EXPONENTIAL DECAY OF TWO-BODY EIGENFUNCTIONS: A REVIEW

Dedicated to Eyvind H. Wichmann

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Abstract

We review various results on the exponential decay of the eigenfunctions of two-body Schrödinger operators. The exponential, isotropic bound results of Slaggie and Wichmann [15] for eigenfunctions of Schrödinger operators corresponding to eigenvalues below the bottom of the essential spectrum are proved. The exponential, isotropic bounds on eigenfunctions for nonthreshold eigenvalues due to Froese and Herbst [5] are reviewed. The exponential, nonisotropic bounds of Agmon [1] for eigenfunctions corresponding to eigenvalues below the bottom of the essential spectrum are developed, beginning with a discussion of the Agmon metric. The analytic method of Combes and Thomas [4], with improvements due to Barbaroux, Combes, and Hislop [2], for proving exponential decay of the resolvent, at energies outside of the spectrum of the operator and localized between two disjoint regions, are presented in detail. These are applied to prove the exponential decay of eigenfunctions corresponding to isolated eigenvalues of Schrödinger and Dirac operators.

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1 Introduction

The decay properties of bound state wave functions of Schrödinger operators have been intensively studied for many years. We are concerned here with the simplest part of the theory: The decay of the wave functions for two-body Schrödinger operators. We consider a Schrödinger operator of the form

$$H = -\Delta + V, \tag{1.1}$$

acting on $L^2(I\!R^n)$. The potential V is a real-valued function assumed to be sufficiently regular so that H is essentially self-adjoint on $C_0^\infty(I\!R^n)$. We will assume that

$$\lim_{\|x\| \to \infty} |V(x)| = 0. \tag{1.2}$$

We also assume that V is well-enough behaved so that the spectrum of H, denoted by $\sigma(H)$, has the standard form

$$\begin{aligned} \sigma(H) &= \sigma_{ess}(H) \cup \sigma_d(H) \\ &= [0, \infty) \cup \{E_j \mid -E_j > 0,\ j = 0, 1, \ldots\} \end{aligned} \tag{1.3}$$

For example, if V is continuous and satisfies (1.2), then the spectrum of H has this form. This is due to the invariance of the essential spectrum under relatively-compact perturbations [9]. In many commonly encountered cases, for example, when V has decaying derivatives, the essential spectrum is purely absolutely continuous. However, it is known that condition (1.2) is not sufficient to guarantee the absolute continuity of the spectrum. There are examples due to Pearson [12] of bounded, decaying potentials for which the Schrödinger operator has purely singular continuous spectrum. We will not need these fine spectral results here.

Suppose that $E < 0$ is an eigenvalue of H with eigenfunction $\psi_E \in L^2(I\!R^n)$ so that $H\psi_E = E\psi_E$. We will always assume that the eigenfuncton is normalized so that

$$\int_{I\!R^n} |\psi_E(x)|^2 \, d^n x = 1.$$

We are interested in the spatial behavior of this function $\psi_E(x)$, as $\|x\| \to \infty$. The well-known example of the eigenfunctions of the hydrogen atom Hamiltonian provides a guide. The hydrogen atom Hamiltonian on $L^2(I\!R^3)$ has the form

$$H = -\Delta - \frac{1}{\|x\|}. \tag{1.4}$$

It is easy to check that the spherically symmetric function

$$\psi_E(x) = \frac{1}{\sqrt{8\pi}} e^{-\sqrt{\frac{1}{4}}\|x\|}, \tag{1.5}$$

is a normalized eigenfunction of H with eigenvalue $E = -1/4$, the ground state energy. We note that the eigenfunction decays exponentially with a factor given by the square root of the distance from the eigenvalue $E = -1/4$ to the bottom of the essential spectrum $\inf \sigma_{ess}(H) = 0$. We will see that this is a characteristic exponential decay behavior.

In general, we do not know if an eigenfunction is continuous, and so pointwise bounds are not meaningful. For the general case, it is convenient to describe the decay of an eigenfunction in the L^2-sense. For a nonnegative function F, we say that ψ decays like e^{-F} *in the* L^2*-sense* if

$$\|e^F \psi\| \leq C_0, \tag{1.6}$$

for some finite constant $C_0 > 0$. Of course, if we know more about the regularity of the potential V, we can use a simple argument to conclude the regularity of the eigenfunction ψ_E corresponding to an eigenvalue $E < 0$. From this regularity and an L^2-exponential decay estimate, we can prove the pointwise decay of the eigenfunction. Simple regularity results are based on the Sobolev Embedding Theorem, which we now state.

Theorem 1.1 *Any function $f \in H^{s+k}(I\!R^n)$, for $s > n/2$ and $k \geq 0$, can be represented by a function $f \in C^k(I\!R^n)$.*

Proposition 1.2 *Suppose that H is a self-adjoint Schrödinger operator and the potential V is bounded and satisfies (1.2). If, additionally, $V \in C^{2k}(I\!R^n)$, with bounded derivatives, then an eigenfunction $\psi_E \in L^2(I\!R^n)$, corresponding to an eigenvalue $E < 0$, satisfies $\psi_E \in H^{2k+2}(I\!R^n)$. If $(2k+2) > n/2 + l$, then the eigenfunction satisfies $\psi_E \in C^l(I\!R^n)$.*

Proof. We note that since $E < 0$, the resolvent of $H_0 = -\Delta$ exists at energy E. Furthermore, the resolvent $R_0(E) = (H_0 - E)^{-1}$ maps $H^s(I\!R^n) \rightarrow H^{s+2}(I\!R^n)$, for all $s \in I\!R$. The eigenvalue equation can be written as

$$\psi_E = -R_0(E) V \psi_E. \tag{1.7}$$

Since V is bounded, the potential is a bounded operator on $L^2(I\!R^n)$. Equation (1.7) then shows that $\psi_E \in H^2(I\!R^n)$. We now repeat this argument

k-times since V is a bounded operator on $H^s(I\!\!R^n)$, provided $s \leq k$. From this, we conclude that $\psi_E \in H^{2k+2}(I\!\!R^n)$. The last statement follows from the Sobolev Embedding Theorem. □

Once regularity of the eigenfunction has been established, the pointwise decay estimate is derived from a local estimate of the following type (cf. [9] for a simple case, or [1], for a general proof). Let $B(y,r)$ denote the ball of radius $r > 0$ about the point $y \in I\!\!R^n$. There exists a constant $C_{E,V}$, depending on the potential V, the energy E, and $\inf \sigma(H)$, but independent of $x_0 \in I\!\!R^n$, so that

$$\max_{x \in B(x_0,1/2)} |\psi_E(x)| \ \leq C_{E,V} \ \|\psi_E\|_{L^2(B(x_0,1))}. \tag{1.8}$$

Given this estimate, we find

$$\begin{aligned} &\max_{x \in B(x_0,1/2)} \ |\psi_E(x) e^{F(x)}| \\ &\leq \ C_{E,V} \left(\max_{x \in B(x_0,1)} e^{F(x)} \right) \ \left(\max_{y \in B(x_0,1)} e^{F(y)} \right) \|\psi_E e^F\|_{L^2(B(x_0,1))} \\ &\leq \ C_1 \|\psi_E e^F\|_{L^2(I\!\!R^n)} \\ &\leq \ C_2, \end{aligned} \tag{1.9}$$

where we used the triangle inequality to combine the exponential terms. This proves that $|\psi_E(x_0)| \leq C_1 e^{-F(x_0)}$, for a constant C_1 independent of x_0. Since x_0 is arbitrary, the eigenfunction satisfies a pointwise exponential bound.

There are two basic types of upper bounds on wave functions as $\|x\| \to \infty$. We will present these as pointwise estimates on the eigenfunction, although they can be formulated in the L^2-sense as described above. We say that a function ϕ satisfies an *isotropic* decay estimate if there exists a nonnegative function $F : I\!\!R^+ \to I\!\!R^+$ so that

$$|\phi(x)| \leq C_\alpha e^{-F(\|x\|)}. \tag{1.10}$$

In many situations, we have $F(\|x\|) = \alpha \|x\|$, for some $0 < \alpha < \infty$. In the situation where $|V(x)| \to 0$ uniformly with respect to $\omega \in S^{n-1}$, as $\|x\| \to \infty$, isotropic decay estimates are optimal. We have seen this from the example of the hydrogen atom ground state wave function. In the situation that the potential has different limits at infinity, depending on the direction, or, the limit at infinity is not achieved uniformly, as in the case of some nonspherically-symmetric potentials, it is more precise to replace the isotropic exponential factor with an anisotropic function which expresses this variation. These anisotropic exponents are described by a function $\rho_E(x) : I\!R^n \to I\!R^+$ that, as we will see, depends on the eigenvalue E and the potential V. An anisotropic upper bound has the form

$$|\phi(x)| \leq C_0 e^{-\rho_E(x)}. \tag{1.11}$$

This is the case for N-body Schrödinger operators when the potential is a sum of pair potentials. Agmon [1] has developed an extensive theory of anisotropic decay estimates.

We will generalize the family of Hamiltonians described so far in order to incorporate Schrödinger operators with gaps in the essential spectrum. The situation we envision is the perturbation of a periodic Schrödinger operator $H_{per} = -\Delta + V_{per}$ by a compactly supported potential W. It is well-known that the spectrum of H_{per} is the union of intervals B_j, called bands, so that

$$\sigma(H_{per}) = \cup_{j\geq 0} B_j. \tag{1.12}$$

For many periodic potentials, there exist two consecutive bands B_j and B_{j+1} that do not overlap. We say that there is an open spectral gap G between the two bands. A local perturbation W, with compact support, preserves the essential spectrum. In the case that W has fixed sign, say $W >\geq 0$, it is easy to show, using the Birman-Schwinger principle, that for $\lambda > 0$ sufficiently large, the perturbed Hamiltonian, $H(\lambda) = H_{per} + \lambda W$, has bound states at energies in the gap G. Suppose that $E \in G$. The existence of an eigenvalue for $H(\lambda) = H_0 + \lambda W$ at E, for some $\lambda \neq 0$, is equivalent to the existence of an eigenvalue of the compact, self-adjoint operator $K(E) \equiv W^{1/2}(H_0 - E)^{-1}W^{1/2}$ equal to $-1/\lambda$. We simply choose $\lambda \in I\!R$ so that $-1/\lambda$ is an eigenvalue of the compact, self-adjoint operator $K(E)$. This argument can be generalized to perturbations W with compact support (or, sufficiently rapid decay) and not necessarily fixed sign [7]. We are interested in the exponential decay of the eigenfunctions corresponding to eigenvalues in open spectral gaps.

The methods used to describe eigenfunction decay below cover three main cases encountered in the study of Schrödinger operators:

1. Isolated eigenvalues below the bottom of the essential spectrum;

2. Eigenvalues embedded in the essential spectrum;

3. Eigenvalues lying in the spectral gap of an unperturbed operator.

As we will discuss in section 3, embedded eigenvalues at positive energies do not occur for most Schrödinger operators. The embedded eigenvalues referred to in point 2 occur at negative energies in the N-body case for $N \geq 3$. A notable exception is the Wigner-von Neumann potential in one-dimension that has an embedded eigenvalue at positive energy. In general, embedded eigenvalues do occur for Schrödinger operators, but they are rare. The methods presented here, especially the Agmon technique, can be extended so as to apply to resonance eigenfunctions (cf. [9]). The methods can also be applied to the study of eigenfunctions for the Laplace-Beltrami operator on noncompact Riemannian manifolds (cf. [8]). Other references on the exponential decay of eigenfunctions can be found in [13].

2 The Slaggie-Wichmann Results on Two-Body Wave Functions

In 1962, Slaggie and Wichmann [15] published a paper in which they studied the decay properties of the eigenfunctions of three-body Schrödinger operators using integral operator methods. Although we will not discuss the many-body problem here, we are interested in their proof of exponential decay of eigenfunctions corresponding to negative energies $E_j < 0$ in the two-body situation. The proof of Slaggie and Wichmann is very simple and requires minimum regularity on the potential. The method capitalizes on a basic fact that will be used again below: The Green's function for the unperturbed operator $H_0 = -\Delta$, in dimensons $n \geq 3$ and at negative energies, decays exponentially in space. In three dimensions, the kernel of the resolvent is given by

$$R_0(z)(x,y) = \{4\pi\|x-y\|\}^{-1} e^{i\sqrt{z}\|x-y\|}, \tag{2.1}$$

with the branch cut for the square root taken along the positive real axis. In higher dimensions, the kernel of the resolvent is given by a Hankel functions of the first kind that exhibits similar exponential decay. Since the spectrum of H_0 is the half-axis $[0,\infty)$, the bound state energies of H lie outside the spectrum of H_0 and, consequently, the free Green's function exhibits exponential decay at those energies. In section 5, we will discuss the exponential decay of the resolvent in more detail.

The hypotheses of Slaggie and Wichmann on the real-valued potential V are rather general.

Hypothesis 1. *There exists a positive, continuous function $Q(s)$, with $s \in \mathbb{R}^+$, having the properties*

$$\lim_{s\to\infty} Q(s) = 0 \tag{2.2}$$

$$\lim_{s\to 0} sQ(s) \leq C_0, \tag{2.3}$$

and such that

$$|V(x)| \leq Q(\|x\|), \text{ for } x \neq 0. \tag{2.4}$$

We also assume that $V \in L^1_{loc}(\mathbb{R}^3)$, and that V is relatively Laplacian bounded with relative bound less than one.

These conditions allow a Coulomb singularity at the origin and slow decay at infinity. It is not difficult to prove, using a Weyl sequence argument, that $\sigma_{ess}(H) = [0, \infty)$. Alternatively, one can show that $|V|^{1/2}(-\Delta+1)^{-1}$ is a compact operator. It follows that $(-\Delta+1)^{-1}V(-\Delta+1)^{-1}$ is compact so that $\sigma_{ess}(H) = \sigma_{ess}(-\Delta) = [0, \infty)$.

Theorem 2.1 *Let $H = -\Delta + V$ be a two-body Schrödinger operator satisfying Hypothesis 1. Let $E_j < 0$ be a negative bound state energy and let ϕ_j be any corresponding normalized eigenfunction satisfying $H\phi_j = E_j\phi_j$. For any $0 < \theta < \sqrt{|E_j|}$, there is a constant $0 < C(\theta) < \infty$, so that*

$$|\phi_j(x)| \leq C(\theta) e^{-\theta\|x\|}. \tag{2.5}$$

Let us note that this bound is saturated for the Coulomb ground state wave function which is $\psi(x) = C_0 e^{-\sqrt{|E_0|}\,\|x\|}$, with $E_0 = -1/4$. The square root in the energy behavior comes from the dependence of the free Green's function on the energy, as seen in (2.1).

Simon [14] proved a similar result on the exponential decay of eigenfunctions corresponding to negative eigenvalues of two-body Schrödinger operators on $L^2(\mathbb{R}^3)$, with $V \in L^2(\mathbb{R}^3)$ (and also for V in the Rollick class), using the integral equation (2.7). Simon used a result, proved in [14], on the solutions of certain integral equations associated with Hilbert-Schmidt kernels.

Suppose that $K(x,y)$ is a Hilbert-Schmidt kernel, that is,

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |K(x,y)|^2 \, d^3x d^3y < \infty,$$

and suppose that $G(x)$ is a nonzero, measurable function, and that $G(x)^{-1}$ exists. Consider the kernel $M(x,y) = G(x)K(x,y)G(y)^{-1}$, and suppose that the kernel $M(x,y)$ is also Hilbert-Schmidt. If $\psi \in L^2(\mathbb{R}^n)$ satisfies $K\psi = \psi$, then $G(x)\psi(x) \in L^2(\mathbb{R}^n)$. In the application of this general result, we note that the kernel of the integral equation (2.7) is Hilbert-Schmidt. For the function $G(x)$, we choose $G(x) = e^{\theta\|x\|}$, for $0 \le \theta < \sqrt{|E_j|}$, as in Theorem 2.1. It is easy to show that the modified kernel $M(x,y)$ is also Hilbert-Schmidt, so the exponential decay of the eigenfunction follows.

Proof of Theorem 2.1. We will repeated use one basic fact below. An L^2-eigenfunction in 3-dimensions is necessarily continuous. This is a consequence of the facts that such an eigenfunction is in the Sobolev space $H^2(\mathbb{R}^3)$, and the Sobolev Embedding Theorem, Theorem 1.1. The eigenvalue equation

$$(-\Delta + V)\psi_j = E_j \psi_j, \tag{2.6}$$

implies the integral equation for ψ_j,

$$\psi_j(x) = -\int_{\mathbb{R}^3} \frac{e^{-\sqrt{|E_j|}\|x-x'\|}}{4\pi\|x-x'\|} V(x')\psi_j(x') \, d^3x'. \tag{2.7}$$

It follows immediately from Hypothesis 1 and (2.7) that

$$|\psi_j(x)| \le \int_{\mathbb{R}^3} \frac{e^{-\sqrt{|E_j|}\|x-x'\|}}{4\pi\|x-x'\|} Q(\|x'\|)|\psi_j(x')| \, d^3x'. \tag{2.8}$$

Let us define a function $m(x)$ by

$$m(x) \equiv \sup_{x'}\{ \, |\psi_j(x')|e^{-\theta\|x-x'\|} \, \}, \tag{2.9}$$

and, motivated by (2.8), another function $h_\theta(x)$ by

$$h_\theta(x) \equiv \int_{\mathbb{R}^3} \frac{e^{-(\sqrt{|E_j|}-\theta)\|x-x'\|}}{4\pi\|x-x'\|} Q(\|x'\|) \, d^3x', \tag{2.10}$$

for $0 < \theta < |E_j|$. It is easy to check that h_θ is continuous, rotationally invariant, and thus a function of $\|x\|$ only. These two definitions and inequality (2.8) imply that

$$|\psi_j(x)| \leq h_\theta(\|x\|)m(x). \tag{2.11}$$

We next prove that

$$\lim_{\|x\| \to \infty} h_\theta(\|x\|) = 0. \tag{2.12}$$

We divide the region of integration $I\!R^3$ into two regions: $\|x - x'\| < \epsilon$ and $\|x - x'\| > \epsilon$, for some $\epsilon > 0$, to be determined below. In the first region, we easily show that $h_\theta(x) \leq C\epsilon^2 \|x\|^{-1}$. In the second region, we use the boundedness of Q and write

$$\int_{\|x-x'\|>\epsilon} \frac{e^{-\lambda\|x-x'\|}}{4\pi\|x-x'\|} Q(\|x\|) d^3x' \leq \frac{C_0}{4\pi\epsilon} \int_{I\!R^3} e^{-\lambda\|u\|} d^3u, \tag{2.13}$$

where $\lambda = \sqrt{|E_j| - \theta} > 0$. If we choose $\epsilon = \|x\|^{1/4}$, for example, property (2.12) follows from these two estimates.

This decay of the function $h_\theta(x)$ as $\|x\| \to \infty$ controls the decay of the eigenfunction in the following sense. Because h_θ vanishes at infinity, there exists a region $\mathcal{R} \subset I\!R^3$ on which $h_\theta(x) < 1$. We can simply take $\mathcal{R} = I\!R^3 \backslash B_R(0)$, for a radius R sufficiently large. We denote by $\mathcal{R}^c$ the complement of this region. We have from (2.11) that $|\psi_j(x)| < m(x)$, for $x \in \mathcal{R}$. On the otherhand, we have for all $x \in I\!R^3$ that

$$m(x) = \max\left(\sup_{x' \in \mathcal{R}} \{|\psi_j(x')|e^{-\theta\|x-x'\|}\}, \sup_{x' \in \mathcal{R}^c} \{|\psi_j(x')|e^{-\theta\|x-x'\|}\} \right). \tag{2.14}$$

Our goal is to show that the maximum is obtained by the $\mathcal{R}^c$-term. This will immediately imply the result. To this end, we first note that from the definition of m, for any $x'' \in I\!R^3$, we have

$$\begin{aligned} m(x) &= \sup_{x'} \{|\psi_j(x')|e^{-\theta\|x-x'\|}\} \\ &= \sup_{x'} \{|\psi_j(x')|(\sup_{x''} e^{-\theta\|x'-x''\|}e^{-\theta\|x''-x\|})\} \\ &= \sup_{x''} \{m(x'')e^{-\theta\|x''-x\|}\}. \end{aligned} \tag{2.15}$$

We have used the identity

$$e^{-\theta\|x-x'\|} = \sup_{x''} e^{-\theta\|x-x''\|} e^{-\theta\|x''-x'\|}, \tag{2.16}$$

that is proved by the triangle inequality and the definition of the supremum. Using (2.15), and the fact that $|\psi_j(x)| < m(x)$, for $x \in \mathcal{R}$, we compute,

$$\begin{aligned}
&\sup_{x' \in \mathcal{R}} \{|\psi_j(x')| e^{-\theta\|x-x'\|}\} \\
&\quad < \sup_{x' \in \mathcal{R}} \{m(x') e^{-\theta\|x-x'\|}\} \\
&\quad \leq \sup_{x' \in I\!R^3} \{m(x') e^{-\theta\|x-x'\|}\} \\
&\quad = m(x).
\end{aligned} \tag{2.17}$$

That is, the supremum over $x' \in \mathcal{R}$ occurring in (2.14) is strictly less that $m(x)$. Hence, we have that

$$m(x) = \sup_{x' \in \mathcal{R}^c} \{|\psi_j(x')| e^{-\theta\|x-x'\|}\}. \tag{2.18}$$

We can take $\mathcal{R}$ to be the exterior of a ball of radius R, for sufficiently large R, due to the vanishing of h_θ. It follows immediately from the continuity of the eigenfunction ψ_j and (2.18) that

$$m(x) \leq C(R, \theta) e^{-\theta\|x\|}, \tag{2.19}$$

for all $x \in I\!R^n$, and for some constant depending on $R > 0$ and θ. Inequality (2.11), that $|\psi_j(x)| \leq h(\|x\|) m(x)$, for all $x \in I\!R^3$, and the boundedness of h, implies that there exists a constant $C_0 > 0$ so that $|\psi_j(x)| \leq C_0 m(x)$. This, together with (2.19), establishes the upper bound on the eigenfunction. $\Box$

As noted by Slaggie and Wichmann, the proof requires less restrictive conditions on the potential V. The potential must satisfy conditions (2.2)–(2.4), and, for each $0 < \theta < \sqrt{|E_j|}$, there must exist an $R_\theta > 0$ so that $h_\theta(\|x\|) < 1$ for $\|x\| > R_\theta$.

3 The Froese-Herbst Method

We indicate the basic ideas of the Froese-Herbst method [5] for proving the decay of eigenfunctions. The authors' main motivation and results concern the exponential decay of the eigenfunctions of N-body Schrödinger operators, and the absence of positive eigenvalues for N-body Schrödinger operators. We will only give the simplest version of the results here. The Froese-Herbst method does not depend upon the explicit properties of the free Green's function, as in the Slaggie-Wichmann method. Consequently, the Froese-Herbst method can be applied to more general classes of differential operators, such as Laplace-Beltrami operators on noncompact manifolds, and to the study of eigenfunctions corresponding to eigenvalues embedded in the essential spectrum.

The Froese-Herbst method is tied to the theory of positive commutators as developed by E. Mourre [10]. We will briefly review the main points of this theory below. The Froese-Herbst method yields L^2-exponential bounds of the form

$$e^F \psi \in L^2(\mathbb{R}^n), \tag{3.1}$$

for some function F. Under more regularity assumptions on V, this L^2-exponential bound can be converted to a pointwise exponential bound, as explained in section 1.

The Froese-Herbst method identifies the *threshhold energies* associated with the Hamiltonian H as controlling the rate of decay of the eigenfunctions. This means the following. Let $\Sigma = \inf \sigma_{ess}(H)$ be the bottom of the essential spectrum. For many-body systems, this can be strictly negative. The bound state energies of subsystems lie between Σ and 0. These energies are called thresholds of the system. More generally, we define threshold energies as those energies at which the Mourre estimate (3.7) fails to hold. For many two-body Schrödinger operators, the only threshold energy is zero, which is also the bottom of the essential spectrum. We mention that there may be an eigenvalue at zero energy, or at any threshold. There is no general method for obtaining estimates on the decay rate of the corresponding eigenfunctions. There are examples for which the decay rate is only inverse polynomial, rather than exponential.

The general Froese-Herbst result states that any eigenfunction $\psi_E \in L^2(\mathbb{R}^n)$, with $H\psi_E = E\psi_E$, decays exponentially at a rate given by the square root of the distance from the eigenvalue to a threshold above the eigenvalue. That is, for some threshold energy $\tau > E$, we have the bound,

$$e^{(\sqrt{\tau - E} - \epsilon)\,\|x\|} \psi_E(x) \in L^2(\mathbb{R}^n), \tag{3.2}$$

for any $\epsilon > 0$. Note that when $\tau = 0$, this is basically the Slaggie-Wichmann result.

In the two-body case studied here, the potential V must satisfy the following hypothesis. We write $R_0(z)$ for the resolvent of the Laplacian, $R_0(z) = (-\Delta - z)^{-1}$.

Hypothesis 2. *We assume that the potential $V \in C^1(\mathbb{R}^n)$, and is relatively $-\Delta$-bounded, with relative bound less than one. Furthermore, we assume that there exists a constant $0 < C_0 < \infty$, so that V satisfies*

$$\|R_0(-1)(x \cdot \nabla V)R_0(-1)\| \leq C_0. \tag{3.3}$$

We can relax the C^1-condition and assume that condition (3.3) holds in the sense of quadratic forms, cf. [6]. The main result of the Froese-Herbst in the two-body case is the following theorem.

Theorem 3.1 *Let $H = -\Delta + V$ be a two-body Schrödinger operator with potential V satisfying Hypothesis 2. Suppose that for $E < 0$, is a bound state energy with eigenfunction $\psi_E \in L^2(\mathbb{R}^n)$, satisfying $H\psi_E = E\psi_E$. Then, we have for any $\epsilon > 0$,*

$$e^{(\sqrt{|E|}-\epsilon)\,\|x\|}\psi_E(x) \in L^2(\mathbb{R}^n). \tag{3.4}$$

If, in addition, we assume that $x \cdot \nabla V$ is relatively Laplacian bounded with relative bound less than 2, then H has no positive eigenvalues.

One of the main applications of the method of proof of this theorem (and its counterpart in the N-body case) is to prove the nonexistence of positive eigenvalues of Schrödinger operators. The idea is to prove that any L^2-eigenfunction ψ_E, corresponding to a positive energy eigenvalue E, must decay faster than any exponential. That is, for all $\theta > 0$, we have

$$e^{\theta\|x\|}\psi_E(x) \in L^2(\mathbb{R}^n). \tag{3.5}$$

Since the decay of an eigenfunction is controlled by the distance to a threshold larger than the eigenvalue, one must prove that an N-body Schrödinger operator has no positive thresholds. For the two-body case, we will show that the Mourre estimate holds at all positive energies, so there are no positive thresholds. Consequently, we see that the eigenfunction for a positive eigenvalue must decay faster than any exponential. A variant of a unique continuation argument then shows that such a function $\psi_E = 0$.

We now give an outline of the proof of the exponential decay part of the Froese-Herbst Theorem. A complete textbook presentation is given in [6]. We will work with the specific case of two-body operators. We begin with the Mourre theory of positive commutators [10]. Let $A = \frac{1}{2}(x \cdot \nabla + \nabla \cdot x)$ be the skew-adjoint operator so that $-iA$ is the self-adjoint generator of the dilation group on $L^2(I\!R^n)$. We assume that the potential V satisfies Hypothesis 2. A simple computation shows that, formally, the commutator $[H, A] \equiv HA - AH$, is

$$[H, A] = 2H - 2V - 2x \cdot \nabla V = 2H + K. \tag{3.6}$$

The operator K is relatively-Laplacian compact. Let $I = [I_0, I_1] \subset I\!R$ be a finite, closed interval, and let $E_H(I)$ be the spectral projection for H and the interval I. Conjugating the commutator relation (3.6) by the spectral projectors $E_H(I)$, we obtain the Mourre estimate,

$$\begin{aligned} E_H(I)[H, A]E_H(I) &= 2E_H(I)H + E_H(I)KE_H(I) \\ &\geq 2I_0 E_H(I) + E_H(I)KE_H(I). \end{aligned} \tag{3.7}$$

This estimate implies a Virial Theorem of the following type. Suppose that the Mourre estimate (3.7) holds in a neighborhood I with compact operator $K = 0$. Then, the operator H cannot have an eigenvalue $E \in I$. Since, if $E \in I$ is an eigenvalue with an eigenfunction ψ_E, we have (neglecting domain considerations),

$$\begin{aligned} \langle \psi_E, [H, A]\psi_E \rangle &= \langle \psi_E, [H - E, A]\psi_E \rangle \\ &= 0. \end{aligned} \tag{3.8}$$

On the otherhand, the Mourre estimate (3.7) with $K = 0$ implies

$$\langle \psi_E, [H, A]\psi_E \rangle \geq 2I_0 > 0. \tag{3.9}$$

This inequality clearly contradicts (3.8). Consequently, the energy E cannot be an eigenvalue for H.

This simple idea lies behind the proof of the Froese-Herbst Theorem. Suppose E is an eigenvalue of H, and define $\langle x \rangle \equiv (1 + \|x\|^2)^{1/2}$. We define

$\tau \equiv \sup\{E + \alpha^2 \mid \alpha > 0, \text{and } e^{\alpha\langle x\rangle}\psi_E \in L^2(I\!R^n)\}$. If $\tau = \alpha_0^2 + E$ is not a threshold of H, then there exist $\alpha_1 \geq 0$ and $\gamma > 0$, with $\alpha_1 < \alpha_0 < \alpha_1 + \gamma$, so that $e^{\alpha_1\langle x\rangle}\psi_E \in L^2(I\!R^n)$, but $e^{(\alpha_1+\gamma)\langle x\rangle}\psi_E$ is not in $L^2(I\!R^n)$. Because τ is not a threshold of H, the Mourre estimate holds in a neighborhood of τ. In particular, it holds in a neighborhood of $E+\alpha_1^2$, for some α_1 sufficiently close to α_0, since the set of thresholds is closed. We will construct a sequence of approximate eigenfunctions Ψ_s for H and the eigenvalue $E+\alpha_1^2$ in the sense that $\|(H - E - \alpha_1^2)\Psi_s\| \leq C_0\gamma$, and Ψ_s converges weakly to zero as $s \to 0$. The Virial Theorem then implies that the matrix element of the $[H, A]$ in the state Ψ_s, which is approximately an eigenfunction with eigenvalue $E+\alpha_1^2$, is very small with respect to γ. On the other hand, the Mourre estimate holds in a small neighborhood $E + \alpha_1^2$, and, since Ψ_s converges weakly to zero, the matrix element $\langle \Psi_s, K\Psi_s\rangle \to 0$. This implies that the matrix element of $[H, A]$ in the state Ψ_s is strictly positive. This gives a contradiction for small γ.

In the first step of the proof, we construct states with shifted energy. For motivation, recall that a translation in momentum space has the effect of shifting the energy. Let ψ_E be an L^2-eigenfunction of H, and assume that F is a differentiable function such that $\psi_F = e^F\psi_E \in L^2(I\!R^n)$. It is a standard calculation (see section 4) to show that

$$H_F \equiv e^F H e^{-F} = H + \nabla F \cdot \nabla + \nabla \cdot \nabla F - |\nabla F|^2. \tag{3.10}$$

It follows from this that the expected value of the Hamiltonian H in the state ψ_F is

$$\langle \psi_F, H\psi_F\rangle = \langle \psi_F, [E + |\nabla F|^2]\psi_F\rangle, \tag{3.11}$$

so the state ψ_F appears as a state with energy $E + |\nabla F|^2$.

Next, we choose a family of functions F_s so that $|\nabla F_s|^2 \sim \alpha_1^2$, and so that the sequence $\psi_{F_s} \equiv \psi_s$ converges weakly to zero. Let $\chi_s(t)$ be a smooth function of compact support satisfying $\lim_{s\to 0}\chi_s(t) = t$. We now define a weight $F_s(x) \equiv \alpha_1 + \gamma\chi_s(\langle x\rangle)$ having the property that $\lim_{s\to 0} F_s(x) = \alpha_1+\gamma$. It then follows that $\psi_s = e^{F_s}\psi_E \in L^2(I\!R^n)$, provided $s > 0$, but that $\|\psi_s\| \to \infty$, as $s \to 0$. Furthermore, a calculation reveals that $|\nabla F_s|^2 \sim \alpha_1^2$, for small γ. We define $\Psi_s \equiv \psi_s\,\|\psi_s\|^{-1}$, so that Ψ_s converges weakly to zero. It is not too difficult to show that Ψ_s is the sequence of approximate eigenfunctions we desire, in the sense that

$$\|(H - E - \alpha_1^2)\Psi_s\| \sim 0, \tag{3.12}$$

for small γ. Finally, it follows from the Virial Theorem (3.8) that the matrix element $\langle \Psi_s, [H, A]\Psi_s \rangle \sim 0$. On the otherhand, since the Mourre estimate holds in a neighborhood of $E + \alpha_1^2$, by the assumption that $E + \alpha_0^2$ is not a threshold, and the sequence Ψ_s converges weakly to zero, we know that this matrix element is bounded from below by a strictly positive constant. This gives a contradiction, so that $\tau = E + \alpha_0^2$ must be a threshold.

Some final comments are in order. The Froese-Herbst technique depends upon the existence of a conjugate operator A for a given Hamiltonian H. It is not always easy to construct a conjugate operator, but this has now been done in a variety of situations. Secondly, if the energy E itself is a threshold, the method gives no information about the rate of decay of a corresponding eigenfuncton. Thirdly, the proof indicates that the rate of decay of the eigenfunction is controlled by the square root of the distance to some threshold above E, similar to the Slaggie-Wichmann result. The proof, however, does not indicate that it is always the nearest threshold above E that controls the exponential decay.

4 Nonisotropic Agmon Decay Estimates

The results that we have discussed so far are exponential decay estimates of the form $e^F \psi \in L^2(I\!R^n)$, with F a function of $\|x\|$ alone. Hence, the resulting bounds are spatially *isotropic*. For the case of a two-body potential, these are optimal when the potential is spherically symmetric. In general, isotropic bounds do not reflect the variation of the potential with direction. In the many-body case, when the total potential is the sum of two-body potentials, the behavior of V at infinity depends crucially on the direction. Hence, one is led to develop *nonisotropic* bounds on the decay of the wave function that more closely reflect the behavior of the potential in each direction. Such bounds and techniques are also crucial for the estimation of the lifetime of quantum resonances in terms of the potential barrier generating the resonance.

A systematic study of the decay of eigenfunctions of second-order partial differential operators, corresponding to eigenvalues below the bottom of the essential spectrum, was performed by Agmon [1]. A key role is played by the Agmon metric on $I\!R^n$. This pseudo-Riemannian metric is constructed directly from the potential and the energy, and thus reflects the variation of the potential with direction. The distance function corresponding to the Agmon metric measures how the potential controls the decay. Explicitly solvable models in one-dimension, and the WKB approximation give some clue as to the form of this metric.

Definition 4.1 *Let V be a bounded, real-valued function on $\mathbb{R}^n$, and let $E \in \mathbb{R}$. For any $x \in \mathbb{R}^n$, and $\xi, \eta \in T_x(\mathbb{R}^n) = \mathbb{R}^n$, the tangent space to $\mathbb{R}^n$ at x, we define a (degenerate) inner product on $T_x(\mathbb{R}^n)$ by*

$$\langle \xi, \eta \rangle_x \equiv (V(x) - E)_+ \langle \xi, \eta \rangle_E, \tag{4.1}$$

where $\langle \cdot, \cdot \rangle_E$ is the usual Euclidean inner product and $f(x)_+ \equiv \max\{f(x), 0\}$. The corresponding pseudo-metric on $\mathbb{R}^n$ is called the Agmon metric induced by the potential V at energy E.

It is important to note that the Agmon metric depends on both the potential and the energy E. The Agmon metric on $\mathbb{R}^n$ is degenerate because there may exist nonempty turning surfaces $\{x \in \mathbb{R}^n \mid V(x) = E\}$, and classically forbidden regions $\{x \in \mathbb{R}^n \mid V(x) < E\}$. These sets play an important role in the theory. The turning surface marks the limits of classical motion for a particle with energy E moving under the influence of the potential V, and such a particle cannot penetrate into the classically forbidden region. Consequently, it is expected that the quantum mechanical wave function is small in the classically forbidden region.

We use the structure given in Definition 4.1 to construct a distance function (or, metric) on $\mathbb{R}^n$. Let $\gamma : \ [0,1] \to \mathbb{R}^n$ be a differentiable path in $\mathbb{R}^n$. The derivative $\dot{\gamma}(t)$ belongs to the tangent space at the point $\gamma(t)$. For any Riemannian metric g on a manifold $\mathbb{R}^n$, the length of γ is given by the integral

$$L(\gamma) = \int_0^1 \| \dot{\gamma}(t) \|_{\gamma(t)} \, dt, \tag{4.2}$$

where $\| \xi \|_x = \langle \xi, \xi \rangle_x^{1/2}$, for $\xi \in T_x(\mathbb{R}^n)$. In the Agmon structure (4.1), the length of the curve γ (4.2) is:

$$L_A(\gamma) = \int_0^1 (V(\gamma(t)) - E)_+^{1/2} \| \dot{\gamma}(t) \|_E \, dt, \tag{4.3}$$

where $\| \cdot \|_E$ denotes the usual Euclidean norm. A path γ is a *geodesic* if it minimizes the energy functional $E(\gamma) \equiv \frac{1}{2} \int_0^1 \| \dot{\gamma}(t) \|_{\gamma(t)}^2 \, dt$.

Definition 4.2 *Given a bounded, real-valued potential V and energy E, the distance between $x, y \in I\!R^n$ in the Agmon metric is*

$$\rho_E(x,y) \equiv \inf_{\gamma \in P_{x,y}} L_A(\gamma), \tag{4.4}$$

where $P_{x,y} \equiv \{\gamma : [0,1] \to I\!R^n \mid \gamma(0) = x, \gamma(1) = y,\ \gamma \in AC[0,1]\}$. Here, the set $AC[0,1]$ is the space of all absolutely continuous functions on $[0,1]$.

The distance between $x, y \in I\!R^n$ with the Agmon metric is the length of the shortest geodesic connecting x to y. The distance function ρ_E in (4.4) reduces to the usual WKB factor for the 1-dimensional case,

$$\rho_E(x,y) = \int_x^y (V(s) - E)_+^{1/2}\, ds. \tag{4.5}$$

The Agmon metric has several nice properties: It satisfies the triangle inequality, and is Lipschitz continuous. The main result of this section is that the Agmon metric at energy E controls the decay of an eigenfunction at energy E, provided $E < \inf \sigma_{ess}(H)$.

Theorem 4.1 *Let $H = -\Delta + V$, with V real and continuous, be a closed operator bounded below with $\sigma(H) \subset I\!R$. Suppose E is an eigenvalue of H, and that the support of the function $(E - V(x))_+ \equiv max\,(0, E - V(x))$ is a compact subset of $I\!R^n$. Let $\psi \in L^2(I\!R^n)$ be an eigenfunction of H such that $H\psi = E\psi$. Then, for any $\epsilon > 0$, there exists a constant C_ϵ, with $0 < C_\epsilon < \infty$, such that*

$$\int e^{2(1-\epsilon)\rho_E(x)} |\psi(x)|^2 dx \leq C_\epsilon, \tag{4.6}$$

where $\rho_E(x) \equiv \rho_E(x, 0)$.

We note that if V satisfies (1.2) uniformly in the sense that $|V(x)| < \epsilon$ for $\|x\|$ large enough, and if $E < 0$, then the support of the positive part of $(E - V)$ is compact.

Sketch of the Proof. We will sketch the proof here. A textbook treatment is given in [9], and the general cases are treated in [1]. The main idea of the Agmon approach is to use the strict positivity of $(V - E)$, outside a compact set, in order to bound the quadratic form $\langle \Phi, (H - E)\Phi \rangle$ from below, for suitably chosen vectors Φ. Note that the set on which $(V - E) > 0$ is the classically forbidden region. A classical particle with energy E cannot penetrate this region. One expects that the corresponding quantum wave function is small in this region. The vector Φ has the form $\Phi = \eta e^F \phi$, where F is a distance function built from the Agmon metric, the function η localizes the eigenfunction to the classically forbidden region, and we will take $\phi = e^F \psi_E$ after some initial calculations. Because Φ is built from an eigenfunction for H, the quadratic form $\langle \Phi, (H-E)\Phi \rangle$ is bounded above by the norm of ψ_E, localized near the support of $\nabla\eta$. Hence, we arrive at an inequality roughly of the form,

$$\|\eta e^F \psi_E\|^2 \;\leq\; C_1 \|g(\nabla\eta) e^F \psi_E\|^2, \tag{4.7}$$

where $g(\nabla\eta)$ represents some combination of $\nabla\eta$. Since e^F will be bounded on the support of $\nabla\eta$, this, in turn, implies the L^2-exponential bound of ψ_E.

We now illustrate how to implement this strategy. Let $F = (1-\epsilon)\rho_E$ and note that almost everywhere,

$$|\nabla F|^2 \leq (1-\epsilon)^2 (V-E)_+ \leq (1-\epsilon)(V-E)_+. \tag{4.8}$$

We first compute a lower bound for the quadratic form $\langle \Phi, (H-E)\Phi \rangle$, for $\Phi = e^F \eta \phi$. We take $\eta \in C^2(I\!\!R^n)$ to be a nonnegative function supported in the region where $(V-E) \geq \delta$, and $\eta = 1$, except near the boundary of this region. A key computation involves the gauge transformation, as in (3.10), given by $H \to H_F \equiv e^F H e^{-F}$. To compute this, we have for any $u \in C_0^\infty(I\!\!R^n)$,

$$\begin{aligned} -e^F \Delta e^{-F} u &= -(e^F \nabla e^{-F})^2 u \\ &= -(\nabla - \nabla F)^2 u, \end{aligned} \tag{4.9}$$

so that

$$e^F H e^{-F} = H + (\nabla \cdot \nabla F + \nabla F \cdot \nabla) - |\nabla F|^2. \tag{4.10}$$

Consequently, for any reasonable function ϕ, we compute a lower bound on the quadratic form,

$$\begin{aligned} & Re\langle e^F \eta\phi, (H-E) e^{-F} \eta\phi \rangle \\ &= Re\langle \eta\phi, (H + (\nabla \cdot \nabla F + \nabla F \cdot \nabla) - |\nabla F|^2 - E)\eta\phi \rangle \\ &\geq \langle \eta\phi, (V - E - |\nabla F|^2)\eta\phi \rangle \\ &\geq \epsilon\delta \|\eta\phi\|^2. \end{aligned} \tag{4.11}$$

We made use of the fact that $Re\langle \phi, (\nabla g \cdot \nabla + \nabla \cdot \nabla g)\phi \rangle = 0$, for any real-valued function g. We use this lower bound by setting $\phi = e^F \psi_E$. After some standard computations, the final formula is

$$Re\langle e^{2F}\eta\psi_E, (H - E)\eta\psi_E \rangle \geq \delta\epsilon \| e^F \eta \psi_E \|^2. \tag{4.12}$$

We now turn to the upper bound. We control the exponentially growing term on the left in (4.12) by the compactness of the support of the gradient of η. Using the fact that ψ_E is an eigenfunction, we have

$$\begin{aligned} (H - E)\eta\psi_E &= [-\Delta, \eta]\psi_E \\ &= (-\Delta\eta - 2\nabla\eta \cdot \nabla)\psi_E. \end{aligned} \tag{4.13}$$

Since $\|\nabla \psi_E\| \leq C_E \|\nabla (H + M)^{-1}\|$, for some M large enough, we obtain an upper bound of the form,

$$|\langle e^{2F}\eta\psi_E, (H - E)\eta\psi_E \rangle| \leq C_E \left(\sup_{x \in supp|\nabla\eta|} e^{2F} \right). \tag{4.14}$$

By arranging the diameter of the support of $|\nabla\eta|$ small enough, we combine (4.12) and (4.14) to obtain

$$\| e^{(1-\epsilon)\rho_E} \eta \psi_E \|^2 \leq C(E, \eta). \tag{4.15}$$

A simple estimate on $\| e^{(1-\epsilon)\rho_E} (1 - \eta)\psi_E \|^2$, using the compactness of the support of $(1 - \eta)$, completes the proof of the result. □

5 Resolvent Decay Estimates and the Combes-Thomas Method

In this final section, we examine another manner of proving exponential decay bounds on eigenfunctions based on the exponential decay of the resolvent at energies outside of the spectrum of the Hamiltonian. The Slaggie-Wichmann proof discussed in section 2 used the decay of the free Green's function at energies below the bottom of the essential spectrum. We will first prove a result, due to Combes and Thomas [4], on the exponential decay of the resolvent of a self-adjoint Schrödinger operator, at energies outside of the spectrum, when localized between two disjoint regions. We will then use this estimate to prove the decay of eigenfunctions corrsponding to eigenvalues outside of the essential spectrum in certain cases. We conclude this section with an application to the exponential decay of eigenfunctions of the Dirac operator corresponding to eigenvalues in the spectral gap $(-m, m)$.

We begin with a form of the Combes-Thomas method [4], due to Barbaroux, Combes, and Hislop [2], which allows an improvement on the rate of decay of the resolvent. Combes and Thomas, motivated by the work of O'-Connor [11] and dilation analyticity, emphasized the use of analytic methods in the study of the decay of eigenfunctions. Their method is more flexible than the Slaggie-Wichmann or O'Connor method in that it can be applied, for example, to Schrödinger operators with nonlocal potentials, to N-body Schrödinger operators, and to other forms of differential operators. As a consequence, one obtains exponential decay for eigenfunctions corresponding to isolated eigenvalues in gaps of the essential spectrum, not just to those below the bottom of the essential spectrum.

The Combes-Thomas method also applies to N-body Schrödinger operators with dilation analytic two-body potentials. For such Schrödinger operators, the Combes-Thomas method allows one to prove the exponential decay on nonthreshold eigenfunctions. The result is similar to that obtained by the Froese-Herbst method. If ψ_E is an eigenfunction of H corresponding to a nonthreshold eigenvalue E, then $e^{a\|x\|}\psi_E \in L^2(I\!R^n)$, for any a satisfying $a^2 < 2\inf\{|E - \mathrm{Re}E_\alpha| + \mathrm{Im}E_\alpha\}$. The infimum is taken over all thresholds of the nonself-adjoint operator $H(i\pi/4)$, obtained from H by dilation analyticity. Since we will not discuss dilation analytic operators here, we refer the reader to [13]. As with the works mentioned above, Combes and Thomas are mainly concerned with the N-body problem. We will discuss the method as applied to two-body problems only.

5.1 A Simple Proof of Resolvent Decay Estimates

The idea of Combes and Thomas is to study the deformation of the Hamiltonian by a unitary representation of an abelian Lie group, and then to analytically continue in the group parameters. Typically, one uses the group of dilations in coordinate space, or boost transformations in momentum space. As an example, let the Hamiltonian $H = -\Delta + V$ be self-adjoint. It follows as in previous sections, that for a constant vector $\lambda \in I\!R^n$, we have

$$H(\lambda) \equiv e^{ix\cdot\lambda} H e^{-ix\cdot\lambda} = H + 2i\lambda \cdot \nabla + |\lambda|^2. \tag{5.1}$$

Provided that the operator ∇ is relatively H-bounded, the operator $H(\lambda)$ extends to an analytic family of type A on $\mathbb{C}^n$.

We next study the resolvent of this analytic type A family of operators. Let us suppose that $E \in \rho(H)$, the resolvent set of H. Then, the operator $(H - E)$ is boundedly invertible, and we can write,

$$(H(\lambda) - E) = (1 + 2i\lambda \cdot \nabla(H - E)^{-1} + |\lambda|^2 (H - E)^{-1})(H - E). \tag{5.2}$$

Let us choose λ so that

$$\|2i\lambda \cdot \nabla(H - E)^{-1}\| \ < \ 1/2. \tag{5.3}$$

We define a constant $C_{V,E} \equiv \|\nabla(H - E)^{-1}\|$, that we assume is finite. We require that $|\lambda|$ satisfies

$$|\lambda| < \frac{1}{4C_{V,E}}. \tag{5.4}$$

Let us write $B \equiv i\nabla(H-E)^{-1}$. Assuming the condition (5.4) for the moment, and returning to (5.2), we see that

$$(H(\lambda) - E) = (1 + 2\lambda B)(1 + (1 + 2\lambda B)^{-1}|\lambda|^2 (H - E)^{-1})(H - E). \tag{5.5}$$

Once again, in order to invert the second factor, we demand $|\lambda|$ also satisfies

$$\|(1 + 2\lambda B)^{-1}|\lambda|^2 (H - E)^{-1}\| < 1/2. \tag{5.6}$$

Since H is self-adjoint, we have $\|(H - E)^{-1}\| \leq \{\text{dist}(\sigma(H), E)\}^{-1}$. Let us define η by $\eta \equiv \text{dist}(\sigma(H), E)$. To satisfy the bound (5.6), we require

$$|\lambda| \ \leq \ \frac{\sqrt{\eta}}{2}. \tag{5.7}$$

Consequently, the inverse of $(H(\lambda) - E)$ satisfies the bound ,

$$\begin{aligned} &\|(H(\lambda) - E)^{-1}\| \\ &\quad \leq \ \|(H - E)^{-1}\| \, \|(1 + B)^{-1}\| \, \|(1 + |\lambda|^2 (1 + B)^{-1}(H - E)^{-1}\| \\ &\quad \leq \ 4 \, \{\text{dist } (\sigma(H), E)\}^{-1}, \end{aligned} \tag{5.8}$$

for $\lambda \in \mathbb{C}^n$ with

$$|\lambda| \leq \min\left(\frac{1}{4C_{V,E}}, \frac{\sqrt{\eta}}{2}\right). \tag{5.9}$$

Let ν denote the minimum of the right side of (5.9). Thus, we have proved that for all $\lambda \in \mathbb{C}^n$ with $|\lambda| < \nu$, the dilated operator $(H(\lambda) - E)$ is invertible, and we have the bound

$$\| e^{i\lambda \cdot x}(H-E)^{-1}e^{-i\lambda \cdot x}\| \leq \frac{4}{\eta}. \tag{5.10}$$

This bound is the key to proving exponential decay of the resolvent. For any $u \in \mathbb{R}^n$, let χ_u be a function with compact support near $u \in \mathbb{R}^n$. We consider a fixed vector $y \in \mathbb{R}^n$, and the origin. First, for any fixed, nonzero unit vector $\hat{e} \in \mathbb{R}^n$, we set $\lambda = \kappa\hat{e} \in \mathbb{R}^n$ and find,

$$\begin{aligned} \chi_y(H-E)^{-1}\chi_0 &= e^{-i\kappa\hat{e}\cdot x}\chi_y(e^{i\kappa\hat{e}\cdot x}(H-E)^{-1}e^{-i\kappa\hat{e}\cdot x})e^{i\kappa\hat{e}\cdot x}\chi_0 \\ &= e^{-i\kappa\hat{e}\cdot x}\chi_y(H(\kappa\hat{e})-E)^{-1}e^{i\kappa\hat{e}\cdot x}\chi_0. \end{aligned} \tag{5.11}$$

Second, we analytically continue the last term in (5.11) to $\kappa = -i\nu$. This is possible because of the type A analyticity proved above, and because the localization functions have compact support. We obtain from (5.10)–(5.11),

$$\begin{aligned} \|\chi_y(H-E)^{-1}\chi_0\| &\leq \|\chi_y e^{-\nu\hat{e}\cdot x}(H(-i\nu)-E)^{-1}e^{\nu\hat{e}\cdot x}\chi_0\| \\ &\leq \frac{C_0}{\eta}e^{-\nu\hat{e}\cdot y}. \end{aligned} \tag{5.12}$$

Taking $\hat{e} = y\|y\|^{-1}$, it follows that

$$\|\chi_y(H-E)^{-1}\chi_0\| \leq \frac{C_1}{\eta}e^{-\nu\|y\|}. \tag{5.13}$$

This is our first resolvent decay estimate. Notice that the estimate holds for any energy that is separated from the spectrum of H. The exponential rate of decay ν is given in (5.9). It is the minimum of $C_2\eta$ and $C_3\sqrt{\eta}$. We will see that this can be improved.

We note an improvement of the above technique when the eigenvalue E satisfies $E < \Sigma \equiv \inf \sigma_{ess}(H)$. In this case, the operator $(H-E)$ is positive in the sense that for all $\phi \in D(H)$,

$$\langle \phi, (H-E)\phi \rangle \geq (\Sigma - E)\|\phi\|^2. \tag{5.14}$$

We are back in the case considered by Agmon. We see that in this case the Combes-Thomas method is the same as an isotropic Agmon estimate with an exponential factor $\sqrt{\Sigma - E}$.

5.2 The Combes-Thomas Method

We now present an optimal version of the Combes-Thomas method [2] improving the presentation in section 5.1. The basic technical result is the following.

Lemma 5.1 *Let A and B be two self-adjoint operators such that $d_\pm \equiv dist(\sigma(A) \cap \mathbb{R}^\pm, 0) > 0$, and $\|B\| \leq 1$. Then,*

(i) For $\beta \in \mathbb{R}$ such that $|\beta| < \frac{1}{2}\sqrt{d_+ d_-}$, one has $0 \in \rho(A + i\beta B)$,

(ii) For $\beta \in \mathbb{R}$ as in (i),

$$\left\|(A + i\beta B)^{-1}\right\| \leq 2 \sup(d_+^{-1}, d_-^{-1}).$$

Proof. Let $P_\pm$ be the spectral projectors for A corresponding to the sets $\sigma(A) \cap \mathbb{R}^\pm$, respectively and define $u_\pm \equiv P_\pm u$. By the Schwarz inequality one has

$$\begin{aligned} \|u\| \, \|(A + i\beta B)u\| &\geq \text{Re } \langle (u_+ - u_-), (A + i\beta B)(u_+ + u_-)\rangle \\ &\geq d_+\|u_+\|^2 + d_-\|u_-\|^2 - 2\beta \text{Im } \langle u_+, Bu_-\rangle \\ &\geq \tfrac{1}{2}(d_+\|u_+\|^2 + d_-\|u_-\|^2), \end{aligned} \tag{5.15}$$

where we again used the Schwarz inequality to estimate the inner product. It follows that

$$\|(A + i\beta B)u\| \geq \frac{1}{2} \min\,(d_+, d_-)\|u\|,$$

and since this is independent of the sign of β, the lemma follows. □

Proposition 5.2 *Let $\widetilde{H}$ be a semibounded self-adjoint operator with a spectral gap $G \equiv (E_-, E_+) \subset \rho(\widetilde{H})$. Let W be a symmetric operator such that $D(W) \supset D((\widetilde{H} + C_0)^{\frac{1}{2}})$ and $\|(\widetilde{H} + C_0)^{-\frac{1}{2}} W (\widetilde{H} + C_0)^{-\frac{1}{2}}\| < 1$, for some C_0 such that $\widetilde{H} + C_0 > 1$. For any $E \in G$, let $\Delta_\pm \equiv dist\ (E_\pm, E)$. Then, we have* *(i) The energy $E \in \rho(\widetilde{H} + i\beta W)$ for all real β satisfying*

$$|\beta| < \frac{1}{2}\left\{\frac{\Delta_+\Delta_-}{(E_+ + C_0)(E_- + C_0)}\right\}^{\frac{1}{2}} ;$$

(ii) for any real β and energy E as in (i),

$$\|(\widetilde{H} + i\beta W - E)^{-1}\| \leq 2 \sup\left(\frac{E_+ + C_0}{\Delta_+}, \frac{E_- + C_0}{\Delta_-}\right) .$$

Proof. Let $E \in G$ and C_0 be as above. Define a self-adjoint operator $A \equiv (\widetilde{H}+C_0)^{-1}(\widetilde{H}-E)$ and $B \equiv (\widetilde{H}+C_0)^{-\frac{1}{2}}W(\widetilde{H}+C_0)^{-\frac{1}{2}}$. By hypothesis, the operator B is self-adjoint and satisfies $\|B\| < 1$. Note that $0 \in \rho(A)$ and

$$d_\pm \equiv \text{dist }(\sigma(A) \cap I\!R^\pm, 0) = \Delta_\pm(E_\pm + C_0)^{-1} > 0 \tag{5.16}$$

Applying Lemma 5.2 to these operators A and B, we see that for β as in (i), $0 \in \rho(A + i\beta B)$ and that

$$\|(A + i\beta B)^{-1}\| \leq 2 \sup\left(\frac{E_+ + C_0}{\Delta_+}, \frac{E_- + C_0}{\Delta_-}\right) .$$

Let $P_\pm$ be as in the proof of Lemma 5.2. For any $w \in D(\widetilde{H})$,

$$\begin{aligned}\|(\widetilde{H} + i\beta W - E)w\| &= \|(\widetilde{H} + C_0)^{\frac{1}{2}}(A + i\beta B)(\widetilde{H} + C_0)^{\frac{1}{2}}w\| \\ &\geq \|(A + i\beta B)(\widetilde{H} + C_0)^{\frac{1}{2}}w\| ,\end{aligned}$$

since $(\widetilde{H} + C_0) \geq 1$. In order to estimate the lower bound, we now repeat estimate (5.20) taking $u \equiv (\widetilde{H} + C_0)^{\frac{1}{2}}w$. This gives

$$\begin{aligned}\|(\widetilde{H} + i\beta W - E)w\| &\geq \tfrac{1}{2}\|(\widetilde{H} + C_0)^{\frac{1}{2}}u\|^{-1}\Big(d_+\|P_+(\widetilde{H} + C_0)^{\frac{1}{2}}w\|^2 \\ &\quad +(d_-\|P_-(\widetilde{H} + C_0)^{\frac{1}{2}}w\|^2\Big) \\ &\geq \tfrac{1}{2}\text{min }(d_+, d_-)\|(\widetilde{H} + C_0)^{\frac{1}{2}}w\| .\end{aligned} \tag{5.17}$$

Since $\|(\widetilde{H} + C_0)^{\frac{1}{2}}w\| \geq \|w\|$ and $d_\pm$ are defined in (5.16), result (ii) follows from (5.17) and Lemma 5.2. □

We now apply these results first to the exponential decay of the localized resolvent, and second, to the decay of eigenfunctions. We let $\rho(x) \equiv \sqrt{1+\|x\|^2}$ be the regularized distance function. We assume that the unperturbed operator H_0 has the form $H_0 = H_A + V_0$, where $H_A \equiv (-i\nabla - A)^2$, and V_0 is relatively H_A bounded. The electric potential V_0 and the vector potential A are assumed to be sufficiently well-behaved so that H_0 is essentially self-adjoint on $C_0^\infty(I\!R^n)$. We also assume that the spectrum of H_0 is semibounded from below. Most importantly, we suppose that the spectrum has an open spectral gap in the sense that there exist constants $-\infty \leq -C_0 \leq B_- < B_+ \leq \infty$ so that

$$\sigma(H_0) \subset [-C_0, B_-] \cup [B_+, \infty). \tag{5.18}$$

Of course, this gap might be the half line $(-\infty, \Sigma_0)$, where $\Sigma_0 = \inf \sigma(H_0)$. For a less trivial example, we can take $H_0 = -\Delta + V_{per}$, where V_{per} is a periodic potential.

Finally, we assume that the perturbation potential V satisfies the following hypothesis.

Hypothesis 3. *The potential V is relatively H_0-compact with relative bound less than one. For each $\epsilon > 0$, the potential V admits a decomposition $V = V_c + V_\epsilon$, where V_c has compact support and $\|V_\epsilon\| < \epsilon$.*

Since the essential spectrum of H_0 is stable under relatively compact perturbations, the effect of the potential V is to create isolated eigenvalues for $H = H_0 + V$ in the spectral gap $G = (B_-, B_+)$. We are interested in the decay of the corresponding eigenfunctions. We first prove that the resolvent of H_0 at energies $E \in G$ decays exponentially when locialized between two disjoint regions.

Theorem 5.3 *Let the unperturbed operator H_0 satisfy the conditions above. Then, the dilated operator $H(\alpha) \equiv e^{i\alpha\rho} H e^{-i\alpha\rho}$, $\alpha \in I\!R$, admits an analytic continuation as a type A family on the strip $S(\alpha_0)$, for any $\alpha_0 > 0$. For any $E \in G = (B_-, B_+)$, define $\Delta_\pm \equiv$ dist $(B_\pm, E)$. Then there exist finite constants C_1, $C_2 > 0$, depending only on H_0 and E, such that*

- *(i) for any real β satisfying $|\beta| <$ min $(\alpha_0, C_1\sqrt{\Delta_+\Delta_-}, \sqrt{\Delta_+/2})$, the energy $E \in \rho(H_0(i\beta))$;*

(ii) for any real β as in (i),

$$\|(H_0(i\beta) - E)^{-1}\| \ \leq \ C_2 \ max(\Delta_+^{-1}, \Delta_-^{-1}) \ ; \tag{5.19}$$

(iii) let χ_u be a function of compact support localized near $u \in I\!R^n$, then for $\beta \in I\!R$ as in (i),

$$\|\chi_y(H_0 - E)^{-1}\chi_0\| \ \leq \ C_3 e^{\beta\rho(y)}. \tag{5.20}$$

Proof. By a calculation similar to that done in section 5.1, we have, for $\alpha \in I\!R$,

$$\begin{aligned} H_0(\alpha) &= e^{i\alpha\rho} H_0 e^{-i\alpha\rho} \\ &= H_0 + \alpha^2 |\nabla\rho|^2 + \alpha W, \end{aligned} \tag{5.21}$$

where $W = -(\nabla\rho \cdot (-i\nabla - A) + (-i\nabla - A) \cdot \nabla\rho)$ is symmetric. Note that $\|\nabla\rho\|_\infty = 1$ and $\|\Delta\rho\|_\infty = 1$. Under the assumption that V_0 is relatively H_A-bounded, it suffices to show that for some $z \in \rho(H_A)$, the operator

$$\{\alpha^2 |\nabla\rho|^2 + W\}(H_A - z)^{-1}, \tag{5.22}$$

is bounded with norm less than one. Let us take $z = -i\eta$, for $\eta > 0$ and sufficiently large. It is then easy to show that the operator in (5.22) is bounded above by $C_0\eta^{-1/2}$, for some constant C_0 depending on $|\alpha|$. Since this bound can be made as small as desired for any fixed α_0, it folows that $H_0(\alpha)$ is an analytic type A family on any strip $S(\alpha_0)$.

Next, we take $\alpha = i\beta, \beta$ real and $|\beta| < \alpha_0$, so from (5.21), we have

$$H_0(i\beta) = H_0 - \beta^2 |\nabla\rho|^2 + i\beta W. \tag{5.23}$$

We apply Proposition 5.2 to this operator taking $\widetilde{H} \equiv H_0 - \beta^2|\nabla\rho|^2$. This operator has a spectral gap which contains $(\widetilde{B}_-, \widetilde{B}_+)$, where $\widetilde{B}_- = B_-$ and $\widetilde{B}_+ = B_+ - \beta^2$. In order that $\tilde{\Delta}_+ \equiv$ dist $(\widetilde{B}_+, E) > (\Delta_+/2)$, we require $|\beta| < \sqrt{\Delta_+/2}$. (Note that $\tilde{\Delta}_- = \Delta_-$). It follows from Proposition 5.2 that $E \in \rho(H_0(i\beta))$ for $|\beta| < \min \left\{\alpha_0, C_1\sqrt{\Delta_+\Delta_-}, \sqrt{\Delta_+/2}\right\}$, and that (ii) holds. Result(iii) follows from (ii) as in section 5.1. □

We now consider the perturbation of H_0 by V. Assuming Hypothesis 3 on V, the operator $H \equiv H_0 + V$ is self adjoint on the same domain as H_0. The perturbation may introduce isolated eigenvalues of finite multiplicity in the spectral gap G. We apply the resolvent bound (5.20) to prove the exponential decay of the corresponding eigenfunctions.

Theorem 5.4 *We assume that H_0 satisfies the hypotheses given above, and that the potential V satisfies Hypothesis 3. Suppose that $H = H_0 + V$ has an eigenvalue $E \in G$, the gap in the spectrum of H_0, with an eigenfunction ψ_E. We assume that $\|\psi_E\| = 1$. For any $\alpha \in I\!R$, with $\alpha < \nu \equiv min\,(C_1\sqrt{\Delta_+\Delta_-}, \sqrt{\Delta_+/2})$, we have*

$$e^{\alpha\rho}\psi_E \in L^2(I\!R^n). \tag{5.24}$$

Proof. Let us first suppose that V has compact support and that supp$V \subset K$, for some compact $K \subset I\!R^n$. We write $R_0(E) \equiv (H_0 - E)^{-1}$. From the eigenvalue equation, we write, for $\lambda \in I\!R$,

$$\begin{aligned} e^{i\lambda\rho}\psi_E &= -(e^{i\lambda\rho}R_0(E)e^{-i\lambda\rho})\,(e^{i\lambda\rho}V\psi_E) \\ &= (H_0(\lambda) - E)^{-1}\,(e^{i\lambda\rho}V\psi_E). \end{aligned} \tag{5.25}$$

Because of the type A analyticity of $H_0(\lambda)$, and the compactness of the support of V, each term on the right in (5.25) admits an analytic continuation onto any the strip $S(\alpha_0)$. We set $\lambda = -i\alpha$, for $\alpha \in I\!R$ with $|\alpha| < \nu$. Taking the norm of of both sides of the equation, and using the bound in (ii) of Proposition 5.3, we find that there exists a constant $C_{E,V} > 0$ so that

$$\|e^{\alpha\rho}\psi_E\| \;\leq\; C_{E,V}. \tag{5.26}$$

When the support of V is not compact, we consider the operator $H_0 + V_\epsilon$, instead of H_0. This operator also extends to an analytic type A family on the same strip as H_0 since V_ϵ is a bounded operator. We choose $\epsilon < \eta \equiv$ dist$(E, \sigma(H_0))$, so that $H_0 + V_\epsilon$ has a spectral gap around E of size at least ϵ. It follows that $(H_0 + V_\epsilon - E)$ is invertible, and its inverse can be computed from the equation

$$(H_0 + V_\epsilon - E) = (1 + V_\epsilon(H_0 - E)^{-1})(H_0 - E), \tag{5.27}$$

since $\|V_\epsilon R_0(E)\| < 1/2$. The eigenvalue equation is now written as

$$\psi_E = -(H_0 + V_\epsilon - e)^{-1} V_c \psi_E. \tag{5.28}$$

The exponential decay bound now follows from Proposition 5.2 applied to $H_0 + V_\epsilon$, and the argument given above. □

5.3 Application: Eigenfunction Decay for the Dirac Operator

As an application of the method of Combes-Thomas, we prove the decay of eigenfunctions corresponding to discrete, isolated eigenvalues of the Dirac operator. The free Dirac operator for a particle of mass $m > 0$ is constructed as follows. The Dirac matrices γ_μ, with $\mu = 0, 1, 2, 3$ are four 4×4 matrices that form a representation of the canonical anticommutation relations,

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu}, \tag{5.29}$$

where $\delta_{\mu\nu}$ is the Kronicker delta function. We write $\gamma = (\gamma_1, \gamma_2, \gamma_3)$ for the three-vector, and $\beta = \gamma_0$. The free Dirac Hamiltonian is

$$H_0 = -i\gamma \cdot \nabla + \beta mc, \tag{5.30}$$

where $c > 0$ is the speed of light. We set $c = 1$. The unperturbed operator H_0 is a first-order, matrix-valued linear operator. It is self-adjoint on its natural domain in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. A simple calculation, based on the relations (5.29), shows that $H_0^2 = -\Delta + m^2$. It follows that the spectrum of H_0 consists of two branches: $\sigma(H_0) = (-\infty, -m] \cup [m, \infty)$. The interval $G = (-m, m)$ is a gap in the spectrum of the free Dirac operator.

We now consider local perturbations V of H_0. Let us suppose that $V > 0$ and that V has compact support. Let I_4 denote the 4×4 identity matrix. An application of the Birman-Schwinger principle shows that $H_\lambda = H_0 + \lambda V \cdot I_4$ has an eigenvalue in the gap G provided λ is suitably chosen. In general, relatively H_0-compact perturbations V will create eigenvalues in the spectral gap of H_0. We are interested in the isotropic exponential decay of the corresponding eigenfunctions.

The simplified argument presented at the beginning of section 5 applies direcly to this situation. Let $\alpha \in \mathbb{R}$ and take $\rho(x) \equiv \sqrt{1 + \|x\|^2}$, as above.

We define $d_\pm(E) = \mathrm{dist}(E, \pm m)$. We apply a standard boost transformation to $H_0 = -i\gamma \cdot \nabla + \beta m$ to obtain

$$\begin{aligned} H_0(\alpha) &\equiv e^{i\alpha\rho} H_0 e^{-i\alpha\rho} \\ &= -i\gamma \cdot (\nabla - i\alpha\nabla\rho) + \beta m \\ &= H_0 - \alpha\gamma \cdot \nabla\rho. \end{aligned} \tag{5.31}$$

We now apply Lemma 5.1 with $A = H_0$ and $B = \nabla\rho \cdot \gamma$. Since $|\nabla\rho| \leq 1$, we have $\|B\| \leq 1$. Hence, with $\alpha = i\eta$, for $\eta \in I\!R$, we require

$$|\eta| \leq (1/2)\sqrt{d_+(E) d_-(E)}. \tag{5.32}$$

Under this condition, we obtain

$$\|(H_0(i\eta) - E)^{-1}\| \leq 2 \max\left(\frac{1}{d_+(E)}, \frac{1}{d_-(E)}\right). \tag{5.33}$$

We now proceed as in Theorem 5.4. First, we suppose that the potential V has compact support, and that $H = H_0 + V$ has an eigenvalue $E \in G$. We write the eigenvalue equation as

$$\psi = -R_0(E) V \psi. \tag{5.34}$$

By analytic continuation from $\alpha \in I\!R$ to $\alpha = -i\eta$, with $\eta \in I\!R$ and satisfying the bound (5.32), we have

$$\|e^{\eta\rho}\psi\| \;\leq\; \|H_0(-i\eta) - E)^{-1}\| \, \|e^{\eta\rho} V\| \;\leq\; C_{E,V}, \tag{5.35}$$

proving the L^2-exponential decay of the eigenfunction for any $\eta \in I\!R$ satisfying (5.32). When V does not have compact support, but vanishes uniformly at infinity, we use the same argument as in the proof of Theorem 5.4. The same exponential decay results hold in the presence of a magnetic field for which $H_0 = \gamma \cdot (-i\nabla - A) + \beta m$, for reasonable magnetic vector potentials A. (A similar result was recently obtained by Breit and Cornean [3]).

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