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Geometrically Induced Spectrum of the Schrödinger Operator

Michael S.P. Eastham

Computer Science Department, Cardiff University Cardiff CF24 3XF, U.K.

ABSTRACT

New and recent results concerning the spectrum of the operator with a boundary condition on a given curve in the $(x, y)-$ *plane are presented. The geometry of the curve influences the nature of the spectrum, and the situations discussed are (i) there is a spectral interval* $[-c^2/4, \infty)$, *(ii) there are discrete eigenvalues in* $[-\infty, -c^2/4)$. *The aim is to present material which avoids some of the technicalities in the literature.*

INTRODUTION

The setting for our topic is the plane R^2, and we have a given piecewise smooth curve (or set of curves) Γ extending to infinity in R^2. We consider the Schrödinger operator

$$H = -\Delta \qquad (1)$$

on a suitable domain $D(H)$ of functions f which satisfy the boundary condition on Γ :

$$\frac{\partial f}{\partial n_1} + \frac{\partial f}{\partial n_2} = -qf \quad on \ \Gamma \qquad (2)$$

Here n_1 and n_2 are the normals on the two sides of Γ in the directions away from Γ, and q is a given real-valued function on Γ. For $D(H)$ we can take

$$D(H) = C_0(R^2) n C^{(2)}(R^2 - \Gamma) \cap (BC),$$

where the subscript zero denotes compact support.

Using a Green's Theorem, we can check that H is a symmetric operator in the Hilbert space $L2(R2)$. That is, $(Hf, g) = (f, Hg)(f, g \in D(H))$ with the inner-product $(f, g) = \int_{R2} \overline{f} g \, dx.$ [Brown B. M,. 2008, 2008b and 2009].

Associated with symmetric operators are certain real numbers λ which are called spectral points (the most familiar being eigenvalues). The set of all spectral points is called the spectrum $\sigma(H)$ of H, and it is the nature of this set which is the subject of this paper.

The spectrum $\sigma(H)$ comprises those numbers λ for which there is a sequence $\{fn\} \in \overline{D(H)}$ (Wey l sequence) such that

$$\|f_n\| = 1 \; and \; |(H - \lambda I) f_n| \to 0 \; (n \to \infty) \qquad (3)$$

The spectrum can be divided into two parts

$$\sigma(H) = \sigma_d(H) U \sigma_e(H)$$

as follows.

The discrete spectrum $\sigma_e(H)$ consists of the eigenvalues, i.e., numbers λ such that the equation

$$(Hf =) - \Delta f = \lambda f \; (f \in \overline{D(H)}) \qquad (4)$$

has a solution $f(\neq 0)$. Here $f_n = i$ for all I_i.

The essential spectrum $\sigma_e(H)$, which is typically formed by one or more λ.-intervals. It is invariant under certain perturbations of the original problem. There is the possibility of eigenvalues being embedded in $\sigma_e(H)$, but this is not our concern here.

The spectral points are important because they are the basis for the "eigenfunction expansion" (or spectral representation) of an arbitrary given function in terms of H. Simple examples from other contexts are Fourier series $\sigma_d = \{m^2\}, \sigma_e = \phi,$ Fourier integrals $\sigma_d = \phi, \sigma_e = (-\infty, \infty)$. Specialists in Functional Analysis will recognize that this is about the Spectral Theorem for a self-adjoint extension of H. However, a specialist knowledge is not assumed in this account.) For our problem with (1.1)+(BC), the nature of $\sigma(H)$ depends on the geometry of Γ, and there is a recent extensive survey paper (Exner,2008). Many of the results in (Exner, 2008) require complicated and technical proofs, but I want to show here that there are some things which can be understood rather more simply.

STAR GRAPHS

A star graph Γ consists of a finite set of infinite rays which start from a point 0 (the origin). There are two basic spectral results (Exner and Ichinose, 2001),(Exner and Ncova, 2003) for the standard case $q(x) = c$, where $c(> 0)$ is a constant.

Theorem 2.1 Let Γ be an infinite straight line. Then

$$\sigma_e = [-c^2/4, \infty)$$

and $\sigma_d = \phi$.

Theorem 2.2 For any other star graph Γ,

$$\sigma_e = [-c^2/4, \infty)$$

and $\sigma_d = \phi$, i.e., there exist eigenvalues below $-c^2/4$.

Example 2.3 Γ is the coordinate axes: 4 rays at right angles. Then the eigenfunction

$$\Psi(x) = exp\{-\frac{1}{2}c(|x|+|y|)\}$$

satisfies

$$-\Delta\Psi = \lambda\Psi$$

and (BC)

when $\lambda = -\frac{1}{2}c^2$. Thus we have an eigenvalue below $-c^2/4$.

Proof of Theorem 2.1 (In the spirit of Weyl and Titchmarsh where we consider an eigenvalue problem in a large square and examine the behavior of the eigenvales as the square expands to the whole of R^2 .) The aim here is to explain the appearance of the number $-c^2/4$. Consider the eigenvalue problem

$$-\Delta\Psi = \lambda\Psi \ (2.1) \qquad (5)$$

in the square $(-T,T)x(-T,T)$ with $y=0$. Now (BC) is

$$\Psi_y(x,0+) - \Psi_y(x,0-) = -c\Psi(x,0) \qquad (6)$$

on $y=0$.

Following Weyl and Titchmarsh, we impose Dirichlet boundary conditions on the sides of the square:

$$\Psi = 0 \ on \ x = \pm T, y = \pm T$$

and we shall let $T \to \infty$.

Now (2.1)-(2.2) is a separable eigenvalue problem which we solve with

$$\Psi(x) = f(x)g(y), \lambda = \mu + V.$$

Then

$$f'' + \mu f = 0, f(\pm T) = 0 \qquad (7)$$

$$g'' + Vg = 0 (y \neq 0), g'(0+) - g'(0-) = -cg(0), g(\pm T) = 0 \qquad (8)$$

Here (2.3) is the elementary S.H.M. problem with μ -eigenvalues

$$\mu = (\frac{N\pi}{2T})^2 \ (N = 1,2,.....)$$

and these become dense in $[0.\infty)$ as $T \to \infty$. For (2.4) we have the eigenvalue equation

$$\tan(w) = \frac{2w}{Tc} \quad (w = \frac{T}{V}). \qquad (9)$$

When $v>0$, w is real. For large T, the solutions of (2.5) are then $v \leftrightharpoons (M\pi/T)^2$ ($M = 1,2,...$), again becoming dense in $[0,\infty)$ as $T \to \infty$. So far, we have $\lambda = \mu + \upsilon$ giving λ -

eigenvalues filling up [0, ∞) as T → ∞ .
But there is another solution of (2.5) when $\upsilon < 0$. Putting $w = iz$, (2.5) becomes

$$tanh\, z = 2z/Tc.$$

Thus there is a single large solution z* with *tanh* z* ⇋ 1, i.e. z* = $\frac{1}{2}$ Tc - € . Thus

$$\sqrt{\upsilon^*} = w^*/T = iz^*/T = i(\frac{1}{2}c - \in /T).$$

giving

$$\upsilon^* = -\frac{1}{4}c^2 + \in' .$$

Hence $\lambda = \mu + \upsilon^*$ fills up [- $\frac{1}{4}$ c ^{2} , ∞) with spectral points as T → ∞.

EXISTENCE OF EIGENVALUES.

The main feature of Theorem 2.2 is that $\sigma_d \neq \phi$ if Γ is anything other than a straight line, and this raises a number of interesting questions about the nature of σ_d . The proof of Theorem 2.2 in (Exner and Ichinose,2001),(Exner and Ncova,2003) is very technical, but there is the possibility of a simpler approach using the variational expression

$$V(f) = (\int_{R^2} |\nabla f|^2 dx - c\int_{\Gamma} |f|^2 ds)/(\int_{R^2} |f|^2 dx)\,(3.1) \qquad (10)$$

The general spectral result which we use is that the least spectral point Λ of H satisfies
$\Lambda < V(f)$ for all f for which $V(f)$ is defined. Hence, if we can identify a function f_0 such that

$$V(f_0) < -\frac{1}{4}c^2, \qquad (11)$$

then we must have a point A_0 in $od(H)$ with the estimate

$$\lambda_0 \leq V(f_0) \qquad (12)$$

Note: (3.3) is most familiar in the context of the mini-max or Rayleigh-Ritz theory for estimating eigenvalues. Our first results depend on the number. N of rays in Γ.

PROPOSITION

If P has $N(> 4)$ rays, then od 4 0.
Proof. In (3.1) and (3.2), we choose $f_0(x) = exp(-ar)$, where a is a parameter to be chosen and $r = |x|$. Then

$$V(f_0) = a^2 - Nac/\pi = (a - \frac{1}{4}Nc/\pi)^2 - \frac{1}{4}(Nc/\pi)^2.$$

Now choose $a = \frac{1}{2} Nc/\pi$ to minimize $V(f_0)$. Then

$$V(f_0) = -(Nc/\pi)^2 < -\frac{1}{2} c2$$

if $N > \pi (i.e., N \geq 4)$.

Note: $N = 4$ gives $\lambda_0 < -4(c/\pi)^2 = -(0.405)c^2$. In Example 2.3 we have $\lambda_0 = -\frac{1}{2}c^2$ for the symmetric graph. We can improve on Proposition 3.1 by choosing an f0 which is more sympathetic to the geometry of Γ (which we now denote by Γ_N to indicate the N rays). We are guided by two examples [Eastham P.M.S.. 1966 and 1967].

(i) For the symmetric Γ_4 in Example 2.3, the level curves of Ψ are $|x| + |y| = const$ giving a contour map consisting of squares with vertices on the axes.

(ii) For the symmetric Γ_6, (Exner and Ncova, 2003) derive computationally a corresponding diagram in which again each level curve is furthest from the origin at points on the rays.

Thus we now consider

$$f_0(x) = exp\{-arg(\phi)\},$$

where $g(6)$ has its minimum value (say 1) on the rays $6 = Q \pm ofFN$. Proceeding as in Prop. 3.1 with a choice of a, we obtain

$$\lambda_{0,N} \leq V(f_0) \leq -N^2 c^2 / I_1 I_2 \tag{13}$$

where

$$I_1 = 2\pi + \int_0^{2\pi} g'^2/g^2 \, d\theta,$$

$$I_2 = \int_0^{2\pi} 1/g^2 \, d\theta.$$

In a typical sector of PN, we define

$$g(\theta) = (1 + p\beta)^{1/2} \{1 + 2p\left|\frac{1}{2}\beta - t\right|\}^{-\frac{1}{2}}$$

symmetric about the bisector, where $t = \theta - \theta_i$ and $p(> 0)$ is a parameter. This choice of g is such that

(i) it has its minimum value 1 on the rays

(ii) the integrals I_1 and I_2 can be evaluated.

When this is done, a good choice of p in (3.4) is $p = \pi/2N$, and then (3.4) gives the following result (Brown, Eastham and Wood).

Theorem 3.2. For any configuration of Γ_N ,

$$\lambda_{0,N} < -2c^2 N^2 (N^2 + \pi^2)^2 / \{\pi^2 (2N^2 + \pi^2)(4N^2 + 5\pi^2)\}.$$

For N = 3, 4, 5, 6,10, the multiples of $-c^2$ here are 0.273, $0.457, 0.689, 0.970, 2.594$. These are all $> \frac{1}{4}$ and show that $\sigma_d \neq \phi$ for $N \geq 3$. For $N = 2$, however, the multiple is only 0.134 (< $\frac{1}{4}$), and so we have not obtained $\lambda_{0,2} < -\frac{1}{4}c^2$

4. The case N = 2. This case presents a number of difficulties (and opportunities) of its own. The general result in Theorem 2.2 is that $\sigma_d \neq \phi$ for $0 < a < 180°$, where α is the angle between the two rays. To get a simple proof using (3.1), we again want an f_0 such that (3.2) holds. With a quite different type of f_0 from that in section 3, (Exner and Ncova,2003) achieved this for the small range

$$0 < a < 5.3°.$$

Then (Brown, Eastham and Wood.,2008) improved this (with a different f0) to

$$0 < a < 53.1°. \qquad (14)$$

This leads on to a number of open questions.

Question 1. Can an f0 be defined to give $V(f_0) < -\frac{1}{4}c^2 (i.e. \sigma d \neq \phi)$ for α in a larger range $0 < \alpha < \alpha_1$ than (4.1)?

Question 2. What is the nature of the lowest eigenf unction Ψ_0 ?

Question 3. Let $\lambda_n(\alpha)(0 \leq n \leq M(\alpha))$ be the discrete eigenvalues of $\Gamma(\alpha)$. We know that $M(\alpha) \to \infty$ as $\alpha \to 0$ (Exner and Ichinose, 2001). But what are the values of α where $M(\alpha)$ increases by unity?

Question 4. Conjecture (Exner ,2008). For small $\alpha' := 180° - \alpha$,

$$\lambda_0(\alpha) = -\frac{1}{4}c^2 - k\alpha'4 + o(\alpha'5).$$

Question 5. Is $\sigma_d \neq \phi$ when Γ_2 consists of two non-straight curves enclosing a corner?

Question 6. Conjecture (Exner ,2008) For a given N, $\lambda_{0,N}$ is maximized when Γ_N is symmetric.

5. Asymptotically straight Γ and σ_e. Moving away from star graphs now, there is another class of graphs P for which again

$$\sigma_e = [-\frac{1}{4}c^2, \infty) \qquad (15)$$

Thus (Exner and Ichinose,2001) introduced a rather technical set of conditions on Γ which include the idea of "asymptotic straightness" (a.s.) - an example of which is that the curvature

$$|k(s)| \le (const.)s^{-\beta}$$

for some $\beta > 5/4$ as s (arc length) $\to \infty$. Here we give a simpler proof of a related result to (5.1) using a different idea of a.s. and a suitable Weyl sequence f_n in (1.2).
Our idea of asymptotic straightness is simply that Γ should lie close to arbitrarily long disjoint line segments as Γ recedes to infinity. The segments can lie arbitrarily in R^2 but, for convenience, we take them to lie along the x-axis. Thus 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, in each I_m , Γ has the equation $y = F(x)$ with

$$F^{(r)}(x) \to 0 \quad (x \to \infty, 0 \le r \le 3).$$

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 Γ near to it) to a position elsewhere in the plane. Thus, Γ has long, nearly straight, segments far away.)
In our theorems, we can allow a non-constant q in (BC), and we write

$$Q(x) = q(x, F(x)) \quad (Q = q \; on \; P)$$

Theorem 5.1 (Brown, Eastham and Wood.,2008) As $x \to \infty$ through the I $_m$ let

$$Q(x) \to c(c > 0), Q'(x) \to 0, Q''(x) \to 0.$$

Then

$$\sigma_e \supset [-\frac{1}{4}c^2, \infty).$$

Note: $\supset$ rather than = as in (5.1), but our Γ is more general with conditions imposed only in the I_m .

Proof. We use the method of Wey1 sequences and show that there is a sequence $\{f_m\} \in$ D(H) such that $\| f_m \| = 1$ and, as in (1.2),

$$\|(\Delta + \lambda I)f_m\| \to 0 (m \to \infty) \qquad (16)$$

for $\lambda \ge -\frac{1}{4}c^2$. We define f $_m$, supported in the large square $S_m := I_m x(-a_m, a_m)$, by

$$f_m(x) = b_m h_m(x - c_m) h_m(y) exp\{-U(x)|y - F(x)| + iV(x)\}.$$

Here b_m is the normalization factor making $\| f_m \| = 1$, and

$h_m(t) = 1(|t| < a_m - 1), = 0(|t| > a_m).$

Also, U and V are real-valued with $U > 0$. The function U is chosen to make fm satisfy (BC), and thus

$$U = \frac{1}{2} Q (l + F'2)^{-\frac{1}{2}} \tag{17}$$

A calculation gives $b \sim (4a_m/c)^{-1/2} (m \to \infty)$. Then, omitting details of the calculation, we have

$$(\Delta + \lambda l) f_m = (U^2 - V'^2 + \lambda) f_m + E_m \tag{18}$$

where $\|E_m\| \to 0 (m \to \infty)$ (using the conditions imposed in the theorem). By (5.3), $U \sim 1/2c$ (m large), and hence

$$(\Delta + \lambda l) f_m = (1/4c^2 + \lambda - V'^2) f_m + E_m.$$

Then $V(x) = (1/4c^2 + \lambda) \frac{1}{2} x$ gives

$$\|(\Delta + \lambda l) f_m\| = \|E_m\| \to 0 \tag{19}$$

as required. Hence $\lambda \in \sigma_e$, and V is real-valued if $\lambda \geq -\frac{1}{4} c^2$. Theorem 5.2 (Brown, Eastham and Wood, 2009) As x $\to \infty$ through the E $_m$, let

$$Q(x) \to \infty, \int_{I_m} 1/Q(x) dx \to \infty$$

and $Q', QQ'', Q^2 F', QF''$ all tend to zero. Then $\sigma = (-\infty, \infty)$.

Proof. In (5.4), we now choose V = $\sqrt{(U^2 + \lambda)}$. Since U $\to \infty$ as x $\to \infty$, V' is real-valued when m is large enough, for any λ in (- ∞, ∞). Hence again (5.5) holds under the conditions stated here.

Examples 5.3. (i) $Q(x) = x^a (x > 1)$, $F(x) = (const.) x^{-b}$, where

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

(ii) $q = q_m$ (const.) in I_m with $q_m \to \infty, a_m/q_m \to \infty$

We note that Theorems 5.1 and 5.2 are reminiscent of those in (Eastham, 1966 and 1967) for the Schrodinger operator $-\Delta + W$ with conditions on the potential W.

Question 7. Is H essentially self-adjoint under the conditions of Theorem 5.2?

Question 8. Is the range $0 < a < 1$ best possible in Example 5.3 (i)?

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الطيف المستحث هندسيا لمؤثرات شرودنجر

ميشيل استيم

قسم علوم الحاسوب (الكمبيوتر)، جامعة كاردف ، المملكة المتحدة

الملخص

فى هذا البحث تم عرض بعض النتائج الحديثة والجديدة المتعلقة لطيف المؤثرات فى وجود شروط حدية على منحنى معطى فى المستوى (x,y) . ووجد أن طبيعة هندسة المنحنى تؤثر على الطيف ، ونوقشت الاوضاع في ظل وجود شروط مثل (1) وجود انعاث فى الفترة $[-c^2/4,\infty)$, (2) وجود قيم مميزة منفصلة فى الفترة $(-\infty,-c^2/4]$ ، والهدف من ذلك هو تقديم بعض النتائج المهمة وتجنب بعض المشاكل الفنية في البحوث السابقة .