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2009 J. Phys. A: Math. Theor. 42 165208

(http://iopscience.iop.org/1751-8121/42/16/165208)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 165208 (13pp) doi:10.1088/1751-8113/42/16/165208

Hermitian boundary conditions at a Dirichlet singularity: the Marletta–Rozenblum model

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Received 10 February 2009, in final form 11 February 2009
Published 27 March 2009
Online at stacks.iop.org/JPhysA/42/165208

Abstract

In domains B with smoothly-varying boundary conditions, points where wavefunctions are required to vanish were recently identified as 'Dirichlet singularities' (D points) where the Hamiltonian $\boldsymbol{H}$ does not define discrete eigenvalues and a scattering phase is undetermined (Berry and Dennis 2008 *J. Phys. A: Math. Theor.* **41** 135203). This is explained (Marletta and Rozenblum 2009 *J. Phys. A: Math. Theor.* **42** 125204) by the observation, illustrated with an exactly-solvable separable model, that a D point requires the specification of an additional parameter defining a family of self-adjoint extensions of $\boldsymbol{H}$. Here the underlying theory is presented in an elementary way, and a D point is identified as a leak, through which current can flow into or out of B. Hermiticity seals the leak, ensuring that no current flows though the D point (as well as across the boundary of B). The solvable model is examined in detail for bound states, where B is a semidisk, and for wave reflections, where B is a half-plane. The quantization condition for a nonseparable billiard is obtained explicitly.

PACS numbers: 02.70.Hm, 02.30.Tb, 02.40.Xx, 03.65.Ge, 03.65.Nk

1. Introduction and the Marletta–Rozenblum model

Recently, Mark Dennis and I [1] considered solutions ψ of the Helmholtz equation in a planar domain B, with mixed (Robin) boundary conditions that vary along the boundary ∂B according to a real function $q(\boldsymbol{r})$, that is

$$\begin{aligned}&\boldsymbol{H}\psi(\boldsymbol{r}) = -\nabla^2\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) = k^2\psi(\boldsymbol{r})\\ &(\boldsymbol{r} = \{x, y\} = r\{\cos\theta, \sin\theta\} \text{ in B}),\\ &\psi(\boldsymbol{r}) + q(\boldsymbol{r})\boldsymbol{n}(\boldsymbol{r})\cdot\nabla\psi(\boldsymbol{r}) = 0(\boldsymbol{r} \text{ on } \partial\text{B}),\end{aligned}\tag{1.1}$$

where $\boldsymbol{n}(\boldsymbol{r})$ is the outward normal on ∂B (in [1] we used the notation $\kappa(\boldsymbol{r}) = 1/q(\boldsymbol{r})$). We identified points where the conditions are locally Dirichlet ($q(\boldsymbol{r}) = 0$, i.e. $\psi = 0$) as singularities ('D points'): for a bounded domain, (1.1) fails to generate a discrete spectrum, and for reflection the phase of an associated scattering function was undetermined. If there are no D points, these difficulties do not arise, and each choice of $q(\boldsymbol{r})$ can be regarded as defining a self-adjoint extension of the differential operator $-\nabla^2$.

In a sophisticated application of operator theory, Marletta and Rozenblum [2] have clarified the situation, by explaining why the arguments in [1] were incomplete. The specification of $q(\boldsymbol{r})$ does not define a self-adjoint (Hermitian) extension of $-\nabla^2$ if ∂B contains a D point: a further boundary condition, defined by an additional parameter, is required. To illustrate the general theory, they considered an ingenious exactly solvable separable model, in which ∂B is the y-axis, with a D point at $y = 0$, defined by

$$\psi - \varepsilon y\,\partial_x\psi = \psi + \varepsilon\partial_\theta\psi = 0 \quad \left(x = 0, \text{i.e.}\ \theta = \pm\tfrac{1}{2}\pi\right), \tag{1.2}$$

and B is the unit semidisk with Dirichlet conditions on the curved part, that is

$$\psi = 0\ (x \geqslant 0,\ r = 1). \tag{1.3}$$

In fact, the family of self-adjoint extensions associated with a D point can be understood using elementary arguments familiar to physicists (section 2). The usual hermiticity requirement that no current flows across ∂B is extended to forbid current flowing through the D point. The quantization condition that this implies for the Marletta–Rozenblum model (1.2) and (1.3) is worth presenting explicitly, in several equivalent forms (section 3). One of the formulations—insisting that states with different eigenvalues are orthogonal—enables the explicit solution (section 4) of the problem outstanding from [1]: determining discrete eigenvalues in the nonseparable model considered there.

If ∂B is the entire y-axis, and B the half-space $x > 0$, the condition (1.2) defines an interesting exactly solvable reflection problem. It suffices to study normal incidence, and since the problem contains no length parameter other than the wavelength $2\pi/k$ there is no loss of generality in choosing $k = 1$; thus the incident wave is

$$\psi_{\text{inc}} = \exp(-\mathrm{i}x). \tag{1.4}$$

The reflected wave is derived in section 5, and it is shown that the phase we were unable to determine in [1] can be interpreted as the additional self-adjoint extension parameter identified by Marletta and Rozenblum.

It has long been recognised that additional parameters are needed to disambiguate operators associated with singular points, for example in the modelling of point contacts [3]. And the self-adjoint extensions associated with radial potentials singular at the origin (see [4, 5], and section 5 of [6]), involving Bessel functions of imaginary order, turn out to be mathematically closely related to the singularities on boundaries considered here.

2. Self-adjoint extensions

The most elementary condition, generalizing the Hermiticity requirement for finite matrices, is

$$H_{12} = -\iint_{\mathrm{B}} \mathrm{d}^2\boldsymbol{r}\,\psi_1^*\nabla^2\psi_2 = H_{21}^* = -\iint_{\mathrm{B}} \mathrm{d}^2\boldsymbol{r}\,\psi_2\nabla^2\psi_1^*, \tag{2.1}$$

where ψ_1 and ψ_2 are any functions in the space on which $\boldsymbol{H}$ acts. Application of Green's theorem gives

$$H_{12} - H_{21}^* = -\oint_{\partial\mathrm{B}'} \mathrm{d}s\,(\psi_1^*\boldsymbol{n}\cdot\nabla\psi_2 - \psi_2\boldsymbol{n}\cdot\nabla\psi_1^*) = 0, \tag{2.2}$$

where $\partial\mathrm{B}'$ is a curve close to the boundary. If there are no D points, $\partial\mathrm{B}'$ can be chosen to coincide with ∂B, and the mixed boundary condition in (1.1) guarantees that (2.2) is satisfied.

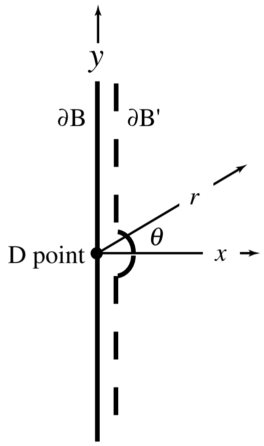

Figure 1. Integration contour $\partial B'$ near a Dirichlet singularity on the boundary ∂B of the domain B.

Even if there is a D point, some of the solutions are regular and the limit $\partial B' \to \partial B$ is still unproblematic. But we shall see that for other solutions the limit is singular, and it is necessary to choose $\partial B'$ avoiding the D point, as in figure 1. Choosing the origin at the D point, the local behaviour of solutions ψ can be determined from singular solutions of the model (1.2), which by application of (1.1) can be confirmed to be

$$\psi = \exp\left(-\frac{\theta}{\varepsilon}\right)\left(\alpha_+ J_{\mathrm{i}/\varepsilon}(kr) + \alpha_- J_{-\mathrm{i}/\varepsilon}(kr)\right). \tag{2.3}$$

The angular part of the integral in (2.2) around the semicircular arc avoiding the D point (figure 1) is nonsingular, so (2.2) requires just the radial condition

$$\lim_{r\to 0} r\left(\psi_1^* \partial_r \psi_2 - \psi_2 \partial_r \psi_1^*\right) = 0. \tag{2.4}$$

Using

$$J_{\mathrm{i}/\varepsilon}(t) \approx \frac{\exp\left\{\frac{\mathrm{i}}{\varepsilon}\log\left(\frac{t}{2}\right)\right\}}{\Gamma(\mathrm{i}/\varepsilon + 1)} \quad (t \ll 1), \tag{2.5}$$

the general solution of the Helmholtz equation near the D point has the form

$$\psi \approx \exp\left(-\frac{\theta}{\varepsilon}\right)\left(A_+ \exp\left(\frac{\mathrm{i}}{\varepsilon}\log r\right) + A_- \exp\left(-\frac{\mathrm{i}}{\varepsilon}\log r\right)\right) \quad (kr \ll 1)). \tag{2.6}$$

In general, the multipliers A_+ and A_- are different for the states ψ_1 and ψ_2. But a short calculation shows that (2.2) is satisfied by choosing

$$A_{\pm 1} = A_1 \exp(\pm \mathrm{i}\Lambda), \quad A_{\pm 2} = A_2 \exp(\pm \mathrm{i}\Lambda), \tag{2.7}$$

in which A_1 and A_2 are arbitrary complex numbers but Λ is common to all states. The local solution (2.6) can now be written

$$\psi \approx 2A \exp\left(-\frac{\theta}{\varepsilon}\right)\cos\left(\frac{1}{\varepsilon}\log r + \Lambda\right). \tag{2.8}$$

This is equivalent to the boundary condition obtained in equation (20) of [2].

As we will see in the next sections, each choice of Λ defines a self-adjoint extension of $\boldsymbol{H} = -\nabla^2$. The restriction to the 'locally real' form (2.8) guarantees the reality of the expectation value of $\boldsymbol{H}$. Moreover it extends the familiar interpretation of the mixed boundary conditions, involving the current

$$\boldsymbol{j} = \mathrm{Im}\psi^* \nabla \psi. \tag{2.9}$$

Even if $|A_+| \neq |A_-|$, i.e. (2.7) is violated, the Robin condition in (1.1) guarantees that there is no current through ∂B away from a D point. We will see that the effect of (2.7) is to prevent current flowing through the D point itself.

3. Bound states with a D point

For the semidisk B, there are nonsingular solutions satisfying (1.2) and (1.3), namely [2]

$$\begin{aligned} &\psi(r,\theta) = (\sin n\theta + D_n \cos n\theta) J_n(k_{mn} r), \qquad n = 1, 2, 3, \ldots, \\ &D_n = -n\varepsilon \quad \text{if} \quad n \text{ is even}, \qquad \frac{1}{n\varepsilon} \text{if } n \text{ is odd}, \qquad J_n(k_{mn}) = 0. \end{aligned} \tag{3.1}$$

These states are unaffected by the D point, and the eigenvalues $E_{mn} = k_{mn}^2$ (all positive) are the same as for the complete circle with Dirichlet boundary conditions, determined by the Bessel zeros.

But there are also solutions singular at the D point, of the form (2.3), which can be made to satisfy the Dirichlet condition (1.3) by choosing the (real) combination

$$\psi = -\mathrm{i} \exp\left(-\frac{\theta}{\varepsilon}\right) [J_{\mathrm{i}/\varepsilon}(kr) J_{-\mathrm{i}/\varepsilon}(k) - J_{-\mathrm{i}/\varepsilon}(kr) J_{\mathrm{i}/\varepsilon}(k)]. \tag{3.2}$$

This separation, between states influenced by the D point and states (3.1) that are not, is an attractive, albeit nongeneric, feature of the Marletta–Rozenblum model; in the model considered in [1], and studied further in section 4, the D point contaminates all the states.

The small-r limiting form of (3.2) is

$$\psi \approx \frac{2\left|J_{\mathrm{i}/\varepsilon}(k)\right|}{|\Gamma(\mathrm{i}/\varepsilon + 1)|} \exp\left(-\frac{\theta}{\varepsilon}\right) \sin\left\{\frac{1}{\varepsilon}\log\frac{kr}{2} - \arg J_{\mathrm{i}/\varepsilon}(k) - \arg\Gamma\left(\frac{\mathrm{i}}{\varepsilon} + 1\right)\right\}. \tag{3.3}$$

To incorporate the additional condition involving the self-adjoint extension parameter Λ, we identify with (2.8), giving

$$\Lambda = \frac{1}{\varepsilon}\log\frac{k}{2} - \arg J_{\mathrm{i}/\varepsilon}(k) - \arg\Gamma\left(\frac{\mathrm{i}}{\varepsilon} + 1\right) - \frac{\pi}{2} \quad (\mathrm{mod}\ 2\pi). \tag{3.4}$$

For each choice of Λ, this determines a spectrum of eigenvalues k. As pointed out in [2], the continuous spectrum we studied in [1] is the union of the discrete spectra of all the different self-adjoint extensions.

An instructive alternative form of the condition is obtained by substituting two solutions of the form (3.2), for candidate eigenvalues k_1 and k_2, into (2.4). A little calculation, using

$$\begin{aligned} &\psi \approx 2\exp\left(-\frac{\theta}{\varepsilon}\right) \mathrm{Im}\left[\frac{\exp\left(\frac{\mathrm{i}}{\varepsilon}\log\frac{kr}{2}\right)}{\Gamma(\mathrm{i}/\varepsilon + 1)} J_{-\mathrm{i}/\varepsilon}(k)\right], \\ &r\partial_r\psi \approx \frac{2}{\varepsilon}\exp\left(-\frac{\theta}{\varepsilon}\right) \mathrm{Re}\left[\frac{\exp\left(\frac{\mathrm{i}}{\varepsilon}\log\frac{kr}{2}\right)}{\Gamma(\mathrm{i}/\varepsilon + 1)} J_{-\mathrm{i}/\varepsilon}(k)\right], \end{aligned} \tag{3.5}$$

leads to

$$\mathrm{Im}\left[\exp\left\{\frac{\mathrm{i}}{\varepsilon}\log\left(\frac{k_1}{k_2}\right)\right\} J_{-\mathrm{i}/\varepsilon}(k_1) J_{\mathrm{i}/\varepsilon}(k_2)\right] = 0. \tag{3.6}$$

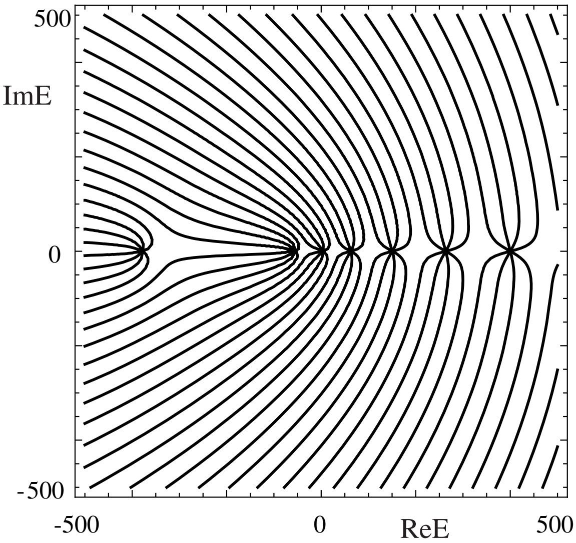

Figure 2. Phase contours of the quantization function (rhs of (3.7)), intersecting at the zeros which are the eigenvalues $E = k^2$, for $\varepsilon = 0.3$ and the additional self-adjoint extension chosen such there is an eigenvalue $E = 2$. Note that there two negative eigenvalues shown, and no complex eigenvalues. The contours are for phases $\pi\left(\frac{1}{6}+\frac{1}{4}n\right)\quad(n = 0, 1, 2, 3)$.

To understand this as a quantization condition, imagine fixing k_2 and solving for k_1, noting that $k_1 = k_2$ is one of the solutions. Thus (3.6) determines the spectrum that includes the specified k_1 as an eigenvalue. We can interpret (3.6) for complex k_1 by writing it as

$$\begin{aligned} 0 = {}& \exp\left\{\frac{\mathrm{i}}{\varepsilon}\log\left(\frac{k_1}{k_2}\right)\right\} J_{-\mathrm{i}/\varepsilon}(k_1)J_{\mathrm{i}/\varepsilon}(k_2) \\ & - \exp\left\{-\frac{\mathrm{i}}{\varepsilon}\log\left(\frac{k_1}{k_2}\right)\right\} J_{\mathrm{i}/\varepsilon}(k_1)J_{-\mathrm{i}/\varepsilon}(k_2). \end{aligned} \tag{3.7}$$

As figure 2 illustrates and as self-adjointness implies, this complex function has all its zeros $E = k_1^2$ on the real axis; there are negative E (k imaginary) as well as positive E.

The asymptotics of the eigenvalues determined by (3.6) can be found from the large-argument asymptotics of the Bessel functions. For large positive E, the asymptotic quantization condition, when there is a zero at $E_0 = k_2^2$, is

$$\mathrm{Im}\left[\exp\left\{\mathrm{i}\left(\frac{1}{2\varepsilon}\log\frac{E}{E_0}+\arg J_{\mathrm{i}/\varepsilon}(\sqrt{E_0})\right)\right\}\cos\left(\sqrt{E}-\frac{1}{4}\pi+\mathrm{i}\frac{\pi}{2\varepsilon}\right)\right]\approx 0. \tag{3.8}$$

For small ε this can be written more explicitly:

$$\sqrt{E}-\frac{1}{2\varepsilon}\log\frac{E}{E_0}-\arg J_{\mathrm{i}/\varepsilon}(\sqrt{E_0})\approx\left(n+\frac{1}{4}\right)\pi. \tag{3.9}$$

For large negative E, (3.6) gives

$$E \approx -E_0\exp\{2\varepsilon(n\pi - \arg J_{\mathrm{i}/\varepsilon}(\sqrt{E_0}))\}. \tag{3.10}$$

Thus the counting function $N(E)$, defined as the number of eigenvalues between 0 and E, is

$$N(E)\sim\begin{cases}\sqrt{E} & (E\gg 0)\\ \log|E| & (E\ll 0).\end{cases} \tag{3.11}$$

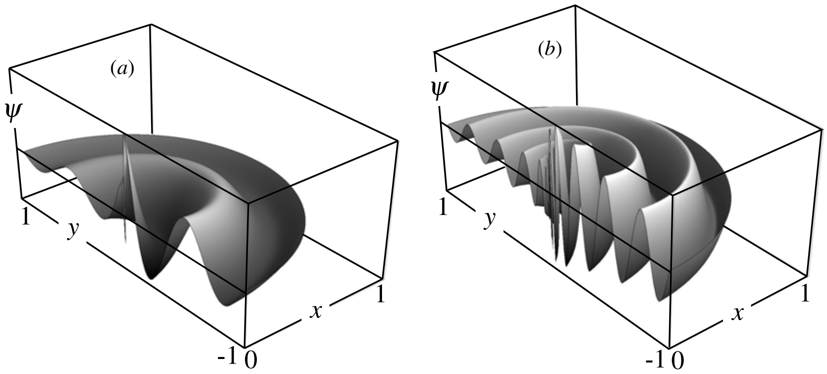

Figure 3. Eigenfunctions (3.2) for (*a*) $\varepsilon = 1$, $k = 10$, (*b*) $\varepsilon = 0.2$, $k = 20$.

The asymptotics (3.8) and (3.10) agree very well with numerical calculations based on the exact quantization formula (3.6).

Figure 3 displays two of the eigenstates (3.2), clearly showing the fast oscillations close to the D point, described by (3.3).

To see the connection between self-adjoint extensions specified by Λ and by k_2, we rewrite (3.6) with $k_1 = k$, and use (3.4):

$$\sin\left\{\frac{1}{\varepsilon}\log\frac{k}{2} - \arg J_{\mathrm{i}/\varepsilon}(k) + \arg J_{\mathrm{i}/\varepsilon}(k_2) - \frac{1}{\varepsilon}\log\frac{k_2}{2}\right\}$$

$$= \sin\left\{\Lambda + \arg J_{\mathrm{i}/\varepsilon}(k_2) - \frac{1}{\varepsilon}\log\frac{k_2}{2} + \arg\Gamma\left(\frac{\mathrm{i}}{\varepsilon}+1\right) + \frac{\pi}{2}\right\} = 0. \tag{3.12}$$

Thus the relation between the two self-adjoint extension parameters is

$$\Lambda = -\arg J_{\mathrm{i}/\varepsilon}(k_2)\frac{1}{\varepsilon}\log\frac{k_2}{2} - \arg\Gamma\left(\frac{\mathrm{i}}{\varepsilon}+1\right) - \frac{\pi}{2}. \tag{3.13}$$

The solutions (3.2), singular at the D point, are orthogonal to the regular solutions (3.1); this follows from the angular integral in the integration over B. And the condition for orthogonality of any two solutions (3.1), with different eigenvalues k_1 and k_2, is precisely the quantization condition (3.6); this can be shown by a careful argument making use of using the indefinite integral [7]

$$\iint \mathrm{d}r r\, J_{\mu\mathrm{i}/\varepsilon}(k_1 r) J_{\nu\mathrm{i}/\varepsilon}(k_2 r)$$

$$= \frac{1}{k_1^2 - k_1^2}\left[k_2 r J_{\mu\mathrm{i}/\varepsilon}(k_1 r) J_{\nu\mathrm{i}/\varepsilon-1}(k_2 r) - k_1 r J_{\mu\mathrm{i}/\varepsilon-1}(k_1 r) J_{\nu\mathrm{i}/\varepsilon}(k_2 r)\right.$$
$$\left. + \frac{\mathrm{i}}{\varepsilon}(\mu-\nu) J_{\mu\mathrm{i}/\varepsilon}(k_1 r) J_{\nu\mathrm{i}/\varepsilon}(k_2 r)\right]. \tag{3.14}$$

For the solutions (3.2), which are real, the current (2.9) is automatically zero everywhere. For the general separable solution (2.3), which almost always violates the self-adjointness condition (2.7), the current is purely radial, that is

$$\boldsymbol{j} = j_r \boldsymbol{e}_r. \tag{3.15}$$

Therefore no current flows across the diameter of the semidisk ($\theta = \pm\pi/2$). Any solution with $|\alpha_+| = |\alpha_-|$ guarantees in addition that no current leaks though the D point, and the particular form (3.2), with $\alpha_+/\alpha_- = -\exp(-2\mathrm{i}\arg J_{\mathrm{i}/\varepsilon}(k))$, ensures compliance with the Dirichlet condition at $r = 1$.

4. Quantization of the nonseparable billiard of [1]

In [1] we considered the case where B is the unit circle with polar coordinates $\{r, \theta\}$ with the boundary condition, of the form (1.1),

$$\psi(1, \theta) + A \tan \tfrac{1}{2}\theta \, \partial_r \psi(1, \theta) = 0. \tag{4.1}$$

(This avoids the choice $A = 1/k$, adopted in [1] for technical reasons explained there.) Solutions of the Helmholtz equations satisfying this condition with eigenvalue E were found to be

$$\psi_E(\boldsymbol{r}) = \sum_{n=-\infty}^{\infty} a_n(E) \exp(\mathrm{i}n\theta) \frac{J_n(r\sqrt{E})}{J_n(\sqrt{E})}, \tag{4.2}$$

where

$$\begin{aligned} &a_0(E) = 1, \\ &a_{n>0}(E) = (-1)^n \frac{(1 - \mathrm{i}kA\rho_0(E))}{(1 + \mathrm{i}kA\rho_n(E))} \prod_{m=1}^{n-1} \frac{(1 - \mathrm{i}kA\rho_m(E))}{(1 + \mathrm{i}kA\rho_m(E))}, \\ &a_{-n}(E) = a_n^*(E), \end{aligned} \tag{4.3}$$

in which

$$\rho_n(E) = \frac{J_n'(\sqrt{E})}{J_n(\sqrt{E})}. \tag{4.4}$$

Now it is possible to supply the quantization condition, missing in [1], for discrete eigenvalues E. Of the several equivalent procedures in the previous section, the simplest is to stipulate that E_c is an eigenvalue and regard this as a self-adjoint extension parameter, and determine the spectrum containing E_c, consisting of eigenvalues $E = E_n(E_\mathrm{c})$, by imposing orthogonality. This requirement is

$$\int_0^1 \mathrm{d}r\, r \int_0^{2\pi} \mathrm{d}\theta\, \psi_{E_\mathrm{c}}^*(\boldsymbol{r}) \psi_E(\boldsymbol{r}) = 0 \quad (E \neq E_\mathrm{c}). \tag{4.5}$$

With the states (4.2), standard Bessel integrals [7] enable this to be evaluated explicitly, with the result (after multiplication by E–E_c, rendering the condition $E \neq E_\mathrm{c}$ redundant)

$$\begin{aligned} 0 = F(E_0, E) &= \sqrt{E}\rho_0(E) - \sqrt{E_\mathrm{c}}\rho_0(E_\mathrm{c}) \\ &\quad + 2\sum_{n=0}^{\infty} \mathrm{Re}[a_n^*(E_\mathrm{c})a_n(E)](\sqrt{E}\rho_n(E) - \sqrt{E_\mathrm{c}}\rho_n(E_\mathrm{c})). \end{aligned} \tag{4.6}$$

This is the explicit quantization condition whose solutions are the eigenvalues $E = E_n(E_\mathrm{c})$. Using the large-n result $|a_n| \sim 1/n$, derived in [1], and Bessel asymptotics for the factor

$$\sqrt{E}\rho_n(E) - \sqrt{E_\mathrm{c}}\rho_n(E_\mathrm{c}) \approx \frac{E_\mathrm{c} - E}{2n} \quad (n \gg 1), \tag{4.7}$$

we see that the summand decays as $1/n^3$, so the sum converges and can easily be evaluated numerically.

Figure 4 shows the quantization condition for $E_\mathrm{c} = 2$, conveniently displayed as a plot of $\log|F|$, so that the eigenvalues $E_n(E_\mathrm{c})$ appear as negative spikes (the positive spikes, at the Bessel zeros, are artefacts of the otherwise convenient choice of denominator in the

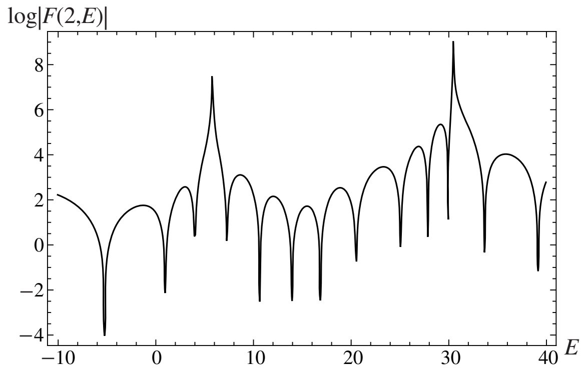

Figure 4. Quantization condition (4.6) for the circle billiard defined by (4.1), with self-adjoint extension parameters $A = 1, E = 2$.

representation (4.2)). Numerics confirms that the same spectrum is obtained starting from any of the eigenvalues $E_n(E_c)$, that is

$$F(E_n(E_c), E_m(E_c)) = 0 \tag{4.8}$$

for all n and m. As figure 4 indicates, the spectrum includes negative as well as positive E. The number of eigenvalues is in good agreement with the Weyl formula for the counting function $N(E)$. Including the boundary term, incorporating the fact that asymptotically the condition (4.1) approaches Neumann, the formula is

$$N(E) = \tfrac{1}{2}E + \tfrac{1}{4}\sqrt{E} + \cdots, \tag{4.9}$$

independent of A and E_c. The corrections incorporate a contribution, so far undetermined, associated with the D singularity. This predicts $N(120) = 35.48$, and I counted 35 numerically determined eigenvalues with $E < 120$.

5. Reflection from a D point

With ∂B consisting of the whole y-axis, we seek the reflected wave generated by the boundary condition (1.2), with the incident wave (1.4). As $y \to \pm\infty$, the boundary condition approaches Neumann ($\partial_x \psi = 0$ on ∂B), so the dominant reflected wave will be +exp(ix). We incorporate this by writing the total wave as the sum of the incident and Neumann-reflected waves, and a scattered wave represented as a superposition of forward-travelling and evanescent plane waves, in the convenient form:

$$\psi = 2\cos x + \int_{-\infty}^{\infty} \frac{\mathrm{d}\kappa}{\sqrt{1-\kappa^2}} b(\kappa) \exp\{\mathrm{i}(y\kappa + x\sqrt{1-\kappa^2})\}. \tag{5.1}$$

Here the square root is positive real if $|\kappa| < 1$, and positive imaginary if $|\kappa| > 1$. The plane-wave amplitude $b(\kappa)$ incorporates the effect of the D point.

Substituting into the boundary condition (1.2) for $x = 0$ gives the equation satisfied by $b(\kappa)$:

$$\frac{b(\kappa)}{\sqrt{1-\kappa^2}} + \varepsilon\partial_\kappa b(\kappa) + 2\delta(\kappa) = 0. \tag{5.2}$$

This has the general solution

$$b(\kappa) = \left(A - \frac{2}{\varepsilon}\Theta(\kappa)\right)\exp\left(-\frac{\sin^{-1}\kappa}{\varepsilon}\right), \tag{5.3}$$

involving the (generally complex) constant A.

To understand how self-adjointness restricts the value of A, we simplify the integral in (5.1) using (5.3). Elementary substitutions and some contour manipulation gives

$$\psi = 2\cos x + \exp\left(-\frac{\theta+\frac{1}{2}\pi}{\varepsilon}\right)\left[A\pi H^{(1)}_{\mathrm{i}/\varepsilon}(r) - \frac{2}{\varepsilon}\int_0^{\theta+\frac{1}{2}\pi}\mathrm{d}t\exp\left(-\frac{t}{\varepsilon}+\mathrm{i}r\sin t\right) + \frac{2\mathrm{i}}{\varepsilon}\int_0^\infty \mathrm{d}w\exp\left(\mathrm{i}\frac{w}{\varepsilon}-r\sinh w\right)\right], \tag{5.4}$$

where H denotes the Hankel function. To find the self-adjoint extensions, we need the small-r asymptotics. Using

$$H^{(1)}_{\mathrm{i}/\varepsilon}(r) = \frac{1}{\sinh\frac{\pi}{\varepsilon}}\left(\exp\frac{\pi}{\varepsilon}J_{\mathrm{i}/\varepsilon}(r) - J_{-\mathrm{i}/\varepsilon}(r)\right) \tag{5.5}$$

and (2.5), and also

$$\left[\frac{\mathrm{i}}{\varepsilon}\int_0^\infty \mathrm{d}w\ \exp\left(\mathrm{i}\frac{w}{\varepsilon}-r\ \sinh\ w\right)\right] \approx -1+\Gamma(\mathrm{i}/\varepsilon+1)\exp\left(-\frac{\mathrm{i}}{\varepsilon}\log\frac{r}{2}\right) \quad (r\ll 1) \tag{5.6}$$

(which can be derived by approximating $\sinh w$ by $(\exp w)/2$ since the small-r behaviour of the integral is dominated by large w), we obtain the singular part of the wave (5.4) as

$$\exp\left(\frac{\mathrm{i}}{\varepsilon}\log\frac{r}{2}\right)\frac{\pi A\exp\frac{\pi}{\varepsilon}}{\Gamma(\mathrm{i}/\varepsilon+1)\sinh\frac{\pi}{\varepsilon}} + \exp\left(-\frac{\mathrm{i}}{\varepsilon}\log\frac{r}{2}\right)\left[-\frac{\pi A}{\Gamma(-\mathrm{i}/\varepsilon+1)\sinh\frac{\pi}{\varepsilon}} + 2\Gamma(\mathrm{i}/\varepsilon+1)\right]. \tag{5.7}$$

The self-adjoint form (2.8) implies that the coefficients of the two terms are equal in modulus. Writing

$$A = |A|\exp(\mathrm{i}\mu) \tag{5.8}$$

leads to the condition

$$\varepsilon^2|A|^2\sinh\frac{\pi}{\varepsilon} + 2\exp\left(-\frac{\pi}{\varepsilon}\right)(\varepsilon|A|\cos\mu - 1) = 0. \tag{5.9}$$

If the phase μ is regarded as fixed, this determines the modulus $|A|$:

$$|A| = \frac{\sqrt{1-\exp\left(-\frac{2\pi}{\varepsilon}\right)\sin^2\mu} - \exp\left(-\frac{\pi}{\varepsilon}\right)\cos\ \mu}{\varepsilon\sinh\frac{\pi}{\varepsilon}}. \tag{5.10}$$

For each choice of ε, this defines a 'hermiticity circle' of self-adjoint extensions in the complex A plane; the circle has radius $1/(\varepsilon\sinh(\pi/\varepsilon))$ and is centred on $A = -2/(\varepsilon(\exp(2\pi/\varepsilon)-1))$.

Thus specifying μ is equivalent to specifying the self-adjoint extension parameter Λ. In [1] we considered a slightly more complicated reflection problem, where $q(\boldsymbol{r})$ varies periodically along ∂B, and were unable to determine the phase of a scattering coefficient; it is now clear that each choice of this parameter, as with μ, determines a different Hermitian scattering problem.

The relation (5.9) can also be obtained from an alternative representation of the self-adjointness condition, also used in [1]: current flowing towards the boundary in the incident

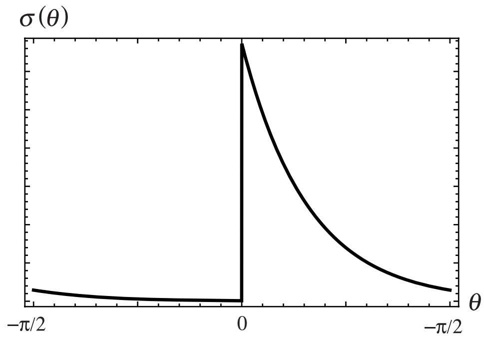

Figure 5. Scattering cross section (5.15) for reflection from a Dirichlet singularity, for $\varepsilon = 1$.

wave must be balanced by current flowing away from the boundary in the Neumann-reflected and scattered waves. Thus

$$I_x = \int_{-\infty}^{\infty} \mathrm{d}y \, \mathrm{Im}\psi^* \partial_x \psi = 0. \tag{5.11}$$

With (5.1), this gives

$$\int_{-1}^{1} \frac{\mathrm{d}\kappa}{\sqrt{1-\kappa^2}} |b(\kappa)|^2 = \int_{-1/2\pi}^{-1/2\pi} \mathrm{d}\theta |b(\sin\theta)|^2 = -2\mathrm{Re}\, b(0), \tag{5.12}$$

which is the form of the optical theorem (unitarity of the scattering operator) for the situation considered here (cf [8]). Substituting (5.3) gives (5.9), as claimed.

It is worth examining the solution (5.1) in a little more detail. The scattered wave is

$$\psi_{\mathrm{sc}} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\kappa}{\sqrt{1-\kappa^2}} b(\kappa) \exp\{\mathrm{i}(y\kappa + x\sqrt{1-\kappa^2})\}. \tag{5.13}$$

In polar coordinates, the large-r asymptotics, obtained by applying the method of stationary phase, is

$$\psi_{\mathrm{sc}} \underset{r\to\infty}{\to} \sqrt{\frac{2\pi}{\mathrm{i}r}} \exp(\mathrm{i}r) b(\sin\theta) = \frac{\exp(\mathrm{i}r)}{\sqrt{r}} f(\theta). \tag{5.14}$$

This defines the scattering amplitude $f(\theta)$, and hence the differential scattering cross section

$$\begin{aligned} \sigma(\theta) &= |f(\theta)|^2 = 2\pi |b(\sin\theta)|^2 \\ &= 2\pi |A|^2 \exp\left(-\frac{2\theta}{\varepsilon}\right) \left(\Theta(-\theta) + \exp\left(\frac{2\pi}{\varepsilon}\right) \Theta(\theta)\right) \end{aligned} \tag{5.15}$$

(in which (5.9) has been used to simplify the formula). Figure 5 shows the unusual scattering pattern corresponding to this function. When the wavenumber k is reinstated, (5.15) remains valid as written; because there is no length scale, the scattering depends only on three dimensionless quantities: the scattering angle θ and the self-adjoint extension parameters ε and (via 5.10) μ.

Figure 6 shows two representations of the wave. In the scattered part ψ_{sc} (figure 6(*a*)), all the current flows away from ∂B, as it must. In the total wave ψ (figure 6(*b*)), interference between the incident and outgoing waves gives rise to a series of wave vortices [9, 10]; this is analogous to what happens in Sommerfeld's wave diffracted by a screen in the form of a half-plane [11], in which vortices arise from interference between the incident plane wave, the plane wave reflected by the screen, and an edge-diffracted wave.

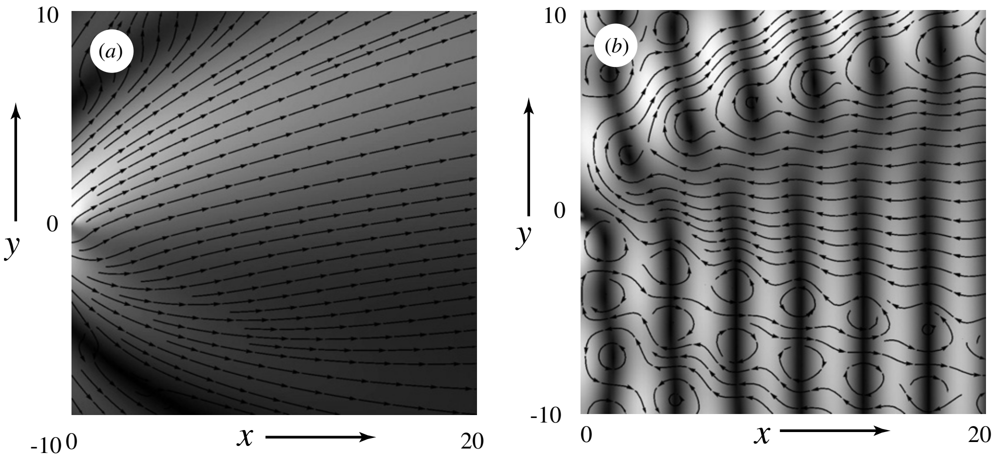

Figure 6. (*a*) Scattered wave $\psi_{\mathrm{sc}} = \psi - 2\cos x$ (equation 5.14) in reflection from a Dirichlet singularity, for $\varepsilon = 1$, $\mu = \arg A = 0$, showing $|\psi_{\mathrm{sc}}|$ as a density plot (with lighter shading representing higher intensity), and streamlines of the current vector $\mathrm{Im}\,\psi_{\mathrm{sc}}^{*}\nabla\psi_{\mathrm{sc}}$. (*b*) As (*a*), for the total wave ψ.

If the self-adjointness condition (5.9) is violated, there will still be no current across ∂B for $y \neq 0$ (though current can flow along ∂B). But there will be current through the D point $x = y = 0$. To explore this, consider real A ($\mu = 0$), for which the hermiticity conditions (5.9) or (5.10) require

$$A = A_1 = \frac{2}{\varepsilon\left(\exp\left(\frac{\pi}{\varepsilon}\right) + 1\right)} \qquad \text{or} \qquad A = A_2 = -\frac{2}{\varepsilon\left(\exp\left(\frac{\pi}{\varepsilon}\right) - 1\right)} \tag{5.16}$$

(intersections of the hermiticity circle with the real axis). For $A_2 < A < A_1$, the current flows into the D point from B; outside this range, the current flows from the D point into B. Therefore we can regard the D point as a portal, though which current can leak between B and the outside world $x < 0$. Hermiticity seals the leak.

To illustrate this, figure 7 shows the total wave for $A = 0$. On a large scale (figure 7(*a*)) this nonhermitian case superficially resembles the Hermitian analogue (figure 6(*b*)). Considerable magnification (figures 7(*b*)–(*e*), with 10,000× for 7(*e*)) is required to unambiguously reveal the current through the D point.

In [1], a more complicated reflection problem was considered: a diffraction grating consisting of the boundary of a half-plane, along which the boundary condition varied periodically, with one D point per period. The solution failed to determine the phase of one of the Bragg-diffracted beams. The simpler model considered here reveals that this was inevitable: the phase is a self-adjoint extension parameter, to be specified in order to define the scattering operator.

6. Concluding remarks

The interpretation of the additional self-adjoint extension parameter as a phase associated with the D point suggests the possibility of a physical implementation. This might take the form of a small hole in ∂B, that could be filled in different ways. If the filling allows current to flow through the hole, this would correspond to not imposing hermiticity. In the Hermitian case,

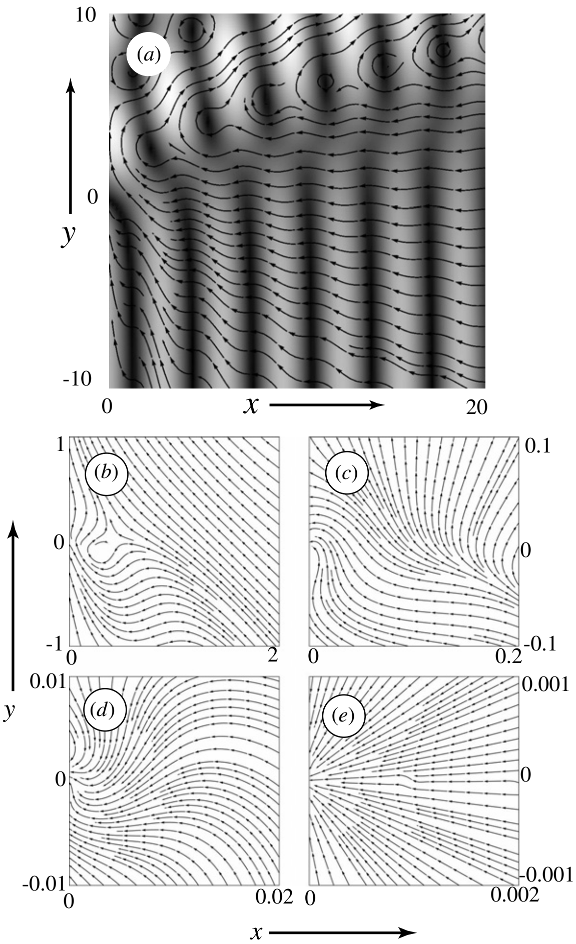

Figure 7. Nonhermitian wave reflection from a D point. (*a*) as figure 6(*b*), with $\varepsilon = 1$, $A = 0$; (*b–e*) magnifications of the current in (*a*), revealing flow into the D point.

the filling would seal the hole, implying a reflected wave whose phase would depend on the type of seal. This deserves further study.

There is an intriguing duality between the D singularities considered here and the more familiar phase singularities (aka optical vortices, nodal points or wave dislocations) [9, 10, 12]. Close to a phase singularity, the azimuthal variation of the phase occurs on scales much smaller than a wavelength (‘superoscillation’, see [13–16]), and, to compensate, the intensity decays radially towards the singularity. By contrast, the solutions (2.6) near a D point are evanescent in azimuth and superoscillate radially. Because azimuthal evanescence is not periodic, this behaviour can occur only in the presence of a boundary, while phase singularities, whose wavefunctions are smooth and single-valued, can occur naturally in free space.

Acknowledgments

I thank Marco Marletta for an instructive correspondence and for sharing several drafts of his paper with Grigori Rozenblum [2], and Mark Dennis, Pragya Shukla and Uzy Smilansky for useful discussions and suggestions.

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