}x = 1$, then indeed $\mathfrak{m} \in L^2(\mathbb{R}^{2n}_{x,v})$.

If $V(x)$ increases slowly, $V(x) \sim c\,\langle x\rangle^{\beta}$ for some constant $c > 0$ and $\beta \in (0,1)$, then zero is an eigenvalue embedded in the essential spectrum of P and it is known that (II.27) still holds with the right-hand side replaced by $O(t^{-\infty})$ ([11]).

The function $\mathfrak{M} = \mathfrak{m}^2$ is conventionally called the Maxwellian ([24]) and represents the equilibrium state of the system. Note that $\mathfrak{m}$ always satisfies the stationary KFP equation

$$P\mathfrak{m} = 0 \tag{II.29}$$

on $\mathbb{R}^{2n}_{x,v}$, regardless whether it lies in $L^2(\mathbb{R}^{2n}_{x,v})$ or not. When the latter is true, it will represent just a resonance of the operator.

In contrast to previous cases, we are interested in the study of potentials verifying

$$|V(x)| + \langle x\rangle\,|\nabla V(x)| \leq C\,\langle x\rangle^{-\rho} \tag{II.30}$$

for $x \in \mathbb{R}^n$ and $\rho \in \mathbb{R}$. It is known that for decreasing potentials ($\rho > 0$), zero is no longer an eigenvalue of P. It is proved in [36] that for $n = 3$ and $\rho > 2$, one has

$$u(t) = \frac{1}{(4\pi t)^{\frac{3}{2}}}\,\langle u_0, \mathfrak{m}\rangle\,\mathfrak{m} + O\left(\frac{1}{t^{\frac{3}{2}+\varepsilon}}\right), \tag{II.31}$$

as $t \to +\infty$, $\varepsilon > 0$ in some weighted spaces. The equation (II.31) shows that for rapidly decreasing potentials, space distribution of particles is still governed by the Maxwellian, but the density of distribution decreases in time in the same rate as heat propagation. Time-decay estimates of local energies are also obtained in [36] for short-range potentials ($\rho > 1$) and in [20] for long-range potentials ($0 < \rho \leq 1$).

The situation of interest here is one dimensional KFP equation with quickly decreasing potential. Our goal was to obtain a result similar to (II.31) – a long-time asymptotic behaviour of solutions of (II.24). From the point of view of spectral analysis, this is closely related to low-energy spectral properties of P. It is known that for Schrödinger operators, low-energy spectral analysis in one and two dimensional cases is more difficult than in higher dimensions and needs specific methods ([3]) because threshold zero is already a resonance of the Laplacian in dimension one and two. For the KFP operator with decreasing potentials, the notions of thresholds and threshold resonances are discussed in [36]. Although $\mathfrak{m}$ always satisfies the stationary KFP equation $P\mathfrak{m} = 0$, a basic fact is that $\langle x \rangle^{-s} \mathfrak{m} \notin L^2(\mathbb{R}^{2n})$ if $n \geq 3$ and $1 < s < \frac{n}{2}$, while $\langle x \rangle^{-s} \mathfrak{m} \in L^2(\mathbb{R}^{2n})$ for any $s > 1$ if $n = 1, 2$. In language of threshold spectral analysis, this means that for $n \geq 3$, zero is not a resonance of P while for $n = 1, 2$, zero is a resonance of P with $\mathfrak{m}$ as a resonant state. This is the main difference between the present work and [36].

We decompose P as $P = P_0 + W$ where

$$\begin{aligned} P_0 &= v \cdot \nabla_x - \Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2} \\ W &= -\nabla_x V(x) \cdot \nabla_v. \end{aligned} \tag{II.32}$$

P_0 and P are regarded as operators in $L^2(\mathbb{R}^{2n})$ with the maximal domain. They are then maximally accretive. Denote e^{-tP_0} and e^{-tP}, $t \geq 0$, the strongly continuous semigroups generated by $-P_0$ and $-P$, respectively. If $\rho > -1$, W is a relatively compact perturbation of the free KFP operator P_0: $W(P_0 + 1)^{-1}$ is a compact operator in $L^2(\mathbb{R}^{2n})$. One can prove that

$$\sigma_{\text{ess}}(P) = \sigma(P_0) = [0, +\infty) \tag{II.33}$$

and that non-zero complex eigenvalues of P have positive real parts and may accumulate only towards points in $[0, +\infty)$. It is unknown for decreasing potentials whether or not the complex eigenvalues do accumulate towards some point in $[0, +\infty)$.

The main result is the following:

Theorem II.3.1 ([27, Prop. 2.1])**.**
Let $n = 1$ and $\rho > 4$. Then for any $s > \frac{5}{2}$, there exists some $\varepsilon > 0$ such that

$$e^{-tP} = \frac{1}{(4\pi t)^{\frac{1}{2}}} \left(\langle \cdot, \mathfrak{m} \rangle \, \mathfrak{m} + O(t^{-\varepsilon}) \right) \tag{II.34}$$

as $t \to +\infty$ as operators from $L^{2,s}$ to $L^{2,-s}$, where

$$L^{2,r} = L^2(\mathbb{R}^{2n}_{x,v}; \langle x \rangle^{2r} \; \mathrm{d}x \, \mathrm{d}v) \tag{II.35}$$

for $r \in \mathbb{R}$.

To prove (II.34), the main task is to show that the resolvent $R(z) = (P - z)^{-1}$ has an asymptotics of the form

$$R(z) = \frac{1}{2\sqrt{z}} \langle \cdot, \mathfrak{m} \rangle + O(|z|^{-\frac{1}{2}+\varepsilon}) \tag{II.36}$$

as operators from $L^{2,s}$ to $L^{2,-s}$, for z near zero and $z \notin \mathbb{R}_+$. Although (II.36) and the decay assumption on the potential look the same as the resolvent asymptotics of one dimensional Schrödinger operators in the case where zero is a resonance but not an eigenvalue ([3]), its proof is quite different from the Schrödinger case. In fact, the known methods for the Schrödinger operator cannot be applied to the KFP operator, mainly because the perturbation W is a first order differential operator. In this work we uses the method of [36] to calculate the low energy asymptotic expansion for the free resolvent $R_0(z) = (P_0 - z)^{-1}$ of the form

$$R_0(z) = \frac{1}{\sqrt{z}} G_{-1} + G_0 + \sqrt{z} G_1 + \dots \tag{II.37}$$

in appropriate spaces, where G_{-1} is an operator of rank one. By a careful analysis of the space $\mathcal{N}$ of resonant states of P defined by

$$\mathcal{N} = \{u; u \in \mathscr{H}^{1,-s}, \forall s > 1 \text{ and } Pu = 0\}, \tag{II.38}$$

we prove that $1 + G_0 W$ is invertible on $L^{2,-s}$, $s > \frac{3}{2}$. (II.36) is derived from the equation

$$R(z) = D(z)(1 + M(z))^{-1} R_0(z) \tag{II.39}$$

for z near zero and $z \notin \mathbb{R}_+$, where

$$\begin{aligned} D(z) &= (1 + R_1(z)W)^{-1}, \\ M(z) &= \frac{1}{\sqrt{z}} G_{-1} W D(z), \end{aligned} \tag{II.40}$$

with $R_1(z) = R_0(z) - \frac{1}{\sqrt{z}} G_{-1}$. As in threshold spectral analysis for Schrödinger operators, non-trivial problem here is to compute the value of some spectral constants involving the resonant state of P. Indeed, in most part of this work only the condition $\rho > 2$ is needed. The stronger assumption $\rho > 4$ is used to show that some number $m(z)$ is nonzero for z near zero and $z \notin \mathbb{R}_+$, which allows to prove the invertibility of $1 + M(z)$ and to calculate its inverse. Note that this result in particular implies that zero is not the accumulation point of complex eigenvalues.

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Publications connected with thesis

This chapter contains full texts of research papers written during the PhD studies. These are (chronologically):

1. Novák R.: *On the Pseudospectrum of the Harmonic Oscillator with Imaginary Cubic Potential*, International Journal of Theoretical Physics 54(11), pp. 4142-4153, 2015
2. Novák R.: *Bound states in waveguides with complex Robin boundary conditions*, Asymptotic Analysis 96(3-4), pp. 251-281, 2016
3. Novák R., Wang X. P.: *On the Kramers-Fokker-Planck equation with decreasing potentials in dimension one*, to appear in Journal of Spectral Theory, 2018

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On the Pseudospectrum of the Harmonic Oscillator with Imaginary Cubic Potential

Radek Novák

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Abstract We study the Schrödinger operator with a potential given by the sum of the potentials for harmonic oscillator and imaginary cubic oscillator and we focus on its pseudospectral properties. A summary of known results about the operator and its spectrum is provided and the importance of examining its pseudospectrum as well is emphasized. This is achieved by employing scaling techniques and treating the operator using semiclassical methods. The existence of pseudoeigenvalues very far from the spectrum is proven, and as a consequence, the spectrum of the operator is unstable with respect to small perturbations and the operator cannot be similar to a self-adjoint operator via a bounded and boundedly invertible transformation. It is shown that its eigenfunctions form a complete set in the Hilbert space of square-integrable functions; however, they do not form a Schauder basis.

Keywords Pseudospectrum · Harmonic oscillator · Imaginary qubic potential · $\mathcal{PT}$-symmetry · Semiclassical method

1 Introduction

One of the first observations of purely real spectrum in a non-self-adjoint Schrödinger operator occured in [6] by Caliceti et al. The authors studied the class of operators $-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \beta x^{2n+1}$ on $L^2(\mathbb{R})$ for a general complex β and noticed that the

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spectrum is real provided $\arg(\beta) = \pi/2$ and β is sufficiently small. This property was later attributed to the PT-symmetry of the considered operator. The so-called $\mathcal{PT}$-symmetric quantum mechanics originated with the numerical observation of a purely real spectrum of an imaginary cubic oscillator Hamiltonian [5] and rapidly developed thenceforth. See e.g. [4, 21] and references therein for a survey of papers in this area. The $\mathcal{PT}$-symmetry property of an operator H should be understood in this paper as the invariance of H with respect to the space inversion and the time reversal on the Hilbert space $L^2(\mathbb{R})$, i.e.

$$[H, \mathcal{PT}] = 0 \tag{1.1}$$

in the operator sense, where $(\mathcal{P}\psi)(x) := \psi(-x)$ stands for spatial reflection and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$ stands for time reversal in quantum mechanics. Such operator possesses a relevant physical interpretation as an observable in quantum mechanics provided it is similar to a self-adjoint operator

$$h = \Omega H \Omega^{-1}, \tag{1.2}$$

where Ω is a bounded and boundedly invertible operator. Then it is ensured that the spectra of h and H are identical and that the corresponding families of eigenfunctions share essential basis properties [19]. The similarity to a self-adjoint operator is in fact equivalent to the quasi-self-adjointness of H,

$$H^*\Theta = \Theta H, \tag{1.3}$$

where the operator Θ is positive, bounded and boundedly invertible [17, 23]. It is often called a metric, since the operator H can be seen as self-adjoint in the space with the modified scalar product $(\cdot, \Theta\cdot)$. The equivalence can be easily seen from the decomposition of a positive operator $\Theta = \Omega^*\Omega$ [18, Prop. 1.8].

In recent years it has been shown that the spectrum is not necessarily the best notion to describe properties of a non-self-adjoint operator and the use of ε-pseudospectrum, denoted here $\sigma_\varepsilon(H)$ and defined as

$$\sigma_\varepsilon(H) := \left\{ \lambda \in \mathbb{C} \;\middle|\; \left\| (H - \lambda)^{-1} \right\| > \varepsilon^{-1} \right\}, \tag{1.4}$$

was suggested instead [7, 11, 16, 18, 19, 25, 27]. In [25] authors studied the operator $-\mathrm{d}^2/\mathrm{d}x^2 + \mathrm{i}x^3$ and derived completeness of its eigenfunctions, found the bounded metric operator Θ and proved that it can not have a bounded inverse. These results were further supplemented in [19] where the existence of points in the pseudospectrum far from the spectrum was established. This paper aims to apply the methods used in these papers to the operator $-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \mathrm{i}x^3$, whose several properties were investigated e.g. in [6, 10, 14, 20]. Our aim is to establish results which can be directly extended to the more general case $-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \mathrm{i}x^{2n+1}$, $n \geq 1$. We choose to study the case $n = 1$ to show its relation to the famous imaginary cubic oscillator.

Let us consider the Hilbert space $L^2(\mathbb{R})$ and define the operator H acting on its maximal domain:

$$\begin{aligned} H &:= -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \mathrm{i}x^3, \\ \mathrm{Dom}(H) &:= \left\{ \psi \in W^{2,2}(\mathbb{R}) \;\middle|\; -\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + x^2\psi + \mathrm{i}x^3\psi \in L^2(\mathbb{R}) \right\}. \end{aligned} \tag{1.5}$$

It was shown in [6] that $\mathrm{Dom}(H)$ coincides with $\left\{ \psi \in W^{2,2}(\mathbb{R}) \;\middle|\; x^3\psi \in L^2(\mathbb{R}) \right\}$ and that H is closed. Furthermore, it is an operator with compact resolvent and therefore its spectrum is discrete (i.e. consists of isolated eigenvalues of finite algebraic multiplicity). The reality and the simplicity of the eigenvalues was established in [24]. Using the approach of

[13, Sec. VII.2] shows that H coincides with the closure of (1.5) defined on smooth functions with compact support and that it is an m-accretive operator. Recall that this means that H is closed and that $\{\lambda \in \mathbb{C} \mid \Re\lambda < 0\} \subset \rho(H)$ and $\|(H-\lambda)^{-1}\| \leq 1/|\Re\lambda|$ for $\Re\lambda < 0$. In this paper we contribute to these results with showing the non-triviality of the pseudospectrum of H and demonstrating its several consequences. The main results are summarised in the following theorem.

Theorem 1 *Let H be the operator defined in* (1.5)*. Then:*

1. *The eigenfunctions of H form a complete set in $L^2(\mathbb{R})$.*
2. *The eigenfunctions of H do not form a (Schauder) basis in $L^2(\mathbb{R})$.*
3. *For any $\delta > 0$ there exist constants $A, B > 0$ such that for all $\varepsilon > 0$ small,*

$$\left\{\lambda \in \mathbb{C} \,\middle|\, |\lambda| > A,\ |\arg\lambda| < \arctan \Re\lambda - \delta,\ |\lambda| \geq B\left(\log\frac{1}{\varepsilon}\right)^{6/5}\right\} \subset \sigma_\varepsilon(H). \quad (1.6)$$

4. *H is not similar to a self-adjoint operator via bounded and boundedly invertible transformation*
5. *H is not quasi-self-adjoint with a bounded and boundedly invertible metric.*
6. *$-\mathrm{i}H$ is not a generator of a bounded semigroup.*

We can see that for any ε the pseudospectrum contains complex points with positive real part, non-negative imaginary part and large magnitude. This result is in particular important in view of the characterisation of pseudospectrum (2.3)—it implies the existence of pseudomodes very far from the spectrum. This non-trivial behaviour of the pseudospectrum was without details announced in [25]. A numerical computation of several of the pseudospectral lines of H can be seen in Fig. 1. As a consequence of the last point in Theorem 1, the time-dependent Schrödinger equation with H does not admit a bounded time-evolution. For more details about establishing a time-evolution of an unbounded non-self-adjoint operator we refer to recent papers [1, 2] and to references therein.

This paper is organised as follows. In Section 2 we formulate some properties of pseudospectrum to emphasize its importance in the study of non-self-adjoint operators. In Section 3 we develop a semiclassical technique applicable in the study of pseudospectrum of the present model. The proof of the main theorem of the paper about pseudospectrum and eigenfunctions of H can be found in Section 4. The Section 5 is devoted to a discussion of the results and of their consequences.

2 General Aspects of the Pseudospectrum

The definition of the pseudospectrum and some of its most prominent properties are presented in this section. The focus is on properties related to this paper, which were already highlighted in [19], where the authors dealt with similar problems. The presented list is far from complete and we refer to the monographs [9, 27] for more details on this subject.

Let H be a closed densely defined operator on a complex Hilbert space $\mathscr{H}$. Its spectrum $\sigma(H)$ is defined as the set of complex points λ for which the operator $(H-\lambda)^{-1}$ does not exist or is not bounded on $\mathscr{H}$. The complement of this set in $\mathbb{C}$ is called the resolvent set of H. It is a well known fact that the spectrum of a bounded linear operator is contained in the closure of its numerical range $\Theta(H) = \{(\psi, H\psi) \mid \psi \in \mathscr{H}, \|\psi\| = 1\}$. Moreover, this holds for closed unbounded operators as well, provided the exterior of the numerical range

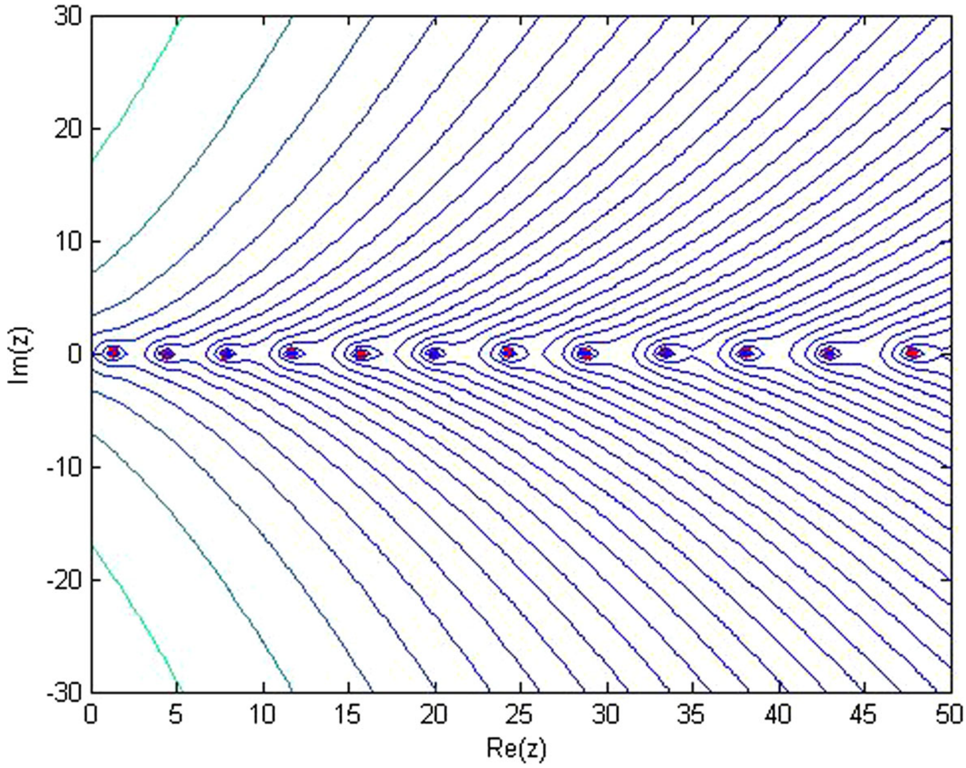

Fig. 1 Spectrum (*red dots*) and ε-pseudospectra (enclosed by *blue-green* contour lines) of harmonic oscillator with imaginary cubic potential. The border of the ε-pseudospectrum is plotted for the values $\varepsilon = 10^{-7}, 10^{-6.75}, 10^{-6.5}, \ldots, 10^{1}$, the green contour lines correspond to large values of ε, the blue ones correspond to smaller values of ε. We notice that for each ε from the selected range the contour lines quickly diverge and therefore the corresponding ε-pseudospectrum contains points very far from the real axes. More details about the used computational method can be found in [26]

in $\mathbb{C}$ is a connected set and has a non-empty intersection with the resolvent set of H. The ε-pseudospectrum (or simply pseudospectrum) of H is defined as

$$\sigma_\varepsilon(H) := \left\{ \lambda \in \mathbb{C} \;\middle|\; \left\| (H-\lambda)^{-1} \right\| > \varepsilon^{-1} \right\}, \tag{2.1}$$

with the convention that $\|(H-\lambda)^{-1}\| = +\infty$ for $\lambda \in \sigma(H)$. In other words, $\sigma(H) \subset \sigma_\varepsilon(H)$ for every ε from the definition and from the inequality $\|(H-\lambda)^{-1}\| \geq \operatorname{dist}(\lambda, \sigma(H))^{-1}$ we can easily see that also an ε-neighbourhood of the spectrum is contained in the pseudospectrum. Similarly as in the previous case, if the exterior of the numerical range in $\mathbb{C}$ is a connected set and has a non-empty intersection with the resolvent set of H, the pseudospectrum is in turn contained in the ε-neighbourhood of the numerical range, i.e. altogether we have

$$\{\lambda \in \mathbb{C} \mid \operatorname{dist}(\lambda, \sigma(H)) < \varepsilon\} \subset \sigma_\varepsilon(H) \subset \left\{ \lambda \in \mathbb{C} \;\middle|\; \operatorname{dist}(\lambda, \overline{\Theta(H)}) < \varepsilon \right\}. \tag{2.2}$$

Perhaps the most striking property of pseudospectrum is provided by the result sometimes known as Roch-Silberman theorem [22]. The ε-pseudospectrum of H may be expressed via the spectra of all perturbations of H of size less than ε:

$$\sigma_\varepsilon(H) = \bigcup_{\|V\| < \varepsilon} \sigma(H+V). \tag{2.3}$$

This result is especially important in the study of non-self-adjoint operators. For operators with highly non-trivial pseudospectrum (i.e. not contained in some bounded neighbourhood of the spectrum) it reveals their spectral instability with respect to small perturbations. It also shows a difficulty in the numerical study of operators with wild pseudospectra—small rounding errors can lead to computing (false) eigenvalues, which are in fact very far from the true spectrum.

The pseudospectrum can also by characterised as the set of all points of the spectrum and of all pseudoeigenvalues (or approximate eigenvalues), i.e.

$$\sigma_\varepsilon(H) = \{\lambda \in \mathbb{C} \mid \lambda \in \sigma(H) \vee (\exists \psi \in \mathrm{Dom}(H)) (\|(H-\lambda)\psi\| < \varepsilon\|\psi\|)\}. \tag{2.4}$$

Any ψ satisfying the inequality in (2.4) is called a pseudoeigenvector (or pseudomode). It can be easily seen that pseudoeigenvalues can be turned into eigenvalues by a small perturbation. If H were to represent a physical observable and V its perturbation, this fact would cause some highly unintuitive behaviour of its energies.

3 Semiclassical Techniques

The use of semiclassical techniques in the study of non-self-adjoint operators was first suggested in [7], and the idea was further developed e.g. in [11, 28]. Let H_h be an operator acting in $L^2(\mathbb{R})$ of the form

$$H_h := -h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_h(x). \tag{3.1}$$

Here V_h are analytic potentials in x for all $h > 0$ small enough which take the form $V_h(x) = V_0(x) + \widetilde{V}(x,h)$, where $\widetilde{V}(x,h) \to 0$ locally uniformly as $h \to 0$. This operator should be understood as some closed extension of an operator originally defined on $C_c^\infty(\mathbb{R})$. The following theorem is an analogue of [7, Thm. 1] for a potential depending on h.

Theorem 2 *Let H_h be defined as above and let λ be from the set*

$$\Lambda := \left\{\xi^2 + V_h(x) \;\middle|\; (x,\xi) \in \mathbb{R}^2, \xi\, \Im V_h'(x) < 0\right\}, \tag{3.2}$$

where the dash denotes standard differentiation with respect to x in $\mathbb{R}$. Then there exists some $C = C(\lambda) > 1$, some $h_0 = h_0(\lambda) > 0$, and an h-dependent family of $C_c^\infty(\mathbb{R})$ functions $\{\psi_h\}_{0<h\le h_0}$ with the property that, for all $0 < h \le h_0$,

$$\|(H_h - \lambda)\psi_h\| < C^{-1/h}\|\psi_h\|. \tag{3.3}$$

The function $f(x,\xi) := \xi^2 + V_h(x)$ is called the symbol associated with H_h. Note that relation (2.4) gives us that $\lambda \in \sigma_\varepsilon(H_h)$ for all $\varepsilon \ge C(\lambda)^{-1/h}$. Here ε can get arbitrarily close to 0, provided h is sufficiently small. The closure of Λ is usually called the semiclassical pseudospectrum [11]. Application of Theorem 2 to non-semiclassical operators is sometimes possible by using scaling techniques and sending the spectral parameter to infinity. This is based on a more general principle that the semiclassical limit is equivalent to the high-energy limit after a change of variables.

Proof The proof is inspired by the proof of [19, 1]. We are interested in the case when h is very close to 0, during the course of the proof we are not going to stress every occasion when this plays a role. We can assume h to be "sufficiently small" when necessary. Let $\lambda = \xi_0^2 + V_h(x_0)$ and assume $\xi_0 \neq 0$, $\Im V_h'(x_0) \neq 0$. Let us notice that λ is dependent on h from definition so changing h in the course of our proof would mean changing λ as well. This problem can be overcome by fixing $\lambda \in \Lambda$ and introduce a dependence of x and ξ on h

in such a way that $\lambda = \tilde{\xi}(h)^2 + V_h(\tilde{x}(h))$, where $\tilde{\xi}(h) \to \xi_0$ and $\tilde{x}(h) \to x_0$ as $h \to 0$. The existence of these functions is ensured by the implicit function theorem. Since we only need to find one function for which (3.3) holds, the main idea is that the sought pseudomode will arise from JWKB approximation of the solution to $(H_h - \lambda)u = 0$ which takes the form

$$u(x,h) := \mathrm{e}^{\mathrm{i}\phi(x,h)/h} \sum_{j=0}^{N(h)} h^j a_j(x,h), \tag{3.4}$$

where $a_j(x,h)$ are functions analytic near x_0. We follow here the procedure of constructing appropriate functions ϕ and a_j as shown e.g. in [12, Chap. 2]. The function ϕ should satisfy the eikonal equation

$$f(x, \phi'(x,h)) - \lambda = 0, \tag{3.5}$$

where f is the symbol associated with H_h. (The dash denotes differentiation with respect to x.) From this equation immediately follows that $\phi'(x,h) = \pm\sqrt{\lambda - V_h(x)}$. The sign is determined by the condition $\xi\, \Im V_h'(x) < 0$ applied in the point $(x_0, \phi'(x_0,h))$ and remains the same for all h. Therefore the sign of $\phi'(x_0,h)$ should be opposite of the sign of $\Im V_h'(x_0)$. Therefore we get

$$\phi(x,h) = -\mathrm{sgn}\left(\Im V_h'(x_0)\right) \int_0^x \sqrt{\lambda - V_h(y)}\, \mathrm{d}y. \tag{3.6}$$

We need to check whether ϕ' is analytic near x_0 for h small. From the assumption we know that $\Im V_h'(x_0) \neq 0$, so there exists $\delta > 0$ such that $\Im V_h'(\tilde{x}) \neq 0$ for $\tilde{x} \in [x_0 - \delta, x_0 + \delta]$. Then for every $\tilde{x} = x_0 + \varepsilon(h)$, where $0 < |\varepsilon| < \delta$ and $\varepsilon(h) \to 0$ as $h \to 0$, we get

$$\Im V_h(\tilde{x}) - \Im\lambda = \Im V_h(\tilde{x}) - \Im V_0(x_0) = \varepsilon(h)\left(\Im V_0'(x_0) + \mathcal{O}(\varepsilon(h))\right) + \widetilde{V}(\tilde{x},h) \tag{3.7}$$

for ε going to 0. Without loss of generality it is possible to assume $\Im V_h'(x_0) > 0$, therefore δ can be fixed so that $\Im V_0'(x_0) + \mathcal{O}(\varepsilon) > C'$ for some $C' > 0$. Taking h small, $\widetilde{V}(\tilde{x},h)$ gets close to 0 uniformly and $|\tilde{x} - x_0| < \delta$, thus $\Im V_h(\tilde{x}) - \Im\lambda > 0$ and consequently the square root in the definition of ϕ' is well-defined. The case $\Im V_h'(x_0) < 0$ is proven in the same manner. After a translation we can assume further on $x_0 = 0$.

The equality

$$\mathrm{e}^{-\mathrm{i}\phi/h}\,(H_h - \lambda)\,\mathrm{e}^{\mathrm{i}\phi/h} = \frac{2h}{\mathrm{i}}\left(\phi'\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2}\phi''\right) - h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{3.8}$$

can be verified with a direct computation. If we set a_j so that they satisfy the transport equations

$$\begin{aligned} \phi'(x,h)a_0'(x,h) + \frac{1}{2}\phi''(x,h)a_0(x,h) &= 0, \\ \phi'(x,h)a_j'(x,h) + \frac{1}{2}\phi''(x,h)a_j(x,h) &= \frac{\mathrm{i}}{2}a_{j-1}''(x,h) \end{aligned} \tag{3.9}$$

for $j > 0$, we get that

$$\mathrm{e}^{-\mathrm{i}\phi(x,h)/h}\,(H_h - \lambda)\,\mathrm{e}^{\mathrm{i}\phi(x,h)/h}\left(\sum_{j=0}^{N} h^j a_j(x,h)\right) = -h^{N+2}a_N''(x,h). \tag{3.10}$$

We can also set $a_0(x_0, h) = 1$ and $a_j(x_0, h) = 0$ for $j > 0$ and all h. The (3.9) can be then solved using the method of integrating factor as

$$\begin{aligned} a_0(x, h) &= \frac{\sqrt{\phi'(x_0, h)}}{\sqrt{\phi'(x, h)}}, \\ a_j(x, h) &= \frac{1}{\sqrt{\phi'(x_0, h)}} \int_0^x \frac{\mathrm{i}\, a_j''(y, h)}{2\sqrt{\phi'(y, h)}} \mathrm{d}y. \end{aligned} \tag{3.11}$$

These functions are well defined and analytic near x_0 thanks to analyticity of ϕ'. We now proceed with estimates of the functions a_j. Note that since the potentials $V_h(x)$ are analytic, we can naturally extend them into the complex plane in the neighbourhood of $x_0 = 0$ and thus the same can be applied on ϕ and all a_j. Our goal is to arrive to the estimate

$$|a_j(x, h)| \leq C_1^{j+1} j^j \tag{3.12}$$

for $C_1 > 0$ and x in some neighbourhood of the origin. Then we will be able to define the h-dependent function

$$a(x, h) := \sum_{0 \leq j \leq (\mathrm{e}C_1 h)^{-1}} h^j a_j(x, h), \tag{3.13}$$

which is uniformly bounded analytic function on the set where (3.12) holds due to the absolute summability of the sum

$$|a(x, h)| \leq C_1 \sum_{0 \leq j \leq (\mathrm{e}C_1 h)^{-1}} C_1^j h^j j^j \leq C_1 \sum_{0 \leq j \leq (\mathrm{e}C_1 h)^{-1}} \mathrm{e}^{-j} < +\infty. \tag{3.14}$$

In the following we will derive the estimate (3.12) for a_j extended to the complex plane (further denoted as $a_j(z, h)$). With the natural choice of the norm

$$\|f\|_{B(R)} := \sup \{z \in B(R) \mid |z| < R\}, \tag{3.15}$$

where $B(R)$ is an open ball in the complex plane with center at 0 and diameter R, we easily see that the estimate obtained for $\|a\|_{B(R)}$ will remained valid for $|a(x, h)|$ in some neighbourhood of the origin. We fix R_0 such that, on $B(R_0)$, ϕ is analytic, $|\phi'|$ is bounded from below and above and $\Im\phi''(x, h) > 1/C_2$ for some $C_2 > 0$. We also employ Cauchy's estimate for the second derivative of an analytic bounded function f defined on $B(R)$:

$$|f''(z)| \leq \frac{2\|f\|_{B(R)}}{(R - |z|)^2}. \tag{3.16}$$

With the use of the formula (3.11) we obtain

$$\begin{aligned} |a_j(z, h)| &= \left| \frac{1}{\sqrt{\phi'(z, h)}} \int_0^z \frac{\mathrm{i} a_{j-1}''(\zeta, h)}{2\sqrt{\phi'(\zeta, h)}} \mathrm{d}\zeta \right| \\ &\leq \|(\phi'(\cdot, h))^{-1}\|_{B(R)} \int_0^{|z|} \frac{\|a_{j-1}(\cdot, h)\|_{B(R)}}{(R - t)^2} \mathrm{d}t \\ &= \|(\phi'(\cdot, h))^{-1}\|_{B(R)} \|a_{j-1}(\cdot, h)\|_{B(R)} \left(\frac{1}{R - |z|} - \frac{1}{R} \right) \\ &= \frac{|z|}{R(R - |z|)} \|(\phi'(\cdot, h))^{-1}\|_{B(R)} \|a_{j-1}(\cdot, h)\|_{B(R)} \end{aligned} \tag{3.17}$$

for $j = 0, 1, \ldots$. We iterate these estimates on balls of radius $R_k := (1 - k/2j)\, R_0$, $k = 0, \ldots, j-1$. Then we have for $|z| < R_j$

$$\frac{|z|}{R_k(R_k - |z|)} \leq \frac{|z|}{R_k(R_k - R_{k+1})} \leq \frac{4j|z|}{R_0^2}. \tag{3.18}$$

Then it follows for a_{k+1} that

$$|a_{k+1}(z,h)| \leq \frac{4j|z|}{R_0^2} \|(\phi'(\cdot,h))^{-1}\|_{B(R_0)} \|a_j(\cdot,h)\|_{B(R)}. \tag{3.19}$$

Subsequently using these estimates for $k = 0, \ldots, j-1$ and taking a supremum we obtain

$$\|a_j(\cdot,h)\|_{B(R_0/2)} \leq \|a_j(\cdot,h)\|_{B(R_j)} \leq \|a_0(\cdot,h)\|_{B(R_0)} \left(\frac{2j}{R_0}\|(\phi'(\cdot,h))^{-1}\|_{B(R_0)}\right)^j. \tag{3.20}$$

We see from (3.11) and our choice of R_0 that $\|a_0(\cdot,h)\|_{B(R_0)} < C_3$ and from the uniform estimate of $|\phi(x,h)|$ from below that $\|(\phi'(\cdot,h))^{-1}\|_{B(R_0)} < C_4$, where the positive constants C_3 and C_4 does not depend on h. The desired estimate (3.12) then follows with the constant

$$C_1 := \max\left\{C_3, \frac{2}{R_0}C_4\right\}. \tag{3.21}$$

We are now able to define the desired pseudomode as

$$\psi_h(x) := \mathrm{e}^{\mathrm{i}\phi(x,h)/h}\chi(x)a(x,h), \tag{3.22}$$

where $a(x,h)$ is the function defined in (3.13) and $\chi \in C_c^\infty(\mathbb{R})$ such that it is identically equal to 1 in some neighbourhood of 0 and its support lies inside the interval $(-R_0/2, R_0/2)$. We divide the calculation of the norm in (3.3) as follows:

$$\|(H_h - \lambda)\psi_h\| = \left\|\chi(H_h - \lambda)\mathrm{e}^{\mathrm{i}\phi/h}a\right\| + \left\|[H_h - \lambda, \chi]\,\mathrm{e}^{\mathrm{i}\phi/h}a\right\|. \tag{3.23}$$

First we focus on the first summand. Since $\phi(0,h) = 0$, $\phi'(0,h)$ is real and $\Im\phi''(x,h) > 1/C_2$ holds, we have

$$\left|\mathrm{e}^{\mathrm{i}\phi(x,h)/h}\right| \leq \exp\left(-\frac{x^2}{2C_2h}\right) \tag{3.24}$$

for all $x \in \operatorname{supp}\chi$. Since $\left|\mathrm{e}^{\mathrm{i}\phi/h}\right| > 1$ on $\operatorname{supp}\chi$, we can use (3.10) to estimate

$$\left\|\chi(H_h - \lambda)\mathrm{e}^{\mathrm{i}\phi/h}a\right\| \leq \left\|\chi\mathrm{e}^{\mathrm{i}\phi/h}(H_h - \lambda)\mathrm{e}^{\mathrm{i}\phi/h}a\right\| = \|h^{N+2}a_N''\chi\|, \tag{3.25}$$

where $N = N(h) = \lfloor(\mathrm{e}C_1h)^{-1}\rfloor$. (Here $\lfloor x\rfloor$ denotes the floor function.) Using the estimate from (3.12) and the Cauchy's estimate (3.16) we obtain for all $x \in \operatorname{supp}\chi$ that $|h^{N+2}a_N''(x,h)| \leq C\mathrm{e}^{-1/(Ch)}$ for $C > 0$ independent of h. From this the estimate

$$\left\|\chi(H_h - \lambda)\mathrm{e}^{\mathrm{i}\phi/h}a\right\| \leq C\mathrm{e}^{-1/(Ch)} \tag{3.26}$$

follows. To estimate the second summand in (3.23) we directly calculate

$$[H_h - \lambda, \chi]\,\mathrm{e}^{\mathrm{i}\phi/h}a = -h^2\mathrm{e}^{\mathrm{i}\phi/h}\left(\chi''a + 2\chi'\left(a' + \frac{\mathrm{i}}{h}\phi'a\right)\right). \tag{3.27}$$

Using (3.14) we have uniform bounds on a and thus on a' after the use of the Cauchy's estimate (3.16), ϕ' is bounded by the choice of R_0, χ' and χ'' are identically equal to 0 on $\operatorname{supp}\chi$ and $\mathrm{e}^{\mathrm{i}\phi/h}$ is again bounded by (3.24) we see that (3.27) is in fact equal to 0 on the neighborhood of 0, where χ is constant.

To complete the proof, it remains to show that ψ_h defined in (3.22) is not exponentially small. Since we have established the estimate (3.12) for $|x| < R_0/2$ and $0 \le j \le N = (\mathrm{e}C_1 h)^{-1}$, we have the estimate

$$\left\| \sum_{j=0}^{N} h^j a_j(x,h) \right\|_{B(r)} \le Cr \tag{3.28}$$

for $0 < r \le r_0$, where r_0 is sufficiently small. We can take r very small and fixed, so because $a_0(x,h)$ is close to 1 and $\Im\phi(x,h)$ is close to $\Im\phi''(0,h)x^2/2$ for x small, we obtain

$$\|u(\cdot,h)\| \ge \|u(\cdot,h)\|_{L^2((-r,r))} \ge \frac{1}{C}\left(\int_{-r}^{r} \exp\left(\frac{x^2}{Ch}\right) \mathrm{d}x\right)^{1/2} \ge \frac{1}{C} h^{1/4}. \tag{3.29}$$

□

4 The Proof of Theorem 1

For the sake of clarity we choose to divide the proof into several lemmas.

Lemma 1 *The eigenfunctions of H form a complete set in $L^2(\mathbb{R})$.*

Proof Let us first briefly recall that completeness of $\{\psi_k\}_{k=1}^{+\infty}$ means that the span of ψ_k is dense in $L^2(\mathbb{R})$. Since H is m-accretive, its resolvent is m-accretive as well. It is also a Hilbert-Schmidt operator [6] and the application of [3, Thm. 1.3] yields that it is trace class as well. The completeness of its eigenfunctions follows from [15, Thm. X.3.1]. The completeness of eigenfunctions of H then follows from the application of the spectral mapping theorem [13, Thm.IX.2.3]. □

Lemma 2 *For any $\delta > 0$ there exist constants $C_1, C_2 > 0$ such that for all $\varepsilon > 0$ small,*

$$\left\{ \lambda \in \mathbb{C} \;\middle|\; |\lambda| > A, |\arg\lambda| < \arctan\Re\lambda - \delta, |\lambda| \ge B\left(\log\frac{1}{\varepsilon}\right)^{6/5} \right\} \subset \sigma_\varepsilon(H). \tag{4.1}$$

Proof Using the unitary transformation

$$(U\psi)(x) := \tau^{1/2}\,\psi(\tau x) \tag{4.2}$$

the semiclassical analogue of H is introduced:

$$UHU^{-1} = \tau^3 H_h, \tag{4.3}$$

where

$$H_h := -h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + h^{2/5}x^2 + \mathrm{i}x^3 \tag{4.4}$$

and $h := \tau^{-5/2}$. For the set Λ from Theorem 2 holds $\Lambda = \{\lambda \in \mathbb{C} \mid \Re\lambda > 0, |\arg\lambda| < \arctan\Re\lambda\}$. This theorem gives us that for any $\lambda \in \Lambda$ and h sufficiently small

$$\left\|\left(H - \tau^3\lambda\right)^{-1}\right\| = \tau^{-3}\left\|(H_h - \lambda)^{-1}\right\| > h^{6/5}C(\lambda)^{1/h} \tag{4.5}$$

holds. Let us define the set

$$A_\delta = \{\lambda \in \mathbb{C} \mid |\lambda| = 1, |\arg \lambda| < \arctan \Re\lambda - \delta\} \tag{4.6}$$

for any $\delta > 0$. Then we see from the inequality (4.5) that $\tau^3 A_\delta \subset \sigma_\varepsilon(H)$ for every δ and every τ sufficiently large, in particular such that the inequality $\tau^{-3} C^{\tau^{5/2}} > \varepsilon^{-1}$ holds. We may then identify the points of Λ in absolute value with τ^3, i.e. $|\lambda| = \tau^3 = h^{-6/5}$. After we take logarithm of the lastly mentioned inequality and neglect the term $\log \tau^{-3}$ which is small compared to $\tau^{5/2}$ for τ large, the statement of the theorem follows after expressing the inequality in terms of $|\lambda|$. ☐

Lemma 3 *The eigenfunctions of H do not form a (Schauder) basis in $L^2(\mathbb{R})$.*

Proof Let us first recall that a Schauder basis is a set $\{\psi_k\}_{k=1}^{+\infty} \subset \mathscr{H}$ such that for every element $\psi \in \mathscr{H}$ can be uniquely expressed as $\psi = \sum_{k=1}^{+\infty} \alpha_k \psi_k$, where $\alpha_k \in \mathbb{C}$ for $k = 1, 2, \dots$. From the inequality (4.5) we can clearly see that the norm of the resolvent $(H - \lambda)^{-1}$ shoots up exponentially fast for $|z|$ large. Therefore the eigenfunctions of H cannot be tame by [8, Thm. 3]. Specifically, if we arrange the eigenvalues λ_k of H in increasing order, the norm of spectral projection P_k corresponding to λ_k cannot satisfy

$$\|P_k\| \leq a k^\alpha \tag{4.7}$$

for some a, α and all k. Therefore $\{\psi_k\}_{k=1}^{+\infty}$ cannot form a basis. ☐

Lemma 4 $-\mathrm{i}H$ *is not a generator of a bounded semigroup.*

Proof As in the previous proof, since the norm of resolvents grows exponentially for $|z|$ large, the claim follows from [9, Thm. 8.2.1]. ☐

The following result is a direct consequence of several propositions about operators with non-trivial pseudospectra from [19] which apply to H as well. We summarise them and provide a compact proof.

Lemma 5 *H is not similar to a self-adjoint operator via bounded and boundedly invertible transformation and H is not quasi-self-adjoint with a bounded and boundedly invertible metric.*

Proof If H were similar to a self-adjoint operator h as in (1.2), its pseudospectrum would have to satisfy

$$\sigma_{\varepsilon/\kappa}(H) \subset \sigma_\varepsilon(h) \subset \sigma_{\varepsilon\kappa}(H), \tag{4.8}$$

where $\kappa = \|\Omega\|\|\Omega^{-1}\|$. However, since the pseudospectrum of h is just the ε-neighbourhood of its spectrum, it cannot contain arbitrarily large points as ε/κ-pseudospectrum of H does. The claim about the quasi-self-adjointness (1.3) follows from the already established equivalence from the decomposition $\Theta = \Omega^*\Omega$. ☐

5 Summary

The harmonic oscillator coupled with an imaginary cubic oscillator potential was the main subject of interest of the present paper and we aimed to provide a detailed study of its basis and pseudospectral properties. The pseudospectrum of H exhibits wild properties and contains points very far from the spectrum, which can be turned into true eigenvalues by a small perturbation of the operator. As a consequence, the eigenfunctions of H do not form a Schauder basis, although they form a dense set in $L^2(\mathbb{R})$. The semigroup associated with the time-dependent Schödinger equation then does not have an expansion in the basis of eigenfunctions and does not admit a bounded time-evolution. The non-trivial pseudospectrum also implies that the considered operator does not have any bounded and boundedly invertible metric and thus it cannot be faithfully represented by any self-adjoint operator in the framework of standard quantum mechanics. In conclusion let us note that all results of this paper can be directly generalised to potentials of the type $x^2 + \mathrm{i}x^{2n+1}$, since all previous cited results apply to this more general case as well.

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Bound states in waveguides with complex Robin boundary conditions

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Abstract. We consider the Laplacian in a tubular neighbourhood of a hyperplane subjected to non-self-adjoint $\mathcal{PT}$-symmetric Robin boundary conditions. Its spectrum is found to be purely essential and real for constant boundary conditions. The influence of the perturbation in the boundary conditions on the threshold of the essential spectrum is studied using the Birman–Schwinger principle. Our aim is to derive a sufficient condition for existence, uniqueness and reality of discrete eigenvalues. We show that discrete spectrum exists when the perturbation acts in the mean against the unperturbed boundary conditions and we are able to obtain the first term in its asymptotic expansion in the weak coupling regime.

Keywords: non-self-adjointness, waveguide, Robin boundary conditions, spectral analysis, essential spectrum, weak coupling, Birman–Schwinger principle, reality of the spectrum

1. Introduction

Quantum waveguides undoubtedly belong among the systems interesting both from the physical and mathematical perspective. This notion customarily denotes long and thin semiconductor tubes or layers produced of very pure and crystalline materials. Usually Hamiltonians describing these models are self-adjoint and the bound states correspond to an electron trapped inside the waveguide. One of the possible ways how to describe a transport inside quantum waveguides is to consider the Laplacian in an unbounded tubular region Ω. Physical relevance of such description have been thoroughly discussed in [14,23,37]. The confinement of the wavefuntion to the spatial region is usually achieved by imposing Dirichlet [18,21], Neumann [13,39] or Robin [17,20,25] boundary conditions on $\partial\Omega$.

In this paper we choose to study properties of a Laplacian in a tubular neighbourhood of a hyperplane $\mathbb{R}^n \times I$, where $I = (0, d)$ is a finite one-dimensional interval. Instead of standard self-adjoint boundary condition we impose on the boundary complex Robin boundary conditions

$$\frac{\partial \Psi}{\partial n} + \mathrm{i}\alpha\Psi = 0, \tag{1.1}$$

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where Ψ is a wavefunction, n denotes the unit normal vector field of the boundary and α is a real-valued function. The selected boundary conditions physically correspond to the imperfect containment of the electron in the waveguide. This type of boundary conditions has been considered before in the description of open quantum systems [26,27] and in the context of quantum waveguides in [9]. (See also [6,7,10,35] for other results in this direction.)

In the paper [9] the authors focused on the case of the planar waveguide, $n = 1$. The spectrum of the waveguide with constant boundary conditions (i.e. $\alpha(x) = \alpha_0$ along the boundary) was found to be purely essential and equal to the half-line $[\mu_0^2, +\infty)$, where $\mu_0^2 := \min\{\alpha_0^2, (\frac{\pi}{d})^2\}$. Furthermore, it is stable under sufficiently smooth compact perturbation β of the function α. In the case of a weakly coupled perturbation $\varepsilon\beta$ the existence and uniqueness of an isolated eigenvalue was established under the condition that $\alpha_0 \int_{\mathbb{R}} \beta(x)\,\mathrm{d}x < 0$ holds and its asymptotic expansion up to the order ε^3 was calculated. The border case $\alpha_0 \int_{\mathbb{R}} \beta(x)\,\mathrm{d}x = 0$ was studied as well. This paper aims to generalise some of the above mentioned results to higher dimensions and to more general perturbations without compact support. In [9] method of matched asymptotic expansions was used, we choose a different approach to the problem based on the Birman–Schwinger principle.

Another reason for choosing complex Robin boundary conditions arises from the context of the so-called $\mathcal{PT}$-symmetric quantum mechanics. Motivated by the numerical observation of purely real spectrum of an imaginary cubic oscillator Hamiltonian [4] it blossomed into a large and rapidly developing field studying non-self-adjoint operators. See e.g. [3,38] and reference therein for a survey of papers in this area. The $\mathcal{PT}$-symmetry property of operator H should be here understood as its invariance on the Hilbert space $L^2(\mathbb{R}^n \times I)$, i.e.

$$[H, \mathcal{PT}] = 0 \tag{1.2}$$

in the operator sense, where $(\mathcal{P}\Psi)(x, u) := \Psi(x, d-u)$ stands for spatial reflection and $(\mathcal{T}\Psi)(x, u) := \overline{\Psi(x, u)}$ stands for time reversal. The relevant physical interpretation of the operators is ensured when they are in addition quasi-self-adjoint, i.e. they are similar to a self-adjoint operator $h = \omega H \omega^{-1}$, where ω is a bounded and boundedly invertible operator. Then it is ensured that spectra of h and H are identical and that the corresponding families of eigenfunctions share essential basis properties [33,34].

This paper is organised as follows. In the following section we summarise main results. Section 3 is devoted to the proper definition of the Hamiltonian outlined in Section 1 and to proof of its basic properties. We study essential spectrum of the model in Section 4. First of all we study the waveguide with constant boundary conditions along its boundary and their perturbations. Finally, Section 5 studies the existence of weakly-coupled bound states in this perturbed waveguide.

2. Main results

Let us consider a region $\Omega := \mathbb{R}^n \times I$ embedded into $\mathbb{R}^{n+1}$, where $I = (0, d)$ is a finite interval. For $n = 1$ it reduces to a planar strip, for $n = 2$ a layer in three dimensions. We study the problem for a general n except for the investigation of the bound states, where a specific form of the resolvent function of the Hamiltonian plays its role. We are interested in the action of the Hamiltonian of a free particle in this region subjected to $\mathcal{PT}$-symmetric Robin boundary condition on $\partial\Omega$ acting in the Hilbert space $L^2(\Omega)$. Elements of this Hilbert space are going to be consistently denoted with capital Greek letters (usually Ψ or Φ). The variables are going to be split as (x, u), where $x \in \mathbb{R}^n$ and $u \in (0, d)$. Given a real-valued function $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ we define the Hamiltonian as

$$\begin{aligned} &H_\alpha \Psi := -\Delta\Psi, \\ &\mathrm{Dom}(H_\alpha) := \left\{\Psi \in W^{2,2}(\Omega) \mid \partial_u\Psi + \mathrm{i}\alpha\Psi = 0 \text{ on } \partial\Omega\right\}, \end{aligned} \tag{2.1}$$

where ∂_u stands for differentiation with respect to u, similarly Δ stands for sum of all second derivatives. The effect of H_α should be understood in a distributional sense and the boundary conditions in the sense of traces.

We can see that the probability current in $\mathbb{R}^{n+1}$ of wavefunction $\Psi \in \mathrm{Dom}(H_\alpha)$ gives in the point (x, u) of $\partial\Omega$

$$\vec{j}(x, u) = \frac{1}{\mathrm{i}}(\overline{\Psi}\,\partial_u\Psi - \Psi\,\partial_u\overline{\Psi})(x, u)\vec{e}_{n+1} = -2\alpha(x)\left|\Psi(x, u)\right|^2\vec{e}_{n+1}, \tag{2.2}$$

where $\vec{e}_{n+1}$ stands for $(n + 1)$th vector of the standard basis in $\mathbb{R}^{n+1}$. Clearly the current is not equal to zero for non-trivial α and general Ψ. However, the influence of the boundary conditions on the current does not depend on whether we are at $u = 0$ or $u = d$ and therefore is the same for both components of $\partial\Omega$ and the gain and loss are balanced.

Using the quadratic form approach and the First Representation theorem, it will be derived in Theorem 3.4 that H_α is an m-sectorial operator if $\alpha \in W^{1,\infty}(\mathbb{R}^n)$. This yields that the operator is closed, therefore its spectrum is well defined and contained in a sector. Furthermore, the spectrum of H_α is localised inside a parabola, more precisely,

$$\sigma(H_\alpha) \subset \left\{z \in \mathbb{C} \mid \mathrm{Re}\, z \geqslant 0, |\mathrm{Im}\, z| \leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)}\sqrt{\mathrm{Re}\, z}\right\}. \tag{2.3}$$

Using the quadratic forms it can be shown for its adjoint operator that $H_\alpha^* = H_{-\alpha}$. Note that H_α is not self-adjoint, unless α is identically equal to 0.

Elementary calculations also lead to the conclusion, that H_α is $\mathcal{PT}$-symmetric, i.e. commutes with operator $\mathcal{PT}$ in operator sense explained in [28, Section III.5.6]. The spatial reflection operator $\mathcal{P}$ and the time reversal operator $\mathcal{T}$ are in our context defined as

$$\begin{aligned} &(\mathcal{P}\Psi)(x, u) := \Psi(x, d - u), \\ &(\mathcal{T}\Psi)(x, u) := \overline{\Psi(x, u)}. \end{aligned} \tag{2.4}$$

Another important property of H_α is $\mathcal{T}$-selfadjointness, i.e. $\mathcal{T}H_\alpha\mathcal{T} = H_\alpha^*$. A major consequence of this is that the residual spectrum of H_α is empty [9, Corollary 2.1], i.e.

$$\sigma_\mathrm{r}(H_\alpha) = \emptyset. \tag{2.5}$$

We emphasize that in our non-self-adjoint case it was impossible to a priori say anything about the residual spectrum, compared to the self-adjoint case, in which it is always empty.

Before approaching deeper results, we focus on a very simple case of the boundary conditions, $\alpha(x) = \alpha_0$ for all $x \in \mathbb{R}^n$, where α_0 is a real constant. Using the decomposition of the resolvent into the transversal basis, it is possible to show that the Hamiltonian H_{α_0} can be written as a sum

$$H_{\alpha_0} = -\Delta' \otimes 1^I + 1^{\mathbb{R}^n} \otimes -\Delta^I_{\alpha_0}, \tag{2.6}$$

where $1^{\mathbb{R}^n}$ and 1^I are identity operators on $L^2(\mathbb{R}^n)$ and $L^2(I)$ respectively, $-\Delta'$ is a self-adjoint Laplacian in $L^2(\mathbb{R}^n)$ and $-\Delta^I_{\alpha_0}$ is a Laplacian in $L^2(I)$ with complex Robin-type boundary conditions (see (4.1) for a precise definition). The latter operator has been extensively studied in [22,24,30–32]. It was shown that it is an m-sectorial and quasi-self-adjoint operator. It has purely discrete spectrum, its lowest lying point we denote as μ_0^2. It holds that $\mu_0^2 := \min\{\alpha_0^2, (\frac{\pi}{d})^2\}$. Our main conclusion about the spectrum of H_{α_0} is the following:

Proposition 2.1. *Let* $\alpha_0 \in \mathbb{R}$. *Then*

$$\sigma(H_{\alpha_0}) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = \left[\mu_0^2, +\infty\right). \tag{2.7}$$

Remark 2.2. There are several different definitions of the essential spectra in literature. For the self-adjoint operators they coincide, however this needs not to be true when the operator is non-self-adjoint and the various essential spectra can differ significantly. We employ the definition via so-called singular sequences – for a closed operator A we say that $\lambda \in \mathbb{C}$ belongs to the essential spectrum of A (denoted $\sigma_{\mathrm{ess}}(T)$) if there exists a sequence $(\psi_n)_{n=1}^{+\infty}$ (called a singular sequence), $\|\psi_n\|_{\mathscr{H}} = 1$ for all n, such that it does not contain any convergent subsequence and $\lim_{n\to+\infty}(T-\lambda)\psi_n = 0$. Other definitions are based e.g. on the violation of the Fredholm property (i.e. range of the studied operator is not closed or its kernel or cokernel are not finite-dimensional). However, many of these definitions coincide, provided A is $\mathcal{T}$-self-adjoint [15, Theorem IX.1.6].

Further on we study the perturbed waveguide, where the function α from the boundary conditions takes the form

$$\alpha(x) = \alpha_0 + \varepsilon\beta(x). \tag{2.8}$$

Here $\beta \in W^{2,\infty}(\mathbb{R}^n)$ and $\varepsilon > 0$. The stability of the essential spectrum is ensured when the boundary conditions approach uniform boundary conditions in infinity.

Theorem 2.3. *Let* $\alpha - \alpha_0 \in W^{1,\infty}(\mathbb{R})$ *with* $\alpha_0 \in \mathbb{R}$ *such that*

$$\lim_{|x|\to+\infty} (\alpha - \alpha_0)(x) = 0. \tag{2.9}$$

Then

$$\sigma_{\mathrm{ess}}(H_\alpha) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = \left[\mu_0^2, +\infty\right). \tag{2.10}$$

In the rest of the paper we search for conditions under which a small perturbation allows the existence of a bound state, i.e. of an isolated eigenvalue with finite geometric multiplicity. Due to the singularity of the resolvent this effect can be expected when the effective infinite dimension of the problem is 1 or 2. (See Remark 5.8 for more details.) Our method of ensuring its existence works under assumption of a sufficiently fast decay of β in infinity, which is summarized in technical conditions (5.23) and (5.34). Using different estimates in the proofs of relevant lemmas it could be probably improved. In further text the mean value of β is denoted as $\langle\beta\rangle := \int_{\mathbb{R}^n} \beta(x)\,\mathrm{d}x$.

Theorem 2.4. *Let us recall* (2.8). *Assume that* $\beta \in W^{2,\infty}(\mathbb{R}^n)$ *such that for* $\alpha = 0, 1, 2$ *and all* $j = 1, \dots, n$ *we have* $\partial_{x_j}^{\alpha}\beta = o(|x|^{-\mu})$ *for* $|x| \to +\infty$ *with* $\mu > 5$ *if* $n = 1$ *and* $\mu > 4$ *if* $n = 2$. *If* $\varepsilon > 0$ *is sufficiently small,* $|\alpha_0| < \pi/d$, *then* H_α *possesses a unique, simple and real eigenvalue* $\lambda = \lambda(\varepsilon) \in \mathbb{C} \setminus [0, +\infty)$ *if* $\alpha_0\langle\beta\rangle < 0$. *The asymptotic expansion*

$$\lambda(\varepsilon) = \begin{cases} \mu_0^2 - \varepsilon^2\alpha_0^2\langle\beta\rangle^2 + \mathcal{O}(\varepsilon^3), \\ \mu_0^2 - \mathrm{e}^{2/w(\varepsilon)}, \end{cases} \tag{2.11}$$

where $w(\varepsilon) = \frac{\varepsilon}{\pi}\alpha_0\langle\beta\rangle + \mathcal{O}(\varepsilon^2)$, *holds as* $\varepsilon \to 0$. *If* $\alpha_0\langle\beta\rangle > 0$, H_α *has no eigenvalues.*

When $\alpha_0 > \pi/d$, (5.51) is equal to zero and we are unable to say anything about the eigenvalue. To do so it would be necessary to take higher terms in the expansion of λ, which shows to be computationally challenging by the present method. We would encounter similar difficulties when trying to obtain more than just the leading term in the asymptotic expansion (2.11) to check the equality situation $\alpha_0\langle\beta\rangle = 0$.

We have just seen that the existence of the weakly coupled bound state is conditioned by fulfilment of $\alpha_0\langle\beta\rangle < 0$. Both α_0 and β play equivalent role in the boundary conditions – they cause a non-zero probability current over each component of the boundary. However, the negative sign of their product means, that they generate the probability current against each other. We may conclude that the weakening of the probability current through the waveguide due to the small perturbation is responsible for the existence of the bound state.

3. Definition of the Hamiltonian

This section is devoted to a proper definition of the Hamiltonian outlined in Sections 1 and 2 and to stating its basic properties. We begin by prescription of the densely defined sesquilinear form

$$\begin{aligned} h_\alpha(\Phi, \Psi) &:= h_\alpha^1(\Phi, \Psi) + \mathrm{i}h_\alpha^2(\Phi, \Psi), \\ \operatorname{Dom}(h_\alpha) &:= W^{1,2}(\Omega), \end{aligned} \tag{3.1}$$

where the real part h_α^1 and the imaginary part h_α^2 are two sesquilinear forms defined on $W^{1,2}(\Omega)$ as

$$\begin{aligned} h_\alpha^1(\Phi, \Psi) &:= \int_\Omega \overline{\nabla\Phi(x, u)} \cdot \nabla\Psi(x, u)\,\mathrm{d}x\,\mathrm{d}u, \\ h_\alpha^2(\Phi, \Psi) &:= \int_{\mathbb{R}^n} \alpha(x)\overline{\Phi(x, d)}\Psi(x, d)\,\mathrm{d}x - \int_{\mathbb{R}^n} \alpha(x)\overline{\Phi(x, 0)}\Psi(x, 0)\,\mathrm{d}x, \end{aligned} \tag{3.2}$$

where the dot stands for the scalar product in $\mathbb{R}^n$ and the boundary term should be again understood in the sense of traces. The form h_α^1 is associated with a Neumann Laplacian in $L^2(\Omega)$, it is therefore densely defined, closed, positive and symmetric. In the spirit of perturbation theory we show that h_α^2 plays a role of a small perturbation of h_α^1. We employ the notation $h[\cdot]$ for the quadratic form associated with the sesquilinear form $h(\cdot, \cdot)$.

Lemma 3.1. *Let $\alpha \in L^\infty(\mathbb{R}^n)$. The h_α^2 is relatively bounded with respect to h_α^1 with arbitrarily small relative bound. We have*

$$\left|h_\alpha^2[\Psi]\right| \leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)}\|\Psi\|_{L^2(\Omega)}\sqrt{h_\alpha^1[\Psi]} \leqslant \delta h_\alpha^1[\Psi] + \frac{1}{\delta}\|\alpha\|_{L^\infty(\mathbb{R}^n)}^2\|\Psi\|_{L^2(\Omega)}^2 \tag{3.3}$$

for every $\Psi \in W^{1,2}(\Omega)$ and $\delta > 0$.

Proof. Since Ω satisfies the segment condition, the set of restrictions of $C_0^\infty(\mathbb{R}^n)$ functions to Ω is dense in $W^{1,2}(\Omega)$ [2, Theorem 3.22]. (To check the condition, it is sufficient to take as U_x a ball with radius strictly smaller than $d/2$ and as the vector y_x any inwards pointing vector not exceeding the length of $d/2$.) We may thus restrict ourselves to the case $\Psi \in C_0^\infty(\mathbb{R}^n)$. Now we are able to differentiate $|\Psi(x)|^2$ and hence we may write

$$\begin{aligned}\left|h_\alpha^2[\Psi]\right| &= \left|\int_\Omega \alpha(x)\frac{\partial|\Psi(x,u)|^2}{\partial u}\,\mathrm{d}x\,\mathrm{d}u\right| \\ &\leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)}\int_\Omega \left|\Psi(x,u)\right|\left|\partial_u\Psi(x,u)\right|\mathrm{d}x\,\mathrm{d}u \\ &\leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)}\|\Psi\|_{L^2(\Omega)}\|\partial_u\Psi\|_{L^2(\Omega)} \\ &\leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)}\|\Psi\|_{L^2(\Omega)}\sqrt{h_\alpha^1[\Psi]},\end{aligned} \tag{3.4}$$

where we used the inequality $\|\partial_u\Psi\|_{L^2(\Omega)} \leqslant \|\nabla\Psi\|_{L^2(\Omega)} = \sqrt{h_\alpha^1[\Psi]}$. On this result we apply the Young inequality and we obtain the other inequality from the claim. □

According to [28, Theorem VI-1.33], the form h_α is closed and sectorial. The First Representation theorem [28, Theorem VI-2.1] states that then there exists a unique m-sectorial operator $\tilde{H}_\alpha$ such that $h_\alpha(\Phi, \Psi) = (\Phi, \tilde{H}_\alpha\Psi)_{L^2(\Omega)}$ for all $\Psi \in \mathrm{Dom}(\tilde{H}_\alpha) \subset \mathrm{Dom}(h_\alpha)$ and $\Phi \in \mathrm{Dom}(h_\alpha)$. The domain of $\tilde{H}_\alpha$ can be expressed as

$$\mathrm{Dom}(\tilde{H}_\alpha) = \left\{\Psi \in W^{1,2}(\Omega) \mid \exists F \in L^2(\Omega), \forall\Phi \in W^{1,2}(\Omega), h_\alpha(\Phi,\Psi) = (\Phi, F)_{L^2(\Omega)}\right\}. \tag{3.5}$$

To prove that $\tilde{H}_\alpha = H_\alpha$, we state first an auxiliary lemma.

Lemma 3.2. *Let $\alpha \in W^{1,\infty}(\mathbb{R}^n)$. For each $F \in L^2(\Omega)$ a solution Ψ to the problem*

$$h_\alpha(\Phi, \Psi) = (\Phi, F)_{L^2(\Omega)} \tag{3.6}$$

for all $\Phi \in W^{1,2}(\Omega)$ belongs to $\mathrm{Dom}(H_\alpha)$.

Remark 3.3. Equivalently, the statement may be formulated that the generalized solution Ψ to the problem

$$\begin{cases} -\Delta\Psi = F & \text{in } \Omega, \\ \partial_u\Psi + \mathrm{i}\alpha\Psi = 0 & \text{on } \partial\Omega \end{cases} \tag{3.7}$$

belongs to $\mathrm{Dom}(H_\alpha)$. This means that for any $\Psi \in W^{1,2}(\Omega)$ satisfying (3.7) we need to check that in fact $\Psi \in W^{2,2}(\Omega)$.

Proof of Lemma 3.2. We introduce the difference quotient [16, Section 5.8.2]

$$\Psi_\delta^j(x,u) := \frac{\Psi(x+\delta e_j,u)-\Psi(x,u)}{\delta} \tag{3.8}$$

for $j = 1,\dots,n$ and any $\Psi \in L^2(\Omega)$ and δ a small real number. Here e_j stands for jth vector of the standard basis in $\mathbb{R}^n$, i.e. $x+\delta e_j = (x_1,\dots,x_{j-1},x_j+\delta,x_{j+1},\dots,x_n)$. We estimate using the Schwarz inequality

$$\bigl|\Psi(x+\delta e_j,u)-\Psi(x,u)\bigr| = \left|\delta\int_0^1 \partial_{x_j}\Psi(x+\delta e_j,u)\,\mathrm{d}t\right| \leqslant |\delta|\sqrt{\int_0^1 \bigl|\partial_{x_j}\Psi(x+\delta e_j t)\bigr|^2\,\mathrm{d}t}, \tag{3.9}$$

which subsequently with the use of Fubini's theorem yields the inequality

$$\|\Psi_\delta^j\|_{L^2(\Omega)}^2 \leqslant \int_\Omega\left(\int_0^1 \bigl|\partial_{x_j}\Psi(x+\delta e_j t)\bigr|^2\,\mathrm{d}t\right)\mathrm{d}x\,\mathrm{d}u = \int_0^1 \|\partial_{x_j}\Psi\|_{L^2(\Omega)}\,\mathrm{d}t \leqslant \|\Psi\|_{W^{1,2}(\Omega)}^2. \tag{3.10}$$

Similarly we estimate α_δ^j:

$$\|\alpha_\delta^j\|_{L^\infty(\mathbb{R}^n)} \leqslant \operatorname*{ess\,sup}_{x\in\mathbb{R}^n}\int_0^1 \bigl|\partial_{x_j}\alpha(x+\delta e_j t)\bigr|\,\mathrm{d}t \leqslant \|\partial_{x_j}\alpha\|_{L^\infty(\mathbb{R}^n)} \leqslant \|\alpha\|_{W^{1,\infty}(\mathbb{R}^n)}. \tag{3.11}$$

If Ψ satisfies (3.6), then Ψ_δ is a solution to

$$h_\alpha(\Phi,\Psi_\delta^j) = (\Phi,F_\delta^j)_{L^2(\Omega)} - \int_{\mathbb{R}^n}\alpha_\delta^j(x)\bigl(\overline{\Phi(x,0)}\Psi(x+\delta e_j,0)-\overline{\Phi(x,d)}\Psi(x+\delta e_j,d)\bigr)\,\mathrm{d}x \tag{3.12}$$

with $\Phi \in W^{1,2}(\Omega)$ arbitrary. It also holds

$$\begin{aligned}(\Phi,F_\delta^j)_{L^2(\Omega)} &= \frac{1}{\delta}\int_\Omega \overline{\Phi(x,u)}\bigl(F(x+\delta e_j,u)-F(x,u)\bigr)\,\mathrm{d}x\,\mathrm{d}u\\ &= \frac{1}{\delta}\int_\Omega\bigl(\overline{\Phi(x-\delta e_j,u)}-\overline{\Phi(x,u)}\bigr)F(x,u)\,\mathrm{d}x\,\mathrm{d}u\\ &= -\bigl(\Phi_{-\delta}^j,F\bigr)_{L^2(\Omega)}\end{aligned} \tag{3.13}$$

and we use it together with setting $\Phi = \Psi_\delta^j$ to obtain from (3.12)

$$\begin{aligned}h_\alpha[\Psi_\delta^j] = &-\bigl((\Psi_\delta^j)_{-\delta},F\bigr)_{L^2(\Omega)}\\ &-\int_{\mathbb{R}^n}\alpha_\delta^j(x)\bigl(\overline{\Psi_\Delta^j(x,0)}\Psi(x+\delta e_j,0)-\overline{\Psi_\Delta^j(x,d)}\Psi(x+\delta e_j,d)\bigr)\,\mathrm{d}x.\end{aligned} \tag{3.14}$$

We employ the estimates

$$\left|\left((\Psi_\delta^j)_{-\delta}^j, F\right)\right| \leqslant \|F\|_{L^2(\Omega)}\left\|(\Psi_\delta^j)_{-\delta}^j\right\|_{L^(\Omega)} \leqslant \frac{1}{2}\|F\|_{L^2(\Omega)} + \frac{1}{2}\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)} \tag{3.15}$$

and

$$\begin{aligned} &\left|\int_{\mathbb{R}^n} \alpha_\delta^j(x)\left(\overline{\Psi_\delta^j(x,0)}\Psi(x+\delta e_j,0) - \overline{\Psi_\delta^j(x,d)}\Psi(x+\delta e_j,d)\right)\mathrm{d}x\right| \\ &\quad \leqslant 2\|\alpha\|_{W^{1,\infty}(\mathbb{R}^n)}\left\|T\Psi_\delta^j\right\|_{L^2(\partial\Omega)}\|T\Psi\|_{L^2(\partial\Omega)} \\ &\quad \leqslant C_1\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}\|\Psi\|_{W^{1,2}(\Omega)}, \end{aligned} \tag{3.16}$$

where T is trace operator $W^{1,2}(\Omega) \to L^2(\partial\Omega)$, together with Young inequality and Lemma 3.1 to obtain

$$\begin{aligned} \left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}^2 &= \|\Psi_\delta\|_{L^2(\Omega)}^2 + \|\nabla\Psi_\delta\|_{L^2(\Omega)}^2 \\ &\leqslant \|\Psi\|_{W^{1,2}(\Omega)}^2 + \frac{1}{2}\|F\|_{L^2(\Omega)} + \frac{1}{2}\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)} + C_1\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}\|\Psi\|_{W^{1,2}(\Omega)} \\ &\quad + 2\|\alpha\|_{W^{1,\infty}(\mathbb{R}^n)}\left\|\Psi_\delta^j\right\|_{L^2(\Omega)}\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)} \\ &\leqslant \|\Psi\|_{W^{1,2}(\Omega)}^2 + \frac{1}{2}\|F\|_{L^2(\Omega)} + \frac{1}{2}\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)} \\ &\quad + C_1\left(\frac{1}{4\tau}\|\Psi\|_{W^{1,2}(\Omega)}^2 + \tau\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}\right) \\ &\quad + C_2\left(\frac{1}{4\tau}\|\Psi\|_{W^{1,2}(\Omega)}^2 + \tau\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}\right) \\ &\leqslant \frac{1}{2}\|F\|_{L^2(\Omega)} + \left(1 + \frac{C_1+C_2}{4\tau}\right)\|\Psi\|_{W^{1,2}(\Omega)}^2 + \left(\frac{1}{2} + (C_1+C_2)\tau\right)\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)}, \end{aligned} \tag{3.17}$$

where $\tau > 0$ can be chosen arbitrarily small. Setting $\tau = 1/(4C_1 + 4C_2)$ we have

$$\left\|\Psi_\delta^j\right\|_{W^{1,2}(\Omega)} \leqslant C, \tag{3.18}$$

where C is independent of δ. This implies that

$$\sup_{\delta\in\mathbb{R}} \|\Psi_\delta\|_{W^{1,2}(\Omega)} < +\infty. \tag{3.19}$$

Since bounded sequences in a reflexive Banach space are weakly precompact [16, Theorem D.4.3], we find a subsequence $(\delta_k)_{k=1}^\infty$, $\lim_{k\to+\infty}\delta_k = 0$, such that $\Psi_{\delta_k}^j$ weakly converges to some f in $W^{1,2}(\Omega)$. As can be expected,

$$
\begin{aligned}
-\int_\Omega \overline{\partial_{x_j}\Psi(x,u)}\Phi(x,u) &= \int_\Omega \overline{\Psi(x,u)} \lim_{\delta_k\to 0} \Phi^j_{-\delta_k}(x,u)\,\mathrm{d}x\,\mathrm{d}u \\
&= \lim_{\delta_n\to 0}\int_\Omega \overline{\Psi(x,u)}\Phi^j_{-\delta_k}(x,u)\,\mathrm{d}x\,\mathrm{d}u \\
&= -\lim_{\delta_k\to 0}\int_\Omega \overline{\Psi^j_{\delta_k}(x,u)}\Phi(x,u)\,\mathrm{d}x\,\mathrm{d}u \\
&= -\int_\Omega \overline{f(x,u)}\Phi(x,u)\,\mathrm{d}x\,\mathrm{d}u.
\end{aligned} \tag{3.20}
$$

Therefore $\partial_{x_j}\Psi = f$ in a weak sense and so $\partial_{x_j}\Psi \in W^{1,2}(\Omega)$ for every j, $j = 1,\dots,n$. From the Interior Regularity theorem [16, Theorem 6.3.1] follows that $\Psi \in W^{2,2}_{\mathrm{loc}}(\Omega)$. Hence, the equation $-\Delta\Psi = F$ holds almost everywhere in Ω. Also, $\partial_u^2\Psi = -F - \Delta'\Psi \in L^2(\Omega)$ and therefore $\Psi \in W^{2,2}(\Omega)$.

Using Gauss–Green theorem we find that

$$
\begin{aligned}
(\Phi, F)_{L^2(\Omega)} = (\Phi, -\Delta\Psi)_{L^2(\Omega)} \\
&+ \int_{\mathbb{R}^n} \big(\partial_u\Psi(x,d) + \mathrm{i}\alpha(x)\Psi(x,d)\big)\overline{\Phi(x,d)}\,\mathrm{d}x \\
&- \int_{\mathbb{R}^n} \big(\partial_u\Psi(x,0) + \mathrm{i}\alpha(x)\Psi(x,0)\big)\overline{\Phi(x,0)}\,\mathrm{d}x
\end{aligned} \tag{3.21}
$$

for all $\Phi \in W^{1,2}(\Omega)$. Using this equality and the fact that $F = -\Delta\Psi$ almost everywhere in Ω we obtain the boundary conditions for Ψ. □

Theorem 3.4. *Let $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ be real-valued. Then H_α is an m-sectorial operator on $L^2(\Omega)$ satisfying*

$$
H_\alpha = \tilde{H}_\alpha. \tag{3.22}
$$

Proof. Using integration by parts it is straightforward to verify that $\tilde{H}_\alpha$ is an extension of H_α, $H_\alpha \subset \tilde{H}_\alpha$. The other inclusion follows from Lemma 3.2 and the uniqueness in the First Representation theorem [28, Theorem VI-2.1]. □

Using the quadratic form approach, we are able to find the adjoint operator to H quite easily.

Theorem 3.5. *Let $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ be real-valued. Then*

$$
H_\alpha^* = H_{-\alpha}. \tag{3.23}
$$

Proof. We find the adjoint operator H_α^* as an operator corresponding to the adjoint form h_α^*. The adjoint form can be obtained from h_α by replacing α for $-\alpha$. Therefore, its corresponding operator is $H_{-\alpha}$. □

Spectrum of H_α is indeed well defined since H_α is a closed operator. Consequence of H_α being m-sectorial is enclosure of its spectrum in a sector in a complex plane. Using the estimate from Lemma 3.1, this estimate can be further improved as follows.

Proposition 3.6. *The spectrum of H_α is localised inside a parabola, more precisely,*

$$\sigma(H_\alpha) \subset \left\{ z \in \mathbb{C} \mid \operatorname{Re} z \geqslant 0, |\operatorname{Im} z| \leqslant 2\|\alpha\|_{L^\infty(\mathbb{R}^n)} \sqrt{\operatorname{Re} z} \right\}. \tag{3.24}$$

The studied Hamiltonian is fundamentally non-self-adjoint, we can however state some symmetry properties, more precisely the $\mathcal{PT}$-symmetry and $\mathcal{T}$-self-adjointness.

Proposition 3.7. *Let $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ be real-valued. Then H_α is $\mathcal{PT}$-symmetric with operators $\mathcal{P}$, $\mathcal{T}$ defined in* (2.4).

Proof. According to our definition (1.2) of $\mathcal{PT}$-symmetry we need to check that $[H_\alpha, \mathcal{PT}] = 0$ holds in the sense $\mathcal{PT} H_\alpha \subset H_\alpha \mathcal{PT}$ [28, Section III.5.6]. For every $\Psi \in \operatorname{Dom}(H_\alpha)$ easily holds that $\mathcal{PT}\Psi \in W^{2,2}(\Omega)$. We can directly check that the action of H_α is invariant under the influence of the operator $\mathcal{PT}$ and that the boundary conditions hold also for $\mathcal{PT}\Psi$. □

Proposition 3.8. *Let $\alpha \in W^{1,\infty}(\mathbb{R}^n)$ be real-valued. Then H_α is $\mathcal{T}$-self-adjoint, i.e.*

$$\mathcal{T} H_\alpha \mathcal{T} = H_\alpha^*. \tag{3.25}$$

Proof. The proof follows in the same way as the proof of Proposition 3.7. □

The $\mathcal{T}$-self-adjointness in particular due to [9, Corollary 2.1] implies that

$$\sigma_{\mathrm{r}}(H_\alpha) = \emptyset. \tag{3.26}$$

4. The essential spectrum

4.1. Uniform boundary conditions

Let us now study the operator H_α with $\alpha(x)$ identically equal to $\alpha_0 \in \mathbb{R}$ for all $x \in \mathbb{R}^n$. We are going to establish some of its basic properties and use them in next subsection to study the perturbed operator $H_{\alpha_0+\varepsilon\beta}$. Our first goal is to prove the decomposition (2.6). Let us summarise some properties of the operator

$$\begin{aligned} &-\Delta_{\alpha_0}^I \psi := -\psi'', \\ &\operatorname{Dom}\left(-\Delta_{\alpha_0}^I\right) := \left\{ \psi \in W^{2,2}(I) \mid \psi' + \mathrm{i}\alpha_0\psi = 0 \text{ at } \partial I \right\}. \end{aligned} \tag{4.1}$$

It has been shown in [31, Proposition 1] that it is an m-sectorial operator therefore it is also closed and the study of its spectrum has a good meaning. The point spectrum of $-\Delta_{\alpha_0}^I$ is the countable set $\{\mu_j^2\}_{j=0}^{+\infty}$ with

$$\mu_{j_0} := \alpha_0, \qquad \mu_{j_1} := \frac{\pi}{d}, \qquad \mu_j := \frac{j\pi}{d}, \tag{4.2}$$

where $j \geqslant 2$, $(j_0, j_1) = (0, 1)$ if $|\alpha_0| \leqslant \pi/d$ and $(j_0, j_1) = (1, 0)$ if $|\alpha_0| > \pi/d$. Making the hypothesis

$$\frac{\alpha_0 d}{\pi} \notin \mathbb{Z} \setminus \{0\} \tag{4.3}$$

the eigenvalues have algebraic multiplicity equal to one. The corresponding set of eigenfunctions $\{\psi_j\}_{j=0}^{+\infty}$ can be chosen as

$$\psi_j(u) := \cos(\mu_j u) - \mathrm{i}\frac{\alpha_0}{\mu_j}\sin(\mu_j u), \quad j \geqslant 0. \tag{4.4}$$

Since the resolvent of the operator $-\Delta_{\alpha_0}^I$ is compact [31, Proposition 2], the spectrum is purely discrete and we have

$$\sigma\left(-\Delta_{\alpha_0}^I\right) = \sigma_{\mathrm{d}}\left(-\Delta_{\alpha_0}^I\right) = \left\{\mu_j^2\right\}_{j=0}^{+\infty}. \tag{4.5}$$

The adjoint operator $(-\Delta_{\alpha_0}^I)^*$ possesses the same spectrum since it can be obtained by interchanging α_0 for $-\alpha_0$ in the boundary conditions because $-\Delta_{\alpha_0}^I$ fulfils the relations analogous to the one in Eq. (3.23), $(-\Delta_{\alpha_0}^I)^* = -\Delta_{-\alpha_0}^I$, and therefore the eigenvalue equation remains unchanged. The corresponding eigenfunction can be selected as

$$\phi_j(u) := \overline{A_j \psi_j(u)}, \tag{4.6}$$

where A_j are normalisation constants defined as

$$A_{j_0} := \frac{2\mathrm{i}\alpha_0}{1 - \exp(-2\mathrm{i}\alpha_0 d)}, \qquad A_{j_1} := \frac{2\mu_{j_1}^2}{(\mu_{j_1}^2 - \alpha_0^2)d}, \qquad A_j := \frac{2\mu_j^2}{(\mu_j^2 - \alpha_0^2)d}, \tag{4.7}$$

where $j \geqslant 2$, $(j_0, j_1) = (0, 1)$ if $|\alpha_0| < \pi/d$ and $(j_0, j_1) = (1, 0)$ if $|\alpha_0| > \pi/d$. (Note that we already ruled out the case $|\alpha_0| = \pi/d$ due to (4.3).) If $\alpha_0 = 0$, A_{j_0} should be understood in the limit sense $\alpha_0 \to 0$. With this choice of normalization constants the both sets of eigenvectors form biorthonormal basis [31, Proposition 3] with the relations

$$(\phi_j, \psi_k)_{L^2(I)} = \delta_{jk} \quad \forall j, k \in \mathbb{N}, \tag{4.8}$$

and

$$\psi = \sum_{j=0}^{+\infty} (\phi_j, \psi)_{L^2(I)} \psi_j \tag{4.9}$$

for every $\psi \in L^2(I)$.

Proposition 4.1. *The identity*

$$\Psi(x,u) = \sum_{j=0}^{+\infty} \Psi_j(x)\psi_j(u), \tag{4.10}$$

where $\Psi_j(x) := (\phi_j, \Psi(x,\cdot))_{L^2(I)}$, *holds for every* $\Psi \in L^2(\Omega)$ *in the sense of* $L^2(\Omega)$*-norm.*

Proof. Let us define $(\Pi_N\psi)(u) := \sum_{j=0}^{N}(\phi_j,\psi)_{L^2(I)}\psi_j(u)$. From (4.9) follows that Π_N strongly converges to identity operator in $L^2(I)$. From Banach principle of uniform boundedness principle [41, Theorem III.9] follows that Π_N is uniformly bounded as $N \to +\infty$. Denote $\Psi^{(N)}(x,u) := \sum_{j=0}^{N}\Psi_j(x)\psi_j(u)$. Then we obtain

$$\int_I \left|\Psi^{(N)}(x,u) - \Psi(x,u)\right|^2 \mathrm{d}u = \int_I \left|(\Pi_N\Psi)(x,u) - \Psi(x,u)\right|^2 \mathrm{d}u \leqslant C\int_I \left|\Psi(x,u)\right|^2 \mathrm{d}u$$

for almost every $x \in \mathbb{R}^n$. Here the positive constant C is independent of N. At the same time we have $\int_I |\Psi^{(N)}(x,u) - \Psi(x,u)|^2\,\mathrm{d}u \to 0$ from the biorthonormal expansion (4.9). The convergence of $\Psi^{(N)}$ to Ψ in $L^2(\Omega)$ then follows from the Lebesgue dominated convergence theorem. □

4.2. Spectrum of the unperturbed Hamiltonian

We aim to proof Proposition 2.1. It is quite straightforward to see that its point spectrum is empty under the hypothesis (4.3), i.e.

Lemma 4.2. *Let* α_0 *satisfy* (4.3). *Then*

$$\sigma_{\mathrm{p}}(H_{\alpha_0}) = \emptyset. \tag{4.11}$$

Proof. For the contradiction let us assume that H_{α_0} possesses an eigenvalue λ with an eigenfunction $\Psi \in L^2(\Omega)$. We then multiply the eigenvalue equation with $\overline{\phi_j}$ and integrate it over I. Adopting the notation $\Psi_j(x) := (\phi_j, \Psi(x,\cdot))_{L^2(I)}$ the equation then reads

$$-\Psi_j'' = \left(\lambda - \mu_j^2\right)\Psi_j \tag{4.12}$$

in $\mathbb{R}^n$ for every $j \geqslant 0$. Using Schwarz inequality and Fubini's theorem we see that $\Psi_j \in L^2(\mathbb{R}^n)$:

$$\|\Psi_j\|^2_{L^2(\mathbb{R}^n)} \leqslant \int_{\mathbb{R}^n} \left\|\phi_j(u)\right\|^2_{L^2(I)} \left\|\Psi(x,u)\right\|^2_{L^2(I)} \mathrm{d}x = \|\phi_j\|^2_{L^2(I)}\|\Psi\|^2_{L^2(\Omega)} < +\infty. \tag{4.13}$$

Since the point spectrum of the Laplacian in $\mathbb{R}^n$ is empty, Eq. (4.12) only has a trivial solution. Therefore, (4.10) yields $\Psi = 0$, which is in contradiction with our hypothesis. □

Remark 4.3. We can further claim that the set of isolated eigenvalues is always empty, even in the case when the condition (4.3) is not satisfied. This is the consequence of the fact that H_{α_0} forms a holomorphic family of operators of type (B) with respect to α_0 and hence all its isolated eigenvalues $\mu_j(\alpha_0)$ are analytic functions in α_0 [28, Section VII.4].

The essential spectrum behaves, as can be expected – it consists of the essential spectrum of the free Laplacian in $\mathbb{R}^n$, shifted by the lowest-lying eigenvalue of $-\Delta^I$.

Lemma 4.4. *Let $\alpha_0 \in \mathbb{R}$. Then $[\mu_0^2, +\infty) \subset \sigma_{\mathrm{ess}}(H_\alpha)$.*

Proof. Let $\lambda \in [\mu_0^2, +\infty)$. It can be expressed as $\lambda = \mu_0^2 + z$, where $z \in [0, +\infty)$. Let $(\Phi_k)_{k=1}^{+\infty} \subset L^2(\mathbb{R}^n)$ be a singular sequence of $-\Delta'$ corresponding to z, i.e. $\|\Phi_k\|_{L^2(\mathbb{R}^n)} = 1$, $(\Phi_k)_{k=1}^{+\infty}$ does not contain converging subsequence and $(-\Delta' - z)\Phi_k \to 0$. We define sequence $(\Psi_k)_{k=1}^{+\infty}$ by $\Psi_k(x, u) := \Phi_k(x)\psi_0(u)/\|\psi_0\|_{L^2(I)}$. It can be easily seen that $\|\Psi_k\|_{L^2(\Omega)} = 1$ for all $k \in \mathbb{N}$ and $\Psi_k \to 0$ and that $(H_{\alpha_0} - \lambda)\Psi_k \to 0$ since

$$\big(H_{\alpha_0} - z - \mu_0^2\big)\Psi_k = \big(\big(-\Delta' - z\big)\Phi_k\big)\psi_0/\|\psi_0\|_{L^2(I)} \to 0. \tag{4.14}$$

In other words, $(\Psi_k)_{k=1}^{+\infty}$ forms a singular sequence for λ and it is therefore part of the essential spectrum. □

The opposite inclusion can be seen by employing the decomposition of the resolvent into the transverse biorthonormal basis.

Lemma 4.5. *Let α_0 satisfy (4.3). Then $\mathbb{C} \setminus [\mu_0^2, +\infty) \subset \rho(H_{\alpha_0})$ and for any $\lambda \in \mathbb{C} \setminus [\mu_0^2, +\infty)$ we have*

$$(H_{\alpha_0} - \lambda)^{-1} = \sum_{j=0}^{+\infty} \big(-\Delta' + \mu_j^2 - \lambda\big)^{-1} B_j. \tag{4.15}$$

Here B_j is a bounded operator on $L^2(\Omega)$ defined by

$$(B_j \Psi)(x, u) := \big(\Psi(x, \cdot), \phi_j\big)_{L^2(\Omega)} \psi_j(u) \tag{4.16}$$

for $\Psi \in L^2(\Omega)$ and $(-\Delta' + \mu_j^2 - \lambda)^{-1}$ abbreviates $(-\Delta' + \mu_j^2 - \lambda)^{-1} \otimes 1$.

Proof. We proceed with the proof as in [9, Lemma 4.3]. Let $\lambda \in \mathbb{C} \setminus [\mu_0^2, +\infty)$ and $\Psi \in L^2(\Omega)$. We denote $\Psi_j(x) := (\phi_j, \Psi(x, \cdot))_{L^2(I)} \in L^2(\mathbb{R}^n)$ and $U_j := (-\Delta' + \mu_j^2 - \lambda)^{-1}\Psi_j \in L^2(\mathbb{R}^n)$ for $j \geqslant 0$. Its norm can be estimated as

$$\|U_j\|_{L^2(\mathbb{R}^n)} \leqslant \frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}}{\operatorname{dist}(\lambda, [\mu_j^2, +\infty))} \leqslant C_1 \frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}}{j^2 + 1}. \tag{4.17}$$

The constant C_1 depends only on $|\alpha_0|$, d and λ. Similarly, we estimate $|\partial_{x_l} U_j|$ for every $j \geqslant 0$, $l \geqslant 1$ by its gradient in $\mathbb{R}^n$ and we obtain

$$\big\|\nabla' U_j\big\|_{L^2(\mathbb{R}^n)}^2 \leqslant C_1 \frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}^2}{j^2 + 1} + C_1^2 \big|\mu_j^2 - \lambda\big| \frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}^2}{(j^2 + 1)^2}. \tag{4.18}$$

We define a function $R_j(x) := U_j(x)\psi_j(u)$ (which is exactly the summand of the sum (4.15)). It belongs to $W^{2,1}(\Omega)$ and this is true for their infinite sum too as we shall see. We use the fact that all $|A_j|$ can be estimated by a constant c depending only on $|\alpha_0|$ and d, and Parseval identity for χ_j^D and χ_j^N to estimate

$$\sum_{j=2}^{+\infty}\left|\Psi_j(x)\right|^2 \leqslant c^2 d\left(\sum_{j=2}^{+\infty}\left|\Psi_j^N\right|^2 + \frac{\alpha_0^2}{\mu_2^2}\sum_{j=2}^{+\infty}\left|\Psi_j^D\right|^2\right) \leqslant c^2 d\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)\left\|\Psi(x,\cdot)\right\|_{L^2(I)}^2. \tag{4.19}$$

Employing this and the estimate (4.17) together with Fubini's theorem yields

$$\begin{aligned}\left\|\sum_{j=2}^{k} R_j\right\|_{L^2(\Omega)}^2 &\leqslant d^2\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)^2 C_1^2 \sum_{j=2}^{k}\frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}}{(j^2+1)^2} \\ &\leqslant d^2\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)^2 C_1^2 \int_{\mathbb{R}^n}\sum_{j=2}^{k}\left|\left(\phi_j,\Psi(x,\cdot)\right)_{L^2(I)}\right|^2 \mathrm{d}x \\ &\leqslant c^2 d^3\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)^3 C_1^2\|\Psi\|_{L^2(\Omega)}. \end{aligned} \tag{4.20}$$

We remind that constant c depends only on $|\alpha_0|$, d and λ, just as C_1. In exactly the same manner we estimate $\|\sum_{j=1}^k \partial_{x_l} R_j\|_{L^2(\Omega)}$ for every $l \geqslant 1$ using the estimate (4.18) instead of (4.17). Employing the estimate $|\partial_u \psi_j| \leqslant \alpha_0^2 + \mu_j^2$ valid for $j \geqslant 1$, we readily estimate the norm of $\sum_{j=2}^k \partial_u R_j$:

$$\begin{aligned}\left\|\sum_{j=1}^{k} \partial_u R_j\right\|_{L^2(\Omega)}^2 &\leqslant d^2 C_1^2 \sum_{j=2}^{k}\left(\frac{\mu_j^2+\alpha_0^2}{j^2+1}\right)^2\|\Psi_j\|_{L^2(\mathbb{R}^n)}^2 \\ &\leqslant d^2 C_1^2 C_2^2 \int_{\mathbb{R}^n}\sum_{j=2}^{k}\left|\left(\phi_j,\Psi(x,\cdot)\right)_{L^2(I)}\right|^2 \mathrm{d}x \\ &\leqslant c^2 d\left(1+\frac{\alpha_0^2}{\mu_2^2}\right) C_1^2 C_2^2\|\Psi\|_{L^2(\Omega)}, \end{aligned} \tag{4.21}$$

where C_2 is a constant bounding the sequence $(\frac{\mu_j^2+\alpha_0^2}{j^2+1})_{j=2}^{+\infty}$, depending only on $|\alpha_0|$ and d. Regarding the sum of the first two terms, we obtain

$$\left\|\sum_{j=0}^{1} R_j\right\|_{L^2(\Omega)}^2 \leqslant d^2\left(1+\frac{\alpha_0^2}{\mu_0^2}\right)^2 C_1^2 \sum_{j=0}^{1}\frac{\|\Psi_j\|_{L^2(\mathbb{R}^n)}^2}{(j^2+1)^2} \leqslant c^2 d^3\left(1+\frac{\alpha_0^2}{\mu_0^2}\right)^3 C_1^2\|\Psi\|_{L^2(\Omega)} \tag{4.22}$$

and similarly for $\partial_{x_l} R_j$ and $\partial_u R_j$. Altogether we uniformly estimated the partial sum of R_j and of its derivatives, and therefore the series $\sum_{j=0}^{+\infty} R_j$ converges in $W^{1,2}(\Omega)$ to a function R and

$$\|R\|_{W^{1,2}(\Omega)} \leqslant K\|\Psi\|_{L^2(\Omega)}, \tag{4.23}$$

where K depends only on $|\alpha_0|$, d and λ. It is easily seen that R satisfies the identity

$$h_{\alpha_0}(R, \Phi) - \lambda(R, \Phi)_{L^2(\Omega)} = (\Psi, \Phi)_{L^2(\Omega)} \tag{4.24}$$

for all $\Phi \in W^{1,2}$. Therefore, $R \in \mathrm{Dom}(H_{\alpha_0})$ and $(H_{\alpha_0} - \lambda)R = \Psi$, i.e. $R = (H_{\alpha_0} - \lambda)^{-1}\Psi$. □

Proof of Proposition 2.1. The first inequality follows from Lemma 4.2. From Lemmas 4.4 and 4.5 we know that the second equality holds for all α_0 satisfying (4.3). This result extends to all α_0 in view of the fact that H_{α_0} forms a holomorphic family of operators of type (B) with respect to α_0 (cf. Remark 4.3). □

4.3. Stability of the essential spectrum

Our goal is to find conditions under which a single bound state arises as a consequence of a perturbation of the boundary conditions. Generally, it could happen that although it appears, the essential spectrum changes in such a way that it is absorbed in it. Therefore, we first investigate the stability of the essential spectrum under perturbations of uniform boundary conditions studied in detail in previous section and conclude with the proof of Theorem 2.3. Let us state an auxiliary lemma.

Lemma 4.6. *Let $\alpha_0 \in \mathbb{R}$ and $\varphi \in L^2(\partial\Omega)$. There exist positive constants c and C, depending on d and $|\alpha_0|$, such that any weak solution $\Psi \in W^{1,2}(\Omega)$ of the boundary value problem*

$$\begin{cases} (-\Delta - \lambda)\Psi = 0 & \text{in } \Omega, \\ (\partial_u + \mathrm{i}\alpha_0)\Psi = \varphi & \text{on } \partial\Omega, \end{cases} \tag{4.25}$$

with any $\lambda \leqslant -c$, satisfies the estimate

$$\|\Psi\|_{W^{1,2}(\Omega)} \leqslant C\|\varphi\|_{L^2(\partial\Omega)}. \tag{4.26}$$

Proof. Multiplying the first equation of (4.25) by $\overline{\Psi}$ and integrating over Ω yields

$$\begin{aligned}
\int_\Omega \overline{\Psi(x,u)}(-\Delta - \lambda)\Psi(x,u)\,\mathrm{d}x\,\mathrm{d}u &= \mathrm{i}\int_{\mathbb{R}^n} \alpha_0\left|\Psi(x,d)\right|^2 \mathrm{d}x - \mathrm{i}\int_\Omega \alpha_0\left|\Psi(x,0)\right|^2 \mathrm{d}x \\
&\quad - \int_{\mathbb{R}^n} \overline{\Psi(x,d)}\varphi(x,d)\,\mathrm{d}x + \int_{\mathbb{R}^n} \overline{\Psi(x,0)}\varphi(x,0)\,\mathrm{d}x \\
&\quad + \|\nabla\Psi\|^2_{L^2(\Omega)} - \lambda\|\Psi\|^2_{L^2(\Omega)} \\
&= 0.
\end{aligned} \tag{4.27}$$

We readily estimate using Schwarz and Young inequality

$$\begin{aligned}
\left|\int_{\mathbb{R}^n} \alpha_0\left|\Psi(x,d)\right|^2 \mathrm{d}x - \int_\Omega \alpha_0\left|\Psi(x,0)\right|^2 \mathrm{d}x\right| &= \left|\int_\Omega \alpha_0\,\partial_u\left|\Psi(x)\right|^2 \mathrm{d}x\right| \\
&= 2|\alpha_0|\left|\mathrm{Re}(\partial_u\Psi, \Psi)\right| \\
&\leqslant 2|\alpha_0|\|\partial_u\Psi\|_{L^2(\Omega)}\|\Psi\|_{L^2(\Omega)} \\
&\leqslant |\alpha_0|\left(\delta\|\nabla\Psi\|^2_{L^2(\Omega)} + \delta^{-1}\|\Psi\|^2_{L^2(\Omega)}\right)
\end{aligned} \tag{4.28}$$

and

$$\left| -\int_{\mathbb{R}^n} \overline{\Psi(x,d)}\varphi(x,d)\,\mathrm{d}x + \int_{\mathbb{R}^n} \overline{\Psi(x,0)}\phi(x,0)\,\mathrm{d}x \right| \leqslant 2\|T\Psi\|_{L^2(\partial\Omega)}\|\varphi\|_{L^2(\partial\Omega)} \leqslant \delta\widetilde{C}\|\Psi\|^2_{W^{1,2}(\Omega)} + \delta^{-1}\|\varphi\|^2_{L^2(\partial\Omega)}, \tag{4.29}$$

where $\delta > 0$ and $\widetilde{C}$ is the constant from the embedding of $W^{1,2}(\Omega)$ in $L^2(\Omega)$ depending only on d. Putting these estimates into (4.27) we get

$$\big(1 - \delta|\alpha_0| - \delta\widetilde{C}\big)\|\Psi\|^2_{W^{1,2}(\Omega)} \leqslant \big(1 - \delta|\alpha_0| + \delta^{-1}|\alpha_0| + \lambda\big)\|\Psi\|^2_{L^2(\Omega)} + \delta^{-1}\|\varphi\|^2_{L^2(\partial\Omega)}. \tag{4.30}$$

Taking δ sufficiently small and λ sufficiently large negative, coefficients standing by $\|\Psi\|_{W^{1,2}(\Omega)}$ and $\|\Psi\|_{L^2(\Omega)}$ are positive and this yields the inequality (4.26). □

Using this lemma we are able to prove the following result.

Proposition 4.7. *Let $\alpha - \alpha_0 \in W^{1,\infty}(\mathbb{R})$ with $\alpha_0 \in \mathbb{R}$ such that (2.9) holds. Then $(H_\alpha - \lambda)^{-1} - (H_{\alpha_0} - \lambda)^{-1}$ is compact in $L^2(\Omega)$ for any $\lambda \in \rho(H_\alpha) \cap \rho(H_{\alpha_0})$.*

Proof. The proof is inspired by the proof of [9, Proposition 5.1]. It suffices to prove the result only for one $\lambda \in \rho(H_\alpha) \cap \rho(H_{\alpha_0})$ sufficiently negative. (Since both H_{α_0} and H_α are m-sectorial, their spectra are bounded from below.) The result can be then extended to any other $\lambda' \in \rho(H_\alpha) \cap \rho(H_{\alpha_0})$ due to the first resolvent identity. Let us denote for this purpose $R(H_\alpha;\lambda) := (H_\alpha - \lambda)^{-1}$ and $R(H_{\alpha_0};\lambda) := (H_{\alpha_0} - \lambda)^{-1}$. Then we have

$$\begin{aligned} &R\big(H_\alpha;\lambda'\big) - R\big(H_{\alpha_0};\lambda'\big) \\ &\quad = R\big(H_\alpha;\lambda'\big)\big(1 + \big(\lambda' - \lambda\big)R\big(H_\alpha;\lambda'\big)\big) - \big(1 + \big(\lambda' - \lambda\big)R\big(H_\alpha;\lambda'\big)\big)R\big(H_{\alpha_0};\lambda'\big) \\ &\quad = \big(1 + \big(\lambda' - \lambda\big)R\big(H_\alpha;\lambda'\big)\big)\big(R(H_\alpha;\lambda) - R(H_{\alpha_0};\lambda)\big)\big(1 + \big(\lambda' - \lambda\big)R\big(H_\alpha;\lambda'\big)\big). \end{aligned} \tag{4.31}$$

From the assumption $R(H_\alpha;\lambda) - R(H_{\alpha_0};\lambda)$ is compact and $1 + (\lambda' - \lambda)R(H_\alpha;\lambda')$ and $1 + (\lambda' - \lambda)R(H_\alpha;\lambda')$ are bounded. The claim then follows from the two side ideal property of compact operators. Given an arbitrary $\Phi \in L^2(\Omega)$, let us define $\Psi := (H_\alpha - \lambda)^{-1}\Phi - (H_{\alpha_0} - \lambda)^{-1}\Phi$. Ψ clearly satisfies the first equation in (4.25). Plugging it into the second one we get

$$(\partial_2 + \mathrm{i}\alpha_0)\Psi = (\partial_2 + \mathrm{i}\alpha_0)\big((H_\alpha - \lambda)^{-1}\Phi - (H_{\alpha_0} - \lambda)^{-1}\Phi\big) = -\mathrm{i}(\alpha - \alpha_0)(H_\alpha - \lambda)^{-1}\Phi, \tag{4.32}$$

therefore our $\varphi = -\mathrm{i}(\alpha - \alpha_0)T(H_\alpha - \lambda)^{-1}\Phi$, where T is a trace operator from $W^{2,2}(\Omega)$ to $W^{1,2}(\partial\Omega)$. Due to the estimate (4.26) it is enough to show that $(\alpha - \alpha_0)T(H_\alpha - \lambda)^{-1}$ is compact. Indeed if this is true then given any sequence $(\Phi_n)_{n=1}^{+\infty} \subset L^2(\Omega)$ we know there is a strictly increasing sequence $(k_n)_{n=1}^{+\infty} \subset \mathbb{N}$ such that for every $\varepsilon > 0$ there is $n_0 \in \mathbb{N}$ such that for all $m, n > n_0$ inequality $\|((\alpha - \alpha_0)T(H_\alpha - \lambda)^{-1})(\Phi_m - \Phi_n)\| < \varepsilon$ holds. It follows the same is true for $(H_\alpha - \lambda)^{-1} - (H_{\alpha_0} - \lambda)^{-1}$ since

$$\big\|\big((H_\alpha - \lambda)^{-1} - (H_{\alpha_0} - \lambda)^{-1}\big)(\Phi_m - \Phi_n)\big\|_{L^2(\Omega)} \leqslant C\big\|\big((\alpha - \alpha_0)T(H_\alpha - \lambda)^{-1}\big)(\Phi_m - \Phi_n)\big\|_{L^2(\Omega)}. \tag{4.33}$$

We denote $\beta := \alpha - \alpha_0$ and define functions

$$\beta_n(x) := \begin{cases} \beta(x), & x \in (-n, n), \\ 0 & \text{otherwise.} \end{cases} \tag{4.34}$$

These bounded continuous functions with compact support converge to $\beta(x)$ in $L^\infty(\mathbb{R}^n)$ norm. $\beta_n T(H_\alpha - \lambda)^{-1}$ is a compact operator since $W^{1,2}(\partial\Omega)$ is compactly embedded in $L^2(\omega)$ for every bounded subset ω of $\partial\Omega$, due to the Rellich–Kondrachov theorem [2, Section VI]. In other words, every set A, which is bounded in the topology of $W^{1,2}(\partial\Omega)$, is precompact in the topology of $L^2(\omega)$. The claim then follows from the two sided ideal property of the set compact operator if we show that the compact operators $\beta_n T(H_\alpha - \lambda)^{-1}$ converge in the uniform $L^2(\partial\Omega)$ topology to our operator $\beta_n T(H_\alpha - \lambda)^{-1}$. We have

$$\left\| \beta T(H_\alpha - \lambda)^{-1} - \beta_n T(H_\alpha - \lambda)^{-1} \right\| \leqslant \|\beta - \beta_n\|_{L^\infty(\mathbb{R}^n)} \left\| T(H_\alpha - \lambda)^{-1} \right\|, \tag{4.35}$$

which converges to 0 for $n \to +\infty$. □

Proof of Theorem 2.3. Since the difference of the resolvents is a compact operator according to Proposition 4.7, it follows from the Weyl's essential spectrum theorem [40, Theorem XIII.14] that the essential spectra of H_α and H_{α_0} are identical. □

5. Weakly coupled bound states

Another possible influence of the perturbation of the boundary conditions on the spectrum is studied in this section. We shall employ the form

$$\alpha(x) = \alpha_0 + \varepsilon\beta(x) \tag{5.1}$$

for α further on. Here $\alpha_0 \in \mathbb{R}$, $\beta \in W^{2,\infty}(\mathbb{R}^n)$ and $\varepsilon > 0$. This section contains some preliminary and auxilliary results and culminates with the proof of Theorem 2.4.

5.1. Unitary transformation of H_α

The form (2.1) is not very convenient for the study of bound states, the unitary transformation is therefore applied to simplify the boundary conditions for the cost of an adding of a differential operator.

Proposition 5.1. *H_α is unitarily equivalent to the operator $H_{\alpha_0} + \varepsilon Z_\varepsilon$, where*

$$Z_\varepsilon := 2\mathrm{i}u\nabla'\beta(x)\cdot\nabla' + 2\mathrm{i}\beta(x)\frac{\partial}{\partial u} + \left(\varepsilon\beta^2(x) + \mathrm{i}\Delta'\beta(x)u + \varepsilon u^2\left|\nabla'\beta\right|^2\right), \tag{5.2}$$

and $\mathrm{Dom}(H_{\alpha_0} + \varepsilon Z_\varepsilon) = \mathrm{Dom}(H_{\alpha_0})$.

Proof. We are going to show that the relation

$$U_\varepsilon^{-1} H_\alpha U_\varepsilon = H_{\alpha_0} + \varepsilon Z_\varepsilon, \tag{5.3}$$

holds in operator sense with the unitary operator of multiplication U_ε acting on $\Psi \in L^2(\Omega)$ as $(U_\varepsilon\Psi)(x,u) := \mathrm{e}^{-\mathrm{i}\varepsilon\beta(x)u}\Psi(x,u)$. First we show that $\mathrm{Dom}(U_\varepsilon^{-1} H_\alpha U_\varepsilon) = \mathrm{Dom}(H_{\alpha_0} + \varepsilon Z_\varepsilon)$. Simple calculations show that $\mathrm{Dom}(H_{\alpha_0}) = \mathrm{Dom}(U_\varepsilon^{-1} H_\alpha U_\varepsilon)$. Further, $U_\varepsilon^{-1} H_\alpha U_\varepsilon$ and $H_{\alpha_0} + \varepsilon Z_\varepsilon$ act in the same on functions from their domain. Now we prove that $\mathrm{Dom}(H_{\alpha_0} + \varepsilon Z_\varepsilon) = \mathrm{Dom}(H_{\alpha_0})$. It is clear that domain of $H_{\alpha_0} + \varepsilon Z_\varepsilon$ is a subset of the domain of H_{α_0}. Taking $\Psi \in \mathrm{Dom}(H_{\alpha_0}) \subset W^{2,2}(\Omega)$ we estimate every action of Z_ε as

$$\begin{aligned}
&\big\|2\mathrm{i}u\big(\nabla'\beta\big)(x)\cdot\nabla'\Psi\big\|_{L^2(\Omega)} \leqslant 2nd\|\beta\|_{W^{2,\infty}(\mathbb{R}^n)}\|\Psi\|_{W^{2,2}(\Omega)},\\
&\|2\mathrm{i}\beta\,\partial_u\Psi\|_{L^2(\Omega)} \leqslant 2\|\beta\|_{W^{2,\infty}(\mathbb{R}^n)}\|\Psi\|_{W^{2,2}(\Omega)},\\
&\big\|\varepsilon\beta^2\Psi\big\|_{L^2(\Omega)} \leqslant \varepsilon\|\beta\|^2_{W^{2,\infty}(\mathbb{R}^n)}\|\Psi\|_{W^{2,2}(\Omega)},\\
&\big\|-\mathrm{i}\Delta'\beta u\Psi\big\|_{L^2(\Omega)} \leqslant d\|\beta\|_{W^{2,\infty}(\mathbb{R}^n)}\|\Psi\|_{W^{2,2}(\Omega)},\\
&\big\|-\varepsilon u^2\big|\nabla'\beta\big|^2\Psi\big\|_{L^2(\Omega)} \leqslant \varepsilon d^2\|\beta\|^2_{W^{2,\infty}(\mathbb{R}^n)}\|\Psi\|^2_{W^{2,2}(\Omega)}.
\end{aligned} \tag{5.4}$$

In other words we just showed that $\mathrm{Dom}(H_{\alpha_0}) \subset \mathrm{Dom}(H_{\alpha_0} + \varepsilon Z_\varepsilon)$ and the equality of domains is proven. □

Overall, we were able to transform away the perturbed boundary conditions at the cost of adding a differential operator to the unperturbed Hamiltonian. Since unitarily equivalent operators possesses identical spectra, further on we are going to study the operator $H_{\alpha_0} + \varepsilon Z_\varepsilon$. Hereafter, a straightforward calculation inspired by [8] proves that

$$Z_\varepsilon = \sum_{i=1}^{n+2} A_i^* B_i + \varepsilon \sum_{i=n+3}^{2n+3} A_i^* B_i, \tag{5.5}$$

where A_i and B_i are first-order differential operators, specifically

$$\begin{aligned}
A_1^* &:= 2\mathrm{i}\big(\partial_{x_1}\beta(x)\big)_{1/2}u, & B_1 &:= \big|\partial_{x_1}\beta(x)\big|^{1/2}\frac{\partial}{\partial x_1},\\
&\vdots & &\vdots\\
A_n^* &:= 2\mathrm{i}\big(\partial_{x_n}\beta(x)\big)_{1/2}u, & B_n &:= \big|\partial_{x_n}\beta(x)\big|^{1/2}\frac{\partial}{\partial x_n},\\
A_{n+1}^* &:= 2\mathrm{i}\beta(x)_{1/2}, & B_{n+1} &:= \big|\beta(x)\big|^{1/2}\frac{\partial}{\partial u},\\
A_{n+2}^* &:= -\mathrm{i}\big(\Delta'\beta(x)\big)_{1/2}u, & B_{n+2} &:= \big|\Delta'\beta(x)\big|^{1/2},\\
A_{n+3}^* &:= \beta(x)u^2, & B_{n+3} &:= \beta(x),\\
A_{n+4}^* &:= \partial_{x_1}\beta(x)u^2, & B_{n+4} &:= \partial_{x_1}\beta(x),\\
&\vdots & &\vdots\\
A_{2n+3}^* &:= \partial_{x_n}\beta(x)u^2, & B_{2n+3} &:= \partial_{x_n}\beta(x),
\end{aligned} \tag{5.6}$$

where $(f(x))_{1/2} := \operatorname{sgn}(f(x))|f(x)|^{1/2}$ for any function f. We define a pair of operators $C_\varepsilon, D : L^2(\Omega) \to L^2(\Omega) \otimes \mathbb{C}^{2n+3}$ by

$$(C_\varepsilon\varphi)_i := \begin{cases} A_i\varphi, & i = 1, 2, \dots, n+2, \\ \varepsilon A_i\varphi, & i = n+3, \dots, 2n+3, \end{cases} \qquad (5.7)$$

$$(D\varphi)_i := B_i\varphi, \quad i = 1, \dots, 2n+3.$$

Then (5.5) finally becomes

$$U_\varepsilon^{-1} H_\alpha U_\varepsilon = H_{\alpha_0} + \varepsilon C_\varepsilon^* D. \qquad (5.8)$$

(Note that C_ε^* project from $L^2(\Omega) \otimes \mathbb{C}^{2n+3}$ to $L^2(\Omega)$ according to the definition of adjoint operator.)

5.2. Birman–Schwinger principle

We introduce a useful technique for studying certain types of partial differential equations, particularly in the analysis of the point spectrum of differential operators. It was developed independently by Russian mathematician M.S. Birman [5] and American physicist J. Schwinger [43] in the year 1961 for estimating the number of negative eigenvalues of a self-adjoint Schrödinger operator. Since its origin it was applied in finding weakly coupled bound states [44], studying behaviour of the resolvent [29], localizing the spectrum [11] and also finding eigenvalue bounds in non-self-adjoint operators [12,19,36]. Generally it enables us to solve an eigenvalue problem for differential operators by solving an eigenvalue problem for integral operators. In this paper we apply it on the non-self-adjoint operator. Since Z_ε is a differential operator, we will have to employ regularity of functions involved and integration by parts to obtain an integral operator (cf. proof of Lemmas 5.5 and 5.6).

Proposition 5.2. *Let* $\lambda \in \mathbb{C} \setminus [0, +\infty)$, $\varepsilon \in \mathbb{R}$, $\beta \in W^{2,\infty}(\mathbb{R}^n)$ *such that*

$$\lim_{|x|\to+\infty} \beta(x) = \lim_{|x|\to+\infty} \partial_{x_j}\beta(x) = \lim_{|x|\to+\infty} \partial_{x_j}^2\beta(x) = 0 \qquad (5.9)$$

for all $j = 1, \dots, n$. *Denoting* $K_\varepsilon^\lambda := \varepsilon D(H_{\alpha_0} - \lambda)^{-1} C_\varepsilon^*$, *then*

$$\lambda \in \sigma_{\mathrm{p}}(H_\alpha) \iff -1 \in \sigma_{\mathrm{p}}\big(K_\varepsilon^\lambda\big). \qquad (5.10)$$

Proof. $\Rightarrow$: Assuming $H_\alpha\Phi = \lambda\Phi$ holds for some $\Phi \in \operatorname{Dom}(H_\alpha)$ we define $\Psi := D\Phi$. $\Psi \in L^2(\Omega) \otimes \mathbb{C}^{2n+3}$ since we have for each $(D\Phi)_i$ the following estimate:

$$\big\|(D\Phi)_i\big\|_{L^2(\Omega)} \leqslant c_1\|\nabla\Phi\|_{L^2(\Omega)} + c_2\|\Phi\|_{L^2(\Omega)} \leqslant (c_1 + c_2)\|\Phi\|_{W^{2,2}(\Omega)} < +\infty, \qquad (5.11)$$

where c_1 and c_2 are constants arising from the boundedness of β, its derivatives and their square roots. For this Ψ we then have

$$K_\varepsilon^\lambda\Psi = \varepsilon D(H_{\alpha_0} - \lambda)^{-1} C_\varepsilon^* D\Phi = -D(H_{\alpha_0} - \lambda)^{-1}(H_{\alpha_0} - \lambda)\Phi = -\Psi. \qquad (5.12)$$

$\Leftarrow$: Let us assume that $\Psi \in L^2(\Omega)\otimes\mathbb{C}^{2n+3}$ is an eigenfunction of K_ε^λ pertaining to the eigenvalue -1. The assumptions imply that β, $\partial_{x_j}\beta$ and $\partial_{x_j}^2\beta$ are bounded for all $j = 1,\dots,n$, therefore the operator C_ε is bounded and the same applies for its adjoint. Then $\Phi := -(H_{\alpha_0}-\lambda)^{-1}C_\varepsilon^*\Psi \in W^{2,2}(\Omega)$ and

$$(H_{\alpha_0}-\lambda)\Phi = (H_{\alpha_0}-\lambda)(H_{\alpha_0}-\lambda)^{-1}C_\varepsilon^*\Psi = -\varepsilon C_\varepsilon^* D(H_{\alpha_0}-\lambda)^{-1}C_\varepsilon^*\Psi = -\varepsilon C_\varepsilon^* D\Phi. \tag{5.13}$$

□

5.3. Structure of K_ε^λ

To analyze the structure of K_ε^λ we take a closer look on the resolvent operator $(H_{\alpha_0}-\lambda)^{-1}$. We have shown in Lemma 4.5 that the biorthonormal-basis-type relations (4.8) enable us to decompose the resolvent of H_{α_0} into the transverse biorthonormal-basis. Its integral kernel then for every $\lambda \in \mathbb{C}\setminus[\mu_0^2,+\infty)$ reads

$$\big((H_{\alpha_0}-\lambda)^{-1}\big)(x,u,x',u') = \sum_{j=0}^{+\infty}\psi_j(u)\mathcal{R}_{\mu_j^2-\lambda}(x,x')\overline{\phi_j(u')}, \tag{5.14}$$

where ψ_j and ϕ_j were defined in (4.4) and (4.6), respectively, and $\mathcal{R}_{\mu_j^2-\lambda}(x,x')$ is the integral kernel of $(-\Delta'+\mu_j^2-\lambda)$. This naturally differs for various "longitudinal" dimensions n. It is an integral operator with the integral kernel

$$\mathcal{R}_z(x,x') = \begin{cases} \frac{e^{-\sqrt{-z}|x-x'|}}{2\sqrt{-z}} & \text{if } n=1,\\ \frac{1}{2\pi}K_0(\sqrt{-z}|x-x'|) & \text{if } n=2,\\ \frac{e^{-\sqrt{-z}|x-x'|}}{4\pi|x-x'|} & \text{if } n\geqslant 3.\end{cases} \tag{5.15}$$

Here K_0 is Macdonald function [1, Eq. (9.6.2)]. In the rest of this paper we are interested only in the case $n = 1,2$, where K_ε^λ possesses a singularity for λ tending to μ_0^2. This singularity will play a key role in the existence of the bound state (cf. Section 5.4.1 and Remark 5.8). We notice that it arises from the first term in the sum (5.14). Hence, following [44] we decompose it into sum of three operators, $K_\varepsilon^\lambda = \varepsilon D(L_\lambda + N_\lambda + R_{\alpha_0}^\perp)C_\varepsilon^*$, separating the diverging part in the operator $L_\varepsilon^\lambda := \varepsilon D L_\lambda C_\varepsilon^*$, where L_λ is an integral operator with the kernel

$$\mathcal{L}_\lambda(x,u,x',u') := \begin{cases} \psi_0(u)\frac{1}{2\sqrt{\mu_0^2-\lambda}}\overline{\phi_0(u')} & \text{if } n=1,\\ -\frac{1}{2\pi}\psi_0(u)\ln\sqrt{\mu_0^2-\lambda}\,\overline{\phi_0(u')} & \text{if } n=2.\end{cases} \tag{5.16}$$

We indeed see that the integral kernel $\mathcal{L}_\lambda$ diverges for λ tending to μ_0^2. The integral kernels of N_λ and $R_{\alpha_0}^\perp(\lambda)$ are

$$\mathcal{N}_\lambda(x,u,x',u') := \begin{cases} \psi_0(u)\frac{e^{-\sqrt{\mu_0^2-\lambda}|x-x'|}-1}{2\sqrt{\mu_0^2-\lambda}}\overline{\phi_0(u')} & \text{if } n=1,\\ \frac{1}{2\pi}\psi_0(u)(K_0(\sqrt{\mu_0^2-\lambda}|x-x'|)+\ln\sqrt{\mu_0^2-\lambda})\overline{\phi_0(u')} & \text{if } n=2,\end{cases} \tag{5.17}$$

and

$$\mathcal{R}_{\alpha_0}^{\perp}(x, u, x', u'; \lambda) := \begin{cases} \sum_{j=1}^{+\infty} \psi_j(u) \frac{e^{-\sqrt{\mu_j^2-\lambda}|x-x'|}}{2\sqrt{\mu_j^2-\lambda}} \overline{\phi_j(u')} & \text{if } n = 1, \\ -\frac{1}{2\pi} \sum_{j=1}^{+\infty} \psi_j(u) K_0(\sqrt{\mu_j^2 - \lambda}|x - x'|) \overline{\phi_j(u')} & \text{if } n = 2, \end{cases} \tag{5.18}$$

respectively. We see that N_λ is the remainder after the singular part L_λ in the first term of the resolvent expansion (5.14) and $R_{\alpha_0}^{\perp}$ is nothing else than the projection of the resolvent of H_{α_0} on higher transversal modes. We collectively denote the regular part $M_\varepsilon^\lambda := \varepsilon D N_\lambda C_\varepsilon^* + \varepsilon D R_{\alpha_0}^{\perp}(\lambda) C_\varepsilon^*$. We define a new variable

$$k := \begin{cases} \sqrt{\mu_0^2 - \lambda} & \text{if } n = 1, \\ (\ln \sqrt{\mu_0^2 - \lambda})^{-1} & \text{if } n = 2, \end{cases} \tag{5.19}$$

and show that M_ε^λ is well-behaved with respect to this variable including the region where $k = 0$ (i.e. where $\lambda = \mu_0^2$). This will hold whenever β and its derivatives decay sufficiently fast in $\pm\infty$. We divide the proof of this fact into several lemmas.

5.3.1. Behaviour of the projected resolvent

Independently on the specific form of the integral kernel (5.18) of the projected resolvent $R_{\alpha_0}^{\perp}(\lambda)$, we are able to establish its boundedness and analyticity.

Lemma 5.3. *$D R_{\alpha_0}^{\perp}(\lambda) C_\varepsilon^*$ as a function of k defined in $\{k \in \mathbb{C} \mid \operatorname{Re} k > 0\}$ for $n = 1$ or in $\{k \in \mathbb{C} \mid \operatorname{Re} k < 0\}$ for $n = 2$ is a bounded operator-valued function.*

Proof. Let Π_0 be the projection on ψ_0 in $L^2(I)$ (ψ_0 was defined in (4.4)) and let us define a projection $\mathcal{P}_0 := 1 \otimes \Pi_0$ onto the subspace in $L^2(\Omega)$. We denote $\mathcal{P}_0^{\perp} := 1 - \mathcal{P}_0$ projection onto its orthogonal complement. Now $R_{\alpha_0}^{\perp}(\lambda) = R_{\alpha_0}(\lambda)\mathcal{P}_0^{\perp}$ has an analytic continuation into the region $\mathbb{C} \setminus [\mu_1^2, +\infty)$ since the lowest point in the spectrum of $H_{\alpha_0}\mathcal{P}_0^{\perp} \restriction \mathcal{P}_0^{\perp} L^2(\Omega)$ is μ_1^2. (Recall that its spectrum lies on the positive real half-line.) This includes the studied region $\mathbb{C} \setminus [\mu_0^2, +\infty)$.

In fact, we need show that $D R_{\alpha_0}^{\perp}(\lambda) C_\varepsilon^*$ is bounded. It is straightforward to see since every action of C_ε on any $\Psi \in L^2(\Omega)$ can be estimated and we see that C_ε is bounded and the same holds for C_ε^*. To show that $D R_{\alpha_0}^{\perp}(\lambda)$ is also bounded we apply the first resolvent formula to obtain

$$D R_{\alpha_0}^{\perp}(\lambda) = D(H_{\alpha_0} - \lambda)^{-1} \mathcal{P}_0^{\perp} = D(H_{\alpha_0} + 1)^{-1} \big(\mathcal{P}_0^{\perp} - (\lambda + 1)(H_{\alpha_0} - \lambda)^{-1} \mathcal{P}_0^{\perp}\big). \tag{5.20}$$

The operator $\mathcal{P}_0^{\perp} - (\lambda + 1)(H_{\alpha_0} - \lambda)^{-1} \mathcal{P}_0^{\perp}$ is clearly bounded. The boundedness of $D(H_{\alpha_0} + 1)^{-1}$ follows from the definition of D in (5.7) and the fact that the image of $(H_{\alpha_0} + 1)^{-1}$ lies in $W^{2,2}(\Omega)$. □

Lemma 5.4. *$(\psi, D R_{\alpha_0}^{\perp}(\lambda) C_\varepsilon^* \phi)$ as a function of k is analytic in $\{k \in \mathbb{C} \mid \operatorname{Re} k > 0\}$ for $n = 1$ or in $\{k \in \mathbb{C} \mid \operatorname{Re} k < 0\}$ for $n = 2$ for every $\psi, \phi \in L^2(\Omega) \otimes \mathbb{C}^{2n+3}$.*

Proof. The analyticity can be showed in the same manner as the boundedness in Lemma 5.3, now using the first resolvent formula. It is equivalent to showing that the sesquilinear form

$$r_\lambda(\Phi, \Psi) := \big(\Phi, D R_{\alpha_0}^{\perp}(\lambda) C_\varepsilon^* \Psi\big) \tag{5.21}$$

is analytic as a function of λ for every Φ and Ψ from the fundamental subset. We are in fact able to show for every $\Phi, \Psi \in L^2(\Omega)$ and every $\lambda_0 \in \mathbb{C} \setminus [\mu_0^2, +\infty)$

$$\begin{aligned} r'_{\lambda_0}(\Phi, \Psi) &:= \lim_{\lambda \to \lambda_0} \frac{r_\lambda(\Phi, \Psi) - r_{\lambda_0}(\Phi, \Psi)}{\lambda - \lambda_0} \\ &= \lim_{\lambda \to \lambda_0} \frac{(\Phi, (DR_{\alpha_0}^{\perp}(\lambda)C_\varepsilon^* - DR_{\alpha_0}^{\perp}(\lambda_0)C_\varepsilon^*)\Psi)}{\lambda - \lambda_0} \\ &= \lim_{\lambda \to \lambda_0} \frac{(\Phi, D((\lambda - \lambda_0)R_{\alpha_0}^{\perp}(\lambda)R_{\alpha_0}^{\perp}(\lambda_0))C_\varepsilon^*\Psi)}{\lambda - \lambda_0} \\ &= \lim_{\lambda \to \lambda_0} \frac{(D^*\Phi, ((\lambda - \lambda_0)R_{\alpha_0}^{\perp}(\lambda)R_{\alpha_0}^{\perp}(\lambda_0))C_\varepsilon^*\Psi)}{\lambda - \lambda_0} \\ &= \left(\Phi, DR_{\alpha_0}^{\perp}(\lambda_0)^2 C_\varepsilon^*\Psi\right). \end{aligned} \tag{5.22}$$

(The dash denotes differentiation with respect to λ.) The next step would be to show boundedness of $DR_{\alpha_0}^{\perp}(\lambda_0)^2 C_\varepsilon^*$ which can be done exactly in the same way as the proof of the boundedness of $DR_{\alpha_0}^{\perp}(\lambda_0)C_\varepsilon^*$. □

5.3.2. Behaviour of N_ε^λ in the strip ($n = 1$)

Let us now assume decay of β and of its derivatives in $\pm\infty$, specifically that for $\alpha = 0, 1, 2$ and $j = 1, \ldots, n$

$$\partial_{x_j}^{\alpha} \beta = o\left(|x|^{-\mu}\right) \quad \text{for } |x| \to +\infty \tag{5.23}$$

holds with $\mu > 5$. Then we are able to show that $DN_\lambda C_\varepsilon^*$ is well-behaved.

Lemma 5.5. *Let us assume* (5.23). *Then $DN_\lambda C_\varepsilon^*$ as a function of k defined in $\{k \in \mathbb{C} \mid \operatorname{Re} k > 0\}$ is a bounded and analytic operator-valued function.*

Proof. We are able to obtain an integral operator from $DN_\lambda C_\varepsilon^*$ by immersing the differentiations in D into the inside of the integral operator $N_\lambda C_\varepsilon^*$. (This operation is justified, if the new integral kernel will be integrable and that is the object of our proof anyway.) Now, in the integral kernel, every part depending on u can be uniformly estimated. Therefore we may check only the boundedness and analyticity of integral operators $h\tilde{N}_\lambda h$ and $h\,\partial\tilde{N}_\lambda h$ with kernels $hn_\lambda h$ and $h\,\partial n_\lambda h$, respectively, where

$$\begin{aligned} n_\lambda(x, x') &:= \frac{e^{-\sqrt{\mu_0^2 - \lambda}|x - x'|} - 1}{2\sqrt{\mu_0^2 - \lambda}}, \\ \partial n_\lambda(x, x') &:= -\frac{1}{2}\frac{x - x'}{|x - x'|} e^{-\sqrt{\mu_0^2 - \lambda}|x - x'|}, \end{aligned} \tag{5.24}$$

with $h(x)$ being a bounded continuous function in $\mathbb{R}$. Its specific form is not important, the main role plays its behaviour in infinity. Since h arises from the terms inside of C_ε and D, h decays in $\pm\infty$ faster than $|x|^{5/2+\delta/2}$. As a consequence, $h \in L^2(\mathbb{R}, (1+x^2+x^4)\,\mathrm{d}x)$ since it is bounded and its absolute value can be estimated near $\pm\infty$ by $1/|x|^{5/2+\delta/2}$. Using the Hilbert–Schmidt norm we get

$$\begin{aligned}\|h\tilde{N}_\lambda h\|^2 &\leqslant \frac{1}{4}\int_{\mathbb{R}^2} \left|h(x)\right|^2 \left|x-x'\right|^2 \left|h(x')\right|^2 \mathrm{d}x\,\mathrm{d}x' \\ &\leqslant \frac{1}{2}\int_{\mathbb{R}^2} \left|h(x)\right|^2 \left(|x|^2+\left|x'\right|^2\right) \left|h(x')\right|^2 \mathrm{d}x\,\mathrm{d}x' \\ &\leqslant \frac{1}{2}\left(\int_{\mathbb{R}} \left|h(x)\right|^2 \left(1+x^2\right)\mathrm{d}x\right)^2 < +\infty. \end{aligned} \tag{5.25}$$

In the same manner the boundedness of $h\,\partial\tilde{N}_\lambda h$ can be shown:

$$\begin{aligned}\left\|h\tilde{N}'_\lambda h\right\| &\leqslant \frac{1}{4}\int_{\mathbb{R}^2} \left|h(x)^2\right| \mathrm{e}^{-2\sqrt{\mu_0^2-\lambda}|x-x'|} \left|h(x')\right|^2 \mathrm{d}x\,\mathrm{d}x' \\ &\leqslant \frac{1}{4}\int_{\mathbb{R}} \left|h(x)^2\right| \mathrm{d}x \int_{\mathbb{R}} \left|h(x')^2\right| \mathrm{d}x' < +\infty. \end{aligned} \tag{5.26}$$

To verify the second inequality in (5.25) it is sufficient to see that

$$\left|\frac{\mathrm{e}^{a+\mathrm{i}b}-1}{-(a+\mathrm{i}b)}\right|^2 \leqslant 1 \tag{5.27}$$

holds for all $a, b \in \mathbb{R}$, $a < 0$. After an explicit calculation of the absolute value on left-hand side of the inequality and a simple algebraic manipulation, we reformulate our problem to verification that

$$1+\mathrm{e}^{2a}-2\mathrm{e}^a\cos b - a^2 - b^2 \leqslant 0 \tag{5.28}$$

holds. We employ the estimate $\cos b \geqslant 1 - b^2/2$ which holds for all $b \in \mathbb{R}$ to get

$$\begin{aligned}1+\mathrm{e}^{2a}-2\mathrm{e}^a\cos b - a^2 - b^2 &\leqslant 1+\mathrm{e}^{2a}-2\mathrm{e}^a\left(1-\frac{b^2}{2}\right) - a^2 - b^2 \\ &\leqslant 1+\mathrm{e}^{2a}-2\mathrm{e}^a 1 + b^2 - a^2 - b^2 \\ &= 1+\mathrm{e}^{2a}-2\mathrm{e}^a - a^2. \end{aligned} \tag{5.29}$$

Using calculus of functions of one variable it is now easy to check that $f(a) := 1+\mathrm{e}^{2a}-2\mathrm{e}^a - a^2 \leqslant 0$.

For proving the analyticity we need to check the finiteness of the norms of derivatives of the integral kernels

$$\begin{aligned}\frac{\mathrm{d}n_\lambda}{\mathrm{d}k}(x,x') &= \frac{-k|x-x'|\mathrm{e}^{-k|x-x'|}-\mathrm{e}^{-k|x-x'|}+1}{2k^2}, \\ \frac{\mathrm{d}n'_\lambda}{\mathrm{d}k}(x,x') &= \frac{1}{2}(x-x')\mathrm{e}^{-k|x-x'|}. \end{aligned} \tag{5.30}$$

We estimate

$$\left|\frac{-k|x-x'|\mathrm{e}^{-k|x-x'|}-\mathrm{e}^{-k|x-x'|}+1}{2k^2}\right| \leqslant \left|x-x'\right|^2. \tag{5.31}$$

(This can be proven in exactly the same way as (5.27).) Similarly as in (5.25) we calculate the bound and we obtain

$$\begin{aligned}\left\|h\frac{\mathrm{d}n'_\lambda}{\mathrm{d}k}h\right\|^2 &\leqslant \int_{\mathbb{R}^2}\left|h(x)\right|^2\left|x-x'\right|^4\left|h(x')\right|^2\,\mathrm{d}x\,\mathrm{d}x' \\ &\leqslant 8\int_{\mathbb{R}^2}\left|h(x)\right|^2\left(|x|^4+\left|x'\right|^4\right)\left|h(x')\right|^2\,\mathrm{d}x\,\mathrm{d}x' \\ &\leqslant 8\left(\left|h(x)\right|^2\left(1+|x|^4\right)\mathrm{d}x\right)^2<+\infty.\end{aligned} \tag{5.32}$$

We conduct the estimate of $\frac{\mathrm{d}n'_\lambda}{\mathrm{d}k}$ in the same way:

$$\begin{aligned}\left\|h\frac{\mathrm{d}n_\lambda}{\mathrm{d}k}h\right\|^2 &\leqslant \int_{\mathbb{R}^2}\left|h(x)\right|^2\left(|x|^2+\left|x'\right|^2\right)\left|h(x')\right|^2\,\mathrm{d}x\,\mathrm{d}x' \\ &\leqslant \left(\left|h(x)\right|^2\left(1+|x|^2\right)\mathrm{d}x\right)^2<+\infty. \qquad \square\end{aligned} \tag{5.33}$$

5.3.3. Behaviour of N_ε^λ in the layer ($n=2$)

For the layer, there is a different requirement on the decay of β and of its derivatives in $\pm\infty$, specifically that for $\alpha=0,1,2$ and $j=1,\dots,n$

$$\partial_{x_j}^\alpha\beta = o\left(|x|^{-\mu}\right) \quad \text{for } |x|\to+\infty \tag{5.34}$$

holds with $\mu>4$. Note that these conditions differ from (5.23). This is caused by both different dimension of the problem and by using a different estimate method.

Lemma 5.6. *Let us assume (5.34). Then $DN_\lambda C_\varepsilon^*$ as a function of k defined in $\{k\in\mathbb{C}\mid \operatorname{Re}k<0\}$ is a bounded and analytic operator-valued function*

Proof. Throughout this proof we employ various properties of the Macdonald function K which can be found e.g. in [1, Section 9.6-7]. Similarly as in the proof of Lemma 5.5 we get rid of the derivatives in D and we may check the boundedness of integral operators $h\tilde{N}_\lambda h$ and $h\,\partial_\mu\tilde{N}_\lambda h$ with kernels $hn_\lambda h$ and $h\,\partial_\mu n_\lambda h$, respectively, where

$$\begin{aligned} n_\lambda(x,x') &:= \frac{1}{2\pi}\left(K_0\left(w_0(\lambda)\left|x-x'\right|\right)+\ln w_0(\lambda)\right), \\ \partial_\mu n_\lambda(x,x') &:= -\frac{1}{2\pi}\frac{x_\mu-x'_\mu}{|x-x'|}w_0(\lambda)K_1\left(w_0(\lambda)\left|x-x'\right|\right),\end{aligned} \tag{5.35}$$

with $\mu = 1, 2$ and ∂_μ means the derivative with respect to x_μ. We adopted the notation $w_0(\lambda) = \sqrt{\mu_0^2 - \lambda}$. We used the differentiation formula for Macdonald functions, $K_0' = -K_1$. For the purpose of the estimates, we use several other formulae, which are valid for any $z \in (0, +\infty)$:

$$\begin{aligned}
&\left|\left(K_0(z) + \ln z\right)\mathrm{e}^{-z}\right| \leqslant c_1,\\
&\left|K_1(z) - 1/z\right| \leqslant c_2,\\
&\left|K_1(z) - z\left(K_0(z) + K_2(z)\right)/2\right| \leqslant c_3,\\
&\left|zK_1(z)\right| \leqslant 1,\\
&\left|\left(K_0(z) + \ln z\right)/z\right| \leqslant c_4.
\end{aligned} \tag{5.36}$$

In the calculation of the integral bounds we make use of the polar coordinates

$$\left(x_1', x_2'\right) = (x_1 - \rho\cos\varphi, x_2 - \rho\sin\varphi) \tag{5.37}$$

and employ the estimate via Schur–Holmgren bound, holding for every integral operator K with the integral kernel $\mathscr{K}(\cdot,\cdot)$ acting on $L^2(M)$, where M is an open subset of $\mathbb{R}^n$ [8, Lemma 2.2]:

$$\|K\| \leqslant \|K\|_{SH} := \left(\sup_{x\in M}\int_M \left|\mathscr{K}(x,y)\right| \mathrm{d}y \sup_{y\in M}\int_M \left|\mathscr{K}(x,y)\right| \mathrm{d}x\right)^{1/2}. \tag{5.38}$$

Since h is continuous, bounded and $|x||h(x)| \leqslant 1/|x|^{1+\delta}$ for sufficiently high $|x|$, then $h \in L^1(\mathbb{R}^2, (1 + |x|)\,\mathrm{d}x)$. We obtain

$$\begin{aligned}
\|h\tilde{N}_\lambda h\| &\leqslant \frac{1}{2\pi}\sup_{x\in\mathbb{R}^2}\left|h(x)\right|\int_{\mathbb{R}^2}\left|\left(K_0\left(w_0(\lambda)\left|x-x'\right|\right) + \ln w_0(\lambda)\left|x-x'\right| - \ln\left|x-x'\right|\right)h\left(x'\right)\right|\mathrm{d}x'\\
&\leqslant c_1\|h\|^2_{L^\infty(\mathbb{R}^2)}\left(\int_0^R \mathrm{e}^{w_0(\lambda)\rho}\rho\,\mathrm{d}\rho + \int_0^R |\ln\rho|\rho\,\mathrm{d}\rho\right)\\
&\quad + \frac{1}{2\pi}\sup_{x\in\mathbb{R}^2}\left|h(x)\right|\sup_{z\in(R,+\infty)}\frac{K_0(w_0(\lambda)z) - \ln w_0(\lambda)z + \ln z}{z}\int_{\mathbb{R}^2}\left(|x| + \left|x'\right|\right)h\left(x'\right)\mathrm{d}x'\\
&\leqslant c_1\|h\|^2_{L^\infty(\mathbb{R}^2)}R\left(R\mathrm{e}^{w_0(\lambda)R} + \max\left\{\mathrm{e}^{-1}, R\ln R\right\}\right)\\
&\quad + (c_4 + c_5)\left(\sup_{x\in\mathbb{R}^2}\left|xh(x)\right|\|h\|_{L^1(\mathbb{R}^2)} + \sup_{x\in\mathbb{R}^2}\left|h(x)\right|\|h\|_{L^1(\mathbb{R}^2,|x|\,\mathrm{d}x)}\right) < +\infty,
\end{aligned} \tag{5.39}$$

where $R > 0$ arbitrary and $c_5 := \sup_{z\in(R,+\infty)} \ln z/z$. The estimates of $\|h\tilde{\partial}_\mu N_\lambda h\|_{SH}$ yield

$$\begin{aligned}
\|h\,\partial_\mu\tilde{N}_\lambda h\|_{SH} &\leqslant \|h\|^2_{L^\infty(\mathbb{R}^2)}\int_0^R\frac{\rho\,\mathrm{d}\rho}{\rho} + \sup_{x\in\mathbb{R}^2}\left|h(x)\right|w_0(\lambda)\sup_{z\in(R,+\infty)}K_1\left(w_0(\lambda)z\right)\|h\|_{L^1(\mathbb{R}^2)}\\
&\leqslant \|h\|^2_{L^\infty(\mathbb{R}^2)}R + \frac{1}{R}\|h\|_{L^\infty(\mathbb{R}^2)}\|h\|_{L^1(\mathbb{R}^2)} < +\infty.
\end{aligned} \tag{5.40}$$

Checking the analyticity means, according to its definition, checking the analyticity of the two sesquilinear forms $(\Phi, N_\lambda \Psi)$ and $(\Phi, \partial_\mu N_\lambda \Psi)$ with arbitrary $\Phi, \Psi \in L^2(\mathbb{R}^2)$, taken as functions of k. This can be done by checking the finiteness of the norms of $\mathrm{d}N_\lambda/\mathrm{d}k$ and $\mathrm{d}(\partial_\mu N_\lambda)/\mathrm{d}k$. Using the formula $K_1'(z) = (K_0(z) + K_2(z))/2$ and employing the notation $z := w_0(\lambda)|x - x'|$ we arrive at

$$\begin{aligned}\frac{\mathrm{d}n_\lambda}{\mathrm{d}k} &= \frac{1}{2\pi}\frac{z}{k^2}\left(K_1(z) - \frac{1}{z}\right),\\ \frac{\mathrm{d}(\partial_\mu n_\lambda)}{\mathrm{d}k} &= \frac{1}{2\pi}\frac{x_\mu - x'_\mu}{|x - x'|}\frac{w_0(\lambda)}{k^2}\left(K_1(z) - z\frac{K_0(z) + K_2(z)}{2}\right).\end{aligned} \tag{5.41}$$

Now we use the inequality $\mathrm{e}^{k^{-1}}/k^2 \leqslant c_6$, valid for all $k \in (-\infty, 0)$ and estimate

$$\begin{aligned}\left\| h\frac{\mathrm{d}n_\lambda}{\mathrm{d}k}h\right\| &\leqslant \frac{c_2 c_6}{2\pi}\sup_{x\in\mathbb{R}^2}\left|h(x)\right|\int_{\mathbb{R}^2}\left(|x| + \left|x'\right|\right)\left|h\left(x'\right)\right|\,\mathrm{d}x'\\ &\leqslant \frac{c_2 c_6}{2\pi}\left(\sup_{x\in\mathbb{R}^2}\left|xh(x)\right|\|h\|_{L^1(\mathbb{R}^2)} + \sup_{x\in\mathbb{R}^2}\left|h(x)\right|\|h\|_{L^1(\mathbb{R}^2, x\,\mathrm{d}x)}\right) < +\infty.\end{aligned} \tag{5.42}$$

The estimate of $\mathrm{d}\partial_\mu n_\lambda/\mathrm{d}k$ can also be carried out without further difficulties:

$$\left\| h\frac{\mathrm{d}(\partial_\mu n_\lambda)}{\mathrm{d}k}h\right\| \leqslant \frac{c_3 c_6}{2\pi}\|h\|_{L^\infty(\mathbb{R}^2)}\|h\|_{L^1(\mathbb{R}^2)} < +\infty. \qquad \square \tag{5.43}$$

5.4. *The bound state*

Now we are able to summarise the results about both parts of M_ε^λ and state that it is well-behaved in the right half-plane, as we suspected.

Lemma 5.7. *Let us assume* (5.23) *if* $n = 1$ *or* (5.34) *if* $n = 2$. *Then* $M_\varepsilon^\lambda(\lambda(k))$ *as a function of* k *defined in* $\{k \in \mathbb{C} \mid \operatorname{Re} k > 0\}$ *for* $n = 1$ *or in* $\{k \in \mathbb{C} \mid \operatorname{Re} k < 0\}$ *for* $n = 2$ *is a bounded and analytic operator-valued function which can be analytically continued to the region* $\{k \in \mathbb{C} \mid \operatorname{Re} k \geqslant 0\}$ *or* $\{k \in \mathbb{C} \mid \operatorname{Re} k \leqslant 0\}$, *respectively.*

Proof. Let us recall that $M_\varepsilon^\lambda = \varepsilon D R_{\alpha_0}^\perp(\lambda) C_\varepsilon^* + \varepsilon D N_\lambda C_\varepsilon^*$. Using Lemmas 5.3 and 5.4 to study the first part of the operator and Lemma 5.5 in the case of the strip ($n = 1$) or Lemma 5.6 in the case of the layer ($n = 2$) for the study of the latter part, we see that $M_\varepsilon^\lambda(\lambda(k))$ and its derivatives are bounded when $\operatorname{Re} k \to 0$, therefore $M_\varepsilon^\lambda(\lambda(k))$ can be analytically continued to the region where $\operatorname{Re} k = 0$. $\square$

Equipped with Lemma 5.7 we may proceed to the main proof of this section.

5.4.1. *Proof of Theorem* 2.4

Our goal is to find the condition to ensure that the operator $\varepsilon K_\varepsilon^\lambda$ has an eigenvalue -1. First we restrict ourselves to the case $n = 1$. Using Lemma 5.7 we may choose ε so small that $\|M_\varepsilon^\lambda\| < 1$ so the operator $(I + M_\varepsilon^\lambda)^{-1}$ exists and is analytic in the region $\{k \in \mathbb{C} \mid \operatorname{Re} k \geqslant 0\}$. We may write

$$\left(I + K_\varepsilon^\lambda\right)^{-1} = \left(\left(I + M_\varepsilon^\lambda\right)\left(I + \left(I + M_\varepsilon^\lambda\right)^{-1}L_\varepsilon^\lambda\right)\right)^{-1} = \left(I + \left(I + M_\varepsilon^\lambda\right)^{-1}L_\varepsilon^\lambda\right)^{-1}\left(I + M_\varepsilon^\lambda\right)^{-1}, \tag{5.44}$$

and therefore only determine whether the operator $P_\varepsilon^\lambda := (I + M_\varepsilon^\lambda)^{-1} L_\varepsilon^\lambda$ has eigenvalue -1. Since L_ε^λ is a rank-one operator by definition, we can write

$$P_\varepsilon^\lambda(\cdot) = \Phi(\Psi, \cdot), \tag{5.45}$$

with

$$\begin{aligned} \overline{\Psi(x,u)} &:= \varepsilon \psi_0(u) \frac{1}{2\sqrt{-\lambda}} C_\varepsilon^*, \\ \Phi(x,u) &:= \big(\big(I + M_\varepsilon^\lambda\big)^{-1} D\overline{\phi_0}\big)(x,u). \end{aligned} \tag{5.46}$$

(Recall that C_ε^* is just an operator of multiplication by a function.) The operator P_ε^λ can have only one eigenvalue, namely (Ψ, Φ). Putting it equal to -1 we get the condition

$$-1 = \frac{\varepsilon}{2\sqrt{\mu_0^2 - \lambda}} \int_\Omega \psi_0(u) \big(C_\varepsilon^* \big(I + M_\varepsilon^\lambda\big)^{-1} D\overline{\phi_0}\big)(x,u)\,\mathrm{d}x\,\mathrm{d}u. \tag{5.47}$$

Let us define the function

$$G(k,\varepsilon) := -\frac{\varepsilon}{2} \int_\Omega \psi_0(u) \big(C_\varepsilon^* \big(I + M_\varepsilon^\lambda\big)^{-1} D\overline{\phi_0}\big)(x,u)\,\mathrm{d}x\,\mathrm{d}u. \tag{5.48}$$

We shall return to the proof of existence of the eigenvalue later on, let us now for a moment assume that there is a solution to the implicit Eq. (5.47). Using the formula

$$\big(I + M_\varepsilon^\lambda\big)^{-1} = I - M_\varepsilon^\lambda \big(I + M_\varepsilon^\lambda\big)^{-1} = I - M_\varepsilon^\lambda + \big(M_\varepsilon^\lambda\big)^2 \big(I + M_\varepsilon^\lambda\big)^{-1} \tag{5.49}$$

we derive its asymptotic expansion in 0:

$$k(\varepsilon) = \frac{\varepsilon}{2} \int_\Omega \psi_0 C_0^* D\overline{\phi_0} + \mathcal{O}\big(\varepsilon^2\big) = \frac{\varepsilon}{2}\big(C_\varepsilon^* D\phi_0, \psi_0\big) + \mathcal{O}\big(\varepsilon^2\big) \tag{5.50}$$

for ε tending to 0. Since $B_j\phi_0 = 0$ for $j = 1, \ldots, n$, $\int_{\mathbb{R}^n} \Delta'\beta(x)\,\mathrm{d}x = 0$ (due to the decay in infinity) and $(C_\varepsilon)_l = \mathcal{O}(\varepsilon)$ for $l = n+3, \ldots, 2n+3$, after simple calculation we have

$$k(\varepsilon) = \frac{\varepsilon}{2}(B_{n+1}\phi_0, A_{n+1}\psi_0) + \mathcal{O}\big(\varepsilon^2\big) = \mathrm{i}\varepsilon\langle\beta\rangle \left(\frac{\partial}{\partial u}\phi_0, \psi_0\right) + \mathcal{O}\big(\varepsilon^2\big) = -\varepsilon\langle\beta\rangle\alpha_0 + \mathcal{O}\big(\varepsilon^2\big). \tag{5.51}$$

Here we used $\alpha_0 < \pi/d$. Clearly $k \to 0$ when $\varepsilon \to 0$ and if λ ought to be an eigenvalue outside the essential spectrum, $\operatorname{Re} k \geqslant 0$ must hold. This is if $\langle\beta\rangle\alpha_0 < 0$. If $\langle\beta\rangle\alpha_0 > 0$ no eigenvalue can exist. The expansion of k reads $k(\varepsilon) = \sqrt{\mu_0^2 - \lambda} = \varepsilon\langle\beta\rangle\alpha_0 + \mathcal{O}(\varepsilon^2)$ and this gives

$$\lambda(\varepsilon) = \mu_0^2 - \varepsilon^2\langle\beta\rangle^2\alpha_0^2 + \mathcal{O}\big(\varepsilon^3\big) \tag{5.52}$$

as ε goes to 0.

So far we only found out what our solution had to meet, if it existed. Equipped with the knowledge of the asymptotic expansion (5.51) we apply the Rouché's theorem [42, Theorem 10.43(b)] in the disc $B(k_0, r)$, where

$$k_0 := -\varepsilon\langle\beta\rangle\alpha_0 \tag{5.53}$$

and the radius r is so small that the whole disc lies in the half-plane $\operatorname{Re} k > 0$. First we show that $G(k,\varepsilon)$ is analytic as a function of k in the region $\operatorname{Re} k \geqslant 0$. We prepare formula for differentiating of $(1+M_\varepsilon^\lambda)^{-1}$:

$$\begin{aligned}\frac{\partial}{\partial k}\big(1+M_\varepsilon^\lambda\big)^{-1} &= \lim_{k'\to k}\frac{(1+M_\varepsilon^\lambda)^{-1}-(1+M_\varepsilon^{\lambda'})^{-1}}{k-k'}\\ &= \lim_{k'\to k}\frac{(1+M_\varepsilon^\lambda)^{-1}(M_\varepsilon^\lambda-\varepsilon M_\varepsilon^{\lambda'})(1+M_\varepsilon^{\lambda'})^{-1}}{k-k'}\\ &= \big(1+M_\varepsilon^\lambda\big)^{-1}\frac{\partial M_\varepsilon^\lambda}{\partial k}\big(1+M_\varepsilon^\lambda\big)^{-1}.\end{aligned} \tag{5.54}$$

And we have for $G(k,\varepsilon)$ in the region $\operatorname{Re} k \geqslant 0$:

$$\begin{aligned}\left|\frac{\partial G(k,\varepsilon)}{\partial k}\right| &= \frac{\varepsilon}{2}\left|\int_\Omega \psi_0(u)\left(C_\varepsilon^*\frac{\partial}{\partial k}\big(1+M_\varepsilon^\lambda\big)^{-1}D\overline{\phi_0}\,\mathrm{d}x\,\mathrm{d}u\right)(x,u)\right|\\ &= \frac{\varepsilon}{2}\left|\int_\Omega \psi_0(u)\left(C_\varepsilon^*\big(1+M_\varepsilon^\lambda\big)^{-1}\frac{\partial M_\varepsilon^\lambda}{\partial k}\big(1+M_\varepsilon^\lambda\big)^{-1}D\overline{\phi_0}\,\mathrm{d}x\,\mathrm{d}u\right)(x,u)\right|\\ &\leqslant \frac{\varepsilon}{2}\|\psi_0\|_{L^2(I)}\big\|C_\varepsilon^*\big\|\big\|\big(1+M_\varepsilon^\lambda\big)^{-1}\big\|^2\left\|\frac{\partial M_\varepsilon^\lambda}{\partial k}\right\|\|D\phi_0\|_{L^2(\Omega)}\\ &= K\varepsilon,\end{aligned} \tag{5.55}$$

where we used analyticity of M_ε^λ in the region $\operatorname{Re} k \geqslant 0$ (Lemma 5.7) and properties of operators C_ε^* and D. With sufficiently small r we can expand $G(k,\varepsilon)$ in Taylor series in the neighbourhood of the point k_0

$$G(k,\varepsilon) = G(k_0,\varepsilon) + (k-k_0)\frac{\partial G(k,\varepsilon)}{\partial k}(k_0) + \mathcal{O}\big((k-k_0)^2\big). \tag{5.56}$$

We employ Rouché's theorem to show that Eq. (5.47) possesses one simple and unique solution in the half-plane $\operatorname{Re} k > 0$. We prove that the holomorphic functions $G(k,\varepsilon) - k$ and $k_0 - k$ have the same number of zeros (counted as many times as their multiplicity) in $B(k_0, r)$ (i.e. one simple zero). It suffices to show that absolute value of their difference, $|G(k,\varepsilon) - k_0|$, is strictly smaller than $|k_0 - k|$. It directly follows for all $k \in B(k_0, r)$ from (5.51), (5.55) and (5.56)

$$\big|G(k,\varepsilon) - k_0\big| \leqslant \left|\frac{\partial G(k,\varepsilon)}{\partial k} + o(1)\right||k-k_0|, \tag{5.57}$$

where $o(1)$ tends to 0 as k tends to k_0. Using (5.55) and setting ε and r sufficiently small, we can make the coefficient by $|k - k_0|$ strictly smaller than 1.

The reality of the obtained eigenvalue is ensured by the $\mathcal{PT}$-symmetry of the operator H_α (cf. Proposition 3.7). Indeed, from the relation (1.2) follows that if λ is an eigenvalue of H_α, then $\overline{\lambda}$ is its eigenvalue as well. From the uniqueness follows that $\lambda = \overline{\lambda}$ and it is therefore real.

The proof for the case $n = 2$ proceeds in the same manner. Equation (5.47) becomes

$$-1 = -\frac{\varepsilon}{2\pi} \ln \sqrt{\mu_0^2 - \lambda} \int_\Omega \psi_0(u)\big(C_\varepsilon^*\big(I + M_\varepsilon^\lambda\big)^{-1} D\overline{\phi_0}\big)(x, u)\, \mathrm{d}x\, \mathrm{d}u \tag{5.58}$$

and solving it yields the asymptotic expansion

$$\begin{aligned} k(\varepsilon) &= -\frac{\varepsilon}{2\pi}\big(C_\varepsilon^* D\phi_0, \psi_0\big) + \mathcal{O}\big(\varepsilon^2\big) \\ &= \frac{\varepsilon}{2\pi}\langle\beta\rangle\alpha_0 + \mathcal{O}\big(\varepsilon^2\big). \end{aligned} \tag{5.59}$$

Now from the requirement that $\operatorname{Re} k \leqslant 0$ must hold, we obtain the condition $\langle\beta\rangle\alpha_0 > 0$ again. The expansion of $\lambda(\varepsilon)$ reads

$$\lambda(\varepsilon) = \mu_0^2 - \mathrm{e}^{2/w(\varepsilon)} + \mathcal{O}\big(\varepsilon^3\big), \tag{5.60}$$

where $w(\varepsilon) = \frac{\varepsilon}{\pi}\langle\beta\rangle\alpha_0$ for $\varepsilon \to 0$. The proof of existence and uniqueness holds without change.

Remark 5.8. Note the important role of the singularity of the resolvent function on the existence of the bound state. For this purpose it was necessary for K_ε^λ to have an eigenvalue -1, a necessity for this is $\|K_\varepsilon^\lambda\| \geqslant 1$. It would not be possible in the limit $\varepsilon \to 0$ if the resolvent function inside K_ε^λ had not a singularity in the limit $\lambda \to \mu_0^2$. Since the resolvent function in dimension $n \geqslant 3$ does not possess a singularity, it cannot be expected that a weak perturbation of the boundary would yield a bound state. More likely there would be a critical value of the parameter ε, giving a lower bound on ε enabling a bound state.

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ON THE KRAMERS-FOKKER-PLANCK EQUATION WITH DECREASING POTENTIALS IN DIMENSION ONE

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Abstract. For quickly decreasing potentials with one position variable, the first threshold zero is always a resonance of the Kramers-Fokker-Planck operator. In this article we study low-energy spectral properties of the operator and calculate large time asymptotics of solutions in terms of the Maxwellian.

1. Introduction

The Kramers equation is a special Fokker-Planck equation describing the Brownian motion in an external field. This equation was derived and used by H. A. Kramers [13] to describe kinetics of chemical reaction. Later on it turned out that it had more general applicability to different fields such as supersonic conductors, Josephson tunnelling junction and relaxation of dipoles ([19]). Mathematical analysis of the Kramers-Fokker-Planck (KFP, in short) equation is initially motivated by trend to equilibrium for confining potentials ([7, 9, 20]). Spectral problems of the KFP operator reveal to be quite interesting, because this operator is neither elliptic nor selfadjoint. After appropriate normalisation of physical constants and a change of unknowns, the KFP equation can be written into the form

$$\partial_t u(t;x,v) + Pu(t;x,v) = 0,\ \ (x,v) \in \mathbb{R}^n \times \mathbb{R}^n, t > 0, \tag{1.1}$$

with initial data

$$u(0;x,v) = u_0(x,v). \tag{1.2}$$

Here x and v represent respectively position and velocity of the particle, P is the KFP operator given by

$$P = -\Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2} + v\cdot\nabla_x - \nabla V(x)\cdot\nabla_v, \tag{1.3}$$

where the potential $V(x)$ is supposed to be a real-valued C^1 function verifying

$$|V(x)| + \langle x\rangle|\nabla V(x)| \le C\langle x\rangle^{-\rho}, \quad x\in\mathbb{R}^n, \tag{1.4}$$

for some $\rho \in \mathbb{R}$ and $\langle x\rangle = (1+|x|^2)^{1/2}$. Let $\mathfrak{m}$ be the function defined by

$$\mathfrak{m}(x,v) = \frac{1}{(2\pi)^{\frac{n}{4}}} e^{-\frac{1}{2}(\frac{v^2}{2}+V(x))}. \tag{1.5}$$

Then $\mathfrak{M} = \mathfrak{m}^2$ is the Maxwellian ([19]) and $\mathfrak{m}$ verifies the stationary KFP equation

$$P\mathfrak{m} = 0 \quad \text{ on } \mathbb{R}^{2n}_{x,v}. \tag{1.6}$$

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From the point of view of spectral analysis, large time behavior of solutions of (1.1) is closely related to low-energy spectral properties of P. If $V(x) \geq C|x|$ for some constant $C > 0$ outside some compact, then $\mathfrak{m} \in L^2(\mathbb{R}^{2n}_{x,v})$ and zero is a discrete eigenvalue of P. This case has been studied by many authors. It is known that

$$u(t) - \langle u_0, \mathfrak{m}\rangle \mathfrak{m} = O(e^{-\sigma t}), \quad t \to +\infty, \tag{1.7}$$

in $L^2(\mathbb{R}^{2n})$, where $\sigma > 0$ can be evaluated in terms of spectral gap between zero eigenvalue and the real part of the other eigenvalues of P and $V(x)$ is normalized by

$$\int_{\mathbb{R}^n} e^{-V(x)} dx = 1.$$

See [7, 9, 10, 20] and references quoted therein. If $V(x)$ increases slowly: $V(x) \sim c\langle x\rangle^\beta$ for some constants $c > 0$ and $\beta \in]0, 1[$, then zero is an eigenvalue embedded in the essential spectrum of P and it is known that (1.7) still holds with the right-hand side replaced by $O(t^{-\infty})$ ([4, 6]) or more precisely by $O(e^{-at^{\frac{\beta}{2-\beta}}})$ for some $a > 0$ ([16]). For decreasing potentials ($\rho > 0$ in (1.4)), zero is no longer an eigenvalue of P. It is proved in [21] that for $n = 3$ and $\rho > 2$, one has

$$u(t) = \frac{1}{(4\pi t)^{\frac{3}{2}}} \langle u_0, \mathfrak{m}\rangle \mathfrak{m} + O(\frac{1}{t^{\frac{3}{2}+\epsilon}}), \quad t \to +\infty, \epsilon > 0, \tag{1.8}$$

in some weighted spaces. (1.8) shows that for rapidly decreasing potentials, space distribution of particles is still governed by the Maxwellian, but the density of distribution decreases in times in the same rate as for heat propagation. Time-decay estimates of local energies are also obtained in [21] for short-range potentials ($\rho > 1$) and in [16] for long-range potentials ($0 < \rho \leq 1$). See also [2, 8, 14, 15, 18] for other related works.

In this work we study one dimensional KFP equation with quickly decreasing potentials. It is known that for Schrödinger operators, low-energy spectral analysis in one and two dimensional cases is more difficult than higher dimensions and needs specific methods ([1, 3, 11]) because zero is already a threshold resonance of the Laplacian in dimension one and two. For the KFP operator with decreasing potentials, the notion of thresholds and threshold resonances is discussed in [21]. Although $\mathfrak{m}$ always verifies the stationary KFP equation $P\mathfrak{m} = 0$, a basic fact is that $\langle x\rangle^{-s}\mathfrak{m} \notin L^2(\mathbb{R}^{2n})$ if $n \geq 3$ and $1 < s < \frac{n}{2}$, while $\langle x\rangle^{-s}\mathfrak{m} \in L^2(\mathbb{R}^{2n})$ for any $s > 1$ if $n = 1, 2$. In language of threshold spectral analysis, this means that for $n \geq 3$, zero is not a resonance of P while for $n = 1, 2$, zero is a resonance of P with $\mathfrak{m}$ as a resonant state. This is the main difference between the present work and [21].

Set $P = P_0 + W$ where

$$P_0 = v \cdot \nabla_x - \Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2} \text{ and } W = -\nabla_x V(x) \cdot \nabla_v. \tag{1.9}$$

P_0 and P are regarded as operators in $L^2(\mathbb{R}^{2n})$ with the maximal domain. They are then maximally accretive. Denote e^{-tP_0} and e^{-tP}, $t \geq 0$, the strongly continuous semigroups generated by $-P_0$ and $-P$, respectively. If $\rho > -1$, W is a relatively compact perturbation of the free KFP operator P_0: $W(P_0 + 1)^{-1}$ is a compact operator in $L^2(\mathbb{R}^{2n})$.

One can prove that

$$\sigma_{\text{ess}}(P) = \sigma(P_0) = [0, +\infty[\tag{1.10}$$

and that non-zero complex eigenvalues of P have positive real parts and may accumulate only towards points in $[0, +\infty[$. It is unknown for decreasing potentials whether or not the complex eigenvalues does accumulate towards some point in $[0, +\infty[$.

The main result of this work is the following

Theorem 1.1. *Let $n = 1$ and $\rho > 4$. Then for any $s > \frac{5}{2}$, there exists some $\epsilon > 0$ such that*

$$e^{-tP} = \frac{1}{(4\pi t)^{\frac{1}{2}}}\left(\langle \cdot, \mathfrak{m}\rangle \mathfrak{m} + O(t^{-\epsilon})\right), \quad t \to +\infty \tag{1.11}$$

as operators from $\mathcal{L}^{2,s}$ to $\mathcal{L}^{2,-s}$, where

$$\mathcal{L}^{2,r} = L^2(\mathbb{R}^2_{x,v}; \langle x\rangle^{2r} dxdv), \quad r \in \mathbb{R}.$$

To prove (1.11), the main task is to show that the resolvent $R(z) = (P - z)^{-1}$ has an asymptotics of the form

$$R(z) = \frac{i}{2\sqrt{z}}\langle \cdot, \mathfrak{m}\rangle \mathfrak{m} + O(|z|^{-\frac{1}{2}+\epsilon}) \tag{1.12}$$

as operators from $\mathcal{L}^{2,s}$ to $\mathcal{L}^{2,-s}$, for z near zero and $z \notin \mathbb{R}_+$. Although (1.12) and the decay assumption on the potential look the same as the resolvent asymptotics of one dimensional Schrödinger operators in the case where zero is a resonance but not an eigenvalue ([1, 3, 11]), its proof is quite different from the Schrödinger case. In fact, the known methods for the Schrödinger operator can not be applied to the KFP operator, mainly because the perturbation W is a first order differential operator. In this work we use the method of [21] to calculate the low energy asymptotic expansion for the free resolvent $R_0(z) = (P_0 - z)^{-1}$ of the form

$$R_0(z) = \frac{1}{\sqrt{z}}G_{-1} + G_0 + \sqrt{z}G_1 + \cdots \tag{1.13}$$

in appropriate spaces, where G_{-1} is an operator of rank one. By a careful analysis of the space $\mathcal{N}$ of resonant states of P defined by (4.2), we prove that $1 + G_0W$ is invertible on $\mathcal{L}^{2,-s}$, $s > \frac{3}{2}$. (1.12) is derived from the equation

$$R(z) = D(z)(1 + M(z))^{-1}R_0(z) \tag{1.14}$$

for z near zero and $z \notin \mathbb{R}_+$, where

$$D(z) = (1 + R_1(z)W)^{-1} \text{ with } R_1(z) = R_0(z) - \frac{1}{\sqrt{z}}G_{-1}$$

and

$$M(z) = \frac{1}{\sqrt{z}}G_{-1}WD(z).$$

As in threshold spectral analysis for Schrödinger operators, a non-trivial problem here is to compute the value of some spectral constants involving the resonant state of P. Indeed, in most part of this work only the condition $\rho > 2$ is needed. The stronger assumption $\rho > 4$ is used to show that some number $m(z)$ is nonzero for z near 0 and $z \notin \mathbb{R}_+$ (see (5.24)), which allows to prove the invertibility of $1 + M(z)$ and to calculate its inverse.

The organisation of this article is as follows. In Section 2, we recall some known results needed in this work. The low-energy asymptotics of the free resolvent in dimension one is calculated in Section 3. The threshold spectral analysis of P is carried out in Section 4. We prove in particular that zero resonance is simple and $1 + G_0W$ is invertible. The low-energy asymptotics of the full resolvent (1.12) is proved in Section 5, which implies in particular that if $\rho > 4$, zero is not an accumulation point of complex eigenvalues of P. Finally, Theorem 1.1 is deduced in Section 6 by using a high-energy resolvent estimate of [21] valid in all dimensions.

Notation. For $r \geq 0$ and $s \in \mathbb{R}$, introduce the weighted Sobolev space

$$\mathcal{H}^{r,s} = \{u \in \mathcal{S}'(\mathbb{R}^{2n}); (1 - \Delta_v + |v|^2 + \langle D_x\rangle^{\frac{2}{3}})^{\frac{r}{2}}\langle x\rangle^s u \in L^2\}.$$

For $r < 0$, $\mathcal{H}^{r,s}$ is defined as the dual space of $\mathcal{H}^{-r,-s}$ with the dual product identified with the scalar product of L^2. The natural norm on $\mathcal{H}^{r,s}$ is denoted by $\|\cdot\|_{r,s}$. When no confusion is possible, we use $\|\cdot\|$ to denote the usual norm of $L^2(\mathbb{R}^{2n})$ or that bounded operators on L^2. Set $\mathcal{H}^r = \mathcal{H}^{r,0}$ and $\mathcal{L}^{2,s} = \mathcal{H}^{0,s}$. Denote $\mathcal{B}(r, s; r', s')$ the space of continuous linear operators from $\mathcal{H}^{r,s}$ to $\mathcal{H}^{r',s'}$. The weighted Sobolev spaces $\mathcal{H}^{r,s}$ are introduced in accordance with the sub-ellipticity of P_0: although P_0 does not map $\mathcal{H}^{1,s}$ to $\mathcal{H}^{-1,s}$, the sub-elliptic estimate of P_0 (Corollary 2.4) implies that $(P_0 + 1)^{-1} \in \mathcal{B}(-1, 0; 1, 0)$ and a commutator argument shows that $(P_0 + 1)^{-1} \in \mathcal{B}(-1, s; 1, s)$ for any $s \in \mathbb{R}$.

2. Preliminaries

In this Section we fix notation and state some known results which will be used in this work. Denote by P_0 the free KFP operator (with $\nabla V = 0$):

$$P_0 = v \cdot \nabla_x - \Delta_v + \frac{1}{4}|v|^2 - \frac{n}{2}, \quad x, v \in \mathbb{R}^n. \tag{2.1}$$

In terms of Fourier transform in x-variables, we have for $u \in D(P_0)$

$$\begin{aligned} (P_0u)(x, v) &= \mathcal{F}^{-1}_{x\to\xi}\hat{P}_0(\xi)\hat{u}(\xi, v), \quad \text{where} && (2.2)\\ \hat{P}_0(\xi) &= -\Delta_v + \frac{v^2}{4} - \frac{n}{2} + iv \cdot \xi, && (2.3)\\ \hat{u}(\xi, v) &= (\mathcal{F}_{x\to\xi}u)(\xi, v) \triangleq \int_{\mathbb{R}^n} e^{-ix\cdot\xi}u(x, v)\, dx. && (2.4)\end{aligned}$$

Denote

$$D(\hat{P}_0) = \{f \in L^2(\mathbb{R}^{2n}_{\xi,v}); \hat{P}_0(\xi)f \in L^2(\mathbb{R}^{2n}_{\xi,v})\}. \tag{2.5}$$

Then $\hat{P}_0 \triangleq \mathcal{F}_{x\to\xi}P_0\mathcal{F}^{-1}_{x\to\xi}$ is a direct integral of the family of complex harmonic operators $\{\hat{P}_0(\xi); \xi \in \mathbb{R}^n\}$.

For fixed $\xi \in \mathbb{R}^n$, $\hat{P}_0(\xi)$ can be written as

$$\hat{P}_0(\xi) = -\Delta_v + \frac{1}{4}\sum_{j=1}^{n}(v_j + 2i\xi_j)^2 - \frac{n}{2} + |\xi|^2.$$

$\{\hat{P}_0(\xi), \xi \in \mathbb{R}^n\}$ is a holomorphic family of type A with constant domain $D = D(-\Delta_v + \frac{v^2}{4})$ in $L^2(\mathbb{R}^n_v)$. Its spectrum and eigenfunctions can be explicitly calculated. Let $F_j(s) = (-1)^j e^{\frac{s^2}{2}} \frac{d^j}{ds^j} e^{-\frac{s^2}{2}}$, $j \in \mathbb{N}$, be the Hermite polynomials and

$$\varphi_j(s) = (j!\sqrt{2\pi})^{-\frac{1}{2}} e^{-\frac{s^2}{4}} F_j(s)$$

the normalized Hermite functions. For $\xi \in \mathbb{R}^n$ and $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_n) \in \mathbb{N}^n$, define

$$\psi_\alpha(v) = \prod_{j=1}^{n} \varphi_{\alpha_j}(v_j) \text{ and } \psi_\alpha^\xi(v) = \psi_\alpha(v + 2i\xi). \tag{2.6}$$

One can check ([21]) that the spectrum of $\hat{P}_0(\xi)$ is given by

$$\sigma(\hat{P}_0(\xi)) = \{l + \xi^2; l \in \mathbb{N}\}. \tag{2.7}$$

Each eigenvalue $l + \xi^2$ is semi-simple (i.e., its algebraic multiplicity and geometric multiplicity are equal) with multiplicity $m_l = \#\{\alpha \in \mathbb{N}^n; |\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_n = l\}$. The Riesz projection associated with the eigenvalue $l + \xi^2$ is given by

$$\Pi_l^\xi \phi = \sum_{\alpha, |\alpha| = l} \langle \phi, \psi_\alpha^{-\xi} \rangle \psi_\alpha^\xi, \quad \phi \in L^2. \tag{2.8}$$

The following result is useful to study the boundary values of the resolvent $R_0(z) = (P_0 - z)^{-1}$. Let $\hat{R}_0(z) = (\hat{P}_0 - z)^{-1}$ and $\hat{R}_0(z, \xi) = (\hat{P}_0(\xi) - z)^{-1}$ for $z \notin \mathbb{R}_+$. Then $R_0(z) = \mathcal{F}^{-1}_{x \to \xi} \hat{R}_0(z) \mathcal{F}_{x \to \xi}$.

Proposition 2.1. *Let $l \in \mathbb{N}$ and $l < a < l + 1$ be fixed. Take $\chi \geq 0$ and $\chi \in C_0^\infty(\mathbb{R}^n_\xi)$ with supp $\chi \subset \{\xi, |\xi| \leq a + 4\}$, $\chi(\xi) = 1$ when $|\xi| \leq a + 3$ and $0 \leq \chi(\xi) \leq 1$. Then one has*

$$\hat{R}_0(z, \xi) = \sum_{k=0}^{l} \chi(\xi) \frac{\Pi_k^\xi}{\xi^2 + k - z} + r_l(z, \xi), \tag{2.9}$$

for any $\xi \in \mathbb{R}^n$ and $z \in \mathbb{C}$ with $\operatorname{Re} z < a$ and $\operatorname{Im} z \neq 0$. Here $r_l(z, \xi)$ is holomorphic in z with $\operatorname{Re} z < a$ verifying the estimate

$$\sup_{\operatorname{Re} z < a, \xi \in \mathbb{R}^n} \|r_l(z, \xi)\|_{\mathcal{L}(L^2(\mathbb{R}^n_v))} < \infty. \tag{2.10}$$

See Proposition 2.7 of [21] for the proof. As a consequence of Proposition 2.1 and known results for the boundary values of the resolvent of $-\Delta_x$, we obtain the following

Corollary 2.2. *Let $n \geq 1$ and $R_0(z) = (P_0 - z)^{-1}$, $z \notin \mathbb{R}_+$.*

(a). With the notation of Proposition 2.1, one has

$$R_0(z) = \sum_{k=0}^{l} b_k^w(v, D_x, D_v)(-\Delta_x + k - z)^{-1} + r_l(z) \tag{2.11}$$

where $r_l(z)$ is $\mathcal{B}(L^2)$-valued holomorphic function for Re $z < a$ *and $b_k^w(v, D_x, D_v)$ is the Weyl pseudo-differential operator with symbol $b_k(x, \xi, \eta)$ given by*

$$b_k(v, \xi, \eta) = \int_{\mathbb{R}^n} e^{-iv'\cdot\eta/2} \left(\sum_{|\alpha|=k} \chi(\xi)\psi_\alpha(v + v' + 2i\xi)\psi_\alpha(v - v' + 2i\xi) \right) dv'. \tag{2.12}$$

In particular,

$$b_0(v, \xi, \eta) = 2^{\frac{n}{2}} e^{-v^2-\eta^2+2iv\cdot\xi+2\xi^2} \chi(\xi). \tag{2.13}$$

(b). Let I be a compact interval of $\mathbb{R}$ which does not contain any non negative integer. Then for any $s > \frac{1}{2}$, one has

$$\sup_{\lambda\in I;\epsilon\in]0,1]} \|R_0(\lambda \pm i\epsilon)\|_{\mathcal{B}(-1,s;1,-s)} < \infty \tag{2.14}$$

The boundary values of the resolvent $R_0(\lambda \pm i0) = \lim_{\epsilon\to 0_+} R_0(\lambda \pm i\epsilon)$ exist in $\mathcal{B}(0, s; 0, -s)$ for $\lambda \in I$ and is Hölder-continuous in λ.

Seeing (2.11), it is natural to define $\mathbb{N}$ as set of thresholds of the KFP operator P ([21]). Note that an exponential upper-bound in λ for $R_0(\lambda \pm i\epsilon)$, $\epsilon > 0$ fixed, is obtained in [16] by method of harmonic analysis in Besov spaces.

For high energy resolvent estimate, we need the following result proved in Appendix A.2 of [18].

Theorem 2.3. *There exists some constant $C > 0$ such that*

$$\|(1 - \Delta_v + v^2 + |\xi|^{\frac{2}{3}} + |\lambda|^{\frac{1}{2}})(\hat{P}_0(\xi) + \frac{n}{2} + 1 - i\lambda)^{-1}\| \leq C \tag{2.15}$$

uniformly in $\xi \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$.

As consequence, we obtain a uniform sub-elliptic estimate for the free KFP operator.

Corollary 2.4. *One has*

$$|\lambda|\|u\|^2 + \|\Delta_v u\|^2 + \||v|^2 u\|^2 + \||D_x|^{\frac{2}{3}} u\|^2 \leq C\|(P_0 + \frac{n+2}{2} - i\lambda)u\|^2, \tag{2.16}$$

for $u \in \mathcal{S}(\mathbb{R}^{2n}_{x,v})$ and $\lambda \in \mathbb{R}$. In addition, P_0 defined on $\mathcal{S}(\mathbb{R}^{2n}_{x,v})$ is essentially maximally accretive.

Let us indicate that the essential maximal accretivity of P_0 is discussed in [17]. Henceforth we still denote by P_0 its closure in L^2 with maximal domain $D(P_0) = \{u \in L^2(\mathbb{R}^{2n}_{x,v}); P_0 u \in L^2(\mathbb{R}^{2n}_{x,v})\}$. To determine the spectrum of P_0 which is unitarily equivalent with a direct integral of $\hat{P}_0(\xi)$, $\xi \in \mathbb{R}^n$, in addition to (2.7), one needs a resolvent estimate uniform with respect to $\xi \in \mathbb{R}^n$ proved in [21]: $\forall z \in \mathbb{C} \setminus \mathbb{R}_+$,

$$\sup_{\xi\in\mathbb{R}^n} \|(\hat{P}_0(\xi) - z)^{-1}\| \leq C_z. \tag{2.17}$$

See [5] for the necessity of such uniform resolvent estimate in order to determine the spectrum of direct integral of a family of non-selfadjoint operators. (2.7) and (2.17) show that

$$\sigma(P_0) = \cup_{\xi\in\mathbb{R}^n}\sigma(\hat{P}_0(\xi)) = [0,+\infty[. \tag{2.18}$$

Under the condition (1.4) on V for some $\rho > -1$, $|\nabla V(x)| \to 0$ as $|x| \to +\infty$. By Corollary 2.4, $W = -\nabla V(x)\cdot\nabla_v$ is relatively compact with respect to P_0. It follows that

$$\sigma_{\rm ess}(P) = [0,+\infty[\tag{2.19}$$

and discrete spectrum of P is at most countable with possible accumulation points included in $[0,+\infty[$.

3. The free resolvent in dimension one

We use (2.11) with $l = 0$ to calculate the asymptotics of $R_0(z)$ near the first threshold zero.

Proposition 3.1. *Let $n = 1$. One has the following low-energy resolvent asymptotics for $R_0(z)$: for $s, s' > \frac{1}{2}$, there exists $\epsilon > 0$ such that*

$$R_0(z) = \frac{1}{\sqrt{z}}(G_{-1} + O(|z|^\epsilon)), \text{ as } z\to 0, z\notin\mathbb{R}_+, \tag{3.1}$$

as operators in $\mathcal{B}(-1,s;1,-s')$. More generally, for any integer $N\geq 0$ and $s > N+\frac{3}{2}$, there exists $\epsilon > 0$

$$R_0(z) = \sum_{j=-1}^{N} z^{\frac{j}{2}} G_j + O(|z|^{\frac{N}{2}+\epsilon}), \text{ as } z\to 0, z\notin\mathbb{R}_+, \tag{3.2}$$

as operators in $\mathcal{B}(-1,s;1,-s)$. Here the branch of $z^{\frac{1}{2}}$ is chosen such that its imaginary part is positive when $z\notin\mathbb{R}_+$ and $G_j\in\mathcal{B}(-1,s;1,-s)$ for $s > j+\frac{3}{2}$, $j\geq 0$. In particular,

$$G_{-1} = \frac{i}{2}\langle\cdot,\mathfrak{m}_0\rangle\mathfrak{m}_0 \tag{3.3}$$

$$G_0 = F_0 + F_1, \tag{3.4}$$

where

$$\mathfrak{m}_0(x,v) = 1\otimes\psi_0(v) \tag{3.5}$$

with $\psi_0(v) = \frac{1}{(2\pi)^{\frac{1}{4}}}e^{-\frac{v^2}{4}}$ the first eigenfunction of harmonic oscillator, F_0 is the operator with integral kernel

$$F_0(x,v;x',v') = -\frac{1}{2}\psi_0(v)\psi_0(v')|x-x'| \tag{3.6}$$

and $F_1\in\mathcal{B}(-1,s;1,-s')$ for any $s,s' > \frac{1}{2}$.

Proof. For $z\notin\mathbb{R}_+$, (2.11) with $l = 0$ shows that

$$R_0(z) = b_0^w(v,D_x,D_v)(-\Delta_x - z)^{-1} + r_0(z), \tag{3.7}$$

with $r_0(z) \in \mathcal{B}(-1,0;1,0)$ holomorphic in z when Re $z < a$ for some $a \in]0,1[$. Here the cut-off $\chi(\xi)$ is chosen such that $\chi \in C_0^\infty(\mathbb{R}^n)$ and $\chi(\xi) = 1$ in a neighbourhood of $\{|\xi|^2 \leq a\}$. Therefore $r_0(z)$ admits a convergent expansion in powers of z for z near 0

$$r_0(z) = r_0(0) + z r_0'(0) + \cdots + z^n \frac{r_0^{(n)}(0)}{n!} + \cdots$$

in $\mathcal{B}(-1,0;1,0)$. It is sufficient to study the lower-energy expansion of $b_0^w(v, D_x, D_v)(-\Delta_x - z)^{-1}$.

Note that in one dimensional case, the integral kernel of the resolvent $(-\Delta_x - z)^{-1}$ is given by

$$\frac{i}{2\sqrt{z}} e^{i\sqrt{z}|x-y|}, z \notin \mathbb{R}_+, x, y \in \mathbb{R} \tag{3.8}$$

where the branch of $\sqrt{z}$ is chosen such that its imaginary part is positive for $z \notin \mathbb{R}_+$. The integral kernel of $b_0^w(v, D_x, D_v)(-\Delta_x - z)^{-1}$, $z \notin \mathbb{R}_+$, is given by

$$K(x, x'; v, v'; z) = \frac{i}{2\sqrt{z}} \int_{\mathbb{R}} e^{i\sqrt{z}|y-(x-x')|} \Phi(v, v', y)\, dy \tag{3.9}$$

with

$$\begin{aligned} \Phi(v, v', y) &= (2\pi)^{-\frac{3}{2}} e^{-\frac{1}{4}(v^2+v'^2)} \int_{\mathbb{R}} e^{i(y-v-v')\cdot\xi + 2\xi^2} \chi(\xi)\, d\xi \\ &= \psi_0(v)\psi_0(v')\Psi(y - v - v') \end{aligned} \tag{3.10}$$

where Ψ is the inverse Fourier transform of $e^{2\xi^2}\chi(\xi)$. Since $\chi \in C_0^\infty$, one has the following asymptotic expansion for $K(x, x'; v, v'; z)$: for any $\epsilon \in [0,1]$ and $N \geq 0$

$$|K(x, x'; v, v'; z) - \sum_{j=-1}^{N} z^{\frac{j}{2}} K_j(x, x', v, v')| \leq C_{N,\epsilon} |z|^{\frac{N+\epsilon}{2}} |x - x'|^{N+1+\epsilon} e^{-\frac{1}{4}(v^2+v'^2)} \tag{3.11}$$

where

$$K_j(x, x'; v, v') = \frac{i^{j+2}}{2\,(j+1)!} \int_{\mathbb{R}} |y - (x - x')|^{j+1} \Phi(v, v', y) dy. \tag{3.12}$$

Remark that for $N \geq 0$, $s', s > N + \frac{1}{2}$ and $0 < \epsilon < \min\{s, s'\} - N - \frac{1}{2}$ and $\epsilon \in]0, \frac{1}{2}]$

$$\langle x\rangle^{-s} \langle x'\rangle^{-s'} |x - x'|^{N+\epsilon} e^{-\frac{1}{4}(v^2+v'^2)} \in L^2(\mathbb{R}^4).$$

We obtain the asymptotic expansion for $b_0^w(v, D_x, D_v)(-\Delta_x - z)^{-1}$ in powers of $z^{\frac{1}{2}}$ for z near 0 and $z \notin \mathbb{R}_+$.

$$b_0^w(v, D_x, D_v)(-\Delta_x - z)^{-1} = \sum_{j=-1}^{N} z^{\frac{j}{2}} K_j + O(|z|^{\frac{N}{2}+\epsilon}), \text{ as} \tag{3.13}$$

as operators in $\mathcal{B}(0, s'; 0, -s)$, $s', s > N + \frac{3}{2}$. By the sub-elliptic estimate of P_0, this expansion still holds in $\mathcal{B}(-1, s'; 1, -s)$. This proves (3.2) with G_k given by

$$G_{2j} = K_{2j} + \frac{r_0^{(j)}(0)}{j!}, \quad G_{2j-1} = K_{2j-1}, \quad j \geq 0. \tag{3.14}$$

To show (3.3) and (3.4), note that since $\chi(0) = 1$, one has

$$\int_{\mathbb{R}} \Phi(v, v', y)\, dy = \psi_0(v)\psi_0(v').$$

The first two terms in the expansion of $K(x, x'; v, v'; z)$ can be simplified as

$$K_{-1}(x, x', v, v') = \frac{i}{2}\int_{\mathbb{R}} \Phi(v, v', y)dy = \frac{i}{2}\psi_0(v)\psi_0(v') \tag{3.15}$$

$$\begin{aligned} K_0(x, x', v, v') &= -\frac{1}{2}\int_{\mathbb{R}} \Phi(v, v', y)|y - (x - x')|dy \qquad (3.16) \\ &= -\frac{1}{2}\psi_0(v)\psi_0(v')|x - x'| - \frac{1}{2}\int (|y - (x - x')| - |x - x'|)\Phi(v, v', y)dy. \end{aligned}$$

Therefore (3.3) is true and G_0 can be decomposed as: $G_0 = F_0 + F_1$ with F_0 defined by (3.6) and $F_1 = K_{0,1} + r_0(0)$, $K_{0,1}$ being the operator with the integral kernel

$$K_{0,1}(x, x', v, v') = -\frac{1}{2}\int_{\mathbb{R}} (|y - (x - x')| - |x - x'|)\Phi(v, v', y)dy,$$

which is a smooth function and

$$K_{0,1}(x, x', v, v') = O(\psi_0(v)\psi_0(v'))$$

for $|x - x'|$ large. Therefore $K_{0,1}$ is bounded in $B(-1, s; 1, -s')$ for any $s, s' > \frac{1}{2}$. This shows that $F_1 = K_{0,1} + r_0(0)$ has the same continuity property, which proves (3.4). □

Corollary 3.2. *Let $n = 1$ and e^{-tP_0}, $t \geq 0$, be the strongly continuous semigroup generated by $-P_0$. Then for any integer $N \geq 0$ and $s > 2N + \frac{1}{2}$, the following asymptotic expansion holds for some $\epsilon > 0$*

$$e^{-tP_0} = \sum_{k=0}^{N} t^{-\frac{2k+1}{2}}\beta_k G_{2k-1} + O(t^{-\frac{2N+1}{2}-\epsilon}), \quad t \to +\infty, \tag{3.17}$$

in $\mathcal{B}(0, s, 0, s)$. Here β_k is some non zero constant. In particular, the leading term $\beta_0 G_{-1}$ is a rank-one operator given by

$$\beta_0 G_{-1} = \frac{1}{(4\pi)^{\frac{1}{2}}}\langle\cdot, \mathfrak{m}_0\rangle\mathfrak{m}_0 : \mathcal{L}^{2,s} \to \mathcal{L}^{2,-s} \tag{3.18}$$

for any $s > \frac{1}{2}$.

The proof of Corollary 3.2 uses Proposition 3.1 and a representation formula of the semigroup e^{-tP_0} as contour integral of the resolvent $R_0(z)$ in the right half-plane. See the proof of Theorem 1.1 for more details.

4. Threshold spectral properties

Assume that $V \in C^1(\mathbb{R}^n; \mathbb{R})$ and

$$|V(x)| + \langle x\rangle|\nabla V(x)| \leq C\langle x\rangle^{-\rho} \tag{4.1}$$

for some $\rho > 0$. Consider the null space of P defined by

$$\mathcal{N} = \{u; u \in \mathcal{H}^{1,-s}, \forall s > 1 \text{ and } Pu = 0\}. \tag{4.2}$$

Since zero is not an eigenvalue of P, $\mathcal{N}$ is the spaces of resonant states of P associated with zero resonance. See [21] for the definitions in general case. Remark that for $n = 1$, one can equally take $s > \frac{1}{2}$ in the above definition, instead of $s > 1$. But the condition $s > 1$ is necessary to define appropriately resonant states for $n = 2$. Clearly, $\mathfrak{m} \in \mathcal{N}$. We want to prove that in one dimensional case, one has: $\dim \mathcal{N} = 1$. In order to calculate the leading term of the resolvent expansion at threshold zero, we need also to calculate solutions of some integral equation.

Lemma 4.1. *Let $\rho > 0$ and $n = 1$. If $u \in \mathcal{H}^{1,-s}$ for some $s < \rho + \frac{1}{2}$ and satisfies the equation $Pu = 0$, then*

$$\langle Wu, \mathfrak{m}_0 \rangle = 0, \tag{4.3}$$

where

$$\mathfrak{m}_0(x, v) = 1 \otimes \psi_0(v).$$

Proof. Suppose for the moment $n \geq 1$. Since $u \in \mathcal{H}^{1,-s}$, one has $Wu \in \mathcal{H}^{0,\rho+1-s} \subset L^2$. Using the equation $Pu = 0$ and the ellipticity of P in velocity variables v, we deduce that $(-\Delta_v + v^2)u(x, \cdot) \in L^2(\mathbb{R}^n_v)$ a.e. in $x \in \mathbb{R}^n$. Taking scalar product of Pu with $\psi_0(v)$ in v-variables, one has

$$\langle (Pu)(x, \cdot), \psi_0 \rangle_v = 0, \quad \text{a. e.} \quad x \in \mathbb{R}^n.$$

Since ψ_0 is the first eigenfunction of the harmonic oscillator in v, one has also

$$\langle Pu, \psi_0 \rangle_v = \langle v \cdot \nabla_x u, \psi_0 \rangle_v - \langle \nabla_x V(x) \cdot \nabla_v u, \psi_0 \rangle_v$$

a. e. in $x \in \mathbb{R}^n$. These two relations imply that

$$2\nabla_x \cdot \langle \nabla_v u, \psi_0 \rangle_v + \nabla_x V(x) \cdot \langle \nabla_v u, \psi_0 \rangle_v = 0. \tag{4.4}$$

The above equation holds for $n \geq 1$. In the case $n = 1$, $\langle \nabla_v u, \psi_0 \rangle_v$ is a scalar function in x and the differential equation (4.4) determines $\langle \nabla_v u, \psi_0 \rangle_v$ up to some constant:

$$\langle \nabla_v u, \psi_0 \rangle_v = C e^{-\frac{V(x)}{2}}, \text{ a. e. in } x \in \mathbb{R} \tag{4.5}$$

for some constant C. It is now clear that in one dimensional case, one has

$$\langle Wu, \mathfrak{m}_0 \rangle = -\int_{\mathbb{R}} V'(x) \langle \partial_v u, \psi_0 \rangle_v dx = -C \int_{\mathbb{R}} V'(x) e^{-\frac{V(x)}{2}} dx = 0, \tag{4.6}$$

because $V(x) \to 0$ as $|x| \to +\infty$. □

Lemma 4.1 is important in threshold spectral analysis of the KFP operator in dimension one. We believe that this result still holds when $n \geq 2$, but the last argument above does not hold if $n \geq 2$. In fact when $n \geq 2$, (4.4) only implies that the vector-valued function $\langle \nabla_v u, \psi_0 \rangle_v$ is of the form

$$\langle \nabla_v u, \psi_0 \rangle_v = e^{-\frac{V(x)}{2}} \overrightarrow{F}(x) \tag{4.7}$$

where $\overrightarrow{F} \in L^2(\mathbb{R}^n; \langle x \rangle^{-2s} dx)$ and $\nabla \cdot \overrightarrow{F} = 0$ in sense of distributions, which are not sufficient to conclude that $\langle Wu, \mathfrak{m}_0 \rangle = 0$.

From now on, assume that $\rho > 2$ and $n = 1$. Then by the sub-elliptic estimate for P_0, G_0W is a compact operator in $\mathcal{H}^{1,-s}$ for $\frac{3}{2} < s < \frac{\rho+1}{2}$. We want to study solutions of the integral equation

$$(1 + G_0W)u = \beta\mathfrak{m}_0 \tag{4.8}$$

for $u \in \mathcal{H}^{1,-s}$ and $\beta \in \mathbb{C}$.

Lemma 4.2. *Let $\rho > 2$ and $u \in \mathcal{H}^{1,-s}$ for some $\frac{3}{2} < s < \frac{\rho+1}{2}$ such that $(1 + G_0W)u = \beta\mathfrak{m}_0$ for some $\beta \in \mathbb{C}$. Then $Pu = 0$. In particular, one has: $\langle Wu, \mathfrak{m}_0\rangle = 0$.*

Proof. One has seen that

$$R_0(z) = \frac{G_{-1}}{\sqrt{z}} + G_0 + o(1)$$

in $\mathcal{B}(-1, r; 1, -r)$ for any $r > \frac{3}{2}$. Therefore,

$$G_0Wu = \lim_{z\to 0, z\notin\mathbb{R}_+}(R_0(z) - \frac{G_{-1}}{\sqrt{z}})Wu$$

in $H^{1,-r}$. Since $P_0G_{-1} = 0$ in $\mathcal{H}^{-1,r}$, one has for $\lambda < 0$

$$P_0(R_0(\lambda) - \frac{G_{-1}}{\sqrt{\lambda}})Wu = Wu + \lambda R_0(\lambda)Wu.$$

The m-accretivity of P_0 implies

$$\|\lambda R_0(\lambda)W\| \le 1, \quad \lambda < 0.$$

It follows that

$$\|\lambda R_0(\lambda)Wu\| \le \|Wu\| \le C\|u\|_{1,-s}, \quad \frac{3}{2} < s < \frac{\rho+1}{2},$$

uniformly in $\lambda < 0$. In addition, if $\frac{1}{2} < s' < \frac{\rho+1}{2}$, one has

$$\|\lambda R_0(\lambda)Wu\|_{1,-s'} \le \|\lambda R_0(\lambda)\|_{\mathcal{B}(0,s';0,-s')}\|Wu\|_{0,s'} \le C|\lambda|^{\frac{1}{2}}\|u\|_{1,-s}$$

for $\lambda < 0$. These two bounds show that

$$w - \lim_{\lambda\to 0_-} \lambda R_0(\lambda)Wu = 0, \quad \text{in } L^2(\mathbb{R}^2). \tag{4.9}$$

Since $u = -G_0Wu + \beta\mathfrak{m}_0$ and $P_0\mathfrak{m}_0 = 0$, the following equalities hold:

$$P_0u = -w - \lim_{\lambda\to 0_-} P_0(R_0(\lambda) - \frac{G_{-1}}{\sqrt{\lambda}})Wu = -Wu$$

in sense of distributions. This proves that $Pu = 0$. In particular Lemma 4.1 shows that $\langle Wu, \mathfrak{m}_0\rangle = 0$. □

Proposition 4.3. *Let $u \in \mathcal{H}^{1,-s}$ for some $\frac{3}{2} < s < \frac{\rho+1}{2}$ such that $(1 + G_0W)u = \beta\mathfrak{m}_0$ for some $\beta \in \mathbb{C}$. Then one has*

$$u(x, v) = (\beta - C_1(x) - vC_2(x))\psi_0(v) + r(x, v) \tag{4.10}$$

where $C_j \in L^\infty$ and $C_j' \in L^1$, $j = 1, 2$, and $(1 + v^2 - \partial_v^2)r \in L^2(\mathbb{R}^2_{x,v})$. In addition,

$$\lim_{x\to\pm\infty} C_1(x) = \pm d_1, \quad \lim_{x\to\pm\infty} C_2(x) = 0 \tag{4.11}$$

where

$$d_1 = -\frac{1}{4}\int\int_{\mathbb{R}^2} (x + \frac{v}{2})\psi_0(v)\nabla V(x)\nabla_v u(x,v)dxdv. \tag{4.12}$$

In particular, $u \in \mathcal{H}^{1,-s}$ *for any* $s > \frac{1}{2}$*.*

Proof. Recall that $G_0 = K_1 + r_0(0)$ where $r_0(0)$ is bounded from $\mathcal{H}^{-1}$ to $\mathcal{H}^1$ and K_1 is an operator of integral kernel

$$K_1(x, x'; v, v') = -\frac{1}{2}\int_{\mathbb{R}} |y - (x - x')|\Phi(v, v'; y)dy \tag{4.13}$$

with

$$\Phi(v, v', y) = \frac{1}{2}\psi_0(v)\psi_0(v')\Psi(y - v - v'),$$

Ψ being the inverse Fourier transform of $e^{2\xi^2}\chi(\xi)$. Let $u \in \mathcal{H}^{1,-s}$, $\frac{3}{2} < s < \frac{\rho+1}{2}$, such that $(1 + G_0W)u = \beta\mathfrak{m}_0$. By Lemma 4.2,

$$\langle Wu, \mathfrak{m}_0\rangle = 0. \tag{4.14}$$

Set $w = K_1Wu$. Then $u + w - \beta\mathfrak{m}_0 = -r_0(0)Wu$ belongs to L^2. Let us study the asymptotic behavior of w as $|x| \to \infty$. Put

$$F(x', y, v, v') = \psi_0(v)\psi_0(v')\Psi(y - v - v')\nabla V(x')\nabla_v u(x', v').$$

Making use of the asymptotic expansion

$$|y - (x - x')| = |x - x'| - \frac{y(x - x')}{|x - x'|} + O(\frac{y^2}{|x - x'|})$$

for $|x - x'|$ large, one obtains that

$$\begin{aligned} w(x, v) &= \frac{1}{4}\int\int_{\mathbb{R}^3} |y - (x - x')|F(x', y, v, v')dydx'dv' \\ &\simeq \frac{1}{4}\int\int_{\mathbb{R}^3} (|x - x'| - \frac{y(x - x')}{|x - x'|})F(x', y, v, v')dydx'dv' \\ &= \frac{1}{4}\int\int_{\mathbb{R}^2} (|x - x'| - \frac{(v + v')(x - x')}{|x - x'|})\psi_0(v)\psi_0(v')\nabla V(x')\nabla_v u(x', v')dx'dv'. \end{aligned} \tag{4.15}$$

Here and in the following, "$\simeq$" means the equality modulo some term in $L^2(\mathbb{R}^2)$.

Recall that since Ψ is the inverse Fourier transform of $e^{2\xi^2}\chi(\xi)$, one has

$$\int_{\mathbb{R}} \Psi(y)dy = 1, \quad \int_{\mathbb{R}} y\Psi(y)dy = 0$$

and that according to Lemma 4.1

$$\int_{\mathbb{R}^2} \psi_0(v')\nabla V(x')\nabla_v u(x', v')dx'dv' = -\langle Wu, \mathfrak{m}_0\rangle = 0. \tag{4.16}$$

The term related to $|x-x'|$ on the right-hand side of (4.15) is equal to

$$\begin{aligned}
&\frac{1}{4}\int\int_{\mathbb{R}^2}(|x-x'|)\psi_0(v)\psi_0(v')\nabla V(x')\nabla_v u(x',v')dx'dv' \\
&= \frac{1}{4}\left(\int_{-\infty}^{x}-\int_{x}^{+\infty}\right)(x-x')\psi_0(v)\nabla V(x')\langle\nabla_{v'}u(x',\cdot),\psi_0\rangle_{v'}dx' \qquad (4.17)
\end{aligned}$$

Applying (4.16), one has for $x\leq 0$

$$\begin{aligned}
&\left|x\left(\int_{-\infty}^{x}-\int_{x}^{+\infty}\right)\psi_0(v)\nabla V(x')\langle\nabla_{v'}u(x',\cdot),\psi_0\rangle_{v'}dx'\right| \\
&= \left|2x\int_{-\infty}^{x}\psi_0(v)\nabla V(x')\langle\nabla_{v'}u(x',\cdot),\psi_0\rangle_{v'}dx'\right| \\
&\leq C|x|\left\{\int_{-\infty}^{x}\langle x'\rangle^{-2(\rho+1-s)}dx'\right\}^{\frac{1}{2}}\psi_0(v)\|u\|_{\mathcal{H}^{1,-s}} \\
&\leq C'\langle x\rangle^{-\rho+s+\frac{1}{2}}\psi_0(v)\|u\|_{\mathcal{H}^{1,-s}} \qquad (4.18)
\end{aligned}$$

Since $\rho>2$ and $s<\frac{\rho+1}{2}$, this proves that the term

$$x\left(\int_{-\infty}^{x}-\int_{x}^{+\infty}\right)\nabla V(x')\langle\nabla_{v'}u(x',\cdot),\psi_0\rangle_{v'}dx'$$

is bounded for $x\leq 0$ and tends to 0 as $x\to-\infty$. The same conclusion also holds as $x\to+\infty$, using once more (4.16). In the same way one can check that

$$\left(\int_{-\infty}^{x}-\int_{x}^{+\infty}\right)x'\nabla V(x')\langle\nabla_{v'}u(x',\cdot),\psi_0\rangle_{v'}dx'$$

is bounded for $x\in\mathbb{R}$. The other terms in (4.15) can be studied in a similar way. Finally we obtain that

$$\begin{aligned}
w(x,v) &\simeq (C_1(x)+vC_2(x))\psi_0(v) \text{ where} \qquad (4.19)\\
C_1(x) &= \frac{1}{4}\int\int_{\mathbb{R}^2}(x-x'-\frac{v'}{2})\text{sgn }(x-x')\psi_0(v')\nabla V(x')\nabla_v u(x',v')dx'dv' \qquad (4.20)\\
C_2(x) &= -\frac{1}{8}\int\int_{\mathbb{R}^2}\text{sgn }(x-x')\psi_0(v')\nabla V(x')\nabla_v u(x',v')dx'dv'. \qquad (4.21)
\end{aligned}$$

It follows from Dominated Convergence Theorem that the limits

$$\lim_{x\to\pm\infty}C_j(x)=\pm d_j \qquad (4.22)$$

exist, where

$$\begin{aligned}
d_1 &= -\frac{1}{4}\int\int_{\mathbb{R}^2}(x'+\frac{v'}{2})\psi_0(v')\nabla V(x')\nabla_v u(x',v')dx'dv' \qquad (4.23)\\
d_2 &= -\frac{1}{8}\int\int_{\mathbb{R}^2}\psi_0(v')\nabla V(x')\nabla_v u(x',v')dx'dv'=0. \qquad (4.24)
\end{aligned}$$

This proves that

$$u\simeq\beta\mathfrak{m}_0-w\simeq(\beta-C_1(x)-vC_2(x))\psi_0(v)$$

modulo some terms in $L^2(\mathbb{R}^2)$. In particular, $u \in \mathcal{H}^{1,-s}$ for any $s > \frac{1}{2}$. Since $\rho > 2$, one can also check that $C_j'(x)$ belongs to $L^1(\mathbb{R})$, $j = 1, 2$. □

Theorem 4.4. *Assume $\rho > 2$. If $u \in \mathcal{H}^{1,-s}$, $\frac{3}{2} < s < \frac{\rho+1}{2}$, satisfies the equation $(1 + G_0 W)u = 0$, then $u = 0$.*

Proof. Let $\chi_1 \in C_0^\infty(\mathbb{R})$ be a cut-off with $\chi_1(\tau) = 1$ for $|\tau| \le 1$ and $\chi_1(\tau) = 0$ for $|\tau| \ge 2$ and $0 \le \chi_1(\tau) \le 1$. Set $\chi_R(x) = \chi_1(\frac{x}{R})$ for $R \ge 1$ and $u_R(x, v) = \chi_R(x)u(x, v)$. Then one has

$$Pu_R = \frac{v}{R}\chi'(\frac{x}{R})u.$$

Taking the real part of the equality $\langle Pu_R, u_R\rangle = \langle \frac{v}{R}\chi'(\frac{x}{R})u, u_R\rangle$, one obtains

$$\int\int_{\mathbb{R}^2} |(\partial_v + \frac{v}{2})u(x, v)|^2 \chi_R(x)^2 \, dxdv = \langle \frac{v}{R}\chi'(\frac{x}{R})u, u_R\rangle. \tag{4.25}$$

According to Proposition 4.3, u can be decomposed as

$$u(x, v) = z(x, v) + r(x, v) \tag{4.26}$$

where $z(x, v) = -(C_1(x) + vC_2(x))\psi_0(v)$ and C_1, C_2 and r are given in Proposition 4.3. Since $\psi_0(v)$ is even in v, the term $\langle \frac{v}{R}\chi'(\frac{x}{R})z, \chi_R z\rangle$ is reduced to

$$2\text{Re}\, \langle \frac{v^2}{R}\chi'(\frac{x}{R})C_1\psi_0, \chi_R C_2\psi_0\rangle \tag{4.27}$$

$$= \; -\text{Re} \int\int_{\mathbb{R}^2} v^2\psi_0(v)^2\chi_R(x)^2 \frac{d}{dx}(C_1(x)\overline{C}_2(x))dxdv \tag{4.28}$$

$$\to \; -\text{Re} \int\int_{\mathbb{R}^2} v^2\psi_0(v)^2 \frac{d}{dx}(C_1(x)\overline{C}_2(x))dxdv = 0 \tag{4.29}$$

as $R \to +\infty$, because $\frac{d}{dx}(C_1(x)\overline{C}_2(x))$ belongs to L^1 and $C_1(x)\overline{C}_2(x) \to 0$ as $|x| \to +\infty$. The term $|\langle \frac{v}{R}\chi'(\frac{x}{R})r, u_R\rangle|$ can be estimated by

$$|\langle \frac{v}{R}\chi'(\frac{x}{R})r, u_R\rangle| \le CR^{-(1-s)}\|u\|_{L^{2,-s}}\|\langle v\rangle r\|_{L^2}$$

for $\frac{1}{2} < s < 1$. Similar estimate also holds for $|\langle \frac{v}{R}\chi'(\frac{x}{R})z, \chi_R r\rangle|$. Summing up, we proved that

$$\lim_{R\to+\infty} \langle \frac{v}{R}\chi'(\frac{x}{R})u, u_R\rangle = 0 \tag{4.30}$$

which implies that $(\partial_v + \frac{v}{2})u(x, v) = 0$ a.e. in x and v. Since $u \in \mathcal{H}^{1,-s}$ for any $s > \frac{1}{2}$ and $Pu = 0$, it follows that u is of the form $u(x, v) = D(x)e^{-\frac{v^2}{4}}$ for some $D \in L^{2,-s}(\mathbb{R})$ verifying the equation

$$D'(x) + \frac{1}{2}V'(x)D(x) = 0 \tag{4.31}$$

in sense of distributions on $\mathbb{R}$. It follows that $D(x) = \alpha e^{-\frac{V(x)}{2}}$ a.e. for some constant α. Hence

$$u(x, v) = \alpha e^{-\frac{v^2}{4} - \frac{V(x)}{2}}.$$

In particular, one has

$$\int_0^R \int_{\mathbb{R}_v} u(x,v)dvdx = \sqrt{\pi}\alpha R + O(1) \quad (4.32)$$

$$\int_{-R}^0 \int_{\mathbb{R}_v} u(x,v)dvdx = \sqrt{\pi}\alpha R + O(1) \quad (4.33)$$

as $R \to +\infty$. But according to Proposition 4.3, one has for some constant d_1

$$\int_0^R \int_{\mathbb{R}_v} u(x,v)dvdx = -\frac{d_1}{\sqrt{2}}R + o(R) \quad (4.34)$$

$$\int_{-R}^0 \int_{\mathbb{R}_v} u(x,v)dvdx = \frac{d_1}{\sqrt{2}}R + o(R). \quad (4.35)$$

as $R \to +\infty$. One concludes that $\alpha = d_1 = 0$. Therefore $u = 0$. □

Since G_0W is a compact operator on $\mathcal{H}^{1,-s}$, $\frac{3}{2} < s < \frac{\rho+1}{2}$, it follows from Theorem 4.4 that $1 + G_0W$ is invertible and

$$(1 + G_0W)^{-1} \in \mathcal{B}(1,-s;1,-s). \quad (4.36)$$

Theorem 4.5. *Let $\rho > 2$. One has:*

$$\mathcal{N} = \{u \in \mathcal{H}^{1,-s}; (1+G_0W)u = \beta\mathfrak{m}_0 \text{ for some } \beta \in \mathbb{C}, \frac{3}{2} < s < \frac{\rho+1}{2}\}. \quad (4.37)$$

In particular, $\mathcal{N}$ is of dimension one and

$$(1 + G_0W)\mathfrak{m} = \mathfrak{m}_0 \quad (4.38)$$

Proof. To prove (4.37), it remains to prove the inclusion

$$\mathcal{N} \subset \left\{u \in \mathcal{H}^{1,-s}; (1+G_0W)u = \beta\mathfrak{m}_0 \text{ for some } \beta \in \mathbb{C}, \frac{3}{2} < s < \frac{\rho+1}{2}\right\}. \quad (4.39)$$

The inclusion in the opposite sense is a consequence of Lemma 4.2 and Proposition 4.3.

Let $u \in \mathcal{N}$ and $\lambda < 0$. Then $u \in \mathcal{H}^{1,-r}$ for $r > 1$ and r close to 1 and $P_0u = -Wu \in \mathcal{L}^{2,\rho+1-r}$. By Corollary 2.2, the resolvent $R_0(\lambda)$ can be decomposed as

$$R_0(\lambda) = b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} + r_0(\lambda) \quad (4.40)$$

where

$$b_0(v,\xi,\eta) = 2^{\frac{3}{2}} e^{-v^2-\eta^2+2iv\cdot\xi+2\xi^2}\chi(\xi)$$

with χ a smooth cut-off around 0 with compact support, and $r_0(\lambda)$ is uniformly bounded as operators in L^2 for $\lambda < a$ for some $a \in]0,1[$. One has

$$u + R_0(\lambda)Wu = -\lambda R_0(\lambda)u = -\lambda\left(b_0^w(v,D_x,D_v)(-\Delta_x - \lambda)^{-1} + r_0(\lambda)\right)u \quad (4.41)$$

for $\lambda < 0$. Recall the following estimate for $r_0(\lambda)$ (see (2.85) in [21]):

$$\|\langle x\rangle^{-s} r_0(\lambda)\langle x\rangle^s f\| \le C(\|f\| + \|H_0 f\|) \quad (4.42)$$

for $f \in D(H_0)$, $\lambda < a$ and $s \in [0,2]$, where $H_0 = -\Delta_v + v^2 - \Delta_x$. It follows from (4.42) that

$$\lambda r_0(\lambda)u = O(|\lambda|), \quad \lambda < 0, \quad (4.43)$$

in $\mathcal{H}^{1,-r}$.

Let $\phi \in \mathcal{S}(\mathbb{R})$ such that $\int_{\mathbb{R}} \phi(x)dx = 1$. Then

$$\Pi = \langle \cdot, \phi \otimes \psi_0 \rangle \mathfrak{m}_0$$

is a projection on $\mathcal{H}^{1,-s}$ for any $s > \frac{1}{2}$ onto the linear span of $\mathfrak{m}_0$. Set $\Pi' = 1 - \Pi$. The term $\Pi' \lambda b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} u$ can be evaluated as follows. Making use of the inequality

$$|e^{-a} - e^{-b}| \le |a - b|(e^{-a} + e^{-b}), \quad a, b \ge 0,$$

the quantity

$$\begin{aligned} &|\lambda \Pi' b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} u(x, v)| \\ &= \frac{\sqrt{|\lambda|}}{2} \left| \int_{\mathbb{R}^4} (e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|}) \phi(y') \Phi(v, v', y) u(x', v') \, dy dy' dx' dv' \right| \end{aligned}$$

is bounded by

$$|\lambda| \int_{\mathbb{R}^4} |x - y'| (e^{-\sqrt{|\lambda|}|y-(x-x')|} + e^{-\sqrt{|\lambda|}|y-(y'-x')|}) |\phi(y') \Phi(v, v', y) u(x', v')| \, dy dy' dx' dv'.$$

The integral involving the term $e^{-\sqrt{|\lambda|}|y-(x-x')|}$ can be evaluated as follows:

$$\begin{aligned} &|\lambda| \int_{\mathbb{R}^4} |x - y'| e^{-\sqrt{|\lambda|}|y-(x-x')|} |\phi(y') \Phi(v, v', y) u(x', v')| \, dy dy' dx' dv' \\ \le\ & C_1(1 + |x|)|\lambda| \int_{\mathbb{R}^3} e^{-\sqrt{|\lambda|}|y-(x-x')|} \big| \Phi(v, v', y) u(x', v') \big| \, dy dx' dv' \\ =\ & C_2(1 + |x|)|\lambda| \int_{\mathbb{R}^3} e^{-\sqrt{|\lambda|}|y-(x-x')|} \big| \psi_0(v) \psi_0(v') \Psi(y - v - v') u(x', v') \big| \, dy dx' dv' \\ \le\ & C_3(1 + |x|)|\lambda| \|u\|_{\mathcal{L}^{2,-r}} \\ & \times \left\{ \int_{\mathbb{R}^3} \big| \langle x' \rangle^r e^{-\sqrt{|\lambda|}|y-(x-x')|} \psi_0(v) \psi_0(v') \Psi(y - v - v') \big|^2 \, dy dx' dv' \right\}^{\frac{1}{2}} \\ \le\ & C_4(1 + |x|)^{1+r} |\lambda| \|u\|_{\mathcal{L}^{2,-r}} \left\{ \int_{\mathbb{R}} \big| \langle x' \rangle^r e^{-\sqrt{|\lambda|}|x'|} \big|^2 \, dx' \right\}^{\frac{1}{2}} \psi_0(v) \\ \le\ & C_5(1 + |x|)^{1+r} |\lambda|^{\frac{3}{4} - \frac{r}{2}} \|u\|_{\mathcal{L}^{2,-r}} \psi_0(v) \end{aligned}$$

for some constants C_j. A similar upper-bound also holds for the integral involving the term $e^{-\sqrt{|\lambda|}|y-(y'-x')|}$. Putting them together, we obtain a point-wise upper-bound

$$|\lambda \left(\Pi' b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} u \right)(x, v)| \le C(1 + |x|)^{1+r} |\lambda|^{\frac{3}{4} - \frac{r}{2}} \psi_0(v) \|u\|_{\mathcal{L}^{2,-r}} \quad (4.44)$$

This proves that for $1 < r < \frac{3}{2}$,

$$\lambda \Pi' b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} u \to 0, \text{ as } \lambda \to 0_- \quad (4.45)$$

in $\mathcal{L}^{2,-(\frac{3}{2}+r+\epsilon)}$, $\epsilon > 0$. Applying Π' to (4.41) and taking the limit $\lambda \to 0_-$, we get

$$\Pi'(1 + G_0 W)u = 0. \quad (4.46)$$

This means that there exists some constant $\beta \in \mathbb{C}$ such that $(1 + G_0W)u = \beta\mathfrak{m}_0$. The proof of (4.37) is complete.

Since $1+G_0W$ is injective, one deduces from (4.37) that $\mathcal{N}$ is of dimension one. It is clear that $\mathfrak{m} \in \mathcal{N}$ and (4.37) implies that

$$(1 + G_0W)\mathfrak{m} = \beta\mathfrak{m}_0 \tag{4.47}$$

for some $\beta \in \mathbb{C}$. Proposition 4.3 applied to $\mathfrak{m}$ shows that $\mathfrak{m}$ has asymptotic behavior

$$\mathfrak{m}(x, v) = (\beta \mp d_1 + o(1))\psi_0(v), \quad x \to \pm\infty$$

with $d_1 \in \mathbb{C}$ given in Proposition 4.3. Comparing these relations with the trivial expansion of $\mathfrak{m}(x, v)$:

$$\mathfrak{m}(x, v) = (1 + O(\langle x\rangle^{-\rho}))\psi_0(v)$$

for $x \to \pm\infty$, one concludes that $\beta = 1$ and $d_1 = 0$, which prove (4.38). □

5. Low-energy expansion of the resolvent

Let $U_\delta = \{z; |z| < \delta, z \notin \mathbb{R}_+\}$, $\delta > 0$, and $\frac{3}{2} < s < \frac{\rho+1}{2}$. Recall that $(1 + G_0W)^{-1}$ exists and is bounded on $\mathcal{L}^{2,-s}$. Since

$$1 + R_0(z)W - \frac{1}{\sqrt{z}}G_{-1}W = 1 + G_0W + O(|z|^\epsilon) \tag{5.1}$$

in $\mathcal{L}^{2,-s}$ for $z \in U_\delta$, $1 + R_0(z)W - \frac{1}{\sqrt{z}}G_{-1}W$ is invertible for $z \in U_\delta$ if $\delta > 0$ is small enough. Denote

$$D(z) = \left(1 + R_0(z)W - \frac{1}{\sqrt{z}}G_{-1}W\right)^{-1}. \tag{5.2}$$

If $\rho > 2k + 2$, one has

$$D(z) = D_0 + \sum_{j=1}^{k} z^{\frac{j}{2}} D_j + O(|z|^{k+\epsilon}) \tag{5.3}$$

in $\mathcal{B}(1, -s; 1, -s)$ for $k + \frac{3}{2} < s < \frac{\rho+1}{2}$, where

$$D_0 = (1 + G_0W)^{-1} \tag{5.4}$$

$$D_1 = -D_0G_1WD_0 \tag{5.5}$$

$$D_2 = (D_0G_1W)^2D_0 - D_0G_2WD_0 \tag{5.6}$$

It follows that

$$(1 + R_0(z)W)^{-1} = D(z)(1 + M(z))^{-1} \tag{5.7}$$

where $M(z) = \frac{1}{\sqrt{z}}G_{-1}WD(z)$. $M(z)$ is an operator of rank one. In order to study the invertibility of $1 + M(z)$, consider the equation

$$(1 + M(z))u = f, \tag{5.8}$$

where $f \in \mathcal{L}^{2,-s}$ is given and $u = u(z)$ is to be determined. Take $\phi^*(x, v) = \chi(x)\psi_0(v)$ with $\chi \in \mathcal{S}(\mathbb{R})$ such that

$$\int_{\mathbb{R}} \chi(x)dx = 1.$$

Let $\Pi_0 = \langle \cdot, \phi^* \rangle \mathfrak{m}_0$. Then $\Pi_0^2 = \Pi_0$. Decompose f and u as $f = f_0 + f_1$ and $u = u_0 + u_1$ where $f_0 = \Pi_0 f$, $f_1 = (1 - \Pi_0) f$, and similarly for u. Equation (5.8) is equivalent with

$$u_1 = f_1 \text{ and} \tag{5.9}$$

$$C(z)(1 + \langle M(z)\mathfrak{m}_0, \phi^* \rangle) = \langle f, \phi^* \rangle - \langle M(z) f_1, \phi^* \rangle \tag{5.10}$$

where $C(z) = \langle u, \phi^* \rangle$ is some constant to be calculated. If $1 + \langle M(z)\mathfrak{m}_0, \phi^* \rangle \neq 0$ for $z \in U_\delta$, as we shall prove below, then $C(z)$ is uniquely determined by (5.10). Consequently, the equation $(1 + M(z))u = f$ has a unique solution given by

$$u = C(z)\mathfrak{m}_0 + f_1. \tag{5.11}$$

This will prove the invertibility of $1 + M(z)$ for $z \in U_\delta$.

Let us now study

$$m(z) = 1 + \langle M(z)\mathfrak{m}_0, \phi^* \rangle \tag{5.12}$$

for $z \in U_\delta$. Applying (5.3) with $k = 1$ (we need here the condition $\rho > 4$), one obtains

$$\langle M(z)\mathfrak{m}_0, \phi^* \rangle = \frac{i}{2\sqrt{z}} \langle W D(z)\mathfrak{m}_0, \mathfrak{m}_0 \rangle = \frac{i}{2\sqrt{z}} \left(\sigma_0 + \sqrt{z}\sigma_1 + O(|z|^{\frac{1}{2}+\epsilon}) \right) \tag{5.13}$$

where $\sigma_j = \langle W D_j \mathfrak{m}_0, \mathfrak{m}_0 \rangle$. By Theorem 4.5,

$$(1 + G_0 W)^{-1}\mathfrak{m}_0 = \mathfrak{m}. \tag{5.14}$$

Consequently

$$\sigma_0 = \langle W\mathfrak{m}, \mathfrak{m}_0 \rangle = 0 \tag{5.15}$$

and

$$\begin{aligned} \sigma_1 &= \langle (1 + G_0 W)^{-1} G_1 W (1 + G_0 W)^{-1} \mathfrak{m}_0, W\mathfrak{m}_0 \rangle \\ &= \langle G_1 W \mathfrak{m}, D_0^* W \mathfrak{m}_0 \rangle \end{aligned}$$

Let J be the symmetry in velocity variable defined by $J : g(x, v) \to (Jg)(x, v) = g(x, -v)$. Then $J^2 = 1$ and

$$JPJ = P^*, \quad JWJ = -W \quad \text{ and } JP_0 J = P_0^*. \tag{5.16}$$

It follows that $(R_0(z)W)^* = JWR_0(\overline{z})J$, hence

$$(1 + G_0 W)^* = J(1 + W G_0)J. \tag{5.17}$$

We derive that

$$\begin{aligned} D_0^* W \mathfrak{m}_0 &= J(1 + W G_0)^{-1} J W \mathfrak{m}_0 \\ &= -J(1 + W G_0)^{-1} W \mathfrak{m}_0 \\ &= -JW(1 + G_0 W)^{-1} \mathfrak{m}_0 = -JW\mathfrak{m} = W\mathfrak{m}. \end{aligned}$$

This shows

$$\sigma_1 = \langle G_1 W \mathfrak{m}, W \mathfrak{m} \rangle. \tag{5.18}$$

Since $G_1 = \frac{1}{\sqrt{z}}(R_0(z) - \frac{1}{\sqrt{z}}G_{-1} - G_0) + O(|z|^\epsilon)$ in $\mathcal{B}(-1, s; 1, -s)$, $s > \frac{5}{2}$, noticing that $G_{-1}W\mathfrak{m} = 0$, $(1 + G_0W)\mathfrak{m} = \mathfrak{m}_0$, one obtains for $z = \lambda < 0$

$$\begin{aligned}\langle G_1W\mathfrak{m}, W\mathfrak{m}\rangle &= -\frac{i}{\sqrt{|\lambda|}}\langle R_0(\lambda)W\mathfrak{m}, W\mathfrak{m}\rangle + O(|\lambda|^\epsilon) &(5.19)\\ &= i\sqrt{|\lambda|}\langle R_0(\lambda)\mathfrak{m}, W\mathfrak{m}\rangle + O(|\lambda|^\epsilon). &(5.20)\end{aligned}$$

Proposition 5.1. *Assume $\rho > 4$. One has*

$$\langle G_1W\mathfrak{m}, W\mathfrak{m}\rangle = i\lim_{\lambda\to 0_-}\sqrt{|\lambda|}\langle R_0(\lambda)\mathfrak{m}, W\mathfrak{m}\rangle = 0. \tag{5.21}$$

Proof. Let $\lambda < 0$ and Π' be defined as in the proof of Theorem 4.5. Then $\langle R_0(\lambda)\mathfrak{m}, W\mathfrak{m}\rangle = \langle \Pi' R_0(\lambda)\mathfrak{m}, W\mathfrak{m}\rangle$, since $\langle \mathfrak{m}_0, W\mathfrak{m}\rangle = 0$. One has

$$R_0(\lambda)\mathfrak{m} = (b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1} + r_0(\lambda))\mathfrak{m} \tag{5.22}$$

in $\mathcal{L}^{2,-r}$ for any $r > \frac{1}{2}$ and it follows from (4.42) that

$$\sqrt{|\lambda|}r_0(\lambda)\mathfrak{m} = O(\sqrt{|\lambda|}) \tag{5.23}$$

in $\mathcal{H}^{1,-r}$. Let us evaluate $\sqrt{|\lambda|}\Pi' b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1}\mathfrak{m}$.

$$\begin{aligned}&\sqrt{|\lambda|}\Pi' b_0^w(v, D_x, D_v)(-\Delta_x - \lambda)^{-1}\mathfrak{m}(x, v)\\ &= \frac{i}{2}\int_{\mathbb{R}^4}(e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|})\phi(y')\Phi(v, v', y)\mathfrak{m}(x', v')\, dydy'dx'dv'\\ &= \frac{i}{2}\int_{\mathbb{R}^4}(e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|})\phi(y')\Phi(v, v', y)\mathfrak{m}_0(v')\, dydy'dx'dv'\\ &+ \frac{i}{2}\int_{\mathbb{R}^4}(e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|})\phi(y')\Phi(v, v', y)(\mathfrak{m}(x', v) - \mathfrak{m}_0(v'))\, dydy'dx'\\ &= \frac{i}{2}\int_{\mathbb{R}^4}(e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|})\phi(y')\Phi(v, v', y)(\mathfrak{m}(x', v) - \mathfrak{m}_0(v'))\, dydy'dx'\\ &= O(\sqrt{|\lambda|}|x|\psi_0(v))\end{aligned}$$

for $(x, v) \in \mathbb{R}^2$. The first term on the right-hand side of the second equality above vanishes by first integrating with respect to x' variable. In the last equality above, we used the upper bound

$$|e^{-\sqrt{|\lambda|}|y-(x-x')|} - e^{-\sqrt{|\lambda|}|y-(y'-x')|}| \le \sqrt{|\lambda|}|x - y'|\left(e^{-\sqrt{|\lambda|}|y-(x-x')|} + e^{-\sqrt{|\lambda|}|y-(y'-x')|}\right)$$

and the fact $\mathfrak{m} - \mathfrak{m}_0 = O(\langle x\rangle^{-\rho})\psi_0(v)$ to evaluate the integral. It follows that

$$\sqrt{|\lambda|}\langle \Pi' R_0(\lambda)\mathfrak{m}, W\mathfrak{m}\rangle = O(\sqrt{|\lambda|}), \quad \lambda \to 0_-$$

which finishes the proof of Proposition 5.1. □

Summing up, we proved that if $\rho > 4$, then $m(z) = 1 + \frac{i}{2\sqrt{z}}\langle WD(z)\mathfrak{m}_0, \mathfrak{m}_0\rangle$ verifies

$$m(z) = 1 + O(|z|^\epsilon), \quad \epsilon > 0, \tag{5.24}$$

for $z \in U_\delta$. Therefore $1 + M(z)$ is invertible for $z \in U_\delta$ with $\delta > 0$ small enough and the solution u to the equation $(1 + M(z))u = f$ is given by

$$\begin{aligned} u &= f_1 + \frac{1}{m(z)}(\langle f, \phi^*\rangle - \langle M(z)f_1, \phi^*\rangle)\varphi_0 \\ &= f - \langle f, \phi^*\rangle \mathfrak{m}_0 + \frac{1}{m(z)}(\langle f, \phi^*\rangle - \langle M(z)(f - \langle f, \phi^*\rangle \mathfrak{m}_0), \phi^*\rangle)\mathfrak{m}_0 \\ &= f - \frac{1}{m(z)}\langle M(z)f, \phi^*\rangle \mathfrak{m}_0. \end{aligned} \quad (5.25)$$

Taking notice that $\langle \mathfrak{m}_0, \phi^*\rangle = 1$, we proved the following

Proposition 5.2. *Let $\rho > 4$. Then $1 + M(z)$ is invertible in $\mathcal{B}(1, -s; -1, s)$, $s > \frac{3}{2}$, for $z \in U_\delta$. Its inverse is given by*

$$(1 + M(z))^{-1} = 1 - \frac{1}{m(z)\sqrt{z}} G_{-1}WD(z). \quad (5.26)$$

In addition, if $\rho > 2k + 2$ for some $k \geq 1$, one has

$$(1 + M(z))^{-1} = 1 - \frac{1}{m(z)\sqrt{z}} G_{-1}W \left(D_0 + \sum_{j=1}^{k} z^{\frac{j}{2}} D_j + O(|z|^{k+\epsilon}) \right) \quad (5.27)$$

in $\mathcal{B}(1, -s; 1, -s)$ for $k + \frac{3}{2} < s < \frac{\rho+1}{2}$, where D_j is given by (5.3).

Theorem 5.3. *Let $\rho > 4$. Then there exists some constant $\delta > 0$ such that if $s > \frac{5}{2}$*

$$R(z) = \frac{i}{2\sqrt{z}}\langle \cdot, \mathfrak{m}\rangle \mathfrak{m} + O(|z|^{-\frac{1}{2}+\epsilon}), \quad z \in U_\delta, \quad (5.28)$$

in $\mathcal{B}(-1, s; 1, -s)$ for some $\epsilon > 0$. In particular, P has no eigenvalues in U_δ. In addition, the boundary values $R(\lambda \pm i0)$ of $R(z)$ exist in $\mathcal{B}(-1, s; 1, -s)$, $s > \frac{3}{2}$, for $\lambda \in]0, \delta[$ and is Hölder continuous in $\lambda \in]0, \delta[$.

Proof. We see from the above calculation that $(1 + M(z))^{-1}$ admits an asymptotic expansion as $z \in U_\delta$ and $z \to 0$. The existence of the asymptotics of the resolvent $R(z)$ follows from the equation

$$R(z) = D(z)(1 + M(z))^{-1}R_0(z) = D(z)\left(1 - \frac{1}{m(z)\sqrt{z}}G_{-1}WD(z)\right)R_0(z). \quad (5.29)$$

Let us calculate its leading term.

$$\begin{aligned} &\left(1 - \frac{1}{m(z)\sqrt{z}}G_{-1}WD(z)\right)R_0(z) \\ \equiv\ &-\frac{1}{m(z)z}G_{-1}WD_0G_{-1} + \frac{1}{\sqrt{z}}\left(G_{-1} - \frac{1}{m(z)}(G_{-1}WD_0G_0 + G_{-1}WD_1G_{-1})\right). \end{aligned}$$

Here and in the following, "$\equiv$" means equality module some term which is of order $O(|z|^{-\frac{1}{2}+\epsilon})$ in $\mathcal{B}(-1, s; 1, -s)$, $s > \frac{5}{2}$. Recall that $G_{-1} = \frac{i}{2}\langle \cdot, \mathfrak{m}_0\rangle \mathfrak{m}_0$, $D_0 = (1 + G_0W)^{-1}$ and $(1 + G_0W)^{-1}\mathfrak{m}_0 = \mathfrak{m}$. It follows that

$$G_{-1}WD_0G_{-1} = \frac{i}{2}\langle W\mathfrak{m}, \mathfrak{m}_0\rangle\langle \cdot, \mathfrak{m}_0\rangle \mathfrak{m}_0 = 0. \quad (5.30)$$

Consequently

$$\begin{aligned} & D(z)\left(1-\frac{1}{m(z)\sqrt{z}}G_{-1}WD(z)\right)R_0(z) \\ \equiv\ & \frac{1}{\sqrt{z}}D_0\left(G_{-1}-\frac{1}{m(z)}(G_{-1}WD_0G_0+G_{-1}WD_1G_{-1})\right) \end{aligned}$$

Noticing that $m(z)=1+O(|z|^\epsilon)$, one obtains

$$\begin{aligned} R(z) &\equiv \frac{1}{\sqrt{z}}D_0G_{-1}(1-W(D_0G_0+D_1G_{-1})) \\ &= \frac{i}{2\sqrt{z}}\langle((1-W(D_0G_0+D_1G_{-1}))\cdot,\mathfrak{m}_0\rangle\mathfrak{m} \end{aligned} \quad (5.31)$$

Recall that $D_0^*W\mathfrak{m}_0=W\mathfrak{m}$ and $\langle G_1W\mathfrak{m},W\mathfrak{m}\rangle=0$ (see Proposition 5.1). One can simplify the leading term as follows:

$$\begin{aligned} & \langle(1-W(D_0G_0))\cdot,\mathfrak{m}_0\rangle \\ =\ & \langle\cdot,\mathfrak{m}_0\rangle+\langle\cdot,G_0^*D_0^*W\mathfrak{m}_0\rangle=\langle\cdot,\mathfrak{m}_0\rangle+\langle\cdot,G_0^*W\mathfrak{m}\rangle \\ =\ & \langle\cdot,\mathfrak{m}_0\rangle+\langle\cdot,JG_0JW\mathfrak{m}\rangle=\langle\cdot,\mathfrak{m}_0\rangle-\langle\cdot,G_0W\mathfrak{m}\rangle=\langle\cdot,\mathfrak{m}\rangle \end{aligned}$$

and

$$\begin{aligned} & \langle WD_1G_{-1}\cdot,\mathfrak{m}_0\rangle \\ =\ & -\langle WD_0G_1WD_0G_{-1}\cdot,\mathfrak{m}_0\rangle=-\frac{i}{2}\langle\cdot,\mathfrak{m}_0\rangle\langle WD_0G_1W\mathfrak{m},\mathfrak{m}_0\rangle \\ =\ & \frac{i}{2}\langle\cdot,\mathfrak{m}_0\rangle\langle G_1W\mathfrak{m},D_0^*W\mathfrak{m}_0\rangle=\frac{i}{2}\langle\cdot,\mathfrak{m}_0\rangle\langle G_1W\mathfrak{m},W\mathfrak{m}\rangle=0. \end{aligned}$$

This finishes the proof of (5.28). (5.28) implies that $R(z)$ has no poles in U_δ, hence P has no eigenvalues there. The last statement of Theorem 5.3 is a consequence of Corollary 2.2 (b) and (5.29), since the boundary values $D(\lambda\pm i0)$ exist in $\mathcal{B}(1,-s;1,-s)$, $s>\frac{3}{2}$, for $\lambda\in]0,\delta[$ and are continuous in λ. □

6. Large time asymptotics of solutions

The following high energy resolvent estimate is proved in [21].

Theorem 6.1. *Let $n\geq 1$ and assume (1.4) with $\rho\geq -1$. Then there exists $C>0$ such that $\sigma(P)\cap\{z;|\mathrm{Im}\ z|>C,\mathrm{Re}\ z\leq\frac{1}{C}|\mathrm{Im}\ z|^{\frac{1}{2}}\}=\emptyset$ and*

$$\|R(z)\|\leq\frac{C}{|z|^{\frac{1}{2}}}, \quad (6.1)$$

and

$$\|(1-\Delta_v+v^2)^{\frac{1}{2}}R(z)\|\leq\frac{C}{|z|^{\frac{1}{4}}}, \quad (6.2)$$

for $|\mathrm{Im}\ z|>C$ and $\mathrm{Re}\ z\leq\frac{1}{C}|\mathrm{Im}\ z|^{\frac{1}{2}}$.

Let $S(t) = e^{-tP}$, $t \geq 0$, be the one-parameter strongly continuous semigroup generated by $-P$. Then one can firstly represent $S(t)$ as

$$S(t)f = \frac{1}{2\pi i} \int_\gamma e^{-tz} R(z) f dz \tag{6.3}$$

for $f \in L^2(\mathbb{R}^2)$ and $t > 0$, where the contour γ is chosen such that

$$\gamma = \gamma_- \cup \gamma_0 \cup \gamma_+$$

with $\gamma_\pm = \{z; z = \pm iC + \lambda \pm iC\lambda^2, \lambda \geq 0\}$ and γ_0 is a curve in the left-half complexe plane joining $-iC$ and iC for some $C > 0$ sufficiently large, γ being oriented from $-i\infty$ to $+i\infty$.

Remark that under the condition (1.4) with $\rho > 0$, P has no eigenvalue on the imaginary axis ([9]). Making use of analytic deformation and Theorem 5.3, one obtains from (6.1) that

$$\langle S(t)f, g\rangle = \frac{1}{2\pi i} \int_\Gamma e^{-tz} \langle R(z)f, g\rangle dz, \quad t > 0, \tag{6.4}$$

for any $f, g \in \mathcal{L}^{2,s}$ with $s > \frac{5}{2}$. Here

$$\Gamma = \Gamma_- \cup \Gamma_0 \cup \Gamma_+$$

with

$$\Gamma_\pm = \{z; z = \delta + \lambda \pm i\delta^{-1}\lambda^2, \lambda \geq 0\}$$

for $\delta > 0$ small enough and

$$\Gamma_0 = \{z = \lambda + i0; \lambda \in [0, \delta]\} \cup \{z = \lambda - i0; \lambda \in [0, \delta]\}.$$

Γ is oriented from $-i\infty$ to $+i\infty$.

Proof of Theorem 1.1. By (6.4), one has for $f, g \in \mathcal{L}^{2,s}(\mathbb{R}^2)$ with $s > \frac{5}{2}$

$$\begin{aligned} \langle S(t)f, g\rangle &= \frac{1}{2\pi i} \left(\int_{\Gamma_0} + \int_{\Gamma_-} + \int_{\Gamma_+} \right) e^{-tz} \langle R(z)f, g\rangle \, dz \\ &\equiv I_1 + I_2 + I_3. \end{aligned}$$

For $\delta > 0$ appropriately small and fixed, it follows from Theorem 6.1 that there exist some constants $C, c > 0$ such that

$$|I_j| \leq Ce^{-ct} \|f\| \, \|g\|, \quad t > 0, \tag{6.5}$$

for $j = 2, 3$. Set

$$F_{-1} = \frac{i}{2} \langle \cdot, \mathfrak{m}\rangle \mathfrak{m}.$$

Applying Theorem 5.3, one has

$$\begin{aligned} I_1 &= \frac{1}{2\pi i}\int_0^\delta e^{-t\lambda}\langle (R(\lambda+i0)-R(\lambda-i0))f,g\rangle\, d\lambda \\ &= \frac{1}{\pi i}\int_0^\delta e^{-t\lambda}\lambda^{-\frac{1}{2}}\langle (F_{-1}+O(\lambda^\epsilon))f,g\rangle\, d\lambda \\ &= \frac{1}{\pi i}\int_0^{+\infty}\frac{1}{\sqrt{\lambda}}e^{-t\lambda}\langle F_{-1}f,g\rangle\, d\lambda + O(t^{-\frac{1}{2}-\epsilon})\|f\|_{0,s}\|g\|_{0,s} \\ &= \frac{1}{i\sqrt{\pi t}}\langle F_{-1}f,g\rangle + O(t^{-\frac{1}{2}-\epsilon}) \end{aligned} \tag{6.6}$$

as $t \to +\infty$ for some $\epsilon > 0$. Using the formula for F_{-1}, we arrive at

$$S(t) = \frac{1}{(4\pi t)^{\frac{1}{2}}}\langle \cdot, \mathfrak{m}\rangle \mathfrak{m} + O(t^{-\frac{1}{2}-\epsilon}), t \to +\infty \tag{6.7}$$

as operators in $\mathcal{B}(0,s;0,-s)$ with $s > \frac{5}{2}$. Theorem 1.1 is proved. □

Remark 6.2. *It remains a natural and interesting open question to study the large-time behavior of solutions to the KFP equation with two space dimensions. Recall that in dimensions one and two, the Maxwellean with a decreasing potential is a threshold resonant state of the KFP operator, while it is not the case if the dimension is greater than or equal to three. We would guess that in dimension two, the Maxwellean is the only resonant state, as proved in this work for one dimensional case (see Theorem 4.5). The argument used in this work is based on Lemma 4.1. While we believe that the same conclusion should hold in any dimensions, the proof given for Lemma 4.1 is special to one dimensional case. See the comments after the proof of Lemma 4.1.*

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UNIVERSITE BRETAGNE LOIRE / MATHSTIC
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Titre : Analyse mathématique de la mécanique quantique avec des opérateurs non auto-adjoints

Mots clés : Mécanique quantique, opérateur non-auto-adjoint, guide d'onde quantique, pseudo-spectre, équation de Kramers-Fokker-Planck

Résumé : L'importance des opérateurs non auto-adjoints dans la physique moderne augmente chaque jour, car ils commencent à jouer un rôle plus important dans la mécanique quantique. Cependant, la signification de leur examen est beaucoup plus récente que l'intérêt pour l'examen des opérateurs auto-adjoints. Ainsi, étant donné que de nombreuses techniques auto-adjointes ne sont pas généralisées à ce contexte, il n'existe pas beaucoup de méthodes bien développées pour examiner leurs propriétés.

Cette thèse vise à contribuer à combler cette lacune et démontre plusieurs modèles non auto-adjoints et les moyens de leur étude. Les sujets comprennent le pseudo-spectre comme un analogue approprié du spectre, un modèle d'une guide d'onde avec un gain et une perte équilibrés à la frontière et l'équation de Kramers-Fokker-Planck avec un potentiel à courte distance.

Title : Mathematical analysis of quantum mechanics with non-self-adjoint operators

Keywords : quantum mechanics, non-self-adjoint operator, quantum waveguide, pseudospectrum, Kramers-Fokker-Planck equation

Abstract : The importance of non-self-adjoint operators in modern physics increases every day as they start to play more prominent role in Quantum mechanics. However, the significance of their examination is much more recent than the interest in the examination of their self-adjoint counterparts. Thus, since many self-adjoint techniques fail to be generalized to this context, there are not many well-developed methods for examining their properties.

This thesis aims to contribute to filling this gap and demonstrates several non-self-adjoint models and the means of their study. The topics include pseudospectrum as a suitable analogue of the spectrum, a model of a quantum layer with balanced gain and loss at the boundary, and the Kramers-Fokker-Planck equation with a short-range potential.