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Norm estimates of complex symmetric operators applied to quantum systems

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Abstract
This paper communicates recent results in the theory of complex symmetric operators and shows, through two non-trivial examples, their potential usefulness in the study of Schrödinger operators. In particular, 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

About half a century ago, Glazman laid the foundations for the theory of unbounded complex symmetric operators [15, 16]. Since then, his fundamental ideas have been successfully tested on several classes of differential operators [7, 20, 27]. Recently, two of the authors discovered an additional structure in the polar decomposition of a complex symmetric operator [14]. 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 paper, we exploit this idea in conjunction with the complex scaling method for Schrödinger operators.

Although quantum mechanics is built on the theory of self-adjoint operators, one must often deal with non-self-adjoint 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], the calculus of resonances and the convergence of time-dependent perturbation theory [31], and asymptotic behaviour of the eigenvectors [10]. As the examples in this paper show, the complex scaling technique naturally leads to complex symmetric operators.

Our first application deals with Schrödinger operators with a spectral gap. 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 [35]. For 1D periodic insulators, exact exponential decays can be derived from Kohn's analytic results [21]. In an attempt to generalize these results to higher dimensions, des Cloizeaux [8, 9] 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 [4, 17, 19, 33]. These results, however, are limited to periodic systems and some of them to the extreme tight-binding limit. In the present paper, 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 periodic systems, it has long been known that the exponential decay of the resolvent, when the energy E is in the gap and close to the gap edges, is proportional to the square root of the distance from E to the gap edge. The theory of the effective mass [22] provides a simple way of estimating this exponential decay constant. Relatively recently, it was proven that this qualitative behaviour is present in any gapped systems [3, 18]. The present paper sharpens these previous estimates. The goal is to find the best quantitative estimate of the exponential decay constant, with the energy spectrum as the only input.

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

2. Complex symmetric operators

This section is a brief account of relevant results (both old and new) about complex symmetric operators. For full details and examples the reader can consult [13, 14].

We first consider bounded operators. Let $\mathcal{H}$ denote a separable complex Hilbert space which carries a *conjugation* $C : \mathcal{H} \longrightarrow \mathcal{H}$, an *antilinear* operator satisfying the conditions $C^2 = I$ and $\langle Cf, Cg\rangle = \langle g, f\rangle$ for all $f, g \in \mathcal{H}$. A bounded operator T on $\mathcal{H}$ is called *C-symmetric* if $T = CT^*C$. More generally, T is called *complex symmetric* if there exists a C such that T is C-symmetric. The terminology arises from the fact that T is complex symmetric if and only if it has a symmetric matrix representation with respect to some orthonormal basis [13].

Examples of bounded complex symmetric operators include normal operators, Hankel operators, finite Toeplitz matrices, Jordan model operators (the infinite-dimensional analogues of Jordan blocks), the Volterra integration operator, and several other classes as well (see [13, 14]). Some of these classes of operators appeared in direct applications like atomic collisions [6] and bound states problems in periodic chains [26].

The following simple factorization theorem (from [14]) is the main ingredient in the proofs contained throughout this paper.

Theorem 2.1 (14). *If $T : \mathcal{H} \longrightarrow \mathcal{H}$ is a bounded C-symmetric operator, then there exists a conjugation $J : \mathcal{H} \longrightarrow \mathcal{H}$, which commutes with the spectral measure of $|T| = \sqrt{T^*T}$, such that $T = CJ|T|$.*

The theorem above asserts the equivalence of the *antilinear* eigenvalue problems

$$Tf = \lambda Cf \quad \Leftrightarrow \quad |T|f = \lambda Jf. \tag{1}$$

We may assume that λ is real and positive, since we may multiply either of these equations by a suitable unimodular constant. This equivalence is important for the following reason: the norm of a compact operator T is equal to the largest eigenvalue of $|T|$. However, working with $|T|$ instead of the original operator T introduces unwanted and potentially serious complications. Equation (1) provides the following convenient alternative: the norm of a compact C-symmetric operator T is equal to the largest positive solution λ of the *antilinear* eigenvalue problem, $Tf = \lambda Cf$. This is because the auxiliary conjugation J fixes an orthonormal basis of each spectral subspace of $|T|$.

We now turn to the case of unbounded operators. A densely defined, closed operator T is *C-symmetric* if $T \subset CT^*C$ and *C-self-adjoint* if $T = CT^*C$, i.e. their domains coincide and, on this common domain, they are equal.

The study of unbounded complex symmetric operators was pioneered by Glazman [15, 16], who established a complex symmetric parallel to von Neumann's theory of self-adjoint extensions of symmetric operators, although certain classes of C-symmetric operators had appeared earlier in von Neumann's work [34]. A renewed interest in Glazman's theory was sparked by its application to certain Dirac-type operators [7] and the realization that the closely related class of *C-unitary* operators is relevant to the study of complex scaling transformations in quantum mechanics [29]. Moreover, certain Sturm–Liouville operators with complex potentials can also be treated similarly [20, 27]. Further examples are furnished by Schrödinger operators $-\Delta + v$ with *complex potentials* v (where C is simply complex conjugation) subject to appropriate boundary conditions [16, 27]. One can also consider Schrödinger operators $-\Delta + v$ with real potentials v, but complex (non-self-adjoint) two-point boundary conditions, in which case the conjugation C is slightly more involved.

From the classical theory of self-adjoint operators, one knows that a symmetric operator has self-adjoint extensions if and only if its deficiency indices are the same. In contrast, *every* C-symmetric unbounded operator admits a C-self-adjoint extension $\widetilde{T}$. Unfortunately, not all unbounded C-self-adjoint operators possess a spectral resolution and a corresponding fine functional calculus. Nevertheless, if an unbounded C-self-adjoint operator has a compact resolvent, then a canonically associated antilinear eigenvalue problem always has a complete set of mutually orthogonal eigenfunctions:

Theorem 2.2 (14)**.** *If $T : \mathcal{D}(T) \longrightarrow H$ is an unbounded C-self-adjoint operator with compact resolvent $(T - z)^{-1}$ 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:*

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

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

This 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 2.3 (14)**.** *If T is a densely-defined C-self-adjoint operator with compact resolvent $(T - z)^{-1}$ for some complex number z, then*

$$\|(T - z)^{-1}\| = \frac{1}{\inf_n \lambda_n} \tag{2}$$

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

$$(T - z)u_n = \lambda_n C u_n. \tag{3}$$

Here $\| \ \|$ *denotes the operator norm:* $\|A\| \equiv \sup_{\|\phi\|=1} \sqrt{\langle A\phi, A\phi\rangle}$.

We also remark that the refined polar decomposition $T = CJ|T|$ applies, under certain circumstances, to unbounded C-self-adjoint operators. The following extension will play a central role in our second application:

Theorem 2.4 (14)**.** *If $T : \mathcal{D}(T) \longrightarrow \mathcal{H}$ is a densely defined C-self-adjoint operator with zero in its resolvent, then $T = CJ|T|$ where $|T|$ is a positive self-adjoint operator (in the von Neumann sense) satisfying $\mathcal{D}(|T|) = \mathcal{D}(T)$ and J is a conjugation on $\mathcal{H}$ which commutes with the spectral measure of $|T|$. Conversely, any operator of the form described above is C-self-adjoint.*

We close this section with a few remarks about the computation of the eigenvalues $\lambda_n = \lambda_n(|T|)$ and associated eigenfunctions via the antilinear problem (1) or (3). If T is a complex C-symmetric operator, then the bilinear (as opposed to sesquilinear) form

$$[Tx, y] = \langle Tx, Cy\rangle = \langle |T|x, Jy\rangle$$

can detect these values via a min–max principle analogous to the corresponding procedure for self-adjoint operators (see [28 XIII.1]). More specifically, if $\lambda_0 \geqslant \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant 0$ are the eigenvalues of the compact positive operator $|T|$, arranged in decreasing order and repeated according to multiplicity, then the evenly indexed eigenvalues λ_{2n} are given by the following variational principle:

$$\lambda_{2n} = \min_{\operatorname{codim} V = n} \ \max_{u \in V, \|u\|=1} \operatorname{Re}[Tu, u]. \tag{4}$$

The same principle applied to a rank one perturbation $T + \xi \otimes C\xi$ (where ξ is any eigenvector of $|T|$, scaled such that $\|\xi\| > \|T\|$) yields the odd eigenvalues. The proof of (4), along with several applications, can be found in [12]. We also remark that (4) generalizes the recently discovered min–max principle for symmetric matrices with complex entries [11].

If one is only concerned with $\|T\|$, then simply take $n = 0$ in (4) and note that

$$\|T\| = \max_{u \in \mathcal{H}, \|u\|=1} \operatorname{Re}[Tu, u].$$

The antilinear eigenproblem $Tf = \lambda Cf$ and min–max principle (4) can be broken into real linear problems and also have the advantage that they do not involve the direct calculation of T^*T. Moreover, one might potentially find numerical approximations to the λ_n via procedures similar to those in [28 XIII.1].

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 for Schrödinger operators with a gap in the spectrum. A short account on the subject has been already given in the introduction.

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) $\Omega \subset \mathbf{R}^d$; 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 $v(\mathbf{x}) \geqslant 0$. We also include a magnetic field, described by a smooth vector potential $\mathbf{A}(\mathbf{x})$. The total Hamiltonian is

$$H_{\mathbf{A}} : \mathcal{D}\big(\nabla_D^2\big) \longrightarrow L^2(\Omega), \qquad H_{\mathbf{A}} = -(\nabla + \mathrm{i}\mathbf{A})^2 + v(\mathbf{x}).$$

The assumption on $H_{\mathbf{A}}$ 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 the upper/lower band. The corresponding spectral projectors are denoted by $P_\pm$.

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

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

where ω_ϵ is the volume of a sphere of radius ϵ in $\mathbf{R}^d$. 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:*

$$|\bar{G}_E(\mathbf{x}_1, \mathbf{x}_2)| \leqslant C_{q,E}\, \mathrm{e}^{-q|\mathbf{x}_1-\mathbf{x}_2|}. \tag{5}$$

$C_{q,E}$ is given by

$$C_{q,E} = \frac{\omega_\epsilon^{-1}\mathrm{e}^{2q\epsilon}}{\min|E_\pm - E - q^2|} \cdot \frac{1}{1 - q/F(q, E)} \tag{6}$$

with

$$F(q, E) = \sqrt{\frac{(E_+ - E - q^2)(E - E_- + q^2)}{4E_-}}. \tag{7}$$

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

Proof. If $\chi_{\mathbf{x}}$ denotes the characteristic function of the ϵ ball centred at $\mathbf{x}$ (i.e., $\chi_{\mathbf{x}}(\mathbf{x}') = 1$ for $|\mathbf{x}' - \mathbf{x}| \leqslant \epsilon$ and 0 otherwise), then one can equivalently write

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

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

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

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

$$H_{\mathbf{q},\mathbf{A}} : \mathcal{D}\big(\nabla_D^2\big) \to L^2(\Omega), \qquad H_{\mathbf{q},\mathbf{A}} = H_{\mathbf{A}} + 2\mathbf{q}(\nabla + \mathrm{i}\mathbf{A}) - q^2. \tag{8}$$

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

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

holds for all $\mathbf{q} \in \mathbf{R}^d$ (this happens only for finite Ω). If $\Omega = \mathbf{R}^d$, the identity holds as long as the continuum spectrum (which moves as $\mathbf{q}$ is increased) does not step over E. We denote

$$\gamma(q, E) = \sup_{|\mathbf{q}|=q} \|(H_{\mathbf{q},\mathbf{A}} - E)^{-1}\|. \tag{9}$$

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

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

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

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

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

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

It is a simple task to check that $\mathbf{H}$ is C-self-adjoint: $\mathbf{H}^* = C\mathbf{H}C$. Moreover,

$$\|(\mathbf{H} - E)^{-1}\| = \|(H_{\mathbf{q},\mathbf{A}} - E)^{-1}\| = \|(H_{-\mathbf{q},-\mathbf{A}} - E)^{-1}\|. \tag{10}$$

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

$$(\mathbf{H} - E)\phi_n = \lambda_n C\phi_n \tag{11}$$

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

$$\|(\mathbf{H} - E)^{-1}\| = \frac{1}{\min_n \lambda_n}. \tag{12}$$

If we write $\phi_n = f_n \oplus g_n$, the antilinear eigenvalue problem equation (11), after we apply a complex conjugation on the second equation, is equivalent to

$$\begin{cases} (H_{\mathbf{q},\mathbf{A}} - E)f_n = \lambda_n \bar{g}_n \\ (H_{-\mathbf{q},\mathbf{A}} - E)\bar{g}_n = \lambda_n f_n. \end{cases} \tag{13}$$

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

$$H_{\mathbf{A}} - E - q^2 = S|H_{\mathbf{A}} - E - q^2|,$$

holds, where $S = P_+ - P_-$. We take the scalar product of the first equation in equation (13) against the vector Sf_n. Keeping only the real part of the result and solving for λ_n, we find

$$\lambda_n = \frac{|\langle f_n, |H_{\mathbf{A}} - E - q^2|f_n\rangle + 2\,\mathrm{Re}\langle Sf_n, \mathbf{q}(\nabla + \mathrm{i}\mathbf{A})f_n\rangle|}{|\mathrm{Re}\langle Sf_n, \bar{g}_n\rangle|}. \tag{14}$$

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

$$\mathrm{Re}\langle Sf_n, \mathbf{q}(\nabla + \mathrm{i}\mathbf{A})f_n\rangle = 2\,\mathrm{Re}\langle f_n, P_+[\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})]P_- f_n\rangle.$$

Moreover, denoting

$$B_{\mathbf{q}} \equiv P_+|H_{\mathbf{A}} - E - q^2|^{-1/2}[\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})]|H_{\mathbf{A}} - E - q^2|^{-1/2}P_-, \tag{15}$$

one obtains

$$|\langle f_n, P_+[\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})]P_- f_n\rangle| \leqslant \tfrac{1}{2}\|B_{\mathbf{q}}\|\langle f_n, |H_{\mathbf{A}} - E - q^2|f_n\rangle.$$

Equation (14) implies

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

Similarly, by taking the scalar product of the second equation of equation (13) against $S\bar{g}_n$, one obtains:

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

The sum of the last two equations yields

$$\lambda_n \geqslant \min\{|E_\pm - E - q^2|\}(1 - 2\|B_\mathbf{q}\|). \tag{16}$$

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

$$q^2(-(\nabla + \mathrm{i}\mathbf{A})^2 + v + a) \geqslant [\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})]^2, \qquad \forall a \geqslant 0,$$

holds true. Consequently

$$\|[\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})]|H_\mathbf{A} + a|^{-1/2}\| \leqslant q, \qquad \forall a > 0.$$

We can then insert $|H_\mathbf{A} + a|^{-1/2}|H_\mathbf{A} + a|^{1/2}$ after $\mathbf{q}(\nabla + \mathrm{i}\mathbf{A})$ in equation (15) and use the above estimate and the spectral theorem to get:

$$\|B_\mathbf{q}\| \leqslant q\sqrt{\frac{E_- + a}{(E_+ - E - q^2)(E - E_- + q^2)}}. \tag{17}$$

Finally, one can pass to the limit $a \to 0$. Equation (12), together with equations (16) and (17) provide the desired estimate of $\gamma(q, E)$. □

We have the following remarks. The reason we considered only finite domains is primarily because the abstract machinery presented in the previous section applies only to complex symmetric operators with compact resolvent. An extension to operators with non-compact resolvent is given in the next section. However, since the constants in theorem 3.1 are independent of the domain Ω, the estimates remain valid when $\Omega \to \mathbf{R}^d$, whenever this limit is well defined. For E close to the gap edges, a brute perturbation theory on $(H_{\mathbf{q},\mathbf{A}} - E)^{-1}$ leads to an exponential decay constant proportional to $|E_\pm - E|$. The correct behaviour of $q_c(E)$ near the band edges is $|E_\pm - E|^{1/2}$, as it was first shown in [3] and later reviewed in [18]. Note that our estimate of $q_c(E)$ does have the correct behaviour near the gap edges.

Corollary 3.2. *Consider 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*

$$\bar{q} \geqslant \frac{G}{4\sqrt{E_-}}. \tag{18}$$

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:

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

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:

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

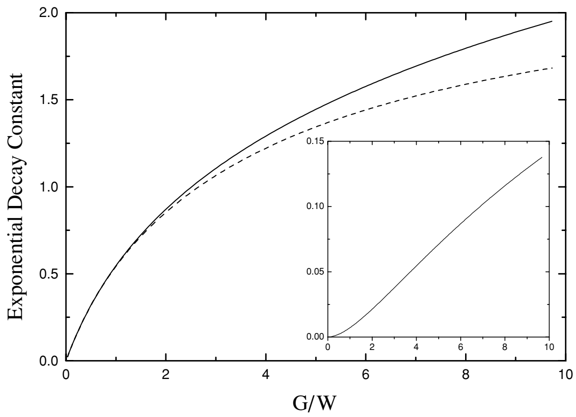

Figure 1. The exponential decay constant of the single-particle density matrix as a function of G/W for the Kronig–Penney insulator. The continuous line represents an exact calculation and the dashed line represents the estimate given in equation (18). The inset shows the relative difference between the two.

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

$$q_c = \sqrt{\frac{\left(E_+ - E - q_c^2\right)\left(E - E_- + q_c^2\right)}{4E_-}} \leqslant \frac{G}{4\sqrt{E_-}} \tag{19}$$

with equality at energy

$$\bar{E} = \frac{E_+ + E_-}{2} - \frac{G^2}{16E_-}. \tag{20}$$

The lower bound of equation (18) is valid as long as $\bar{E}$ is in the gap. □

The lower bound on $\bar{q}$ given in equation (18) can be calculated entirely from the energy spectrum. What is the best lower bound on the exponential decay constant that one can get by only using the information contained in the energy spectrum? We illustrate by an example that equation (18) comes close to such an optimal estimate. In figure 1, we consider a comparison between our estimate equation (18) and the exact value of $\bar{q}$, for a one-dimensional insulator described by the Kronig–Penney model [23]:

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

with the first band completely filled. The Dirac-delta potential is not ∇^2 relatively bounded so the above example is not formally covered by theorem 3.1. However, this potential is a relatively bounded form perturbation and our arguments can be extended to this larger class of potentials. 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 $G/W < 5$), equation (18) estimates the exponential decay to within a 15% error. Note 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 operators. 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

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

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

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

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

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

where θ runs in the finite strip $|\mathrm{Im}\,\theta| < I_0$. As a function of θ, it is well known that [1, 2, 30]:

(a) the discrete spectrum σ_d remains invariant,
(b) the essential spectrum σ_{ess} rotates down by an angle $-2\,\mathrm{Im}\,\theta$,
(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 [5, 24, 25, 32]. 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-self-adjoint 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 $v_\theta(\mathbf{x}) \equiv v(\mathrm{e}^{\theta}\mathbf{x})$ and $w_\theta(\mathbf{x}) \equiv w(\mathrm{e}^{\theta}\mathbf{x})$ are ∇^2-relatively bounded for $|\mathrm{Im}\,\theta| < I_0$, with bound less than 1. For z close to a resonance z_0 of H and γ sufficiently small, the following are true:*

(i) $\sigma_{\mathrm{ess}}(|H_\theta(\gamma) - z|) = [\mathrm{d}(z,\theta), \infty)$.
(ii) $\sigma_d(|H_\theta(\gamma) - z|) \cap [0,\ \mathrm{d}(z,\theta)] \neq \emptyset$.
(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, $\mathrm{d}(z,\theta) = |z \sin(2\,\mathrm{Im}\,\theta - \alpha)|$ *denotes the distance from* z *to* $\sigma_{\mathrm{ess}}(H_\theta)$ *(where* $z = |z|\,\mathrm{e}^{-i\alpha}$*).*

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 $\mathcal{D}(A)$. Then $\sigma_{\mathrm{ess}}|A + B| = \sigma_{\mathrm{ess}}|A|$.*

Proof. Let $K = |A + B|^2$, defined on $|A|^{-2}\mathcal{H}$. We show that $(K - \zeta^2)^{-1}$ is a meromorphic operator-valued function on $\zeta \in \mathbb{C}\backslash[\sigma(|A|) \cup \sigma(-|A|)]$. This follows from the identity

$$(K - \zeta^2)^{-1} = (|A| + \zeta)^{-1}[1 + N(\zeta)]^{-1}(|A| - \zeta)^{-1}, \tag{21}$$

where

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

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

Proof of theorem 4.1. (i) Taking $A = -\mathrm{e}^{-2\theta}\nabla^2 - z$ and $B = v_\theta + \gamma w_\theta$, it follows that the essential spectrum of $|H_\theta(\gamma) - z|$ is contained in $\sigma(|-\mathrm{e}^{-2\theta}\nabla^2 - z|)$, which is $[d(z,\theta), \infty)$.

(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

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

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

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

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.

(iii) Since the operator $H_\theta(\gamma) - z$ is C-self-adjoint, 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 self-adjoint 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. □

5. Conclusions

The goal of this paper was to introduce recent results in the theory of complex symmetric operators and to show, through two non-trivial examples, their potential usefulness in the study of Schrödinger operators. It was shown that, for C-self-adjoint operators with compact resolvent, a certain antilinear eigenvalue problem can be used in a similar way to how the spectral decomposition for self-adjoint operators is used to estimate the norm of the resolvent. We combined this observation with the complex scaling technique, to obtain sharp lower bounds on the exponential decay of the resolvent and density matrix for Schrödinger operators with a gap in the energy spectrum. We have also shown that these techniques can be applied to C-self-adjoint operators with non-compact resolvent, in particular, to Schrödinger appearing in the complex scaling theory of resonances.

In concrete applications, we believe that one can go beyond the approximations made in this paper and use either the newly developed min–max principle for complex-symmetric operators [11, 12], or direct, numerical integration of the antilinear eigenvalue problem to obtain sharper, problem specific estimates of the exponential decay constant or to evaluate the resolvent norm in our second application.

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