Norm estimates of complex symmetric operators applied to quantum systems

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Abstract. Following an old and simple idea of Takagi we propose a formula for computing the norm of a compact complex symmetric operator. This observation is applied to two concrete problems related to quantum mechanical systems. First, we give sharp estimates on the exponential decay of the resolvent and the single-particle density matrix for Schrödinger operators with spectral gaps. Second, we provide new ways of evaluating the resolvent norm for Schrödinger operators appearing in the complex scaling theory of resonances.

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1. Introduction

Although complex symmetric matrices (complex matrices coinciding with their transposes) are as ubiquitous as Hermitian matrices (those coinciding with their complex adjoint), the first class is less well-known than the second. Indeed, the spectral decomposition of a Hermitian matrix remains one of the main tools of modern mathematics. The canonical diagonal form of a complex symmetric matrix was (re)discovered during the last century, for quite different aims, at least by Takagi, Wellstein, Siegel, Schur, and Jacobson (see [11, 17]). In equivalent terms, the difference between complex symmetric and Hermitian matrices corresponds to the distinction between symmetric bilinear and sesquilinear forms (over the complex field).

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It was Takagi [29] who first remarked that the antilinear eigenvalue problem $Tf = \lambda \overline{f}$, where T is a complex symmetric matrix and $\overline{f}$ denotes complex conjugation, entry by entry, of the vector f, solves a fundamental interpolation problem for bounded analytic functions in the disk. He remarked there that the largest such positive skew-eigenvalue λ coincides with the operator norm of T. Later on, this observation was extended to bounded linear operators with certain symmetries. About half a century ago, Glazman [12, 13] laid the foundations of the theory of unbounded complex symmetric operators. Since then, Glazman's fundamental ideas have been successfully tested on several classes of differential operators (see [5, 19, 24]). Recently, two of the authors discovered an additional structure in the polar decomposition of a complex symmetric operator [10]. For certain unbounded operators with compact resolvent, the refined polar decomposition leads to a new method for estimating the norm of their resolvent. In the present note, we exploit this idea in conjunction with the (complex) scaling method for Schrödinger operators.

Dealing with non-selfadjoint operators is much more difficult than with selfadjoint operators due to the lack of an equivalent spectral decomposition and fine functional calculus. In particular, situations where the norms would have been trivially estimated using the spectral theorem can become extremely difficult, often forcing us to make rough approximations. Although Quantum Mechanics is built on the theory of selfadjoint operators, it is not rare when we have to deal with non-selfadjoint operators. For instance, this is the case when appealing to the complex scaling technique. This method became a standard tool in the theory of Schrödinger operators and turned out to be the key to several problems such as: the absence of singular continuous spectrum [1, 2], calculus of resonances and convergence of time-dependent perturbation theory [27], and asymptotic behavior of the eigenvectors [8]. As the examples in this paper will show, the complex scaling technique naturally leads to complex symmetric operators.

Our first application deals with Schrödinger operators with a spectral gap. Using complex scaling and recent results on complex symmetric operators, we provide sharp exponential decay estimates on the resolvent and the single-particle density matrix. Such estimates became increasingly important since it was realized that the localization of the single-particle density matrix provides the key to efficient numerical electronic structure algorithms for systems with large number of particles [32]. For 1D periodic insulators, exact exponential decays can be derived from Kohn's analytic results [20]. In an attempt to generalize these results to higher dimensions, des Cloizeaux [6, 7] developed a method which can be regarded as the first application of the complex scaling idea. He proved the exponential decay of the single-particle density matrix for a class of 3D insulators. Relatively recently, we have seen a renewed interest in the subject and remarkable new exact results in dimensions higher than one [3, 15, 18, 30]. These results, however, are limited to periodic systems and some of them to the extreme tight-binding limit. In the present note, we treat the general case of gapped Schrödinger operators, which find applications, in addition to the periodic insulators, to amorphous insulators, molecular liquids, or large molecules. For recent results and the state of the matters in this subject, one can consult the survey [16].

In our second application, we show that the technique of estimating the norms of complex symmetric operators also extends to operators with non-compact resolvent, such as the scaled Hamiltonians appearing in the problem of resonances.

2. Complex symmetric operators

The aim of this section is to recall a few definitions and facts about complex symmetric operators. For full details and examples the reader can consult [9, 10].

2.1. Bounded complex symmetric operators

We consider a separable Hilbert space $\mathcal{H}$ which carries a *conjugation operator* $C : \mathcal{H} \longrightarrow \mathcal{H}$ (an *antilinear* operator satisfying the conditions $C^2 = I$ and $\langle Cf, Cg\rangle = \langle g, f\rangle$ for all $f, g \in \mathcal{H}$). For a fixed C, we *define* the transpose T^t of a bounded linear operator T to be

$$T^t \equiv CT^*C.$$

Definition 2.1. We say that T is *C-symmetric* if $T = T^t$ (equivalently, if $CT = T^*C$). More generally, we say that T is *complex symmetric* if there exists a C such that T is C-symmetric.

Complex symmetry has a simple interpretation in terms of two forms on $\mathcal{H}$, the standard sesquilinear form $\langle f, g\rangle$ and the symmetric bilinear form $[f, g] \equiv \langle f, Cg\rangle$ induced by the conjugation operator C. It is easy to show that T is C-symmetric if and only if T is symmetric with respect to the corresponding bilinear form: $[Tf, g] = [f, Tg]$ for all f, g in $\mathcal{H}$.

The following simple factorization theorem will be the main ingredient in the proofs contained throughout this note.

Theorem 2.2. [10] *If $T : \mathcal{H} \longrightarrow \mathcal{H}$ is a bounded C-symmetric operator, then there exists a conjugation operator $J : \mathcal{H} \longrightarrow \mathcal{H}$, which commutes with the spectral measure of $|T| = \sqrt{T^*T}$, such that $T = CJ|T|$.*

The proof of this and several related results can be found in [10]. The preceding theorem generalizes an early observation of Godič and Lucenko [14] which asserts that every unitary operator U on a Hilbert space $\mathcal{H}$ can be expressed as the product of two conjugation operators: $U = CJ$. This in turn generalizes the simple fact that a planar rotation is the product of two reflections.

The theorem above asserts, among other things, the equivalence of the *antilinear* eigenvalue problems $Tf = \lambda Cf$ and $|T|f = \lambda Jf$. Here we may assume that $\lambda \geq 0$ since we may multiply either of the above equations by a suitable unimodular constant.

Given that the norm of a compact operator T is equal to the largest eigenvalue of $|T|$, the norm of a compact C-symmetric operator T can be characterized in terms of the *antilinear* eigenvalue problem $Tf = \lambda Cf$:

$$\|T\| = \sup\{\lambda > 0 : (\exists f)(f \neq 0,\ Tf = \lambda Cf)\}$$

The classical motivation for such antilinear eigenvalue problems lies in the consideration of the corresponding variational problem:

$$\|T\| = \sup_{\|f\|=1} \operatorname{Re}\langle Tf, Cf\rangle.$$

This problem is entirely analogous to Takagi's inductive process for computing the singular numbers of a complex Hankel matrix, [29].

Examples of bounded complex symmetric operators include all normal operators (due to the symmetry contained in their diagonalization), Hankel operators, finite Toeplitz matrices, all Jordan model operators (the infinite dimensional analogs of Jordan blocks), Volterra's operator (integration with a free end), and quite a few other classes. It is also worth mentioning that on a finite dimensional Hilbert space, any linear operator is similar to a complex symmetric one. However, the unilateral shift S is not complex symmetric, because the identity $CS = S^*C$ would imply the equality of Fredholm indices $\operatorname{ind} S = \operatorname{ind} S^*$, and the latter is not true.

2.2. Unbounded complex symmetric operators

The study of unbounded complex symmetric operators was pioneered by Glazman [12, 13], who established a complex symmetric parallel to von Neumann's theory of selfadjoint extensions of symmetric operators, although real unbounded symmetric operators (that is C-symmetric operators with respect to the standard complex conjugation symmetry) had appeared earlier in von Neumann's work [31]. A renewed interest in Glazman's theory was sparked by its application to certain Dirac-type operators [5] and the realization that the closely related class of C-*unitary* operators is relevant to the study of complex scaling transformations in quantum mechanics [25]. Moreover, certain Sturm-Liouville operators with complex potentials can also be treated similarly [19, 24]. Further examples are furnished by Schrödinger operators $-\Delta + q$ with *complex potentials* q (where C is simply complex conjugation) subject to appropriate boundary conditions [13, 24]. One can also consider Schrödinger operators $-\Delta + q$ with real potentials q, but complex (non-selfadjoint) two point boundary conditions, in which case the conjugation C is slightly more involved.

Definition 2.3. We say that a densely defined, closed graph operator is C-*symmetric* if $T \subset CT^*C$ and C-*selfadjoint* if $T = CT^*C$.

From the classical theory of selfadjoint operators, one knows that a symmetric operator has selfadjoint extensions if and only if the deficiency indices are the same. In contrast, *every* C-symmetric unbounded operator admits a C-selfadjoint extension $\widetilde{T}$. Indeed, it suffices to observe that the maximal *antilinear* symmetric operators S (in the sense that $\langle Sf, g\rangle = \langle Sg, f\rangle$ for all f, g in $\mathcal{D}(S)$) produce C-selfadjoint operators CS.

There are several practical criteria for determining whether a C-symmetric operator T is C-selfadjoint. For example, the explicit formula

$$\mathcal{D}(CT^*C) = \mathcal{D}(T) \oplus \{f \in \mathcal{D}(T^*CT^*C) : \; T^*CT^*Cf + f = 0\}$$

from [24] provides one method. A different criterion goes back to Zhikhar [33]: if a C-symmetric operator T satisfies $\mathcal{H} = (T - zI)\mathcal{D}(T)$ for some complex number z, then T is C-selfadjoint. The resolvent set of T consists of exactly those z fulfilling the latter condition. We denote the inverse (to the right) of $(T - zI)$ by $(T - zI)^{-1}$ and note that it is a bounded linear operator defined on all of $\mathcal{H}$.

Unfortunately, not all unbounded C-selfadjoint operators possess a spectral resolution and a corresponding fine functional calculus. Nevertheless, if an unbounded C-selfadjoint operator has a compact resolvent, then a canonically associated antilinear eigenvalue problem always has a complete set of mutually orthogonal eigenfunctions:

Theorem 2.4. [10] *If $T : \mathcal{D}(T) \longrightarrow H$ is an unbounded C-selfadjoint operator with compact resolvent $(T - zI)^{-1}$ for some complex number z, then there exists an orthonormal basis $(u_n)_{n=1}^{\infty}$ of $\mathcal{H}$ consisting of solutions of the antilinear eigenvalue problem:*

$$(T - zI)u_n = \lambda_n C u_n$$

where $(\lambda_n)_{n=1}^{\infty}$ is an increasing sequence of positive numbers tending to ∞.

We remark that the preceding result is a direct consequence of the refined polar decomposition $T = CJ|T|$ for *bounded* C-symmetric operators described in Theorem 2.1. Our main technical tool in estimating the norms of resolvents of certain unbounded operators is contained in the following corollary:

Corollary 2.5. [10] *If T is a densely-defined C-selfadjoint operator with compact resolvent $(T - zI)^{-1}$ for some complex number z, then*

$$\| (T - zI)^{-1} \| = \frac{1}{\inf_n \lambda_n} \tag{1}$$

where the λ_n are the positive solutions to the antilinear eigenvalue problem:

$$(T - zI)u_n = \lambda_n C u_n. \tag{2}$$

Finally, we remark that the refined polar decomposition $T = CJ|T|$ applies, under certain circumstances, to unbounded C-selfadjoint operators:

Theorem 2.6. [10] *If $T : \mathcal{D}(T) \longrightarrow \mathcal{H}$ is a densely defined C-selfadjoint operator with zero in its resolvent, then $T = CJ|T|$ where $|T|$ is a positive selfadjoint operator (in the von Neumann sense) satisfying $\mathcal{D}(|T|) = \mathcal{D}(T)$ and J is a conjugation operator on $\mathcal{H}$ which commutes with the spectral measure of $|T|$. Conversely, any operator of the form described above is C-selfadjoint.*

The preceding factorization can be used, for example, in the study of the semigroup generated by the antilinear transformation CT (see [10] for details).

3. Exponential Decay of the Resolvent for Gapped Systems

In this section, we consider the problem of finding sharp estimates on the exponential decay of the resolvent of a Schrödinger operator with a gap in the spectrum. A short account on the subject has been already given in the Introduction.

Our approach relies on the complex scaling technique which reduces the problem to finding sharp norm estimates on the resolvent of a complex symmetric operator. This last part is solved by employing the general theory presented in the previous section.

We now formulate the problem and the main result. Let $-\nabla_D^2$ denote the Laplace operator with zero (Dirichlet) boundary conditions over a finite domain (with smooth boundary) $\Omega \subset \mathbb{R}^d$; let $v(\mathbf{x})$ be a scalar potential, which is ∇_D^2-relatively bounded, with relative bound less than one. Throughout this section all potentials v are presumed to be bounded from below. By measuring the energy from the bottom of the potential, we can assume without loss of generality that $v(\mathbf{x}) \geq 0$. Let

$$H : \mathcal{D}(\nabla_D^2) \longrightarrow L^2(\Omega); \quad H = -\nabla_D^2 + v(\mathbf{x}),$$

be the associated selfadjoint Hamiltonian with compact resolvent. The assumption on H is that its energy spectrum σ consists of two parts, $\sigma \subset [0, E_-] \cup [E_+, \infty)$, which are separated by a gap $G \equiv E_+ - E_- > 0$. We refer to the spectrum $\sigma_\pm$ above/below the gap as as the upper/lower band. The corresponding spectral projectors are denoted by $P_\pm$.

Let $E \in (E_-, E_+)$ and $G_E = (H - E)^{-1}$ be the resolvent. We are interested in the behavior of the kernel $G_E(\mathbf{x}, \mathbf{y})$ for large separations $|\mathbf{x} - \mathbf{y}|$. Instead of looking directly at the pointwise behavior, we take the average

$$\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2) \equiv \frac{1}{\omega_\epsilon^2} \int_{|\mathbf{x}-\mathbf{x}_1| \leq \epsilon} d\mathbf{x} \int_{|\mathbf{y}-\mathbf{x}_2| \leq \epsilon} d\mathbf{y}\ G_E(\mathbf{x}, \mathbf{y}),$$

where ω_ϵ is the volume of a sphere of radius ϵ in $\mathbb{R}^d$. The main result of this section is stated below.

Theorem 3.1. *For q smaller than a critical value $q_c(E)$, there exists a constant $C_{q,E}$, independent of Ω, such that:*

$$|\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2)| \leq C_{q,E} e^{-q|\mathbf{x}_1 - \mathbf{x}_2|}. \tag{3}$$

$C_{q,E}$ is given by:

$$C_{q,E} = \frac{\omega_\epsilon^{-1} e^{2q\epsilon}}{\min |E_\pm - E - q^2|} \ \frac{1}{1 - q/F(q, E)} \tag{4}$$

with

$$F(q, E) = \sqrt{\frac{(E_+ - E - q^2)(E - E_- + q^2)}{4E_-}}. \tag{5}$$

The critical value $q_c(E)$ is the positive solution of the equation $q = F(q, E)$.

Proof. The complex scaling formalism reduces the problem to norm estimates on the resolvent of a scaled Schrödinger operator. It is at this point where the results about C-symmetric operators come in handy.

If $\chi_{\mathbf{x}}$ denotes the characteristic function of the ϵ ball centered in $\mathbf{x}$, then one can equivalently write

$$\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2) = \omega_\epsilon^{-2} \langle \chi_{\mathbf{x}_1}, (H-E)^{-1} \chi_{\mathbf{x}_2} \rangle.$$

Given a vector $\mathbf{q} \in \mathbb{R}^d$ ($q \equiv |\mathbf{q}|$) of arbitrary orientation and magnitude, let $U_{\mathbf{q}}$ denote the following bounded and invertible map

$$U_{\mathbf{q}} : L^2(\Omega) \to L^2(\Omega), \quad [U_{\mathbf{q}} f](\mathbf{x}) = e^{\mathbf{q}\mathbf{x}} f(\mathbf{x}),$$

which leaves the domain of H unchanged. Let $H_{\mathbf{q}} \equiv U_{\mathbf{q}} H U_{\mathbf{q}}^{-1}$ be the family of scaled Hamiltonians. Explicitly, they are given by

$$H_{\mathbf{q}} : \mathcal{D}(\nabla_D^2) \to L^2(\Omega), \quad H_{\mathbf{q}} = H + 2\mathbf{q}\nabla - q^2. \tag{6}$$

We notice that for $\mathbf{q} \neq 0$, these are non-selfadjoint and not even complex symmetric operators (with respect to any natural conjugation). The identity

$$U_{\mathbf{q}}(H-E)^{-1} U_{\mathbf{q}}^{-1} = (H_{\mathbf{q}} - E)^{-1}$$

holds true for all $\mathbf{q} \in \mathbb{R}^d$ (this happens only for finite Ω). We denote

$$\gamma(q, E) = \sup_{|\mathbf{q}|=q} \|(H_{\mathbf{q}} - E)^{-1}\|. \tag{7}$$

As the following lines show, the entire problem can be reduced to estimating $\gamma(q, E)$. Indeed, if $\varphi_1(\mathbf{x}) \equiv e^{-\mathbf{q}(\mathbf{x}-\mathbf{x}_1)} \chi_{\mathbf{x}_1}(\mathbf{x})$ and $\varphi_2(\mathbf{x}) \equiv e^{\mathbf{q}(\mathbf{x}-\mathbf{x}_2)} \chi_{\mathbf{x}_2}(\mathbf{x})$, then

$$\begin{aligned} |\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2)| &= \omega_\epsilon^{-2} |\langle \varphi_1, (H_{\mathbf{q}} - E)^{-1} \varphi_2 \rangle| e^{-\mathbf{q}(\mathbf{x}_1 - \mathbf{x}_2)} \\ &\leq \omega_\epsilon^{-1} e^{2q\epsilon} \gamma(q, E) e^{-\mathbf{q}(\mathbf{x}_1 - \mathbf{x}_2)}. \end{aligned}$$

Choosing $\mathbf{q}$ parallel to $\mathbf{x}_1 - \mathbf{x}_2$, we infer at this step that

$$|\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2)| \leq \omega_\epsilon^{-1} e^{2q\epsilon} \gamma(q, E) e^{-q|\mathbf{x}_1 - \mathbf{x}_2|}.$$

Next we estimate $\gamma(q, E)$ using the results on C-symmetric operators presented in the previous section. As we already mentioned, $H_{\mathbf{q}}$ is not complex symmetric. However, note that the operators $H_{\mathbf{q}}$ and $H_{-\mathbf{q}}$ are dual: $H_{\mathbf{q}}^* = H_{-\mathbf{q}}$ and that $H_{\mathbf{q}}$ commutes with complex conjugation $\mathcal{C}$: $\mathcal{C} H_{\mathbf{q}} = H_{\mathbf{q}} \mathcal{C}$. We define the following block-matrix operator $\mathbb{H}$ and conjugation C on $L^2(\Omega) \oplus L^2(\Omega)$:

$$\mathbb{H} = \begin{pmatrix} H_{\mathbf{q}} & 0 \\ 0 & H_{-\mathbf{q}} \end{pmatrix}, \quad C = \begin{pmatrix} 0 & \mathcal{C} \\ \mathcal{C} & 0 \end{pmatrix}.$$

It is a simple task to check that $\mathbb{H}$ is C-selfadjoint: $\mathbb{H}^* = C\mathbb{H}C$. Moreover, given that $H_{\mathbf{q}}$ and $H_{-\mathbf{q}}$ are adjoints,

$$\|(\mathbb{H} - E)^{-1}\| = \|(H_{\mathbf{q}} - E)^{-1}\| = \|(H_{-\mathbf{q}} - E)^{-1}\|. \tag{8}$$

According to the previous section, the antilinear eigenvalue problem (with $\lambda_n \geq 0$)

$$(\mathbb{H} - E)\phi_n = \lambda_n C \phi_n \tag{9}$$

generates an orthonormal basis in $L^2(\Omega) \oplus L^2(\Omega)$ and

$$\|(\mathbb{H} - E)^{-1}\| = \frac{1}{\min_n \lambda_n}. \tag{10}$$

If we write $\phi_n = f_n \oplus g_n$, the antilinear eigenvalue problem Eq. (9) is equivalent to

$$\begin{cases} (H_{\mathbf{q}} - E)f_n = \lambda_n \bar{g}_n \\ (H_{-\mathbf{q}} - E)g_n = \lambda_n \bar{f}_n. \end{cases} \tag{11}$$

With q small, such that $E + q^2$ lies in the spectral gap, the polar decomposition

$$H - E - q^2 = S|H - E - q^2|,$$

holds, where $S = P_+ - P_-$. We take the scalar product of the first equation in Eq. (11) against the vector Sf_n. Keeping only the real part of the result and solving for λ_n, we find

$$\lambda_n = \frac{|\langle f_n, |H - E - q^2| f_n\rangle - 2\operatorname{Re}\langle Sf_n, \mathbf{q}\nabla f_n\rangle|}{|\operatorname{Re}\langle Sf_n, \bar{g}_n\rangle|}. \tag{12}$$

After elementary manipulations, the second term in the numerator can be rewritten as

$$\operatorname{Re}\langle Sf_n, \mathbf{q}\nabla f_n\rangle = 2\operatorname{Re}\langle f_n, P_+(\mathbf{q}\nabla)P_- f_n\rangle.$$

Moreover, denoting

$$B_{\mathbf{q}} \equiv P_+|H - E - q^2|^{-1/2}(\mathbf{q}\nabla)|H - E - q^2|^{-1/2}P_-,$$

one obtains

$$|\langle f_n, P_+(\mathbf{q}\nabla)P_- f_n\rangle| \le \tfrac{1}{2}\|B_{\mathbf{q}}\|\langle f_n, |H - E - q^2| f_n\rangle.$$

Eq. (12) implies

$$\lambda_n \ge \min\{\,|E_\pm - E - q^2|\,\}(1 - 2\|B_{\mathbf{q}}\|)\frac{\|f_n\|^2}{\|f_n\|\|g_n\|}.$$

Similarly, by taking the scalar product of the second equation of Eq. (11) against Sg_n, one obtains:

$$\lambda_n \ge \min\{\,|E_\pm - E - q^2|\,\}(1 - 2\|B_{\mathbf{q}}\|)\frac{\|g_n\|^2}{\|f_n\|\|g_n\|}.$$

The sum of the last two equations yields

$$\lambda_n \ge \min\{\,|E_\pm - E - q^2|\,\}(1 - 2\|B_{\mathbf{q}}\|). \tag{13}$$

It remains to evaluate $\|B_{\mathbf{q}}\|$. Since the potential is positive and we work with zero boundary conditions, the following inequality between quadratic forms

$$q^2(-\nabla^2 + v + a) \ge (\mathbf{q}\nabla)^2, \quad \forall\, a \ge 0,$$

holds true. Consequently

$$\|(\mathbf{q}\nabla)|H + a|^{-1/2}\| \le q, \quad \forall\, a > 0.$$

The norm of $\|B_{\mathbf{q}}\|$ can be calculated as $\|B_{\mathbf{q}}\| = \sup_{\eta_\pm} |\langle \eta_+, B_{\mathbf{q}} \eta_- \rangle|$, where the supremum is taken over all unit vectors $\eta_\pm \in P_\pm \mathcal{H}$. Denoting

$$\psi_- \equiv |(H+a)(H-E-q^2)^{-1}|^{1/2} \eta_-, \quad \psi_+ \equiv |(H-E-q^2)|^{-1/2} \eta_+,$$

one has

$$\|\psi_-\| \leq \sqrt{\frac{E_- + a}{|E_- - E - q^2|}}, \quad \|\psi_+\| \leq \sqrt{\frac{1}{E_+ - E - q^2}}$$

and

$$\begin{aligned} \|B_{\mathbf{q}}\| &= \sup_{\eta_\pm} |\langle \psi_+, (\mathbf{q}\nabla)|H+a|^{-1/2} \psi_- \rangle| \\ &\leq q \sqrt{\frac{E_- + a}{(E_+ - E - q^2)(E - E_- + q^2)}}. \end{aligned} \tag{14}$$

Finally one can pass to the limit $a \to 0$. Eq. (10), together with Eqs. (13) and (14) provide the desired estimate of $\gamma(q, E)$. □

Corollary 3.2. *Consider an insulator with the lower band completely filled. Then the single-particle density matrix (i.e. the projector onto the occupied states P_-) decays exponentially, with a rate $\bar{q}$ satisfying*

$$\bar{q} \geq \frac{G}{4\sqrt{E_-}}. \tag{15}$$

Proof. Again, we look at the average

$$\bar{P}_-(\mathbf{x}_1, \mathbf{x}_2) = \omega_\epsilon^{-2} \langle \chi_{\mathbf{x}_1}, P_- \chi_{\mathbf{x}_2} \rangle,$$

which has the following representation:

$$\bar{P}_-(\mathbf{x}_1, \mathbf{x}_2) = \frac{i}{2\pi} \int_\Gamma \bar{G}_E(\mathbf{x}_1, \mathbf{x}_2)\, dE,$$

where Γ is a contour in the complex energy plane, surrounding the lower band. The estimates given in the preceding Theorem trivially extend to the case of complex energies:

$$|\bar{G}_{E+i\zeta}(\mathbf{x}_1, \mathbf{x}_2)| \leq C_{q,E} e^{-q|\mathbf{x}_1 - \mathbf{x}_2|}, \quad \forall\ q < q_c(E).$$

Given that Γ can be deformed so as to intersect the real axis at any point in (E_-, E_+), we need to find the energy where $q_c(E)$ is maximum. We have

$$q_c = \sqrt{\frac{(E_+ - E - q_c^2)(E - E_- + q_c^2)}{4E_-}} \leq \frac{G}{4\sqrt{E_-}} \tag{16}$$

with equality at energy

$$\bar{E} = \frac{E_+ + E_-}{2} - \frac{G^2}{16 E_-}. \tag{17}$$

□

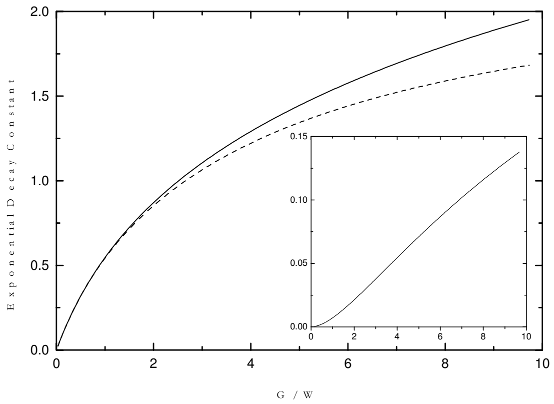

FIGURE 1. The exponential decay constant of the single-particle density matrix as a function of G/W for the Kronig-Penney insulator. The continuous line represents an exact calculation and the dashed line represents the estimate given in Eq. (15). The inset shows the relative difference between the two.

We mention that (see also the remarks in [16]) for E close to the gap edges: $E \to E_{\pm}$, a brute perturbation theory on $(H_{\mathbf{q}} - E)^{-1}$ leads to an exponential decay constant of the resolvent proportional to $|E_{\pm} - E|$. Using physical arguments (see the theory of effective mass [21]), Kohn showed a long time ago that the decay constant is actually proportional to $|E_{\pm} - E|^{1/2}$. Note that the constant $q_c(E)$ of Theorem 3.1 has the correct behavior for $E \to E_{\pm}$. Moreover, at least for 1D periodic systems, we know that the energy where the resolvent has the fastest exponential decay moves toward the lower band as the gap increases. We remark that $\bar{E}$ of Corollary 3.2 has this qualitative feature.

The lower bound on $\bar{q}$ given in Eq. (15) can be calculated entirely from the energy spectrum. What is the best estimate of the exponential decay constant that one can get by only using the information contained in the energy spectrum? In what follows, we illustrate by an example that Eq. (15) comes close to such an optimal estimate. Namely, for 1D periodic systems, the exact exponential decay of the single-particle density matrix can be derived from the analytic properties of the Bloch functions [20]. In Fig. 1, we consider a comparison between our estimate Eq. (15) and an exact result for a one dimensional insulator described by the Kronig-Penney model [22]:

$$H = -\partial_x^2 + v_0 \sum_n \delta(x - n), \;\; v_0 > 0,$$

with the first band completely filled. By varying the strength of the potential v_0, we sweep from a weak to strong insulating regime, which we quantified by the ratio between the gap G and the width of the valence band W. One can see that even in the extreme insulating regime (typically $G/W < 5$), Eq. (15) estimates the exponential decay to within a 15% error. Notice that for $G/W < 5$, the error is less than 5%.

4. Norm Estimates on Resolvents Near Resonances

In this section, we extend the results concerning norm estimates to not necessarily compact resolvents of unbounded complex symmetric. At the same time, we apply this technique to the problem of locating the resonances of a specific class of Hamiltonians.

We first formulate the problem in precise terms. Let

$$H : \mathcal{D}(\nabla^2) \longrightarrow L^2(\mathbb{R}^d), \quad H = -\nabla^2 + v(\mathbf{x})$$

be a Hamiltonian with $v(\mathbf{x})$ a dilation analytic potential in a finite strip $|\operatorname{Im}\theta| < I_0$ and ∇^2-relatively compact. We consider the usual dilation operation:

$$(U(\theta)\psi)(\mathbf{x}) = e^{d\theta/2}\psi(e^{\theta}\mathbf{x})$$

and define the analytic family (of type A) of operators:

$$H_\theta \equiv U(\theta)HU(\theta)^{-1} = -e^{-2\theta}\nabla^2 + v(e^{\theta}\mathbf{x}),$$

where θ runs in the finite strip $|\operatorname{Im}\theta| < I_0$. As a function of θ, it is well known that [1, 2, 26]:

(a) the discrete spectrum σ_d remains invariant,
(b) the essential spectrum σ_{ess} rotates down by an angle $-2\operatorname{Im}\theta$,
(c) as the continuum rotates, it uncovers additional discrete spectrum (the resonances).

In many practical situations, it is desired not only to locate the resonances but also to know how they move under different perturbations [4, 23, 28]. Here we are concerned with the second problem, where norm estimates on the resolvent $(z-H_\theta)^{-1}$ for z near the resonances become especially important either for probing the stability of the spectrum or for building perturbation series.

The Hamiltonians H_θ are C-selfadjoint relative to the complex conjugation $Cf = \bar{f}$. The question that we want to answer is if one can provide an exact norm estimate of $(z - H_\theta)^{-1}$ for z near a resonance, using the theory of complex symmetric operators. The answer is contained in the following theorem:

Theorem 4.1. *Let $\gamma w(\mathbf{x})$ represent the change in $v(\mathbf{x})$ and $H(\gamma) = H + \gamma w$ denote the perturbed Hamiltonian. We assume that both $v_\theta(\mathbf{x}) \equiv v(e^{\theta}\mathbf{x})$ and $w_\theta(\mathbf{x}) \equiv w(e^{\theta}\mathbf{x})$ are ∇^2-relatively bounded for $|\operatorname{Im}\theta| < I_0$, with bound less than one. For z close to a resonance z_0 of H and γ sufficiently small, the following are true:*

(i) $\sigma_{ess}(\,|H_\theta(\gamma) - z|\,) = [d(z,\theta), \infty)$.

(ii) $\sigma_d(\,|H_\theta(\gamma)-z|\,)\cap[0,d(z,\theta)]\neq\emptyset$.
(iii) $\lambda_n\in\sigma_d(|H_\theta(\gamma)-z|)$ *if and only if there exists* $\psi_n\in\mathcal{D}(\nabla^2)$ *such that:*

$$(H_\theta(\gamma)-z)\psi_n=\lambda_n C\psi_n.$$

Moreover

$$\|(H_\theta(\gamma)-z)^{-1}\|=\frac{1}{\min_n\lambda_n}.$$

Above, $d(z,\theta)=|z\sin(2\operatorname{Im}\theta-\alpha)|$ *denotes the distance from* z *to* $\sigma_{ess}(H_\theta)$ *(where* $z=|z|e^{-i\alpha}$*).*

We require the following lemma:

Lemma 4.2. *Let* A *and* B *be two closed operators such that* $\mathcal{D}(A)\subset\mathcal{D}(B)$ *and* $B|A|^{-1}$ *is compact. Let* $A+B$ *be the closed sum on* $\mathcal{D}(A)$ *and* $C=|A+B|^2$*, defined on* $|A|^{-2}\mathcal{H}$*. Then* $(C-\zeta^2)^{-1}$ *is a meromorphic operator valued function on* $\zeta\in\mathbb{C}\backslash[\sigma(|A|)\cup\sigma(-|A|)]$*.*

Proof of Lemma 4.2. This follows from the identity

$$(C-\zeta^2)^{-1}=(|A|+\zeta)^{-1}[1+N(\zeta)]^{-1}(|A|-\zeta)^{-1} \tag{18}$$

where

$$N(\zeta)=(|A|-\zeta)^{-1}[A^*B+B^*A+B^*B](|A|+\zeta)^{-1}$$

is an analytic family of compact operators on $\zeta\in\mathbb{C}\backslash[\sigma(|A|)\cup\sigma(-|A|)]$. □

Proof of (i). Taking $A=-e^{-2\theta}\nabla^2-z$ and $B=v_\theta(\mathbf{x})+\gamma w_\theta(\mathbf{x})$, it follows that the essential spectrum of $|H_\theta(\gamma)-z|$ is contained in $\sigma(|-e^{-2\theta}\nabla^2-z|)$, which is $[d(z,\theta),\infty)$. □

Proof of (ii). We need to show that $|H_\theta(\gamma)-z|$ has spectrum below $d(z,\theta)$. Let ψ_0 be the eigenvector corresponding to the resonance, $H_\theta\psi_0=z_0\psi_0$. Remark that

$$(H_\theta(\gamma)-z)\psi_0=(z_0-z)[1+\gamma w_\theta(H_\theta-z)^{-1}]\psi_0$$

and consequently

$$\||H_\theta(\gamma)-z|\psi_0\|\le|z_0-z|(1+\gamma\|w_\theta(H_\theta-z)^{-1}\|\,).$$

With our assumptions, there exists $0<a<1$ and $b>0$ such that $\|w_\theta\psi\|\le a\|\nabla^2\psi\|+b\|\psi\|$ and similarly for v_θ, for any $\psi\in\mathcal{D}(\nabla^2)$. A relatively elementary manipulation then yields:

$$\|w_\theta(H_\theta-z)^{-1}\|\le\frac{a}{1-a}+\frac{b+a|z|}{1-a}\|(H_\theta-z)^{-1}\|.$$

The conclusion is that we can make $\||H_\theta(\gamma)-z|\psi_0\|$ arbitrarily small, in particular, smaller than $d(z,\theta)$, by taking the limit $z\to z_0$ and $\gamma\to 0$. Consequently, $\inf\sigma(|H_\theta(\gamma)-z|)<d(z,\theta)$ for γ small enough and z close enough to the resonance. □

Proof of (iii). Since the operator $H_\theta(\gamma) - z$ is C-selfadjoint, it admits the decomposition stated by Theorem 2.4:

$$H_\theta(\gamma) - z = CJ|H_\theta(\gamma) - z|,$$

where the second conjugation J commutes, in the strong sense, with the selfadjoint operator $|H_\theta(\gamma) - z|$. In particular J leaves invariant the spectral subspaces of $|H_\theta(\gamma) - z|$. Thus if λ_n belongs to the discrete spectrum of $|H_\theta(\gamma) - z|$, then the vector space consisting of the eigenvectors $\phi_n \in \mathcal{D}(\nabla^2)$:

$$|H_\theta(\gamma) - z|\phi_n = \lambda_n \phi_n$$

is left invariant by J. Thus, either $\phi_n = -J\phi_n$ or $\phi'_n = \phi_n + J\phi_n$ provide a new eigenvector ψ_n satisfying $J\psi_n = \psi_n$. Therefore,

$$C(H_\theta(\gamma) - z)\psi_n = J|H_\theta(\gamma) - z|\psi_n = |H_\theta(\gamma) - z|\psi_n = \lambda_n \psi_n.$$

This proves the last assertion in the statement. □

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