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Conditions for the spectrum associated with an asymptotically straight leaky wire to comprise the interval $(-\infty, \infty)$

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Abstract
We consider a quantum (or leaky) wire in the plane, and the wire supports a singular attraction which becomes large at distant points on the wire. An analogous regular potential arises from the motion of a hydrogen atom in an electric field. We prove that, as in the regular case, the spectrum is the whole of $(-\infty, \infty)$.

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1. Introduction

Let Γ be a continuous and piecewise smooth curve extending to infinity in the plane $\mathbf{R}^2$, and let q be a given real-valued continuous function defined on Γ. We consider the operator H defined by

$$H\psi(\mathbf{x}) = -\Delta\psi(\mathbf{x}) \qquad (\mathbf{x} \in \mathbf{R}^2\backslash\Gamma) \tag{1}$$

with domain $D(H)$ consisting of functions $\psi \in W^{2,2}(\mathbf{R}^2\backslash\Gamma)$ which are continuous at Γ and with the normal derivatives having a jump in the sense that

$$\frac{\partial\psi}{\partial n_1}(\mathbf{x}) + \frac{\partial\psi}{\partial n_2}(\mathbf{x}) = -q(\mathbf{x})\psi(\mathbf{x}) \quad (\mathbf{x} \in \Gamma). \tag{2}$$

Here n_1 and n_2 denote the normals directed away from Γ on the two sides of Γ.

If q is bounded and Γ has no cusps, it is known that H is essentially self-adjoint, and its closure H_1 can be expressed in terms of distributions as

$$H_1 = -\Delta - q(\mathbf{x})\delta(\mathbf{x} - \Gamma),$$

where δ is the Dirac delta function and $D(H_1) \subseteq W^{1,2}(\mathbf{R}^2)$ [6, section 2.1], [9, section 2.1]. The spectral properties of H_1 have been much investigated in recent years, a principal feature being the influence which the geometry of Γ has on the nature of the spectrum $\sigma(H_1)$ of H_1. We refer to the comprehensive survey [6] for the current position.

The physical motivation for this setting is that the Hamiltonian H_1 represents the motion of a particle under the influence of a singular attraction (when $q(\mathbf{x}) \geqslant 0$) along Γ. Unlike other models for this situation, like quantum graphs and fat graphs, the particle is no longer confined to the wire, but lives in the whole space, allowing for quantum tunneling. For this reason, in this context, Γ is called a leaky wire. We again refer to [6] for a more detailed discussion of the physical motivation.

An example of a spectral property which depends on the geometry of Γ is given in [8]. Here $q(\mathbf{x})$ is a positive constant c and, subject to certain conditions on Γ, $\sigma(H_1) = \left[-\frac{1}{4}c^2, \infty\right)$. One of the conditions is that Γ should be asymptotically straight (a.s.) in the sense that, in terms of the arc length s along Γ, the curvature $k(s)$ satisfies $|k(s)| \leqslant (\text{const})|s|^{-\beta}$ for large s and some $\beta > 5/4$ [8, remark 5.6].

A similar result concerning $\sigma(H_1)$ was proved in [1] using the singular (or Weyl) sequence method. This requires Γ to be a.s. in the different but similar sense that Γ should lie close to arbitrarily long disjoint line segments as Γ recedes to infinity. We refer to [1, section 3] for the details, but this idea of a.s. will also appear in this paper in section 2 below.

A second example of a spectral property of $\sigma(H_1)$ is the band structure associated with the periodicity of either q or Γ [6, section 6.1], [7, 10]. This structure is of course well known for the classical Schrödinger operator with a regular periodic potential which reflects the crystalline nature of matter [3], [12, pp 279–315]. There is however a quite different type of regular potential which is relevant to this paper. The motion of a hydrogen atom in the presence of an electric field is described by a regular potential which is unbounded and for which the associated spectrum is the whole of $(-\infty, \infty)$ [14, sections 15.16–15.19]. The question therefore arises whether there is a corresponding spectral property for an unbounded singular potential q supported on Γ.

Similar models also arise when dealing with interface crack problems in fracture mechanics (cf [11] and references therein).

In this paper therefore, we allow q to be unbounded, and it is no longer clear that H is essentially self-adjoint. However, in order to access spectral theory, we begin by adding the requirement that

$$q\psi \in L^2(\Gamma, \mathrm{d}s) \tag{3}$$

for functions $\psi \in D(H)$. Then a simple application of Green's theorem gives

$$(H\psi, \phi) = \int_{\mathbf{R}^2} (\nabla\psi) \cdot (\nabla\overline{\phi})\, \mathrm{d}\mathbf{x} - \int_\Gamma q\psi\overline{\phi}\, \mathrm{d}s$$

for ψ and ϕ in $D(H)$. Thus H is symmetric in $L^2(\mathbf{R}^2)$. Since q is real valued, the deficiency spaces of H are isomorphic, and hence H has at least one self-adjoint extension T [5, p 114]. We denote by σ the spectrum of any such self-adjoint T. Our purpose in this paper is to allow q to be large and positive as $\mathbf{x}$ recedes to infinity, and to give conditions on Γ and q which imply that $\sigma = (-\infty, \infty)$. This property of σ appears to be new in this paper.

2. Asymptotic straightness

Let us first recall the definition of a singular (or Weyl) sequence in the spectral theory of a self-adjoint operator T. A consequence of the spectral theorem for T is that a real number λ is in the essential spectrum σ_e of T if there is a sequence f_m in $D(T)$ such that

$$\|f_m\| = 1, \qquad f_m \rightharpoonup 0 \quad \text{(weak convergence)}$$

and

$$\|(T - \lambda I)f_m\| \to 0 \tag{4}$$

as $m \to \infty$ [5, p 415]. Such a sequence is called a singular (or Weyl) sequence. Our choice of f_m in this paper will have compact support and lie in $D(H)$. Thus (3) is satisfied, and (4) becomes simply

$$\int_{R_1 \cup R_2} |(\Delta + \lambda I)f_m|^2 \, \mathrm{d}\mathbf{x} \to 0 \tag{5}$$

by (1), subject to f_m satisfying the normal derivative condition (2). Here R_1 and R_2 denote the (open) portions of the support of f_m which lie on the two sides of Γ.

Our choice of f_m also relies on Γ being a.s. in the sense that Γ should lie close to arbitrarily long disjoint line segments as Γ recedes to infinity. The segments can be located without restriction in $\mathbf{R}^2$ but, purely for convenience, we take them to lie along the x-axis. Thus we assume that there are disjoint intervals $I_m = (c_m - a_m, c_m + a_m)$ on the x-axis with $c_m - a_m \to \infty$ and $a_m \to \infty$ and, for x in each I_m, Γ has the equation $y = F(x)$ with

$$F^{(r)}(x) \to 0 \ (0 \leqslant r \leqslant 3) \tag{6}$$

as $x \to \infty$ through the I_m. The most general a.s. Γ which is covered by our methods is obtained by rotating and translating each I_m (and the portion of the curve near to it) to a position elsewhere in the plane.

We can now proceed to the definition of f_m, which is a modification of that given in [1, (3.3)] to cope with an unbounded q. In the square $S_m = (c_m - a_m, c_m + a_m) \times (-a_m, a_m)$, we define

$$f_m(\mathbf{x}) = b_m h_m(x - c_m) h_m(y) \exp\{-P(x)|y - F(x)| + \mathrm{i}Q(x)\}, \tag{7}$$

where b_m is the normalization factor making $\|f_m\| = 1$, and h_m is as usual a $\mathbf{C}^{(2)}(-\infty, \infty)$ function such that

$$h_m(t) = 1 (|t| \leqslant a_m - 1), = 0 \quad (|t| \geqslant a_m) \tag{8}$$

and with derivatives independent of m. Next, as in [1, (3.4)], the choice of $P(x)$ is

$$P(x) = \tfrac{1}{2} q(x)(1 + F'^2)^{-1/2}, \tag{9}$$

where $q(x) := q(x, F(x))$, this choice making f_m satisfy (2). Finally, $Q(x)$ is a real-valued function still to be chosen.

Next in this section, we use the a.s. property (6) to estimate the size of b_m as $m \to \infty$ subject to the following two conditions on q:

$$q(x) > 0 \quad \text{in} \quad I_m \quad \text{and} \quad \int_{I_m} 1/q(x) \, \mathrm{d}x \to \infty \tag{10}$$

as $m \to \infty$. Then, by (7) and (8), we have

$$1 = \|f_m\|^2 \sim b_m^2 \int_{I_m} \cdot \int_{-a_m}^{a_m} \exp\{-2P(x)|y - F(x)|\} \, \mathrm{d}y \, \mathrm{d}x.$$

We split the y-integration into the pieces over $y \geqslant F(x)$ and $y \leqslant F(x)$ to obtain

$$1 \sim 2b_m^2 \int_{I_m} 1/\{2P(x)\} \, \mathrm{d}x \sim 2b_m^2 \int_{I_m} 1/q(x) \, \mathrm{d}x$$

by (6) and (9). Thus

$$b_m \sim \left(2 \int_{I_m} 1/q(x) \, \mathrm{d}x \right)^{-\frac{1}{2}}. \tag{11}$$

We also note that (10) and (11) imply that $f_m \rightharpoonup 0$.

3. The spectrum

We can now use (5) to prove our main theorem that $\sigma = (-\infty, \infty)$ under a suitable set of conditions on F and q.

Theorem 3.1. *Let $q(x)$ and $F(x)$ have continuous derivatives up to order 2 and 3 (respectively) in each I_m. In addition to (6) and (10), let*

$$q(x) \to \infty \tag{12}$$

as $x \to \infty$ through the I_m, and let the functions

$$q', \quad qq'', \quad q^2F', \quad qF'' \tag{13}$$

all tend to zero, again as $x \to \infty$ through the I_m. Then $\sigma = (-\infty, \infty)$.

Proof. We use (5) with an arbitrary λ in $(-\infty, \infty)$. When $x \in S_m \backslash \Gamma$, (7) gives

$$\begin{aligned}(\Delta + \lambda) f_m = [&P^2 - Q'^2 + \lambda + P'^2(y - F)^2 + P^2F'^2 \\ &\pm 2PP'|y - F|F' + 2iQ'\{\pm PF' - P'|y - F|\} \\ &- P''|y - F| \pm 2P'F' \pm PF'' + iQ'']f_m + E_m,\end{aligned} \tag{14}$$

where E_m denotes terms containing derivatives of h_m, and $\pm$ refers to the two sides of Γ. Now $h'_m(t)$ and $h''_m(t)$ are by (8) only non-zero when $a_m - 1 < |t| < a_m$, and it then follows from (10) and (11) that $\|E_m\| = o(1)(m \to \infty)$.

We now choose Q so that

$$Q' = \sqrt{(P^2 + \lambda)} \tag{15}$$

in I_m, this giving a real-valued Q for any λ if m is large enough, by (9), (6) and (12). Thus the first three terms on the right-hand side of (14) cancel. We have now to show that the remaining terms there have $o(1)$ norms as $m \to \infty$.

Let us begin with the fourth (and first remaining) term on the right-hand side of (14). We have from (7)

$$\begin{aligned}\|P'^2(y - F)^2 f_m\|^2 &= b_m^2 \int_{I_m} P'^4(x) h_m^2(x - c_m) \\ &\quad \times \int_{-a_m}^{a_m} h_m^2(y)\{y - F(x)\}^4 \exp\{-2P(x)|y - F(x)|\}\,\mathrm{d}y\,\mathrm{d}x \\ &\sim b_m^2 \int_{I_m} P'^4(x) \int_{-a_m}^{a_m} \{y - F(x)\}^4 \exp\{-2P(x)|y - F(x)|\}\,\mathrm{d}y\,\mathrm{d}x\end{aligned}$$

by (8). We again split the y-integration into the pieces over $y \geqslant F(x)$ and $y \leqslant F(x)$, and then carry out the integration to obtain

$$\|P'^2(y - F)^2 f_m\|^2 \sim \frac{3}{2} b_m^2 \int_{I_m} P'^4(x)/P^5(x)\,\mathrm{d}x. \tag{16}$$

By (11), the right-hand side here is $o(1)(m \to \infty)$ if

$$P'^4/P^5 = o(1/q)$$

i.e. if $q' = o(q)$ and $F'F'' = o(1)$, by (6) and (9), and these requirements are certainly covered by (6), (12) and (13).

The next term to consider in (14) is $\|P^2F'^2 f_m\|$, and this is $o(1)$ if $PF' = o(1)$, i.e. if $qF' = o(1)$, and this is also covered by (13). Next again, we have $\|PP'|y - F|F' f_m\|$, and this is dealt with similarly to (16), in place of which we now have

$$\|PP'|y - F|F'f_m\|^2 \sim \frac{1}{2}b_m^2 \int_{I_m} P'^2 F'^2/P\,\mathrm{d}x.$$

By (11) and (9), this is $o(1)$ if $q'F'$ and $qF''F'^2$ are both $o(1)$, again covered by (6) and (13).

We continue in this vein with the remaining six terms on the right-hand side of (14), using (15) where necessary. The conditions for each of these terms to have a $o(1)$ norm are, in order, that the following functions should be $o(1)$:

$$q^2F'; \qquad q' \text{ and } qF'F'';$$
$$qq'', \qquad qq'F'F'', \qquad q(F'F'')' \text{ and } qF'F'';$$
$$q'F' \text{ and } qF'^2F''; \qquad qF''; \qquad q' \text{ and } qF'F''.$$

These conditions are all covered by (6) and (13), and the proof of the theorem is now complete.

We note that the idea of introducing Q into the definition of f_m in (7), together with the choice (15), is reminiscent of the method in [2] in the different context of the Schrödinger operator $-\Delta + V$ in $\mathbf{R}^N$.

4. Examples

As an example on theorem 3.1, we cite

$$q(\mathbf{x}) = |\mathbf{x}|^a (x > 1), \qquad F(x) = (\mathrm{const})x^{-b}$$

with $a > 0$ and $b > 0$. Here

$$q(x, F(x)) = \{x^2 + F^2(x)\}^{a/2}.$$

Then we take $I_m = (a_m, 3a_m)$(i.e.$c_m = 2a_m$), and (10) holds if $a < 1$. The conditions involving F in (13) also hold if $2a < b + 1$. Thus, altogether,

$$0 < a < 1, \qquad b > \max\{0, 2a - 1\}.$$

For a second example, suppose that Γ contains distant disjoint line segments obtained by rotating and translating the I_m, and $q = q_m$ (a constant) in each I_m. Then $P' = F' = Q'' = 0$ in (14). Hence (12) and (10) give $\sigma = (-\infty, \infty)$ if as $m \to \infty$

$$q_m \to \infty \qquad \text{and} \qquad a_m/q_m \to \infty.$$

These two examples raise the question whether there is a continuous/discrete spectrum dichotomy corresponding to the limit-point/limit-circle dichotomy for the Sturm–Liouville equation [13, sections 5.10–5.11] [4], the dividing value for $q(x) = -x^a$ now being $a = 1$ rather than $a = 2$ in [13].

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