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L^2-Exponential Lower Bounds to Solutions of the Schrödinger Equation

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Abstract. We study decay properties of solutions ψ of the Schrödinger equation $(-\Delta+V)\psi=E\psi$. Typical of our results is one which shows that if $V=o(|x|^{-1/2})$ at infinity or if V is a homogenous N-body potential (for example atomic or molecular), then if $E<0$ and $\alpha>\sqrt{-E}$, $e^{\alpha|x|}\psi\notin L^2(\mathbb{R}^n)$. We also construct examples to show that previous essential spectrum-dependent upper bounds can be far from optimal if ψ is not the ground state.

I. Introduction

In recent years there has been much interest in the asymptotic behavior of L^2-solutions to the Schrödinger equation

$$(-\Delta+V)\psi=E\psi. \tag{1.1}$$

By far, most of the effort has gone into proving upper bounds to solutions of (1.1) with E outside the essential spectrum of $-\Delta+V$. Recent work on this subject can be found in [1–3, 12, 19]. The results of Agmon [1, 2] for the N-body problem are the most general. Agmon shows that solutions ψ of (1.1) satisfy (under certain conditions)

$$|\psi(x)|\leqq C_\varepsilon \exp(-(1-\varepsilon)\varrho_E(x)) \tag{1.2}$$

for $\varepsilon>0$, where $\varrho_E(x)$ is (in principle) an explicitly computable function. This generalizes the earlier result in [25] which states that for N-body potentials

$$|\psi(x)|\leqq C_\varepsilon \exp(-(1-\varepsilon)\sqrt{\Sigma-E}|x|), \tag{1.3}$$

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where Σ is the bottom of the essential spectrum. (Actually, (1.3) is only proved in an L^2 sense in [25]. This defect was remedied in [32]. For more recent work on going from L^2-bounds to pointwise bounds the reader should consult [1, 4].)

Obtaining lower bounds to solutions of (1.1) has proved to be a more difficult endeavor. However for the positive groundstate of $-\Delta+V$ with V an N-body potential, a recent result [8] shows that (1.2) is best possible in the sense that

$$\lim_{|x|\to\infty} -(\ln\psi(x))/\varrho_E(x)=1\,. \tag{1.4}$$

For earlier results of this nature on special systems the reader should consult [3, 10, 20, 23].

One of the difficulties in obtaining lower bounds to solutions of (1.1) is the fact that in general the set $\{x:\psi(x)=0\}$ is unbounded and very poorly understood. This difficulty was dealt with in the one-body problem by Bardos and Merigot [6] who proved lower bounds on the quantity

$$F(r)=(\int|\psi(r\omega)|^2d\omega)^{1/2}\,, \tag{1.5}$$

where $d\omega$ is Lebesgue measure on the unit sphere. The naturalness of this quantity is shown by the fact that if E is below the essential spectrum of $-\Delta+V$, $F(r)>0$ for all large r unless ψ has compact support. This follows from the fact that [1, 27]

$$\Sigma=\lim_{R\to\infty}\inf\{(\varphi,(-\Delta+V)\varphi):\varphi\in C_0^\infty(\{x:|x|>R\}),\ \|\varphi\|=1\}\,, \tag{1.6}$$

so that we can choose $\varepsilon>0$ with $\Sigma-E-\varepsilon>0$ and R large enough that

$$(\varphi,(-\Delta+V-E)\varphi)\geqq(\Sigma-\varepsilon-E)\|\varphi\|^2 \tag{1.7}$$

for all $\varphi\in C_0^\infty(\mathbb{R}^n\backslash\bar{B}_R)$. (Here and in what follows, $B_R=\{x:|x|<R\}$ and $\bar{B}_R$ is its closure.) Thus the Dirichlet problem in the region $\mathbb{R}^n\backslash\bar{B}_R$ is uniquely solvable given ψ on ∂B_R. Hence if $\psi=0$ on ∂B_R, $\psi=0$ in $\mathbb{R}^n\backslash\bar{B}_R$.

For $V\in C^\infty(\mathbb{R}^n)$ with $\lim\limits_{|x|\to\infty}(|V(x)|+|x\cdot\nabla V(x)|)=0$, Bardos and Merigot [6] show that for large r and $E<0$

$$F(r)\geqq C_\varepsilon\exp(-(\sqrt{-E-\varepsilon})r)\,, \tag{1.8}$$

for all small $\varepsilon>0$.

Our approach to the problem gives results which say that under certain circumstances

$$\exp(\alpha r)\psi\notin L^2\,. \tag{1.9}$$

This is a rather crude result in comparison to (1.8), however we can prove it in more general situations than those considered by Bardos and Merigot. In addition, it may be the case that a result such as (1.9) in combination with other information yields a statement such as (1.8). This will be the subject of further study.

In Sect. II we consider the one dimensional Schrödinger equation. We develop techniques not available in higher dimensions which enable us to prove rather strong results. One of our results may have application to random Schrödinger operators.

In Sect. III we extend the virial theorem to show that for certain potentials (including homogeneous N-body potentials), each negative energy eigenfunction ψ satisfies

$$\exp(\alpha r)\psi \notin L^2\,; \qquad \alpha > \sqrt{-E}\,. \tag{1.10}$$

We also show that no solution to $(-\Delta + V)\psi = E\psi$, where V is a "reasonable" N-body potential, can decay faster than at some explicitly computable (at least in principle) exponential rate.

In Sect. IV we give examples of solutions to the Schrödinger equation which decay more rapidly than existing upper bounds might lead one to think. One of our examples shows that in a certain sense (1.10) is optimal.

Our methods show that to a very large degree the three problems of unique continuation, embedded eigenvalues, and L^2-exponential lower bounds are intimately related. Indeed the techniques used here and in [14] to deal with the latter problem are to a large extent motivated by techniques which have been used previously to deal with the former problem. This is especially evident in Sect. III.

This is the first of three related papers. In the second paper [15] the methods of Sect. III are used to extend the Kato-Agmon-Simon [27] theorem on non-existence of positive eigenvalues while in the third [14], related methods are used to prove a variety of lower bounds to solutions of the 1-body Schrödinger equation including the case of nonnegative eigenvalues.

II. One Dimension

The Schrödinger equation in one dimension is special because it is an ordinary differential equation. In this section we will use two techniques, one based directly on the differential equation and the other on ideas of Combes and Thomas [11].

Let $p = -id/dx$ in $L^2(\mathbb{R})$ and $H_0(i\alpha) = e^{i\alpha x}p^2 e^{-i\alpha x} = (p-\alpha)^2$, $\alpha \in \mathbb{R}$. Define the analytic family of operators

$$\{H_0(\alpha) = (p + i\alpha)^2 : \alpha \in \mathbb{C}\},\ \mathscr{D}(H_0(\alpha)) = \mathscr{D}(d^2/dx^2)\,. \tag{2.1}$$

Then an easy computation shows that for α real, the spectrum of $H_0(\alpha)$ is a parabola:

$$\sigma(H_0(\alpha)) = \{z \in \mathbb{C} : \operatorname{Re} z = -\alpha^2 + (\operatorname{Im} z)^2/4\alpha^2\}\,. \tag{2.2}$$

In this context, the difference between one and higher dimensions is that an analogous computation in more than one dimension shows that if $H_0(\boldsymbol{\alpha}) = (\mathbf{p} + i\boldsymbol{\alpha})^2$ and $\boldsymbol{\alpha}$ is real, $\sigma(H_0(\boldsymbol{\alpha}))$ also contains the inside of the above parabola [11]. One of the ways in which (2.2) can be used for the purpose of proving L^2 exponential lower bounds is to note that if V is bounded (in some rough sense), then adding V to $H_0(\alpha)$ should not change the spectrum much, at least for large α. If ψ is an L^2 solution of the Schrödinger equation with eigenvalue E and $e^{\alpha x}\psi \in L^2$, then assuming we can show $e^{\alpha x}\psi \in \mathscr{D}(H_0(\alpha) + V)$, we have $E \in \sigma(H_0(\alpha) + V)$, since formally $(H_0(\alpha) + V)e^{\alpha x}\psi = Ee^{\alpha x}\psi$. For large α it is plausible that $E \notin \sigma(H_0(\alpha) + V)$ and this is in fact what we will prove.

We will assume in what follows that V is a (not necessarily real) tempered distribution such that for some $\beta > 0$, the quadratic form

$(p^2+\beta^2)^{-1/2}V(p^2+\beta^2)^{-1/2}$ with domain $\mathscr{S}(\mathbb{R})\times\mathscr{S}(\mathbb{R})$ extends to a bounded operator with bound smaller than one. It is a standard matter to use form techniques [21] to construct an m-sectorial operator H with

$$(\varphi, H\psi)=\int\bar{\varphi}'\psi' dx+V(\bar{\varphi}\psi)$$

for $\varphi,\psi\in\mathscr{S}(\mathbb{R})$. We abuse notation and write $H=-d^2/dx^2+V=p^2+V$.

Theorem II.1. *Define $H=-d^2/dx^2+V$ as above and suppose $H\psi=E\psi$ with ψ not identically zero. Then*

(i) $\operatorname{Re}E+\beta^2>0$ *and if* $\gamma(E)=(\beta^2+|E|)^{1/2}$, *then* $\exp(\gamma(E)x)\psi\notin L^2(\mathbb{R})$.

(ii) *If* $(p^2+1)^{-1/2}V(p^2+1)^{-1/2}$ *is compact, then* $\exp(\alpha x)\psi\notin L^2(\mathbb{R})$ *whenever* $\alpha>|\operatorname{Im}\sqrt{E}|$.

Remarks. (1) V can be rather wild looking and still satisfy the compactness criterion in (ii). For example, let $\{x_n: n=1,\ldots\}$ be dense in $\mathbb{R}$ and $\{c_n\}_{n=1}^{\infty}$ a sequence of complex numbers with $\sum_{n=1}^{\infty}|c_n|<\infty$. Then if $V(x)=\sum_{n=1}^{\infty}c_n\delta(x-x_n)$, $(p^2+1)^{-1/2}V(p^2+1)^{-1/2}$ is compact. If, however, V is a reasonable real-valued function, then comparison methods for ordinary differential equations should suffice to prove (ii).

(2) It also follows from the Combes-Thomas method [11] that in case (ii), if $0\leqq\alpha<|\operatorname{Im}\sqrt{E}|$, then $\exp(\alpha x)\psi\in L^2(\mathbb{R})$.

In the next result we single out real-valued bounded potentials which do not necessarily approach zero at infinity. We do this partially because such potentials occur naturally in the study of random media. Certain bounded "random potentials" have been shown [9, 18, 24] to produce pure point spectrum dense in an interval $[E_0,\infty)$ almost surely, with exponentially decaying eigenfunctions. In the following theorem we find explicit bounds on the rate of exponential decay which can be much better than those in Theorem II.1.

Theorem II.2. *Suppose V is a real-valued function on $[0,\infty)$ with $\|V\|_\infty<\infty$. Define*

$$V_0=\lim_{x_0\to\infty}\|V\chi_{[x_0,\infty)}\|_\infty,$$

where χ_A is the characteristic function of A. Suppose ψ is a real-valued function on $(0,\infty)$ satisfying $(-d^2/dx^2+V)\psi=E\psi$ and that ψ is not identically zero. Define

$$\alpha(V_0,E)=\begin{cases}\sqrt{V_0-E}\,; & E\leqq V_0/2\\ V_0/2\sqrt{E}\,; & V_0/2<E,\end{cases}\tag{2.3}$$

and let $\varrho(x)=(|\psi(x)|^2+|\psi'(x)|^2)^{1/2}$. Then

(i) $$\liminf_{x\to\infty}x^{-1}\ln\varrho(x)\geqq-\alpha(V_0,E),$$

and

(ii) $$e^{\alpha x}\psi\notin L^2((0,\infty))\quad \textit{if}\quad \alpha>\alpha(V_0,E).$$

Proof of Theorem II.1. Since $-\operatorname{Re}V\leqq a(p^2+\beta^2)$ for some $a<1$, it is clear that $\operatorname{Re}E+\beta^2\geqq(1-a)\beta^2>0$.

Define the analytic family $\{H_0(\alpha):\alpha\in\mathbb{C}\}$ as in (2.1). For φ_1 and φ_2 in $\mathscr{S}(\mathbb{R})$ define the sesquilinear form $Q(\varphi_1,\varphi_2;\alpha)=(\varphi_1,H_0(\alpha)\varphi_2)+V(\bar{\varphi}_1\varphi_2)$. Because $(p^2+\beta^2)^{-1/2}V(p^2+\beta^2)^{-1/2}$ extends from $\mathscr{S}(\mathbb{R})\times\mathscr{S}(\mathbb{R})$ to a bounded operator with bound less than one, it is easy to see that Q is sectorial, closable, and that its closure $\bar{Q}$ has domain $\mathscr{D}(d/dx)\times\mathscr{D}(d/dx)$. It is a standard result [21] that there is a unique m-sectorial operator $H(\alpha)$ such that $\mathscr{D}(H(\alpha))\subset\mathscr{D}(d/dx)$ and $\bar{Q}(\varphi_1,\varphi_2;\alpha)=(\varphi_1,H(\alpha)\varphi_2)$ for all $\varphi_1\in\mathscr{D}(d/dx)$ and $\varphi_2\in\mathscr{D}(H(\alpha))$. In addition $\varphi_2\in\mathscr{D}(H(\alpha))$ if and only if $\varphi_2\in\mathscr{D}(d/dx)$ and there is an $h\in L^2(\mathbb{R})$ such that $\bar{Q}(\varphi_1,\varphi_2;\alpha)=(\varphi_1,h)$ for all $\varphi_1\in\mathscr{S}(\mathbb{R})$. In this case $h=H(\alpha)\varphi_2$.

Let ψ be as in the theorem and suppose $\exp(\alpha_0x)\psi\equiv\psi_{\alpha_0}\in L^2(\mathbb{R})$ with $\alpha_0=\gamma(E)$. We will show this leads to a contradiction. Our first task is to show that $\psi_{\alpha_0}\in\mathscr{D}(H(\alpha_0))$ and

$$H(\alpha_0)\psi_{\alpha_0}=E\psi_{\alpha_0}\,. \tag{2.4}$$

Suppose $\chi\in C_0^\infty(\mathbb{R})$ and $\varphi_1,\varphi_2\in\mathscr{D}(d/dx)$. Then it is easy to see that

$$\bar{Q}(\varphi_1,\chi\varphi_2;\alpha)=\bar{Q}(\bar{\chi}\varphi_1,\varphi_2;\alpha)+(\varphi_1,\{-2\chi'\varphi_2'+(2\alpha\chi'-\chi'')\varphi_2\})\,.$$

Suppose $\varphi_2\in\mathscr{D}(H(\alpha))$. Then for all $\varphi_1\in\mathscr{D}(d/dx)$,

$$\bar{Q}(\varphi_1,\chi\varphi_2;\alpha)=(\varphi_1,\chi H(\alpha)\varphi_2)+(\varphi_1,\{-2\chi'\varphi_2'+(2\alpha\chi'-\chi'')\varphi_2\})\,,$$

and hence $\chi\varphi_2\in\mathscr{D}(H(\alpha))$ with

$$H(\alpha)\chi\varphi_2=\chi H(\alpha)\varphi_2-2\chi'\varphi_2'+(2\alpha\chi'-\chi'')\varphi_2\,.$$

Thus if $\chi\in C_0^\infty(\mathbb{R})$, we have $\chi\psi_{\alpha_0}\in\mathscr{D}(H(\alpha_0))$ and

$$H(\alpha_0)\chi\psi_{\alpha_0}=E\chi\psi_{\alpha_0}-\chi''\psi_{\alpha_0}-2\chi'\exp(\alpha_0x)\psi'\,. \tag{2.5}$$

From (2.5) it is easy to calculate that for χ real

$$\operatorname{Re}\bar{Q}(\chi\psi_{\alpha_0},\chi\psi_{\alpha_0};\alpha_0)=\int|\psi_{\alpha_0}|^2\{\operatorname{Re}E\chi^2+(\chi')^2+2\alpha_0\chi\chi'\}dx\,.$$

Let $\chi(x)=\chi_m(x)=\chi_1(x/m)$ with $\chi_1(x)=1$ if $|x|<1$ and $\chi_1\in C_0^\infty$. Then clearly $\chi_m\psi_{\alpha_0}\to\psi_{\alpha_0}$ and $\operatorname{Re}\bar{Q}(\chi_m\psi_{\alpha_0},\chi_m\psi_{\alpha 0};\alpha_0)$ is bounded. Thus [21] $\psi_{\alpha_0}\in\mathscr{D}(d/dx)$. If we similarly take $\chi=\chi_m$ in (2.5) and let $m\to\infty$, we see that $\psi_{\alpha_0}\in\mathscr{D}(H(\alpha_0))$ and that (2.4) holds.

Now let $N^{1/2}$ be some square root of $H_0(\alpha_0)-E=(p+i\alpha_0)^2-E$ which commutes with p. It is not difficult to justify the formula

$$H(\alpha_0)-E=N^{1/2}(1+N^{-1/2}VN^{-1/2})N^{1/2}\,, \tag{2.6}$$

as long as $\min\{|(\xi+i\alpha_0)^2-E|:\xi\in\mathbb{R}\}>0$, so that $N^{1/2}$ is invertible. We will prove that

$$\|(p^2+\beta^2)^{1/2}N^{-1/2}\|\leqq 1\,, \tag{2.7}$$

so that

$$\begin{aligned}&\|N^{-1/2}VN^{-1/2}\|\\&\quad=\|(p^2+\beta^2)^{1/2}N^{-1/2}((p^2+\beta^2)^{-1/2}V(p^2+\beta^2)^{-1/2})(p^2+\beta^2)^{1/2}N^{-1/2}\|<1\,.\end{aligned}$$

This will show that $H(\alpha_0)-E$ is invertible, contradicting (2.4). The proof of (2.7) is a calculation to show that

$$\sup\{|(\xi^2+\beta^2)((\xi+i\alpha_0)^2-E)^{-1}|:\xi\in\mathbb{R}\}\leqq 1.$$

The calculation is simple and we omit it.

To prove the second result of the theorem, suppose $e^{\alpha_0 x}\psi\in L^2(\mathbb{R})$ for some α_0 with $\alpha_0>|\mathrm{Im}\sqrt{E}|$. Then as in (2.4), ψ_α is an eigenvector of $H(\alpha)$ with eigenvalue E for all $\alpha\in[0,\alpha_0]$. Consider the operator

$$K(\alpha)=((p+i\alpha)^2-E)^{-1/2}V((p+i\alpha)^2-E)^{-1/2}, \tag{2.8}$$

where $\alpha\in\Gamma_E=\{\alpha\in\mathbb{C}:\mathrm{Re}\,\alpha>|\mathrm{Im}\sqrt{E}|\}$. We define the operator $((p+i\alpha)^2-E)^{-1/2}$ in this region by

$$((p+i\alpha)^2-E)^{-1/2}f=\mathscr{F}^{-1}((\xi+i\alpha)^2-E)^{-1/2}\mathscr{F}f,$$

where $\mathscr{F}$ is the Fourier transform and the branch of the square root with positive imaginary part is taken. Then $K(\alpha)$ is an analytic compact operator-valued function on Γ_E so that by the analytic Fredholm theorem [28], $1+K(\alpha)$ is either nowhere invertible on Γ_E or has a meromorphic inverse there. We know from our previous considerations that if $\mathrm{Re}\,\alpha$ is large enough, $\|K(\alpha)\|<1$ so that $1+K(\alpha)$ is invertible except for a discrete set in Γ_E. Thus from (2.6) E cannot be an eigenvalue of $H(\alpha)$ except for a discrete set of $\alpha\in\Gamma_E$. However, by assumption $H(\alpha)\psi_\alpha=E\psi_\alpha$ for all $\alpha\in[0,\alpha_0]$, where $\alpha_0>|\mathrm{Im}\sqrt{E}|$. This contradiction proves the result. □

Proof of Theorem II.2. To prove (i) it is enough to show that for each $\varepsilon>0$, $\varrho(x)\geqq c_\varepsilon\exp(-\alpha(V_0+\varepsilon,E)x)$ for some $c_\varepsilon>0$. Choose $x_0>0$ so that $\|V\chi_{[x_0,\infty)}\|_\infty\leqq V_0+\varepsilon$. By changing the definition of V_0 it is enough to show that $\varrho(x)\geqq ce^{-\alpha(V_0,E)x}$ for some $c>0$ under the assumption that $|V(x)|\leqq V_0$ for $x\geqq x_0$ and some $V_0>0$.

Let $h_\beta(x)=|\psi(x)|^2+\beta^{-1}|\psi'(x)|^2$. We will choose $\beta>0$ so that $(\exp(2x\alpha(V_0,E))h_\beta(x))'\geqq 0$ for $x\geqq x_0$. This gives $h_\beta(x)\geqq\exp(-2\alpha(V_0,E)(x-x_0))\cdot h_\beta(x_0)$, which clearly implies the result because $\varrho(x)^2\geqq(1+\beta^{-1})^{-1}h_\beta(x)$. Now

$$\begin{aligned}(e^{2\alpha x}h_\beta)'&=(2\alpha h_\beta+h_\beta')e^{2\alpha x}\\&=(2\alpha h_\beta+2\psi\psi'(1+\beta^{-1}(V-E)))e^{2\alpha x}\\&\geqq(2\alpha-|\beta^{1/2}+\beta^{-1/2}(V-E)|)h_\beta e^{2\alpha x},\end{aligned}\tag{2.9}$$

where we have used $|2\psi\psi'|\leqq\beta^{1/2}|\psi|^2+\beta^{-1/2}|\psi'|^2=\beta^{1/2}h_\beta$. Define

$$f(\beta)=\sup_{-V_0\leqq t\leqq V_0}|\beta^{1/2}+\beta^{-1/2}(t-E)|.$$

A short calculation gives

$$f(\beta)=\begin{cases}\beta^{-1/2}(E+V_0)-\beta^{1/2}; & 0<\beta\leqq E\\ \beta^{-1/2}(V_0-E)+\beta^{1/2}; & E\leqq\beta\end{cases}$$

and

$$\inf_{0<\beta<\infty}f(\beta)=f(\beta_0),$$

where

$$\beta_0 = \begin{cases} V_0 - E; & E \leqq V_0/2 \\ E; & E > V_0/2. \end{cases}$$

Since evidently $f(\beta_0) = 2\alpha(V_0, E)$, (2.9) implies $(\exp(2x\alpha(V_0, E))h_{\beta_0})' \geqq 0$ and thus (i) is proved.

To prove (ii) assume $e^{\alpha x}\psi \in L^2((0,\infty))$ for some $\alpha > \alpha(V_0, E)$ and note that from (i)

$$\int_0^\infty (|\psi(x)|^2 + |\psi'(x)|^2) e^{2\alpha x} dx = \infty. \tag{2.10}$$

Choose $\varphi \in C^\infty((0,\infty))$ with $\varphi = 1$ for large x. Then

$$\{(-id/dx + i\alpha)^2 + V - E\}\varphi e^{\alpha x}\psi = f,$$

where $f = -(\varphi''\psi + 2\varphi'\psi')e^{\alpha x} \in L^2(\mathbb{R})$. Thus elementary considerations show that $\varphi e^{\alpha x}\psi \in \mathcal{D}(d/dx)$ which implies $\varphi e^{\alpha x}\psi' \in L^2(\mathbb{R})$. This contradicts (2.10) and hence the proof is complete. □

III. An Extended Virial Theorem

The virial theorem, which says that under certain conditions $(-\Delta + V)\psi = E\psi$ implies $(\psi, (2\Delta + x \cdot \nabla V)\psi) = 0$, has been an important tool in understanding the nature of the spectrum of Schrödinger operators. We mention only the recent work in [26] where it is used to prove discreteness of $\sigma_{\text{p.p.}}(-\Delta + V)$ away from thresholds in N-body systems and to prove $\sigma_{\text{s.c.}}(H) = \emptyset$ and in addition its use in proving absence of positive eigenvalues. References to the latter work can be traced from [29]. Recent proofs of the virial theorem under general conditions can be found in [22, 26].

In the following we will use the notation D for the *operator* ∇. Let $H = -\Delta + V$ and for $\alpha > 0$ define $H(\alpha) = H + \alpha B - \alpha^2$, where $B = D \cdot (x/r) + (x/r) \cdot D$. Formally, $H(\alpha) = \exp(\alpha r)\, H \exp(-\alpha r)$, and thus if $\psi_\alpha \equiv \exp(\alpha r)\psi \in L^2$ and $H\psi = E\psi$ we have (again formally) $H(\alpha)\psi_\alpha = E\psi_\alpha$. If V is a relatively compact perturbation of Δ, then it is not difficult to show that $\sigma_{\text{ess}}(H(\alpha))$ is the closure of the interior of the parabola given in (2.2). If $E + \alpha^2 > 0$ we thus see that E is an eigenvalue embedded in the essential spectrum of $H(\alpha)$. Similar considerations lead to the same result in the N-body problem. It is not surprising then that an extension of the virial theorem can be used to prove non-existence of such eigenvalues. [However, one must not push this analogy too far because for example if $V = 0$, $\sigma(H(-\alpha)) = \sigma(H(\alpha)) = \sigma_{\text{p.p.}}(H(-\alpha))$ as is easily seen.]

The above idea is exploited in its simplest form in Theorem III.1 and Corollary III.2. In Theorem III.4 we expand on the idea to prove more general results.

Theorem III.1. *Suppose V is a real-valued function on $\mathbb{R}^n$, $n \geqq 2$, which is Δ-bounded with bound less than one. Suppose the distribution $W = x \cdot \nabla V$ has the property that $(-\Delta + 1)^{-1} W(-\Delta + 1)^{-1}$ extends to a bounded operator on $L^2(\mathbb{R}^n)$. Suppose ψ is an eigenfunction of $H = -\Delta + V$ with $e^{\alpha r}\psi \in L^2(\mathbb{R}^n)$ for some $\alpha \geqq 0$. If $n \geqq 3$ let $\psi_\alpha = e^{\alpha r}\psi$*

and if $n=2$, $\psi_\alpha = e^{\alpha\varrho_\varepsilon}\psi$ *with* $\varrho_\varepsilon = (r^2+\varepsilon^2)^{1/2}$ *and* $\varepsilon>0$. *Let* $A=(x\cdot D + D\cdot x)/2$. *Then* $\psi_\alpha \in \mathscr{D}(\Delta)$, $(\alpha/r)^{1/2}\psi_\alpha \in \mathscr{D}(A)$ *and*

$$(\psi_\alpha, (2\Delta + W)\psi_\alpha) = \begin{cases} 4\|A(\alpha/r)^{1/2}\psi_\alpha\|^2, & n \geqq 3 \\ 4\|(r/\varrho_\varepsilon)^{1/2}A(\alpha/r)^{1/2}\psi_\alpha\|^2 + (\psi_\alpha, f\psi_\alpha), & n=2, \end{cases} \tag{3.1}$$

where $f = \alpha\varepsilon^2(2r^2-\varepsilon^2)\varrho_\varepsilon^{-5} + 2\alpha^2\varepsilon^2 r^2 \varrho_\varepsilon^{-4}$.

Proof. We first give the proof for $n \geqq 3$ where it is simpler and then indicate the modifications for $n=2$. Define $B = D\cdot(x/r) + (x/r)\cdot D = 2(x/r)\cdot D + (n-1)/r$. A simple computation shows that ψ_α satisfies the differential equation

$$(-\Delta + V + \alpha B - \alpha^2)\psi_\alpha = E\psi_\alpha \tag{3.2}$$

in the sense of distributions. Since B is Δ-bounded with bound zero (here we use $n \geqq 3$), the operator

$$H(\gamma) = -\Delta + V + \gamma B - \gamma^2, \qquad \mathscr{D}(H(\gamma)) = \mathscr{D}(\Delta)$$

is closed and $C_0^\infty(\mathbb{R}^n)$ is a core for $H(\gamma)$. In addition $H(\gamma)^* = H(-\gamma)$ for γ real. The fact that (3.2) is satisfied in the distributional sense means that $(H(-\alpha)\varphi, \psi_\alpha) = (H(\alpha)^*\varphi, \psi_\alpha) = E(\varphi, \psi_\alpha)$ for all $\varphi \in C_0^\infty(\mathbb{R}^n)$ so that since C_0^∞ is a core for $H(-\alpha)$, $\psi_\alpha \in \mathscr{D}(H(\alpha)) = \mathscr{D}(\Delta)$ and

$$H(\alpha)\psi_\alpha = E\psi_\alpha. \tag{3.3}$$

For $\beta>0$, let $\mathscr{H}_\beta = \mathscr{D}((-\Delta+1)^{\beta/2})$ with inner product $(f,g)_\beta = ((-\Delta+1)^{\beta/2}f, (-\Delta+1)^{\beta/2}g)$ and denote its dual by $\mathscr{H}_{-\beta}$. Our assumption on the distribution W means that we can consider W as a bounded map of $\mathscr{H}_{+2}$ into $\mathscr{H}_{-2}$. Let $U(\theta) = e^{\theta A}$ be the dilation given by $U(\theta)\varphi(x) = e^{n\theta/2}\varphi(e^\theta x)$. Define $W(\theta) = U(\theta)WU(-\theta)$. Since $U(\theta): \mathscr{H}_\beta \to \mathscr{H}_\beta$ is bounded for any β, $W(\theta)$ is well defined as a bounded map from $\mathscr{H}_{+2} \to \mathscr{H}_{-2}$. Let $V(\theta) = U(\theta)VU(-\theta)$ [as a bounded map from $\mathscr{H}_{+2} \to L^2(\mathbb{R}^n)$]. An easy computation gives $\frac{d}{d\theta}(f, V(\theta)g) = (f, W(\theta)g)$ for $f, g \in \mathscr{S}(\mathbb{R}^n)$, so that

$$(f, V(\theta)g) = (f, Vg) + \int_0^\theta (f, W(s)g)ds. \tag{3.4}$$

We now note that because $U(\theta)$ is strongly continuous in θ as a map from $\mathscr{H}_\beta \to \mathscr{H}_\beta$, $W(\theta)$ is strongly continuous as a map from $\mathscr{H}_{+2} \to \mathscr{H}_{-2}$. Since (3.4) clearly extends to $f, g \in \mathscr{H}_{+2}$ we have the identity between operators from $\mathscr{H}_{+2} \to \mathscr{H}_{-2}$,

$$V(\theta) = V + \int_0^\theta W(s)ds.$$

Hence as an equation between operators from $\mathscr{H}_{+2} \to \mathscr{H}_{-2}$

$$\operatorname*{s-lim}_{\theta\to 0}(V(\theta) - V)/\theta = W. \tag{3.5}$$

We now assume $\alpha>0$. The case $\alpha=0$ corresponds to the usual virial theorem the proof of which we omit. Let $0<\gamma<\alpha$ and note that since $e^{\alpha r}\nabla\psi \in L^2$, $r^{-1/2}\psi_\gamma \in \mathscr{D}(A)$. Suppose that we have proved (3.1) with α replaced by γ for all $\gamma \in (0,\alpha)$. It is easy to see that $\lim_{\gamma\uparrow\alpha} \Delta\psi_\gamma = \Delta\psi_\alpha$ so that

$(\psi_\gamma, (2\Delta + W)\psi_\gamma) \to (\psi_\alpha, (2\Delta + W)\psi_\alpha)$. Thus $\lim_{\gamma\uparrow\alpha} \|Ar^{-1/2}\psi_\gamma\|$ exists. Since $r^{-1/2}\psi_\gamma \to r^{-1/2}\psi_\alpha$, this implies in particular that $r^{-1/2}\psi_\alpha \in \mathscr{D}(A)$. From this one easily sees that $Ar^{-1/2}\psi_\gamma \to Ar^{-1/2}\psi_\alpha$ and hence that (3.1) holds.

It remains to prove (3.1) with α replaced by γ and $0<\gamma<\alpha$. Since $H(\gamma)\psi_\gamma = E\psi_\gamma$,

$$\begin{aligned}\theta^{-1}(\psi_\gamma, [U(\theta)H(\gamma)U(-\theta) - H(-\gamma)]U(\theta)\psi_\gamma) = 0 \\ = (\psi_\gamma, [-\Delta(e^{-2\theta}-1)/\theta + (V(\theta)-V)/\theta + \gamma(B(\theta)+B)/\theta]U(\theta)\psi_\gamma),\end{aligned} \tag{3.6}$$

where $B(\theta) = e^{-\theta}B$. Since B is antisymmetric, $\operatorname{Re}(\psi_\gamma, B\psi_\gamma) = 0$, and thus

$$\operatorname{Re}(\psi_\gamma, (\gamma(B(\theta)+B)/\theta)U(\theta)\psi_\gamma) = -\gamma \operatorname{Re}((B(\theta)+B)\psi_\gamma, (U(\theta)-1)\theta^{-1}\psi_\gamma),$$

which converges to $-2\gamma \operatorname{Re}(B\psi_\gamma, A\psi_\gamma)$ as $\theta \to 0$. Here $\psi_\gamma \in \mathscr{D}(A)$ because $\gamma < \alpha$. Taking the limit of the real part of (3.6) as $\theta \to 0$ and using (3.5) thus gives

$$(\psi_\gamma, (2\Delta + W)\psi_\gamma) = \gamma \operatorname{Re}(B\psi_\gamma, 2A\psi_\gamma).$$

We now notice that $2A = rB + 1$ so that $\operatorname{Re}(B\psi_\gamma, 2A\psi_\gamma) = \|r^{1/2}B\psi_\gamma\|^2 = 4\|r^{-1/2}(A-1/2)\psi_\gamma\|^2 = 4\|Ar^{-1/2}\psi_\gamma\|^2$.

For $n=2$ define $g = r/\varrho_\varepsilon$, $B = \frac{g}{r}x\cdot D + D\cdot xg/r$ and $H(\gamma) = -\Delta + \gamma B + V - \gamma^2 g^2$, for $\gamma \in [0,\alpha]$. Then $B = 2g(x/r)\cdot D + (n/\varrho_\varepsilon) - r^2/\varrho_\varepsilon^3$ is Δ-bounded with bound zero so that as before it is easy to show that $\psi_\gamma = e^{\gamma\varrho_\varepsilon} \in \mathscr{D}(\Delta)$ for $\gamma \in [0,\alpha]$ and

$$H(\gamma)\psi_\gamma = E\psi_\gamma.$$

A calculation similar to the one above gives for $\gamma \in (0,\alpha)$ $(\alpha > 0)$

$$(\psi_\gamma, (2\Delta + W)\psi_\gamma) = 4\gamma\|g^{1/2}Ar^{-1/2}\psi_\alpha\|^2 + (\psi_\gamma, f_\gamma\psi_\gamma), \tag{3.7}$$

where $f_\gamma(r) = \gamma\varepsilon^2(2r^2 - \varepsilon^2)\varrho_\varepsilon^{-5} + 2\gamma^2\varepsilon^2 r^2\varrho_\varepsilon^{-4}$. Note that

$$g^{1/2}Ar^{-1/2}\psi_\gamma = A\varrho_\varepsilon^{-1/2}\psi_\gamma - (\tfrac{1}{2}\varrho_\varepsilon^{-1/2} + x\cdot\nabla\varrho_\varepsilon^{-1/2})\psi_\gamma.$$

Since $(-\Delta+1)\psi_\gamma \to (-\Delta+1)\psi_\alpha$ as $\gamma\uparrow\alpha$ we conclude from (3.7) that $\varrho_\varepsilon^{-1/2}\psi_\alpha \in \mathscr{D}(A)$. From this it is easy to conclude that $r^{-1/2}\psi_\alpha \in \mathscr{D}(A)$ and that $Ar^{-1/2}\psi_\gamma \to Ar^{-1/2}\psi_\alpha$. Now letting $\gamma\uparrow\alpha$ in (3.7) gives (3.1). $\square$

Remark. If $(-\Delta+1)^{-1/2}W(-\Delta+1)^{-1/2}$ extends to a bounded operator, we can take $\varepsilon\downarrow 0$ in (3.1) (for $n=2$) and the equation which holds for $n=3$ also holds for $n=2$ in a quadratic form sense.

Corollary III.2. *Suppose V and W satisfy the hypotheses of Theorem III.1 and $n \geqq 2$. Suppose in addition that for some $b \in (-\infty, 2]$ and $\Lambda \in \mathbb{R}$*

$$(\varphi, [(2-b)\Delta + W + bV]\varphi) \leqq b\Lambda\|\varphi\|^2 \tag{3.8}$$

for all $\varphi \in \mathscr{D}(\Delta)$. Suppose ψ is a non-zero eigenfunction of $H = -\Delta + V$ with eigenvalue E such that $\exp(\alpha r)\psi \in L^2(\mathbb{R}^n)$ *for some* $\alpha > 0$. *Then*

$$b\Lambda > b(\alpha^2 + E). \tag{3.9}$$

In particular if V is homogeneous of degree $-\beta$ with $\beta \in (0,2]$ and $E<0$, then for any non-zero solution to $(-\Delta+V)\psi = E\psi$ we have $\exp(\sqrt{-E}r)\psi \notin L^2(\mathbb{R})$.

Proof. The proof is basically that in [29]. For $n \geqq 3$, (3.1) implies

$$(\psi_\alpha, (2\Delta + W)\psi_\alpha) > 0. \tag{3.10}$$

The strict inequality holds because $\alpha > 0$ and because $Ar^{-1/2}\psi_\alpha = 0$ implies $\psi_\alpha = 0$. For $n=2$, (3.10) also holds for small $\varepsilon > 0$ as can be seen as follows: Since $|f(r)| \leqq \mathrm{const}/r$ uniformly in $\varepsilon > 0$ and $\lim_{\varepsilon \to 0} f(r) = 0$, we conclude from the dominated convergence theorem that $\lim_{\varepsilon \to 0} (\psi_\alpha, f\psi_\alpha) = 0$. It is also easy to show that

$$\lim_{\varepsilon \downarrow 0} \|(r/\varrho_\varepsilon)^{1/2} A r^{-1/2} e^{\alpha \varrho_\varepsilon} \psi\| = \|A r^{-1/2} e^{\alpha r} \psi\|.$$

Thus for small $\varepsilon > 0$, (3.10) holds. Since $H(\alpha)\psi_\alpha = E\psi_\alpha$ we have

$$(\psi_\alpha, (-\Delta + V + \alpha B)\psi_\alpha) = (E + \alpha^2)\|\psi_\alpha\|^2,$$

which in view of the antisymmetry of B implies

$$(\psi_\alpha, (-\Delta + V)\psi_\alpha) = (E + \alpha^2)\|\psi_\alpha\|^2. \tag{3.11}$$

Multiplying (3.11) by b and adding the result to (3.10) gives

$$(\psi_\alpha, [(2-b)\Delta + W + bV]\psi_\alpha) > b(E + \alpha^2)\|\psi_\alpha\|^2,$$

which together with (3.8) yields (3.9).

To prove the last part of the corollary just note that $W = -\beta V$ so that (3.8) holds with $b = \beta$ and $\Lambda = 0$. □

We remark that Corollary III.2 applies to atomic and molecular systems.

Let $n \geqq 2$ and suppose $\pi_1, \ldots, \pi_M$ are non-zero orthogonal projections on $\mathbb{R}^n$ with $\dim(\mathrm{Range}\,\pi_i) = n_i$. Following Agmon [1] we introduce a Schrödinger operator somewhat more general than that encountered in the N-body problem. Let v_i be a real-valued measurable function on $\mathbb{R}^{n_i}$ such that $v_i(-\Delta_i + 1)^{-1}$ is compact on $L^2(\mathbb{R}^{n_i})$, and define

$$V(x) = \sum_{i=1}^{M} v_i(\pi_i x); \qquad H = -\Delta + V. \tag{3.12}$$

We give the following general result about such operators:

Corollary III.3. *Suppose H is as in* (3.12) *and each $v_i = v_i^{(1)} + v_i^{(2)}$ with*

(1) *$v_i^{(1)}$ and $v_i^{(2)}$ Δ_i-bounded with bound zero and real-valued,*

(2) $\lim_{\gamma \to \infty} \| |y| v_i^{(1)} (-\Delta_i + \gamma^2)^{-1/2} \| = 0,$

(3) $\lim_{\gamma \to \infty} \| |y \cdot \nabla_i v_i^{(2)}|^{1/2} (-\Delta_i + \gamma^2)^{-1/2} \| = 0,$

then there exists a Λ_0 so that all eigenvalues of H are $\leqq \Lambda_0$ and if we denote $\alpha(E) = \sqrt{(\Lambda_0 - E)}$, then $H\psi = E\psi$ implies that either $\psi = 0$ or

$$\exp(\alpha|x|)\psi \notin L^2(\mathbb{R}^n) \quad \textit{for all} \quad \alpha > \alpha(E).$$

Proof. Let $b = 1$ in Corollary III.2. Tracing through the proof of this corollary we see that if as quadratic forms on $\mathcal{D}(\Delta) \times \mathcal{D}(\Delta)$

$$-\Delta - x \cdot \nabla V - V \geqq -\Lambda_0, \tag{3.13}$$

then if $H\psi=E\psi$ with $\psi\neq 0$ we must have $\exp(\alpha|x|)\psi\notin L^2(\mathbb{R}^n)$ if $\alpha\geqq 0$ and $\alpha^2+E>\Lambda_0$. To show that (3.45) is satisfied for some Λ_0 it is sufficient to show that for each $\varepsilon>0$

$$x\cdot\nabla V_i\leqq-\varepsilon\Delta+c_\varepsilon, \tag{3.14}$$

$$V_i\leqq-\varepsilon\Delta+c_\varepsilon. \tag{3.15}$$

Inequality (3.15) follows from (1) and to see (3.14) note that $x\cdot\nabla V_i(x)=(\pi_i x)\cdot(\nabla v_i)(\pi_i x)$, so that it is sufficient to have $y\cdot\nabla v_i\leqq-\varepsilon\Delta_i+c_\varepsilon$. From (3) this is clearly true for $v_i^{(2)}$. To see the result for $v_i^{(1)}$ note

$$\begin{aligned}
y\cdot\nabla_i v_i^{(1)}&=[y\cdot D,v_i^{(1)}]=y\cdot Dv_i^{(1)}-v_i^{(1)}y\cdot D\\
&=D\cdot yv_i^{(1)}-v_i^{(1)}y\cdot D-n_i v_i^{(1)}\\
&=\sum_{j=1}^{n_i}[(D_j(y_jv_i^{(1)})-(y_jv_i^{(1)}D_j)-v_i^{(1)}]\\
&\leqq-\varepsilon\Delta_i/2+(2/\varepsilon)|y|^2|v_i^{(1)}|^2-n_iv_i^{(1)}\\
&\leqq-\varepsilon\Delta_i+c_\varepsilon.
\end{aligned}$$

Here we have used (1), (2), and the inequality $[D_j,f]\leqq-\varepsilon D_j^2/2+(2/\varepsilon)f^2$ for f a real-valued function. The latter follows from

$$(\varphi,[D_j,f]\varphi)\leqq 2\|D_j\varphi\|\,\|f\varphi\|\leqq\varepsilon\|D_j\varphi\|^2/2+(2/\varepsilon)\|f\varphi\|^2. \quad\square$$

The next result is in some ways a generalization of Theorem III.1. Here we consider solutions to $(-\Delta+V)\psi=E\psi$ outside a compact set and introduce form hypotheses:

Theorem III.4. *Suppose $V=V_1+V_2$ is a complex-valued function on $\Omega_{R_0}=\{x:|x|>R_0\}$ with V_2 real-valued. Denote by Δ_D the Dirichlet Laplacian in $L^2(\Omega_{R_0})$, and let $\mathscr{H}_{+1}=\{f:\|(\Delta_D+1)^{1/2}f\|<\infty\}$ with $\mathscr{H}_{-1}$ its dual. Let χ_R be the characteristic function of $\Omega_R=\{x:|x|>R\}$. Suppose $b\in(1,\infty)$ and*

(a) *$|x|^{1/2}\chi_R V_1(-\Delta_D+1)^{-1/2}$ is bounded for all $R\geqq R_0$ and converges to zero in norm as $R\to\infty$.*

(b) *$|V_2|$ is $-\Delta_D$ form bounded with form-bound zero.*

(c) *The distribution $x\cdot\nabla V_2$ extends from $C_0^\infty(\Omega_{R_0})\times C_0^\infty(\Omega_{R_0})$ to a bounded operator from $\mathscr{H}_{+1}\to\mathscr{H}_{-1}$ with $x\cdot\nabla V_2\leqq-\varepsilon\Delta_D+C_\varepsilon$ for all $\varepsilon>0$.*

Define the self-adjoint operator

$$h(b)=-(b-1)\Delta_D-\tfrac{1}{2}bx\cdot\nabla V_2-V_2$$

by means of quadratic forms. Let $\Sigma(b)=\inf\sigma_{\mathrm{ess}}(h(b))$. Suppose ψ is a distribution solution to $(-\Delta+V)\psi=E\psi$ with $E\in\mathbb{R}$ in the sense that $\psi\in H^1_{\mathrm{loc}}(\Omega_{R_0})$ and for each $\varphi\in C_0^\infty(\Omega_{R_0})$

$$\int(\nabla\varphi\cdot\nabla\psi+\varphi(V-E)\psi)d^nx=0. \tag{3.16}$$

Suppose $\alpha>0$, $\alpha^2+E+\Sigma(b)>0$, and $\exp(\alpha|x|)\psi\in L^2(\Omega_{R_0})$. Then ψ must vanish outside a compact set.

We supplement this result with a unique continuation theorem which is tailored for Theorem III.4.

Theorem III.5. *Suppose V is a complex-valued function on $\mathbb{R}^n$ which is Laplacian bounded with bound less than one. Suppose $V=V_1+V_2$ with V_2 real-valued and for each real-valued $\eta\in C_0^\infty(\mathbb{R}^n)$ with $\eta\leqq 1$*

(a) $\lim_{\gamma\to\infty}\|\eta V_1(-\Delta+\gamma^2)^{-3/4}\|=0$.

(b) *The distribution $x\cdot\nabla V_2$ satisfies $\eta^2 x\cdot\nabla V_2\leqq -2\Delta+c_\eta$.*

Suppose $(-\Delta+V)\psi=E\psi$ and that ψ has compact support. Then $\psi=0$.

Remark. Condition (a) of Theorem III.5 is implied by $V_1\in L^p_{\mathrm{loc}}(\mathbb{R}^n)$, $p=\mathrm{Max}(2,2n/3)$. Georgescu [17], using other methods, has shown that Theorem III.5 is valid under the assumption that $V\in L^p_{\mathrm{loc}}(\mathbb{R}^n)$, $p=\mathrm{Max}(2,(2n-1)/3)$. See also [5, 7, 30, 31] for other unique continuation theorems.

Proof of Theorem III.4. Suppose that $\exp(\alpha|x|)\psi\in L^2(\Omega_{R_0})$ for some $\alpha>0$ with $\alpha^2+E+\Sigma(b)>0$. By decreasing α if necessary we can assume that with $F(x)=\alpha|x| +\beta|x|^{1-\delta}/(1-\delta)$, $\exp(F)\psi\in L^2(\Omega_{R_0})$ for all $\beta>0$ and $\delta\in(0,1)$. Define $H=-\Delta_D+V$ as a sum of forms and let γ be a real function in $C^\infty(\Omega_{R_0})$ with $\gamma(x)=1$ for $|x|>R_2$ and $\gamma(x)=0$ for $|x|<R_1$, where $R_0<R_1<R_2$. Let η be in $C_0^\infty(\mathbb{R}^n)$, real, and $\eta(x)=1$ if $|x|<1$, $\eta(x)=0$ if $|x|>2$. Define $\eta_R(x)=\eta(x/R)$ and $\tilde{\xi}=\gamma\eta_R\exp(F)$.

As distributions, it is easy to compute

$$(-\Delta+V-\tilde{E})\xi\psi=(-\Delta\tilde{\xi})\psi-2\nabla\tilde{\xi}\cdot(\nabla\psi). \tag{3.17}$$

Note that by assumption $\partial_i(\tilde{\xi}\psi)\in L^2(\Omega_{R_0})$, so that by (a) and (b) $|V|^{1/2}\tilde{\xi}\psi\in L^2(\Omega_{R_0})$. Hence by (3.16), $\tilde{\xi}\psi\in\mathscr{D}(H)$, and since $-(\Delta\tilde{\xi})-2\nabla\tilde{\xi}\cdot D=-(\nabla\tilde{\xi}\cdot D+D\cdot\nabla\tilde{\xi})$, we have from (3.17)

$$(H-E)\tilde{\xi}\psi=-((\nabla\tilde{\xi})\cdot D+D\cdot(\nabla\tilde{\xi}))\psi. \tag{3.18}$$

We thus have

$$(\tilde{\xi}\psi,(H-E)\tilde{\xi}\psi)=-(\tilde{\xi}\psi,(\nabla\tilde{\xi}\cdot D+D\cdot\nabla\tilde{\xi})\psi),$$

and taking the real part of both sides we find

$$\mathrm{Re}(\tilde{\xi}\psi,(H-E)\tilde{\xi}\psi)=\int(\nabla\tilde{\xi})^2|\psi|^2d^nx. \tag{3.19}$$

If we take $R\to\infty$, the right side of (3.19) remains bounded while $\tilde{\xi}\psi\to\xi\psi$ in $L^2(\Omega_{R_0})$, where we have set $\xi=\gamma\exp(F)$. Thus $\nabla(\xi\psi)\in L^2(\Omega_{R_0})$. We now rewrite (3.18) as

$$\begin{aligned}(H-E)&\tilde{\xi}\psi\\ &=-\{D\cdot\nabla(\gamma\eta_R)+\nabla(\gamma\eta_R)\cdot D+(D\cdot\nabla F+\nabla F\cdot D)\gamma\eta_R-2\nabla(\gamma\eta_R)\cdot\nabla F-\gamma\eta_R(\nabla F)^2\}\\ &\quad\cdot\exp(F)\psi,\end{aligned} \tag{3.20}$$

and take $R\to\infty$. Using the fact that $\exp(F)\psi$ and $\nabla(\gamma\exp(F)\psi)$ are in $L^2(\Omega_{R_0})$, it is not hard to see that the right side of (3.20) converges in $L^2(\Omega_{R_0})$. Since $\tilde{\xi}\psi\to\xi\psi$ and H is closed, we have $\xi\psi\in\mathscr{D}(H)$ and $(H-E)\tilde{\xi}\psi\to(H-E)\xi\psi$. Thus from (3.19) we have the important equation

$$\mathrm{Re}(\xi\psi,H\xi\psi)=(\psi,(E\xi^2+(\nabla\xi)^2)\psi). \tag{3.21}$$

Let $H(F)=H+\nabla F\cdot D+D\cdot\nabla F-(\nabla F)^2=H+B-(\nabla F)^2$ with $\mathscr{D}(H(F))=\mathscr{D}(H)$. From (3.20) we have

$$(H(F)-E)\xi\psi=-\{D\cdot\nabla\gamma+\nabla\gamma\cdot D\}\exp(F)\psi+2\nabla\gamma\cdot\nabla F(\exp(F))\psi\,. \tag{3.22}$$

We now claim that with $\nabla F=xg$ and $\psi_F=\exp(F)\psi$ we have

$$\begin{aligned}2\,\mathrm{Re}(A\xi\psi,V_1\xi\psi)=&(\xi\psi,(2\Delta_D+W_2)\xi\psi)-4\|g^{1/2}A\xi\psi\|^2\\&+(\xi\psi,\{(x\cdot\nabla)^2g-(x\cdot\nabla)(\nabla F)^2\}\xi\psi)\\&-\sum_{i,j}2(\partial_i\psi_F,x_i(\nabla\gamma^2)_j\partial_j\psi_F)+(\psi_F,G\psi_F)\,,\end{aligned} \tag{3.23}$$

where $W_2=x\cdot\nabla V_2$, $(\xi\psi,(2\Delta_D+W_2)\xi\psi)$ is interpreted in the form sense and

$$\begin{aligned}G=&(2x\cdot\nabla\gamma)(\nabla\gamma\cdot\nabla F)-2\gamma x\cdot\nabla(\nabla\gamma\cdot\nabla F)\\&+n(\gamma\Delta\gamma+(\nabla\gamma)^2)+x\cdot\nabla(\gamma\Delta\gamma)+2\nabla\gamma\cdot\nabla(x\cdot\nabla\gamma)\,.\end{aligned} \tag{3.24}$$

We remark here that the reason for the condition that $|V_1|$ be essentially $o(|x|^{-1/2})$ is that $g^{1/2}$ behaves like $|x|^{-1/2}$ at infinity. The relevant estimate occurs in Eq. (3.30).

The proof of (3.23) is similar to the proof of Eq. (3.1) so it will only be sketched. First note that because ψ is always multiplied by γ or $\nabla\gamma$ the Dirichlet boundary conditions in (3.22) and (3.23) are irrelevant. The method of proof of (3.1) can thus be used here. Note also that since $\nabla\xi\psi$ is in L^2 for all β, $\xi\psi\in\mathscr{D}(A)$. We have

$$\begin{aligned}&\lim_{\theta\downarrow 0}\theta^{-1}\,\mathrm{Re}\{(\xi\psi,U(\theta)(H(F)-E)\xi\psi)-((H(F)-E)\xi\psi,U(\theta)\xi\psi)\}\\&\quad=\lim_{\theta\downarrow 0}\theta^{-1}\,\mathrm{Re}(\xi\psi,(U(\theta)-U(-\theta))(H(F)-E)\xi\psi)\\&\quad=-2\,\mathrm{Re}(A\xi\psi,(H(F)-E)\xi\psi)\\&\quad=2\,\mathrm{Re}(A\xi\psi,(D\cdot\nabla\gamma+\nabla\gamma\cdot D-2\nabla\gamma\cdot\nabla F)\psi_F)\,.\end{aligned} \tag{3.25}$$

A short calculation gives

$$\begin{aligned}&2\,\mathrm{Re}(A\xi\psi,(D\cdot\nabla\gamma+\nabla\gamma\cdot D-2\nabla\gamma\cdot\nabla F)\psi_F)\\&\quad=2\sum_{i,j}(\partial_i\psi_F,x_i(\nabla\gamma^2)_j\partial_j\psi_F)-(\psi_F,G\psi_F)\,.\end{aligned} \tag{3.26}$$

Going back to the first line of (3.25) we isolate the contribution from V_1:

$$\begin{aligned}&\lim_{\theta\downarrow 0}\theta^{-1}\,\mathrm{Re}\{(\xi\psi,U(\theta)V_1\xi\psi)-(V_1\xi\psi,U(\theta)\xi\psi)\}\\&\quad=\lim_{\theta\downarrow 0}\theta^{-1}\,\mathrm{Re}((U(-\theta)-U(\theta))\xi\psi,V_1\xi\psi)\\&\quad=-2\,\mathrm{Re}(A\xi\psi,V_1\xi\psi)\,.\end{aligned} \tag{3.27}$$

We must now calculate

$$\begin{aligned}&\lim_{\theta\downarrow 0}\theta^{-1}\,\mathrm{Re}(\xi\psi,\{U(\theta)(-\Delta+V_2+B-(\nabla F)^2)U(-\theta)\\&\qquad-(-\Delta+V_2-B-(\nabla F)^2)\}U(\theta)\xi\psi)\\&\quad=\lim_{\theta\downarrow 0}\mathrm{Re}(\xi\psi,(\Delta(1-e^{-2\theta})/\theta+(V_2(\theta)-V_2)/\theta\\&\qquad-((\nabla F)^2(\theta)-(\nabla F)^2)/\theta+(B(\theta)+B)/\theta)U(\theta)\xi\psi)\\&\quad=(\xi\psi,(2\Delta+W_2-x\cdot\nabla(\nabla F)^2)\xi\psi)-2\,\mathrm{Re}(B\xi\psi,A\xi\psi)\,.\end{aligned} \tag{3.28}$$

Since $B = \nabla F \cdot D + D \cdot \nabla F = gx \cdot D + x \cdot Dg = 2gA + (x \cdot \nabla g)$, we easily find

$$2\,\mathrm{Re}(B\xi\psi, A\xi\psi) = 4\|g^{1/2}A\xi\psi\|^2 - (\xi\psi, ((x\cdot\nabla)^2 g)\xi\psi). \tag{3.29}$$

Combining (3.25) through (3.29) yields (3.23). We remark that in deriving (3.23) we have only calculated the formal expression $(\psi, [\xi A\xi, H - V_1]\psi)$ in two different ways.

We now assume that γ is a radially symmetric increasing function. Then the matrix $(x_i(\nabla\gamma^2)_j)$ is positive semidefinite so that the corresponding term in (3.23) is negative. We also use the Schwarz inequality to find

$$\begin{aligned}|2\,\mathrm{Re}(A\xi\psi, V_1\xi\psi)| &\leqq 2\|g^{1/2}A\xi\psi\|\cdot\|g^{-1/2}V_1\xi\psi\| \\ &\leqq 4\|g^{1/2}A\xi\psi\|^2 + \tfrac{1}{4}\|g^{-1/2}V_1\xi\psi\|^2.\end{aligned} \tag{3.30}$$

Combining (3.30) with (3.23) we have

$$(\xi\psi, (-2\Delta_D - W_2 - g^{-1}|V_1|^2/4 + x\cdot\nabla(\nabla F)^2 - (x\cdot\nabla)^2 g)\xi\psi) \leqq (\psi_F, G\psi_F). \tag{3.31}$$

From (3.21) we have

$$(\xi\psi, (-\Delta_D + \mathrm{Re}\,V)\xi\psi) \geqq (\xi\psi, ((\nabla F)^2 + E)\xi\psi). \tag{3.32}$$

Multiplying (3.31) by $b/2$ and subtracting (3.32) gives

$$\begin{aligned}&(\xi\psi, [(h(b) - \mathrm{Re}\,V_1 - bg^{-1}|V_1|^2/8) + ((\nabla F)^2 + E + b\{x\cdot\nabla(\nabla F)^2 - (x\cdot\nabla)^2 g\}/2)]\xi\psi) \\ &\quad\leqq b(\psi_F, G\psi_F)/2.\end{aligned} \tag{3.33}$$

Choose δ so that $b\delta < 1$. Then a short calculation shows that in Ω_{R_0}, for large enough β,

$$(\nabla F)^2 + b\{x\cdot\nabla(\nabla F)^2 - (x\cdot\nabla)^2 g\}/2 \geqq \alpha^2.$$

Since $g = \alpha|x|^{-1} + \beta\langle x\rangle^{-1-\delta} > \alpha|x|^{-1}$ we have

$$(\xi\psi, (h(b) - \mathrm{Re}\,V_1 - b\alpha^{-1}|x|\,|V_1|^2/8)\xi\psi) + (\alpha^2 + E)\|\xi\psi\|^2 \leqq b(\psi_F, G\psi_F)/2. \tag{3.34}$$

Given $\varepsilon > 0$ we can choose $R > R_0$ so that if $\mathrm{supp}\,\gamma \subset \Omega_R$

$$(\xi\psi, (h(b) - \mathrm{Re}\,V_1 - b\alpha^{-1}|x|\,|V_1|^2/8)\xi\psi) \geqq (\Sigma(b) - \varepsilon)\|\xi\psi\|^2. \tag{3.35}$$

To see this choose Λ so that $\tilde{h} + \Lambda = h(b) - \mathrm{Re}\,V_1 + \Lambda \geqq 1$. By assumption $(\tilde{h}+\Lambda)^{-1/2}\chi_R|x|\,|V_1|^2(\tilde{h}+\Lambda)^{-1/2} \to 0$ in norm as $R \to \infty$. Thus given $\varepsilon_0 > 0$ we can find R_1 so that for $\mathrm{supp}\,\gamma \subset \Omega_{R_1}$

$$(\xi\psi, (\tilde{h} + \Lambda - b\alpha^{-1}|x|\,|V_1|^2/8)\xi\psi \geqq (1-\varepsilon_0)(\xi\psi, (\tilde{h}+\Lambda)\xi\psi). \tag{3.36}$$

It is easy to see that $(-\Delta_D + 1)^{-1/2}|V_1|(-\Delta_D + 1)^{-1/2}$ is compact and thus $\sigma_{\mathrm{ess}}(\tilde{h}) = \sigma_{\mathrm{ess}}(h(b))$. Hence we can find an $R_2 \geqq R_1$ so that if $R \geqq R_2$

$$(\xi\psi, \tilde{h}\xi\psi) \geqq (\Sigma(b) - \varepsilon_0)\|\xi\psi\|^2 \tag{3.37}$$

if $\mathrm{supp}\,\gamma \subset \Omega_R$. Combining (3.36) and (3.37) we find

$$\begin{aligned}&(\xi\psi, (h(b) - \mathrm{Re}\,V_1 - b\alpha^{-1}|x|\,|V_1|^2/8)\xi\psi) \\ &\quad\geqq [(1-\varepsilon_0)(\Sigma(b) - \varepsilon_0) - \varepsilon_0\Lambda]\,\|\xi\psi\|^2,\end{aligned}$$

which for small enough $\varepsilon_0 > 0$, yields (3.35).

Choose $\varepsilon > 0$ small enough so that $\alpha^2 + E + \Sigma(b) - \varepsilon = c_0 > 0$. Then combining (3.34) and (3.35) gives

$$2c_0 \|\xi\psi\|^2 \leqq b(\psi_F, G\psi_F). \tag{3.38}$$

We now take β to infinity. If $\gamma(x) = 1$ for $|x| \geqq R_3$ then from (3.38) we have for large β and $R_4 = R_3 + 1$

$$2c_0 \int_{|x| \geqq R_4} |e^{\tilde{F}}\psi|^2 d^n x \leqq c_1 \beta \int_{|x| \leqq R_3} |e^{\tilde{F}}\psi|^2 d^n x, \tag{3.39}$$

where $\tilde{F}(x) = F(x) - F(R_4 x/|x|)$. If $\int_{|x| \geqq R_4} |\psi|^2 d^n x > 0$ then the left side of (3.39) converges to $+\infty$ as $\beta \to \infty$ while the right side converges to zero. Hence $\int_{|x| \geqq R_4} |\psi|^2 d^n x = 0$. □

Proof of Theorem III.5. By replacing V_1 by $V_1 - E$ we can assume that $E = 0$. Suppose Ω is a bounded open set with $\operatorname{supp}\psi \subset \Omega$. Let $\eta \in C_0^\infty(\mathbb{R}^n)$ with $\eta \leqq 1$ and $\eta = 1$ on Ω. Let $\varphi \in C_0^\infty(\Omega)$ and define $\xi = \exp(\alpha|x|^2/2)$. Let $W_2 = x \cdot \nabla V_2$. We compute

$$\begin{aligned}
&2\operatorname{Re}(A\xi\varphi, \xi H\varphi) \\
&\quad = 2\operatorname{Re}(A\xi\varphi, \eta V_1 \xi\varphi) + 2\operatorname{Re}(A\xi\varphi, (-\Delta + V_2 + 2\alpha A - \alpha^2|x|^2)\xi\varphi) \\
&\quad = 2\operatorname{Re}(A\xi\varphi, V_1\xi\varphi) + 4\alpha\|A\xi\varphi\|^2 + (\xi\varphi, (-2\Delta - W_2 + 2\alpha^2|x|^2)\xi\varphi) \\
&\quad \geqq 4\alpha\|A\xi\varphi\|^2 - 2\|A\xi\varphi\| \cdot \|V_1\xi\varphi\| - C_\eta\|\xi\varphi\|^2 + 2\alpha^2\| \, |x|\xi\varphi\|^2 \\
&\quad \geqq 2\alpha^2\| \, |x|\xi\varphi\|^2 - \|V_1\xi\varphi\|^2/4\alpha - C_\eta\|\xi\varphi\|^2.
\end{aligned} \tag{3.40}$$

Since V is Δ-bounded with bound less than one, C_0^∞ is a core for H. It is thus not difficult to see that we can choose $\varphi_n \in C_0^\infty(\Omega)$ so that $\varphi_n \to \psi$, $\xi H\varphi_n \to \xi H\psi = 0$, $A\xi\varphi_n \to A\xi\psi$, and $V_1\xi\varphi_n \to V_1\xi\psi$. Thus from (3.40) we have

$$\|V_1\xi\psi\|^2/4\alpha \geqq 2\alpha^2\|\xi|x|\psi\|^2 - C\|\xi\psi\|^2. \tag{3.41}$$

Suppose $\psi \neq 0$, and define $\Psi_\alpha = \xi\psi/\|\xi\psi\|$. It is easy to see that for some $\delta > 0$, $\| \, |x|\Psi_\alpha\| \geqq \delta$ so that from (3.41)

$$\|V_1\Psi_\alpha\| \geqq c_1\alpha^{3/2} \tag{3.42}$$

for some $c_1 > 0$ and all large α. On the other hand, just as in (3.19) we have

$$(\Psi_\alpha, (-\Delta + \operatorname{Re} V)\Psi_\alpha) = \alpha^2(\Psi_\alpha, |x|^2\Psi_\alpha),$$

so that again for large α

$$\|\nabla\Psi_\alpha\| \leqq c_2\alpha. \tag{3.43}$$

In addition,

$$(-\Delta + V)\Psi_\alpha = (-2\alpha A + \alpha^2|x|^2)\Psi_\alpha,$$

so that from (3.43)

$$\|\Delta\Psi_\alpha\| \leqq c_3\alpha^2 \tag{3.44}$$

for all large α. From (3.44) we have for all $\gamma>0$ and all large α

$$\|\Psi_\alpha\|=1\,, \tag{3.45}$$

$$\|(-\Delta+\gamma^2)\Psi_\alpha\|\leqq c_4^{4/3}(\alpha^2+\gamma^2)\,. \tag{3.46}$$

Interpolating between (3.45) and (3.46) we have

$$\|(-\Delta+\gamma^2)^{3/4}\Psi_\alpha\|\leqq c_4(\alpha^2+\gamma^2)^{3/4}\,,$$

and thus

$$\|V_1\Psi_\alpha\|\leqq\|\eta V_1(-\Delta+\gamma^2)^{-3/4}\|c_4(\alpha^2+\gamma^2)^{3/4}\,. \tag{3.47}$$

If we choose γ so that $c_4\|\eta V_1(-\Delta+\gamma^2)^{-3/4}\|<c_1$, (3.47) contradicts (3.42) for all large α. □

If we combine Theorems III.4 and III.5 we have the following corollary:

Theorem III.6. *Suppose $V=V_1+V_2$ is a complex-valued function on $\mathbb{R}^n$ which is Δ-bounded with bound less than one. Suppose V_2 is real-valued. Let χ_R be the characteristic function of $\{x:|x|>R\}$. Suppose*

(a) $\|V_1(-\Delta+\gamma^2)^{-3/4}\|\to 0$ *as* $\gamma\to\infty$,

(b) *there is an $R_0>0$ so that the operator $|x|^{1/2}\chi_R V_1(-\Delta+1)^{-1/2}$ is bounded for all $R>R_0$ and converges to zero in norm as $R\to\infty$.*

(c) $|V_2|$ *is* $-\Delta$ *form-compact.*

(d) $\pm x\cdot\nabla V_2\leqq c(-\Delta+1)$ *for some $c>0$ and the positive part of the operator $(-\Delta+1)^{-1/2}\,x\cdot\nabla V_2(-\Delta+1)^{-1/2}$ is compact.*

Suppose $(-\Delta+V)\psi=E\psi$ with $E\in\mathbb{R}$ and $\psi\neq 0$. If $\alpha>0$ and $\alpha^2>-E$, then $\exp(\alpha|x|)\psi\notin L^2(\mathbb{R}^n)$.

Proof. Because of (b), (c), and (d) the assumptions of Theorem III.4 are satisfied. It is also not difficult to see that our compactness assumptions imply $\Sigma(b)\geqq 0$. Thus if $\exp(\alpha|x|)\psi\in L^2(\mathbb{R}^n)$ with $\alpha>0$ and $\alpha^2>-E$ we conclude that ψ has compact support. In view of assumption (a) above and Theorem III.5, $\psi=0$. This contradiction proves the result. □

The question of whether $|V(x)|=o(|x|^{-1/2})$ is a border-line case or whether in fact $|V(x)|\to 0$ as $|x|\to\infty$ implies the result of Theorem III.6 as in one dimension is still open. Note that if $x\cdot\nabla V_2\in L^1_{\mathrm{loc}}$ and $\pm x\cdot\nabla V_2\leqq c(-\Delta+1)$ then form compactness of $(x\cdot\nabla V_2)_+$ implies condition (d).

IV. Examples

Let $H=-\Delta+V$ be the Schrödinger operator introduced in (3.12) and suppose ψ is defined on $\Omega_R=\{x\in\mathbb{R}^n:|x|>R\}$ and satisfies

$$(-\Delta+V)\psi=E\psi \tag{4.1}$$

in the distributional sense. Suppose in addition that $\psi\in L^2(\Omega_R)$. Then according to a result of Agmon [1, 2], if $E<\Sigma=\inf\sigma_{\mathrm{ess}}(H)$, then

$$\exp(\alpha|x|)\psi\in L^2(\Omega_R)\,,\qquad \alpha<\sqrt{\Sigma-E}\,. \tag{4.2}$$

Actually Agmon proves stronger results [1, 2] which we will discuss later.

One might conjecture that (4.2) is best possible in the sense that

$$\exp(\alpha|x|)\psi \notin L^2(\Omega_R), \qquad \alpha > \sqrt{\Sigma - E}, \tag{4.3}$$

but this is not the case. We give two examples to illustrate how (4.3) can go wrong. The first example is trivial but must be taken into account in thinking about (4.3). (The example was known to Simon [33] and perhaps to many others.)

Example 4.1. Let $H_1 = -\Delta + V_1$ where $V_1 \in C_0^\infty(\mathbb{R}^n)$. Suppose $E_0 = \inf\sigma(H_1) < 0$ and that H_1 has an eigenvalue E_1 with $E_0 > 2E_1$. Suppose $H_1\psi_1 = E_1\psi_1$ with $\psi_1 \neq 0$. Let $H = H_1 \otimes I + I \otimes H_1$ and $\psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$. Then $H\psi = E\psi$ with $E = 2E_1$. Note $\Sigma = \inf\sigma_{\text{ess}}(H) = E_0$ so that $\sqrt{\Sigma - E} = \sqrt{E_0 - 2E_1}$. It is easy to see that

$$\exp(\alpha|x|)\psi \in L^2, \qquad \alpha < \sqrt{-E_1},$$

$$\exp(\alpha|x|)\psi \notin L^2, \qquad \alpha > \sqrt{-E_1},$$

so that (4.3) is violated because $\sqrt{-E_1} > \sqrt{E_0 - 2E_1}$.

To understand example (4.1) from the viewpoint of embedded eigenvalues, consider the operator

$$H(\alpha) = -(\nabla_1 - \alpha)^2 - (\nabla_2 - \alpha)^2 + V_1(x_1) + V_1(x_2).$$

It is not difficult to see that if $|\alpha|^2 < -E_0$, then

$$\sigma_{\text{ess}}(H(\alpha)) \cap \mathbb{R} = \{E_0 - |\alpha|^2 + t : t \geqq 0\}.$$

Suppose $|\alpha| < \sqrt{-E_1}$. Then $\exp(\alpha \cdot x_1 + \alpha \cdot x_2)\psi \in \mathscr{D}(H(\alpha))$ and

$$(H(\alpha) - 2E_1)\exp(\alpha \cdot x_1 + \alpha \cdot x_2)\psi = 0.$$

Thus while $E = 2E_1$ is not an *embedded* eigenvalue of H, it is embedded in the essential spectrum of $H(\alpha)$ whenever $-E_1 > |\alpha|^2 > E_0 - 2E_1$.

We know that while negative eigenvalues embedded in the continuous spectrum of (self-adjoint) N-body Schrödinger operators can exist (see [29]), it is widely believed (and has been proved in some cases [29]) that positive eigenvalues do not exist for a large class of such operators. In analogy with this situation we make the following conjecture.

Conjecture. Suppose H is the Schrödinger operator defined by (3.12) and $(1+|y|)^{1/2} v_i(-\Delta_i + 1)^{-1/2}$ is compact on $L^2(\mathbb{R}^{n_i})$. Suppose ψ is a non-zero solution of $(-\Delta + V)\psi = E\psi$ in Ω_R with $E < 0$. Then if $\alpha > \sqrt{-E}$

$$\exp(\alpha|x|)\psi \notin L^2(\Omega_R).$$

Note Added. After completion of this work, special cases of this conjecture along with absence of positive eigenvalues were established in [13].

We will show in Example 4.3 that in some sense one cannot do better than the conjecture. For now note that Example 4.1 is not sufficient to show this, for if $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$ with $(-\Delta_j + V_j)\psi_j = E_j\psi_j$, then we always have $\exp(\alpha|x|)\psi \notin L^2(\mathbb{R}^{2n})$ if $\alpha > \sqrt{-E/2}$ where $E = E_1 + E_2$. This follows from the fact that if for example $|E_1| \leqq |E_2|$, then when $x = (x_1, 0)$ ψ decays as $\exp(-\sqrt{-E_1}|x|)$

$\geqq \exp(-\sqrt{-E/2}|x|)$. In the example we are about to construct the decay is arbitrarily close to $\exp(-\sqrt{-E}|x|)$ in all directions even though Σ is arbitrarily close to (but perhaps greater than) E. To prepare for this example we need the following lemma:

Lemma 4.2. *If α and β are given numbers with $\beta > \alpha > 0$, then there exists a real-valued even function $q \in C_0^\infty(\mathbb{R})$ so that if the point spectrum of $-d^2/dx^2 + q$ is labelled $E_0 < E_1 < E_2 < \ldots < E_m$, we have $E_0 = -\beta^2$, $E_2 = -\alpha^2$.*

Proof. The following short proof was kindly supplied by Simon [33] to replace our original longer proof: Suppose we find a real-valued even C_0^∞ function q_1 so that $E_2/E_0 = (\alpha/\beta)^2$. Then we can easily arrange the result in the lemma by scaling, since under the latter transformation the operator

$$\gamma^2(-d^2/dx^2 + q_1(x))$$

with point spectrum $\{\gamma^2 E_0, \gamma^2 E_1, \gamma^2 E_2, \ldots\}$ is unitarily equivalent to

$$-d^2/dx^2 + \gamma^2 q_1(\gamma x).$$

For $\lambda > 0$, let $E_j(\lambda)$, $j = 0, 1, 2, \ldots$ be the eigenvalues of $h_\lambda = -d^2/dx^2 + \lambda q$, where q is a non-zero even function in $C_0^\infty(\mathbb{R})$ with $q \leqq 0$. If h_λ has only j eigenvalues, let $E_l(\lambda) = 0$ for $l > j-1$. Define $r(\lambda) = E_2(\lambda)/E_0(\lambda)$. Then for small enough $\lambda > 0$ $r(\lambda) = 0$ while a simple min-max argument gives $\lim\limits_{\lambda \to \infty} E_j(\lambda)/\lambda = \min\{q(x) : x \in \mathbb{R}\}$ and thus $\lim\limits_{\lambda \to \infty} r(\lambda) = 1$. Since r is continuous, $r(\lambda_0) = (\alpha/\beta)^2$ for some $\lambda_0 > 0$. $\square$

Example 4.3. Suppose E and Σ are two given negative numbers and $0 < \varepsilon < 1$. Then there exists

(a) a real-valued function $q \in C_0^\infty(\mathbb{R})$,

(b) an integer M and orthogonal projections $\pi_1, \ldots, \pi_M$ mapping $\mathbb{R}^2 \to \mathbb{R}$ which define a potential $V(x) = \sum\limits_{i=1}^{M} q(\pi_i x)$ on $\mathbb{R}^2$,

(c) a number $L > 0$ and a function $\psi \in C^\infty(\{x : |x| > L\})$, such that

$$\text{(i)} \qquad (-\Delta + V)\psi = E\psi \quad \text{for} \quad |x| > L,$$

$$\text{(ii)} \qquad |\psi(x)| \leqq C \exp(-(1-\varepsilon)\sqrt{-E}|x|), \tag{4.4}$$

$$\text{(iii)} \qquad \Sigma = \inf \sigma_{\text{ess}}(-\Delta + V).$$

The construction proceeds as follows. Let $\beta^2 = -\Sigma$ and $\alpha_1 = \sqrt{-E}\sin(\pi/N)$, where N is an even integer >2 chosen so that $\cos(\pi/N) \geqq 1 - \varepsilon$, and $\alpha_1^2 < \beta^2$. Let $\alpha_2 = \sqrt{-E}\cos(\pi/N)$ so that $\alpha_1^2 + \alpha_2^2 = -E$. Choose q as in Lemma 4.2 so that the lowest eigenvalue of $-d^2/dx^2 + q$ is $-\beta^2$ and $-d^2/dx^2 + q$ has an even eigenfunction $\varphi(x)$ satisfying

$$(-d^2/dx^2 + q)\varphi = -\alpha_1^2 \varphi. \tag{4.5}$$

Note that we can choose $A > 0$ so that $\operatorname{supp} q \subsetneqq (-A, A)$ and

$$\varphi(x) = e^{-\alpha_1 |x|}, \qquad |x| \geqq A. \tag{4.6}$$

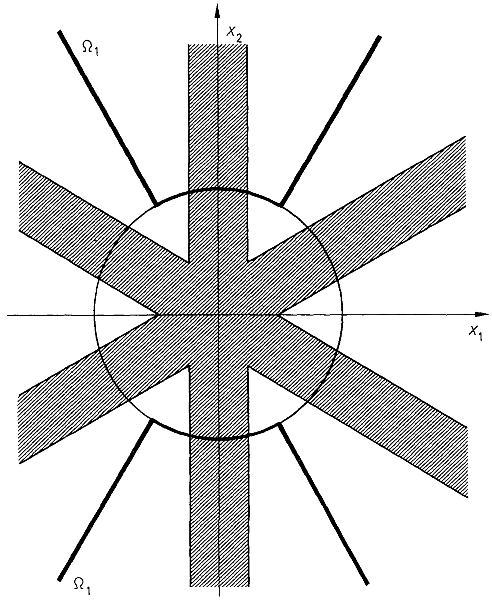

Fig. 1. The region Ω_1 is shown for the case $N=6$. Outside the shaded area $V \equiv 0$

In (4.6) we have chosen a particular normalization for φ. Let $R(\theta)$ be a clockwise rotation by θ in the plane. Thus $R(\theta)$ is given by

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$

Let π_j be the orthogonal projection onto the line

$$R(2\pi(j-1)/N)\{(x_1, x_2) \in \mathbb{R}^2 : x_2 = 0\}$$

for $j = 1, 2, \ldots, N/2$. Thus the number of potentials is $M = N/2$, and if $R_j = R(2\pi(j-1)/N)$ and $e_1 = (1, 0)$ we have

$$q(\pi_j x) = q(\langle R_j e_1, x\rangle); \quad j = 1, 2, \ldots, M, \tag{4.7}$$

where $\langle x, y\rangle = x_1 y_1 + x_2 y_2$. Let

$$\Omega = \{x \in \mathbb{R}^2 : |x| > 2A/\sin(\pi/N)\},$$

$$\Omega_1 = \Omega \cap \{x \in \mathbb{R}^2 : |\langle e_1, x\rangle| \leqq |x| \sin(\pi/N)\},$$

and $\Omega_j = R_j \Omega_1$, $j = 1, 2, \ldots, N/2$. The situation is depicted in Fig. 1. Define

$$\begin{aligned} \psi_1(x_1, x_2) &= e^{-\alpha_2 |x_2|} \varphi(x_1), \\ \psi(x) &= \psi_1(R_j^{-1} x), \qquad x \in \Omega_j. \end{aligned} \tag{4.8}$$

To see that ψ is well defined and smooth on $\Omega = \bigcup_j \Omega_j$, first note that $\varphi \in C^\infty(\mathbb{R})$ and thus ψ_1 is smooth in a neighborhood of Ω_1. Clearly ψ is smooth in the interior

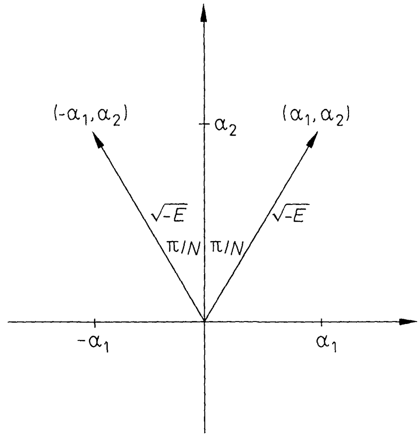

Fig. 2.

of Ω_j. Suppose $x_0 \in \Omega_1 \cap \Omega_2$. Then $x_0 = \lambda w$ with $w = (\sin(\pi/N), \cos(\pi/N))$ and $|\lambda| > 2A/\sin(\pi/N)$. If $\lambda > 0$ then for x in a neighborhood of x_0

$$\begin{aligned} \psi_1(x) &= \exp\{-\langle(\alpha_1, \alpha_2), (x_1, x_2)\rangle\}, \\ \psi(R_2^{-1}x) &= \exp\{-\langle(-\alpha_1, \alpha_2), R(-2\pi/N)(x_1, x_2)\rangle\}. \end{aligned} \tag{4.9}$$

Since $R(2\pi/N)(-\alpha_1, \alpha_2) = (\alpha_1, \alpha_2)$ by our choice of α_1 (see Fig. 2), $\psi_1(x) = \psi_1(R_2^{-1}x)$ in a neighborhood of x_0 if $\lambda > 0$. A similar argument works for all points $x_0 \in \Omega_i \cap \Omega_j$ if $i \neq j$, and hence $\psi \in C^\infty(\Omega)$. If $x_0 \in \Omega_i \cap \Omega_j$, $i \neq j$ then in a neighborhood of x_0

$$\psi = \exp\{\langle(\pm\alpha_1, \pm\alpha_2), R_j^{-1}(x_1, x_2)\rangle\}$$

for some choice of signs so that $-\Delta\psi = E\psi$. Since $V(x) = \sum_{i=1}^{M} q(\pi_i x) = 0$ in a neighborhood of such a point we have $(-\Delta + V)\psi = E\psi$ in a neighborhood of x_0. By construction, if $x \in \Omega_j$, $q(\pi_i x) = 0$ unless $i = j$ so that for $x \in \Omega_j$

$$\begin{aligned} (-\Delta + V)\psi(x) &= (-\Delta + q(\langle e_1, R_j^{-1}x\rangle))\psi_1(R_j^{-1}x), \\ &= (-\Delta + q(y))\ \psi_1(y), \quad \text{where} \quad y = R_j^{-1}x, \\ &= E\psi(x). \end{aligned}$$

Thus $(-\Delta + V)\psi = E\psi$ in Ω.

In Ω_1 we have

$$\begin{aligned} |\psi(x)| &= e^{-\alpha_2|x_2|}|\varphi(x_1)| \leqq Ce^{-\alpha_1|x_1|}e^{-\alpha_2|x_2|} \\ &= C\exp\{-\langle(\alpha_1, \alpha_2), (|x_1|, |x_2|)\rangle \\ &\leqq C\exp\{-\sqrt{\alpha_1^2 + \alpha_2^2}\,|x|\cos(\pi/N)\} \\ &= C\exp\{-\sqrt{-E}\,|x|\cos(\pi/N)\} \\ &\leqq C\exp\{-(1-\varepsilon)|x|\sqrt{-E}\}. \end{aligned} \tag{4.10}$$

By symmetry, (4.10) holds in all of Ω giving (4.4).

It remains to show that $\Sigma = \inf\sigma_{\text{ess}}(-\Delta + V)$. This follows easily from (1.6) [1]. We omit the proof.

A few comments about Example 4.3 are in order:

1. Note that we need not have $E < \Sigma$. In fact Σ does not play an essential role. If we demand, however, that $E < \Sigma$, then Agmon [1, 2] gives an upper bound

$$|\psi(x)| \leqq c_\delta e^{-(1-\delta)\varrho(\omega)|x|}; \quad x = |x|\omega, \quad \delta > 0. \tag{4.11}$$

One might expect that at least for some $\omega \in S^1$, the bound (4.11) may give a good estimate. To see that this need not be the case we calculate $\varrho(x)$. From [1, 2], $\varrho(x)$ is the distance from x to the origin in the metric

$$(ds)^2 = (\Sigma(x/|x|) - E)((dx_1)^2 + (dx_2)^2), \tag{4.12}$$

where

$$\Sigma(\omega) = \lim_{\theta \to 0} \lim_{R \to \infty} \inf\{(\varphi, (-\Delta + V)\varphi) : \varphi \in C_0^\infty(\Gamma_{R,\theta}), \ \|\varphi\| = 1\}.$$

Here $\Gamma_{R,\theta}$ is the truncated cone $\{x : |x| > R, \ \langle x, \omega \rangle > (\cos\theta)|x|\}$. $\Sigma(\omega)$ is easily calculated [1, 2]. We give the result for $\omega = (\sin\theta, \cos\theta)$ with $|\theta| \leqq \pi/N$. The function $\Sigma(\omega)$ can be calculated for other values of ω by symmetry:

$$\Sigma(\omega) = \begin{cases} \Sigma; & \theta = 0 \\ 0; & 0 < |\theta| \leqq \pi/N. \end{cases}$$

With the parametrization $x = |x|(\sin\theta, \cos\theta)$ (note we are measuring θ from the x_2 axis) a simple calculation using (4.12) gives for $|\theta| \leqq \pi/N$

$$\varrho(x) = \begin{cases} \sqrt{-E}|x|; & \cos\theta \leqq \sqrt{(\Sigma - E)}/\sqrt{-E} \\ (\sqrt{-\Sigma}|\sin\theta| + \sqrt{(\Sigma - E)}\cos\theta)|x|; & \cos\theta \geqq \sqrt{(\Sigma - E)}/\sqrt{-E}. \end{cases} \tag{4.13}$$

Choose N large enough so that $\cos(\pi/N) \geqq \sqrt{(\Sigma - E)}/\sqrt{-E}$, and so that

$$\sqrt{-\Sigma}\sin(\pi/N) + \sqrt{(\Sigma - E)}\cos(\pi/N) < \cos(\pi/N)\sqrt{-E}.$$

By symmetry and (4.13) these conditions imply $\varrho(x) < |x|\sqrt{-E}\cos(\pi/N)$ for all $x \neq 0$. From (4.10), $|\psi(x)| \leqq C\exp(-|x|\sqrt{-E}\cos(\pi/N))$ so that $\psi(x)\exp(\varrho(x))$ decays exponentially in all directions.

2. As it stands Example 4.3 suffers from the (slight) defect that $(-\Delta + V)\psi = E\psi$ is satisfied only outside a ball. In a preliminary version of this paper we conjectured that a bounded potential V_1 of compact support and a function $\tilde{\psi} : \mathbb{R}^2 \to \mathbb{R}$ with $\tilde{\psi} = \psi$ for large $|x|$ could be found so that $(-\Delta + V + V_1)\tilde{\psi} = E\tilde{\psi}$. This has now been proved by Gårding [16].

3. The high degree of symmetry in this example is not really necessary. One can produce the same result, for example, by changing $q(\pi_i x)$ to $q_i(\pi_i x)$ if

(1) $q_i \in C_0^\infty(\mathbb{R})$,

(2) $\inf\sigma(-d^2/dx^2 + q_i) = -\beta^2$,

(3) $-d^2/dx^2 + q_i$ has an even eigenfunction with eigenvalue $-\alpha_1^2$.

4. The fact that the region where $|V|$ is large disconnects $\mathbb{R}^2$ may be an important factor in examples of this type.

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