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Spectral asymptotics for the semiclassical Dirichlet to Neumann operator

Andrew Hassell[1] and Victor Ivrii[2]

Abstract. Let M be a compact Riemannian manifold with smooth boundary, and let $R(\lambda)$ be the Dirichlet–to–Neumann operator at frequency λ. The semiclassical Dirichlet–to–Neumann operator $R_{\mathrm{scl}}(\lambda)$ is defined to be $\lambda^{-1}R(\lambda)$. We obtain a leading asymptotic for the spectral counting function for $R_{\mathrm{scl}}(\lambda)$ in an interval $[a_1, a_2)$ as $\lambda \to \infty$, under the assumption that the measure of periodic billiards on T^*M is zero. The asymptotic takes the form

$$\mathsf{N}(\lambda; a_1, a_2) = (\kappa(a_2) - \kappa(a_1))\,\mathrm{vol}'(\partial M)\lambda^{d-1} + o(\lambda^{d-1}),$$

where $\kappa(a)$ is given explicitly by

$$\kappa(a) = \frac{\omega_{d-1}}{(2\pi)^{d-1}}\Big(-\frac{1}{2\pi}\int_{-1}^{1} (1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta - \frac{1}{4} + H(a)(1+a^2)^{(d-1)/2}\Big).$$

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1. Introduction

Let M be a Riemannian manifold with boundary. The Dirichlet–to–Neumann operator is a family of operators defined on $L^2(\partial M)$ depending on the parameter $\lambda \geq 0$. It is defined as follows: given $f \in L^2(\partial M)$, we solve the equation (if possible)

$$(\Delta - \lambda^2)u = 0 \text{ on } M, \quad u|_{\partial M} = f. \tag{1.1}$$

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Then the Dirichlet–to–Neumann operator at frequency λ is the map

$$R(\lambda)\colon f \longmapsto -\partial_\nu u|_{\partial M}. \tag{1.2}$$

Here ∂_ν is the interior unit normal derivative, and Δ is the positive Laplacian on M.

It is well known that $R(\lambda)$ is a self-adjoint, semi-bounded from below pseudodifferential operator of order 1 on $L^2(\partial M)$, with domain $H^1(\partial M)$. It therefore has discrete spectrum accumulating only at $+\infty$. The Dirichlet–to–Neumann operator and closely related operators are important in a number of areas of mathematical analysis including inverse problems (such as Calderón's problem [3]), domain decomposition problems (such as the determinant gluing formula of Burghelea, Friedlander, and Kappeler [2]), and spectral asymptotics (see e.g. [7]).

In this paper, we are interested in the spectral asymptotics of $R(\lambda)$ in the high-frequency limit, $\lambda \to \infty$. Let us recall standard spectral asymptotics for elliptic differential operators, for simplicity in the simplest case of a positive self-adjoint second order scalar operator. Suppose that Q is such an operator on a manifold M of dimension d, with principal symbol q. Then in the case that M is closed, we have an asymptotic for the number $\mathsf{N}(\lambda)$ of eigenvalues of Q (counted with multiplicity) less than λ^2:

$$\begin{aligned} \mathsf{N}(\lambda) &= (2\pi)^{-d}\,\mathsf{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \le \lambda^2\} + O(\lambda^{d-1}) \\ &= \Big(\frac{\lambda}{2\pi}\Big)^d \mathsf{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \le 1\} + O(\lambda^{d-1}), \end{aligned} \tag{1.3}$$

where the equality of the two expressions on the RHS is a simple consequence of the homogeneity of q. Moreover, if the set of periodic geodesics has measure zero, then there is a two-term expansion of the form

$$\Big(\frac{\lambda}{2\pi}\Big)^d \mathsf{vol}\{(x,\xi) \in T^*M \mid q(x,\xi) \le 1\} + \frac{\lambda^{d-1}}{(2\pi)^d}\int_{\{q=1\}} \mathsf{sub}(Q) + o(\lambda^{d-1})$$

where $\mathsf{sub}(Q)$ is the subprincipal symbol of Q, see [5]. This was generalised to the case of manifolds with boundary by the second author [11]. For simplicity we state the result in the case that $Q = \Delta$ is the (positive) metric Laplacian, which satisfies $\mathsf{sub}(\Delta) = 0$. Then Δ is a self-adjoint operator under either Dirichlet $(-)$ or Neumann $(+)$ boundary conditions, and if the set of periodic generalised bicharacteristics has measure zero, we get a two-term expansion for $\mathsf{N}_\Delta(\lambda)$ of the form

$$\Big(\frac{\lambda}{2\pi}\Big)^d \mathsf{vol}\, B^*M \pm \frac{1}{4}\Big(\frac{\lambda}{2\pi}\Big)^{d-1} \mathsf{vol}\, B^*\partial M + o(\lambda^{d-1}). \tag{1.4}$$

These statements can be generalized to the semiclassical setting. Consider a classical Schrödinger operator on M, $P = h^2\Delta + V(x) - 1$, where $h > 0$ is a small parameter ("Planck's constant") and V is a smooth real-valued function. We consider the asymptotic behaviour $\mathsf{N}_h^-(P)$ of the number of negative eigenvalues of P as $h \to 0$. This is equivalent to the problem above if $h = \lambda^{-1}$ and V is identically zero. Define $p(x,\xi)$ to be the semiclassical symbol of P, i.e. $p = |\xi|^2_{g(x)} + V(x) - 1$. Then, if M is closed, under the assumption that the measure of periodic bicharacteristics of P is zero in T^*M, and that 0 is a regular value for p, we have

$$\mathsf{N}_h^-(P) = (2\pi h)^{-d}\operatorname{vol}\{(x,\xi) \in T^*M \mid p(x,\xi) \leq 0\} + O(h^{1-d}). \tag{1.5}$$

Moreover, for manifolds with boundary, we have an analogue of (1.4): under either Dirichlet ($-$) or Neumann ($+$) boundary conditions, if the set of periodic generalised bicharacteristics has measure zero, we get a two-term expansion for $\mathsf{N}_h^-(P)$ (where here we understand the self-adjoint realization of P with either Dirichlet or Neumann boundary condition) of the form

$$(2\pi h)^{-d}\operatorname{vol}\{(x,\xi) \in T^*M \mid p(x,\xi) \leq 0\} \pm \frac{1}{4}(2\pi h)^{1-d}\operatorname{vol}\mathcal{H} + o(h^{1-d}), \tag{1.6}$$

where $\mathcal{H} \subset T^*(\partial M)$ is the hyperbolic region in the boundary, that is, the projection of the set $\{(x,\xi) \mid p(x,\xi) \leq 0\} \cap T^*_{\partial M}M$ to $T^*\partial M$.

From the semiclassical point of view, since $R(\lambda)$ is a first order operator, it makes sense to consider $R_{\mathrm{scl}}(\lambda) := \lambda^{-1}R(\lambda)$ (for $\lambda > 0$), which we call the semiclassical Dirichlet–to–Neumann operator. Like $R(\lambda)$, it is a self-adjoint, semi-bounded from below operator on $L^2(\partial M)$, with discrete spectrum accumulating only at $+\infty$. The goal of this paper is to investigate the spectral asymptotics of $R_{\mathrm{scl}}(\lambda)$, that is, the asymptotics of

$$\mathsf{N}(\lambda; a_1, a_2) := \#\{\beta\colon \beta \text{ is an eigenvalue of } R_{\mathrm{scl}}(\lambda),\ a_1 \leq \beta < a_2\}, \tag{1.7}$$

the number of eigenvalues of $R_{\mathrm{scl}}(\lambda)$ in the interval $[a_1, a_2)$, as $\lambda \to \infty$.

Both $R(\lambda)$ and $R_{\mathrm{scl}}(\lambda)$ have the disadvantage that they are undefined whenever λ^2 is a Dirichlet eigenvalue, since then (1.1) is not solvable for arbitrary $f \in H^1(M)$. Indeed, when λ^2 is a Dirichlet eigenvalue, a necessary condition for solvability of (1.1) is that f is orthogonal to the normal derivatives of Dirichlet eigenfunctions at frequency λ. To overcome this issue, we introduce the *Cayley transform* of $R_{\mathrm{scl}}(\lambda)$: we define

$$C(\lambda) = (R_{\mathrm{scl}}(\lambda) - i)(R_{\mathrm{scl}}(\lambda) + i)^{-1}. \tag{1.8}$$

This family of operators is related to impedance boundary conditions: we have $C(\lambda)f = g$ if and only if there is a function u on M satisfying

$$(\Delta - \lambda^2)u = 0 \tag{1.9}$$

and

$$\frac{1}{2}(\lambda^{-1}\partial_\nu u - iu) = f, \quad \frac{1}{2}(\lambda^{-1}\partial_\nu u + iu) = g. \tag{1.10}$$

As observed in [1], $C(\lambda)$ is a well-defined analytic family of operators for λ in a neighbourhood of the positive real axis, which is unitary on the real axis. In particular, it is well-defined even when λ^2 is a Dirichlet eigenvalue of the Laplacian on M. As a unitary operator, $C(\lambda)$, $\lambda > 0$, has its spectrum on the unit circle, and as $R_{\mathrm{scl}}(\lambda)$ has discrete spectrum accumulating only at ∞, it follows that the spectrum of $C(\lambda)$ is discrete on the unit circle except at the point 1. Our question can be formulated in terms of $C(\lambda)$: given two angles θ_1, θ_2 satisfying $0 < \theta_1 < \theta_2 < 2\pi$, what is the leading asymptotic for

$$\tilde{\mathsf{N}}(\lambda;\theta_1,\theta_2) := \#\{e^{i\theta} : e^{i\theta} \text{ is an eigenvalue of } C(\lambda),\ \theta_1 \le \theta < \theta_2\} \tag{1.12}$$

the number of eigenvalues of $C(\lambda)$ in the interval $\{e^{i\theta} : \theta \in [\theta_1, \theta_2)\}$ of the unit circle, as $\lambda \to \infty$. Clearly, we have

$$\tilde{\mathsf{N}}(\lambda;\theta_1,\theta_2) = \mathsf{N}(\lambda; a_1, a_2), \quad \text{where } e^{i\theta_j} = \frac{a_j - i}{a_j + i}, \text{ i.e. } a_j = -\cot\Bigl(\frac{\theta_j}{2}\Bigr). \tag{1.13}$$

To answer this question we relate it to a standard semiclassical eigenvalue counting problem on M. To state the next result, we first define the self-adjoint operator $P_{a,h}$ on $L^2(M)$ by

$$\mathfrak{D}(P_{a,h}) = \{u \in H^2(M) : (h\partial_\nu + a)u = 0 \text{ at } \partial M\}, \tag{1.14}$$

$$P_{a,h}(u) = (h^2\Delta - 1)u, \quad u \in \mathfrak{D}(P_{a,h}). \tag{1.15}$$

It is the self-adjoint operator associated to the semi-bounded quadratic form

$$h^2\|\nabla u\|_M^2 - \|u\|_M^2 - ha\|u\|_{\partial M}^2. \tag{1.16}$$

The operator $P_{a,h}$ is linked with the semiclassical Dirichlet–to–Neumann operator as follows: if f is an eigenfunction of $R_{\mathrm{scl}}(\lambda)$ with eigenvalue a, then the corresponding Helmholtz function u defined by (1.1) is in the domain (1.14) of $P_{a,h}$, and $P_{a,h}u = 0$ (where $h = \lambda^{-1}$).

Then we have the following result, proved in Section 2.

Proposition 1.1. *Let* $h = \lambda^{-1}$. *Assume* $0 < \theta_1 < \theta_2 < 2\pi$. *Then the number of eigenvalues of* $C(\lambda)$ *in the interval* $J_{\theta_1,\theta_2} := \{e^{i\theta} : \theta \in [\theta_1, \theta_2)\}$ *is equal to*

$$\tilde{N}(\lambda; \theta_1, \theta_2) = N(\lambda; a_1, a_2) = N_h^-(a_2) - N_h^-(a_1), \tag{1.17}$$

where $a_j = -\cot(\theta_j/2)$ *and*

$$N_h^-(a) := \#\{\mu : \mu \text{ is an eigenvalue of } P_{a,h},\ \mu < 0\}. \tag{1.18}$$

Having thus reduced the problem to a standard question about semiclassical spectral asymptotics, we obtain (after some calculations in Section 3) our main result.

Theorem 1.2. (i) *The following estimate for the quantity* (1.12) *holds*:

$$N(\lambda; a_1, a_2) = O(\lambda^{d-1}); \tag{1.19}$$

(ii) *Further, if the set of periodic billiards on* M *has measure* 0 *then the following asymptotic holds as* $\lambda \to +\infty$:

$$N(\lambda; a_1, a_2) = (\kappa(a_2) - \kappa(a_1)) \operatorname{vol}'(\partial M)\lambda^{d-1} + o(\lambda^{d-1}), \tag{1.20}$$

where $\kappa(a)$ *is given explicitly by*

$$\begin{aligned}\kappa(a) = \frac{\omega_{d-1}}{(2\pi)^{d-1}}\Big(&-\frac{1}{2\pi}\int_{-1}^{1}(1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta \\ &-\frac{1}{4} + H(a)(1+a^2)^{(d-1)/2}\Big).\end{aligned} \tag{1.21}$$

Here $H(\cdot)$ *is the Heaviside function,* ω_d *is the volume of the unit ball in* $\mathbb{R}^d$, *and* $\operatorname{vol}(M)$ *and* $\operatorname{vol}'(\partial M)$ *are d-dimensional volume of* M *and* $(d-1)$*-dimensional volume of* ∂M *respectively.*
In the case $d = 3$, *we can evaluate this integral exactly and we find that*

$$\kappa(a) = \frac{1}{4\pi}\Big(-\frac{1}{4} - \frac{1}{\pi}\operatorname{arccot}(a)(1+a^2) + (1+a^2) + \frac{1}{\pi}a\Big) \tag{1.22}$$

where arccot *has range* $(0, \pi)$. *This is simpler expressed in terms of* θ. *Defining* $\tilde{\kappa}(\theta) = \kappa(a)$ *where* $a = -\cot(\theta/2) = \cot(\pi - \theta/2)$, *we have (still under the zero-measure assumption on periodic billiards)*

$$\tilde{N}(\lambda; \theta_1, \theta_2) = (\tilde{\kappa}(\theta_2) - \tilde{\kappa}(\theta_1)) \operatorname{vol}'(\partial M)\lambda^2 + o(\lambda^2), \tag{1.23}$$

$$\tilde{\kappa}(\theta) = \frac{1}{4\pi}\Big(-\frac{1}{4} + \frac{1}{2\pi}\Big(\frac{\theta - \sin\theta}{\sin^2(\theta/2)}\Big)\Big). \tag{1.24}$$

Remark 1.3. It looks disheartening that we only get an upper bound in case (i) and only a "o" remainder under a global geometric condition, but it is the nature of the beast.

In regards to case (i), consider M a hemisphere; then for $\lambda_n^2 = n(n+d-1)$ with $n \in \mathbb{Z}^+$ the operator $R(\lambda)$ has eigenvalue 0 of multiplicity $\asymp n^{d-1}$, hence $N(\lambda; a_1, a_2)$ jumps by at least $c\lambda^{d-1}$ as a_1 or a_2 crosses zero. Therefore, in this case, we do not have an asymptotic, but only an estimate.

In regards to case (ii), we believe that the "o" remainder is the best that can be achieved using current technology. To justify this, consider the problem of finding the spectral asymptotics of the semiclassical Dirichlet–to–Neumann operator for the operator $\Delta + \lambda^2$, instead of $\Delta - \lambda^2$ (for real λ). In this case, one can readily check that the semiclassical Dirichlet–to–Neumann operator is a semiclassically elliptic pseudodifferential operator on the boundary, with principal symbol $\sqrt{1 + h^2\Delta_{\partial M}}$. Then standard spectral asymptotics hold for this operator, and we would get a remainder term $O(\lambda^{d-2})$. However, for the operator $\Delta - \lambda^2$, the semiclassical Dirichlet–to–Neumann operator is only microlocally elliptic in the region $\{(y, \eta) \mid |\eta|_{g'} > 1\} \subset T^*\partial M$, where g' is the induced metric on the boundary. It is hyperbolic in the region where $|\eta|_{g'} < 1$, and that means there is (currently) no machinery for *directly* tackling its spectral asymptotics. Instead, we proceed by relating it to the spectral asymptotics for the interior problem with a family of boundary conditions depending on the spectral parameter a. This means that the problem is in some sense really d-dimensional, and our $o(\lambda^{d-1})$ remainder is the "ghost" of d-dimensional spectral asymptotics, in which the principal, Weyl term cancels under taking the difference (1.17), and all we are left with is the second term – and only under the global geometric assumption of measure zero periodic billiard trajectories.

We note that under stronger assumptions on the billiard flow, the remainder could be improved, for example to $O(\lambda^{d-1-\delta})$ for some $\delta > 0$ in the case of a Euclidean ellipse or elliptical annulus – see Section 7.4 of [14].

Remark 1.4. One can consider eigenvalues of operator $\rho\lambda^{-1}R(\lambda)$ with $\rho > 0$ smooth on ∂M; then estimates (3.1), (1.19) and asymptotics (3.2), (1.20) hold in the frameworks of statements (i) and (ii) of Theorem 1.2 respectively albeit with $\kappa(a)\,\mathrm{vol}'(\partial M)$ replaced by

$$\int_{\partial M} \kappa(\rho(x')a)\, d\sigma$$

where $d\sigma$ is a natural measure on ∂M; however without this condition $\rho > 0$ problem may be much more challenging; even self-adjointness is by no means guaranteed.

Remark 1.5. Operators of the form $P_{a,h}$ were considered by Frank and Geisinger in [6]. They showed that the trace of the negative part of $P_{a,h}$ has a two-term expansion as $h \to 0$ regardless of dynamical assumptions[1], and the second term in their expansion (the $L_d^{(2)}$ term of [6, Theorem 1.1]) is closely related to $\kappa(a)$, see Remark 3.4.

Remark 1.6. We can rephrase Theorem 1.2 in terms of a limiting measure on the unit circle. For each $\lambda > 0$, let $\mu(h)$, $h = \lambda^{-1}$, denote the atomic measure determined by the spectrum of $C(\lambda)$:

$$\mu(h) = (2\pi h)^{d-1} \sum_{e^{i\theta_j} \in \operatorname{spec} C(h^{-1})} \delta(\theta - \theta_j), \tag{1.25}$$

where we include each eigenvalue according to its multiplicity as usual. Then Theorem 1.2 can be expressed in the following way: the measures $\mu(h)$ converge in the weak-$*$ topology as $h \to 0$ to the measure

$$\omega_{d-1} \operatorname{vol}'(\partial M) \frac{d}{d\theta} \tilde{\kappa}(\theta) d\theta \quad \text{on } (0, 2\pi), \text{ that is on } S^1 \setminus \{1\}.$$

In particular, this measure is absolutely continuous, and finite away from $e^{i\theta} = 1$ with an infinite accumulation of mass as $\theta \uparrow 2\pi$. In this form, we can compare our result with results on the semiclassical spectral asymptotics of scattering matrices. In [4] and [8], the scattering matrix $S_h(E)$ at energy E for the Schrödinger operator $h^2\Delta + V(x)$ on $\mathbb{R}^d$ was studied in the semiclassical limit $h \to 0$. Assuming that V is smooth and compactly supported, that E is a nontrapping energy level, and that the set of periodic trajectories of the classical scattering transformation on T^*S^{d-1} has measure zero, it was shown that the measure $\mu(h)$ defined by (1.25) converged weak-$*$ to a uniform measure on $S^1 \setminus \{1\}$, with an atom of infinite mass at the point 1. On the other hand, for polynomially decaying potentials, it was shown by Sobolev and Yafaev [17] in the case of central potentials and by Gell-Redman and the first author more generally [9] that there is a limiting measure which is nonuniform, and is qualitatively similar to the measure for $C(h^{-1})$ above in that it is finite away from 1, with an infinite accumulation of mass at 1 from one side.

[1] The fact that Frank and Geisinger obtain a second term regardless of dynamical assumptions is simply due to the fact that they study $\operatorname{Tr} f(P_{a,h})$ with $f(\lambda) = -\lambda H(-\lambda)$ (H is the Heaviside function), which is one order smoother than $f(\lambda) = H(-\lambda)$.

2. Reduction to semiclassical spectral asymptotics

In this section we prove Proposition 1.1. This result actually follows directly from the Birman-Schwinger principle. As some readers may not be familiar with this, we give the details.

Proof of Proposition 1.1. We begin by recalling that the operator $P_{a,h}$ is the self-adjoint operator associated to the quadratic form (1.16), that is,

$$Q_{a,h}(u) := h^2\|\nabla u\|_M^2 - \|u\|_M^2 - ha\|u\|_{\partial M}^2.$$

We recall the min-max characterization of eigenvalues: the nth eigenvalue $\mu_n(a,h)$ of $P_{a,h}$ is equal to the infimum of

$$\sup_{v\in V, \|v\|=1} Q_{a,h}(v)$$

over all subspaces $V \in H^1(M)$ of dimension n. The monotonicity of $Q_{a,h}$ in a, for fixed h, shows that the eigenvalues are monotone nonincreasing with a. In fact, they are strictly decreasing, which follows from the fact that eigenfunctions of $P_{a,h}$ cannot vanish at the boundary. Indeed, the eigenfunctions satisfy the boundary condition $h\partial_\nu u = -au$, which shows that if u vanishes at the boundary, so does $\partial_\nu u$, which is impossible.

The eigenvalues $\mu_n(a,h)$ are thus continuous, strictly decreasing functions of a. Let $a_1 < a_2$ be real numbers. The Birman-Schwinger principle [13, Proposition 9.2.7] says that the number of negative eigenvalues of $P_{a_2,h}$ is equal to the number of negative eigenvalues of $P_{a_1,h}$, plus the number of eigenvalues $\mu_n(a,h)$ of $P_{a,h}$ that change from nonnegative to negative as a varies from a_1 to a_2. A diagram makes this clear: see Figure 1.

The strict monotonicity of $\mu(a,h)$ in a shows that the number of eigenvalues $\mu_n(a,h)$ of $P_{a,h}$ that change from nonnegative to negative as a varies from a_1 to a_2 is the same as the number of $\mu(a,h)$ (counted with multiplicity) equal to zero, for $a \in [a_1, a_2)$. Next, we observe that the space of eigenfunctions $u_n(a,h)$ of $P_{a,h}$ with zero eigenvalue, i.e. $\mu_n(a,h) = 0$ is in one–to–one correspondence with the space of eigenfunctions of $C(\lambda)$, $\lambda = h^{-1}$, with eigenvalue $(a-i)(a+i)^{-1}$, or equivalently $e^{i\theta}$ where $a = -\cot(\theta/2)$. Indeed, whenever u_n is such an eigenfunction of $P_{a,h}$, then

$$f := \frac{1}{2}(h\partial_\nu u - iu)\big|_{\partial M} \tag{2.1}$$

is an eigenfunction of $C(\lambda)$, with eigenvalue $(a-i)(a+i)^{-1}$. Conversely, if f is an eigenfunction of $C(\lambda)$ with eigenvalue $(a-i)(a+i)^{-1}$, then by definition there exists a Helmholtz function u such that u is related to f according to (2.1), and we have $(h\partial_\nu + a)u = 0$ at ∂M. This completes the proof. □

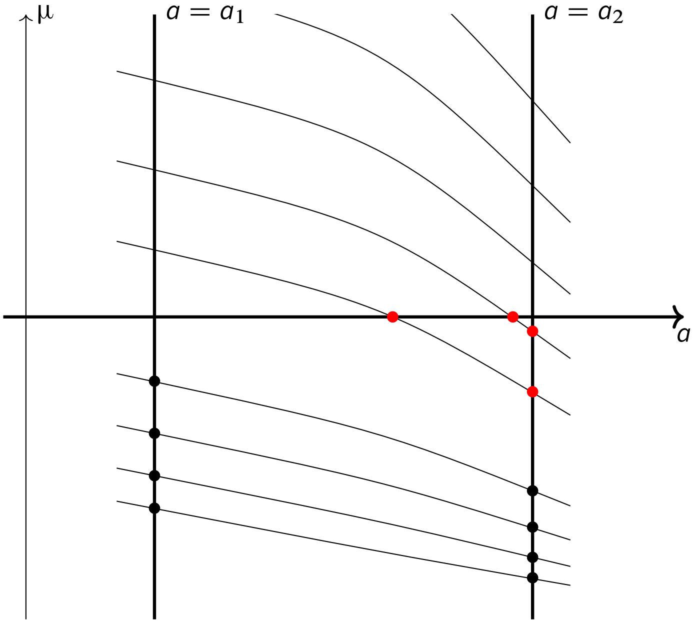

Figure 1. Diagram showing the variation of eigenvalues $\mu(a,h)$ of $P_{a,h}$ as a function of a for fixed h. The eigenvalues are strictly decreasing in a. Consequently, the number of negative eigenvalues of $P_{a_2,h}$ is equal to the number of negative eigenvalues of $P_{a_1,h}$ together with the number that cross the a-axis between $a = a_1$ and $a = a_2$.

Remark 2.1. We can apply similar arguments for $\lambda^{-\delta}\rho^{-1}R(\lambda)$ as $\rho > 0$ is a smooth function on ∂M and then plug corresponding parameters in the boundary conditions coming again to equality (1.17).

We next digress to prove that the eigenvalues of $C(\lambda)$ are monotonic (that is, they move monotonically around the unit circle) in λ. This plays no role in the remainder of our proof, but is (in the authors' opinion) of independent interest.

Proposition 2.2. *The eigenvalues of $C(\lambda)$ rotate clockwise around the unit circle as λ increases.*

Remark 2.3. This implies that the eigenvalues of $R_{\mathrm{scl}}(\lambda)$ are monotone decreasing in λ.

Proof. As discussed in the previous proof, $C(\lambda)$ has eigenvalue $e^{i\theta}$ if and only if $P_{a,h}$ has a zero eigenvalue, where $a = a(\theta) = -\cot(\theta/2)$. Thus, as a function of $h = \lambda^{-1}$, $\theta(h)$ is defined implicitly by the condition

$$\mu(a(\theta), h) = 0.$$

Since a is a strictly increasing function of θ, and we have just seen that μ is a strictly decreasing function of a, it suffices to show that when $\mu = 0$, μ is a strictly increasing function of h, hence a strictly decreasing function of λ.

We now compute the derivative of μ with respect to h, at a value of a and h where $\mu(a,h) = 0$. We have

$$\begin{aligned}\frac{d}{dh}\mu(a,h) &= \frac{d}{dh}((h^2\Delta - 1)u(h), u(h))_M \\ &= 2h(\Delta u, u)_M + ((h^2\Delta - 1)u'(h), u(h))_M + ((h^2\Delta - 1)u(h), u'(h))_M \\ &= 2h(\Delta u, u)_M + ((h^2\Delta - 1)u', u)_M - (u', (h^2\Delta - 1)u)_M.\end{aligned}$$

In the third line, we used the fact that $(h^2\Delta - 1)u = 0$ when $\mu(h) = 0$. Note the second term is not zero, as u' is not in the domain of the operator due to the changing boundary condition, so we cannot move the operator to the right hand side of the inner product without incurring boundary terms. We use the Gauss–Green formula to express the last two terms as a boundary integral:

$$\begin{aligned}\mu'(h) &= 2h(\Delta u, u)_M + h(h\partial_\nu u', u)_{\partial M} - h(u', h\partial_\nu u)_{\partial M} \\ &= 2h(\Delta u, u)_M + h(h\partial_\nu u', u)_{\partial M} + ha(u', u)_{\partial M}.\end{aligned}$$

Differentiating the boundary condition we find that

$$(h\partial_\nu + a)u' = -h\partial_\nu u \text{ at } \partial M.$$

Substituting that in we get

$$\mu'(h) = 2h(\Delta u, u)_M - h(u, \partial_\nu u)_{\partial M}.$$

Applying Gauss–Green again, we get

$$\begin{aligned}\mu'(h) &= h(\Delta u, u)_M + h\|\nabla u\|_M^2 \\ &= h^{-1}(\|u\|_{L^2(M)}^2 + \|h\nabla u\|_{L^2(M)}^2) \\ &> 0.\end{aligned}$$

□

3. Semiclassical spectral asymptotics

In this section, we prove Theorem 1.2. Essentially, we have arrived at a rather standard semiclassical spectral asymptotics problem and results are due to [13], Chapter 5 or [14], Chapter 7. See the appendix to this paper for further discussion.

Proposition 3.1. (i) *Let* $\mathsf{N}^-_h(a)$ *be as in* (1.18)*. The following asymptotic holds as* $h \to +0$:

$$\mathsf{N}^-_h(a) = (2\pi h)^{-d}\omega_d \operatorname{vol}(M) + O(h^{1-d}) \tag{3.1}$$

(ii) *Further, if the set of periodic billiards on* M *has measure* 0 *then as* $h \to +0$:

$$\mathsf{N}^-_h(a) = (2\pi h)^{-d}\omega_d \operatorname{vol}(M) + h^{1-d}\kappa(a)\operatorname{vol}'(\partial M) + o(h^{1-d}) \tag{3.2}$$

with $\kappa(a)$ *given by* (1.21)*.*

Proof. One can check easily that the operator $P_{a,h}$ is microhyperbolic at energy level 0 at each point $(x,\xi) \in T^*M$ in the direction ξ; further, the boundary value problem is microhyperbolic at each point $(x';\xi') \in T^*\partial M$ at energy level 0 in the multidirection (ξ',ξ_1^-,ξ_1^+) with $\xi_1 = \xi_1^\pm$ roots of $\sum g^{jk}\xi_j\xi_k = 0$; finally, the boundary value problem is elliptic at each point of the elliptic zone ($\subset T^*\partial M$) if $a \le 0$, and either elliptic or microhyperbolic in the direction ξ' at each point of the elliptic zone ($\subset T^*\partial M$) if $a > 0$ – see definitions in Chapters 2 and 3 of [14]. Then statements (1.19) and (1.20) follow from Theorems 7.3.11 and 7.4.1 of [14].

We now assume that the set of periodic billiards on M has measure zero, and compute the second term in the spectral asymptotic explicitly. Similar calculations appear in [6].

To do this, one can use method of freezing coefficients (see the appendix, or [14], Section 7.2) which results in

$$h^{1-d}\kappa(a) = \int_{\mathbb{R}^+} \bigl(e(0,x_1;0,x_1;1) - (2\pi h)^{-d}\omega_d\bigr)\,dx_1 \tag{3.3}$$

where $e(x',x_1;y',y_1;\tau)$ is the Schwartz kernel of the spectral projector $E(\tau)$ of the operator $H_a = h^2\Delta$ in half-space $\mathbb{R}^{d-1}\times\mathbb{R}^+ \ni (x',x_1)$ with domain $\mathfrak{D}(H_a) = \{u \in H^2 \colon (h\partial_{x_1} + a)u|_{x_1=0} = 0\}$.

We obtain this spectral projector by integrating the spectral measure. This in turn is obtained via Stone's formula

$$dE_L(\sigma) = \frac{1}{2\pi i}\bigl((L-(\sigma+i0))^{-1} - (L-(\sigma-i0))^{-1}\bigr)\,d\sigma. \tag{3.4}$$

Consider the resolvent for H_a, $(H_a-\sigma)^{-1}$, for $\sigma \in \mathbb{C}\setminus\mathbb{R}$. Using the Fourier transform in the x' variables, we can write the Schwartz kernel of this resolvent in the form

$$(2\pi h)^{1-d}\int e^{i(x'-y')\cdot\xi'}(T_a + |\xi'|^2 - \sigma)^{-1}(x_1,y_1)\,d\xi'. \tag{3.5}$$

Here T_a is the one-dimensional operator $T_a = -h^2\partial^2 + |\xi'|^2$ on $L^2(\mathbb{R}_+)$ under the boundary condition $(h\partial + a)u|_{x_1=0} = 0$. The spectral projector $E_{H_a}(1)$ is therefore given by

$$(2\pi h)^{1-d} \int_{-\infty}^{1} \int e^{i(x'-y')\cdot\xi'} dE_{T_a}(\sigma - |\xi'|^2)(x_1, y_1)\, d\xi'\, d\sigma. \tag{3.6}$$

Thus, we need to find the spectral measure for T_a. Write $\sigma - |\xi'|^2 = \eta^2$, where we take η to be in the first quadrant of $\mathbb{C}$ for $\operatorname{Im}\sigma > 0$, and in the fourth quadrant for $\operatorname{Im}\sigma < 0$.

Lemma 3.2. *Suppose that* $\operatorname{Im}\eta > 0$ *and* $\operatorname{Re}\eta \geq 0$. *Then the resolvent kernel* $(T_a - \eta^2)^{-1}$ *takes the form*

$$(T_a - \eta^2)(x,y) = \begin{cases} \dfrac{i}{2h\eta}\Big(e^{i\eta(x-y)/h} + \dfrac{i\eta - a}{i\eta + a} e^{i\eta(x+y)/h}\Big), & x > y, \\ \dfrac{i}{2h\eta}\Big(e^{i\eta(y-x)/h} + \dfrac{i\eta - a}{i\eta + a} e^{i\eta(x+y)/h}\Big), & x < y. \end{cases} \tag{3.7}$$

If $\operatorname{Im}\eta < 0$ *and* $\operatorname{Re}\eta \geq 0$, *then the resolvent kernel* $(T_a - \eta^2)^{-1}$ *takes the form*

$$(T_a - \eta^2)(x,y) = \begin{cases} -\dfrac{i}{2h\eta}\Big(e^{i\eta(y-x)/h} + \dfrac{i\eta + a}{i\eta - a} e^{-i\eta(x+y)/h}\Big), & x > y, \\ -\dfrac{i}{2h\eta}\Big(e^{i\eta(x-y)/h} + \dfrac{i\eta + a}{i\eta - a} e^{-i\eta(x+y)/h}\Big), & x < y. \end{cases} \tag{3.8}$$

Proof. In the regions $x < y$ and $x > y$, the resolvent kernel must be a linear combination of $e^{i\eta x/h}$ and $e^{-i\eta x/h}$. Moreover, for $\operatorname{Im}\eta > 0$, we can only have the $e^{+i\eta x/h}$ term, as $x \to \infty$, as the other would be exponentially increasing. So we can write the kernel in the form

$$\begin{cases} c_1 e^{+i\eta x/h}, & x > y, \\ c_2 e^{+i\eta x/h} + c_3 e^{-i\eta x/h}, & x < y. \end{cases} \tag{3.9}$$

We apply the boundary condition, and the two connection conditions at $x = y$, namely continuity, and a jump in the derivative of $-1/h$, in order to obtain the delta function $\delta(x-y)$ after applying T_a. These three conditions determine the c_i uniquely, and we find that, in the case $\operatorname{Im}\eta > 0$,

$$c_1 = \frac{i}{2h\eta}\big(e^{-i\eta y/h} + \frac{i\eta - a}{i\eta + a} e^{+i\eta y/h}\big), \tag{3.10$_1$}$$

$$c_2 = \frac{i}{2h\eta}\frac{i\eta - a}{i\eta + a} e^{+i\eta y/h}, \qquad c_3 = \frac{i}{2h\eta} e^{+i\eta y/h}, \tag{3.10$_{2,3}$}$$

yielding (3.7). A similar calculation yields (3.8). △

We now apply (3.4) to find the Schwartz kernel of the spectral measure for T_a.

Lemma 3.3. *The spectral measure $dE_{T_a}(\tau)$ is given by the following.*

(i) *For $\tau \ge 0$, $\tau = \eta^2$*

$$dE_{T_a}(\tau) = \frac{1}{4\pi h\eta}\Big(e^{i\eta(x-y)/h} + e^{i\eta(y-x)/h} + \frac{i\eta - a}{i\eta + a}e^{i\eta(x+y)/h} + \frac{i\eta + a}{i\eta - a}e^{-i\eta(x+y)/h}\Big)\, 2\eta d\eta. \tag{3.11}$$

(ii) *For $\tau < 0$, the spectral measure $dE(\tau)$ vanishes for $a \le 0$, while for $a > 0$*

$$dE_{T_a}(\tau) = \frac{2a}{h}e^{-ax/h}e^{-ay/h}\delta(\tau + a^2)d\tau. \tag{3.12}$$

Proof. This follows directly from Lemma 3.2 and Stone's formula, (3.4). The extra term for $a > 0$ arises from the pole in the denominator, $i\eta + a$ for $\operatorname{Im}\eta > 0$ and $i\eta - a$ for $\operatorname{Im}\eta < 0$ in the expressions (3.7), (3.8), which only occurs for $a > 0$. For τ negative, we need to set $\eta = i\sqrt{-\tau} + 0$ in (3.7) and $\eta = -i\sqrt{-\tau} + 0$ in (3.8), and subtract. Then everything cancels except at the pole, where we obtain a delta function $-2\pi i\delta(\sqrt{-\tau} - a)$, which arises from $(\sqrt{-\tau} + i0 + a)^{-1} - (\sqrt{-\tau} - i0 + a)^{-1}$. This term arises from the negative eigenvalue $-a^2$ which occurs for $a > 0$, corresponding to the eigenfunction $\sqrt{2a/h}\, e^{-ax/h}$. △

Plugging this into (3.6), and making use of the fact that $d\sigma d\xi' = 2\eta d\eta d\xi'$, we find that the Schwartz kernel of $E_{H_a}(1)$ is given by

$$(2\pi h)^{-d}\int_0^1 \int H(1 - |\xi'|^2 - \eta^2)e^{i(x'-y')\cdot\xi'}\Big(e^{i\eta(x_1-y_1)/h} + e^{i\eta(y_1-x_1)/h} + \frac{i\eta - a}{i\eta + a}e^{i\eta(x_1+y_1)/h} + \frac{i\eta + a}{i\eta - a}e^{-i\eta(x_1+y_1)/h}\Big)\, d\xi'\, d\eta \tag{3.13}$$

for $a \le 0$ while for $a > 0$, it is given by the sum of (3.13) and

$$(2\pi h)^{1-d}\frac{2a}{h}e^{-ax_1/h}e^{-ay_1/h}\int_{-\infty}^1 \int e^{i(x'-y')\cdot\xi'}\delta(\sigma - |\xi'|^2 + a^2)\, d\xi'\, d\sigma. \tag{3.14}$$

We are actually interested in the value on the diagonal. Setting $x = y$, and performing the trivial ξ' integral, we find that the Schwartz kernel of the spectral projector $E_{H_a}(1)(x,x)$ on the diagonal is given by

$$\begin{aligned}&\frac{\omega_{d-1}}{(2\pi h)^d}\int_0^1 (1-\eta^2)^{(d-1)/2}\Big(2+\frac{i\eta-a}{i\eta+a}e^{2i\eta x_1/h}+\frac{i\eta+a}{i\eta-a}e^{-2i\eta x_1/h}\Big)\,d\eta\\ &\quad + H(a)\frac{(d-1)\omega_{d-1}}{(2\pi h)^{d-1}}\frac{a}{h}e^{-2ax_1/h}\int_{-a^2}^1 (\sigma+a^2)^{(d-3)/2}\,d\sigma.\end{aligned} \tag{3.15}$$

Since

$$\omega_{d-1}\int_0^1 2(1-\eta^2)^{(d-1)/2}\,d\eta=\omega_d,$$

we see by comparing with (3.3) that this term disappears in the expression for $\kappa(a)$ and we have, after performing the x_1 integral as in (3.3)

$$\begin{aligned}h^{1-d}\kappa(a)=\frac{\omega_{d-1}}{(2\pi h)^d}\int_0^1(1-\eta^2)^{(d-1)/2}\Big(&\frac{i\eta-a}{i\eta+a}\Big(\frac{ih}{2}(\eta+i0)^{-1}\Big)\\ &-\frac{i\eta+a}{i\eta-a}\Big(\frac{ih}{2}(\eta-i0)^{-1}\Big)\Big)\,d\eta\\ +H(a)\frac{(d-1)\omega_{d-1}}{2(2\pi h)^{d-1}}&\int_{-a^2}^1(\sigma+a^2)^{(d-3)/2}\,d\sigma.\end{aligned} \tag{3.16}$$

Simplifying a bit, and performing the σ integral, we have

$$\begin{aligned}\kappa(a)=&-\frac{i\omega_{d-1}}{2(2\pi)^d}\int_{-1}^1(1-\eta^2)^{(d-1)/2}\frac{(i\eta-a)^2}{a^2+\eta^2}(\eta+i0)^{-1}\,d\eta\\ &+H(a)\frac{\omega_{d-1}}{(2\pi)^{d-1}}(1+a^2)^{(d-1)/2}.\end{aligned} \tag{3.17}$$

We further simplify this expression by expanding $(i\eta-a)^2=a^2-2ia\eta-\eta^2$, and noting that the contribution of the $-\eta^2$ term is zero, as this gives an odd integrand in the η integral. A similar statement can be made for the a^2 term, except that there is a contribution from the pole in this case. This leads to the expression

$$\begin{aligned}\kappa(a)=\frac{\omega_{d-1}}{(2\pi)^{d-1}}\Big(&-\frac{1}{2\pi}\int_{-1}^1(1-\eta^2)^{(d-1)/2}\frac{a}{a^2+\eta^2}\,d\eta\\ &-\frac{1}{4}+H(a)(1+a^2)^{(d-1)/2}\Big).\end{aligned} \tag{3.18}$$

Although not immediately apparent, this formula is continuous at $a=0$. In fact, the function $a(a^2+\eta^2)^{-1}$ has a distributional limit $(\operatorname{sgn} a)\pi\delta(\eta)$ as a tends to zero from above or below. The change of sign as a crosses 0 means that the integral in (3.18) has a jump of -1 as a crosses zero from negative to positive. That exactly compensates the jump in the final term.

In odd dimensions, we can compute this integral exactly. In particular, in dimension $d = 3$, we find that

$$\kappa(a) = \frac{\omega_2}{(2\pi)^2}\Big(-\frac{1}{4} + \frac{a}{\pi} + (1+a^2)\Big(1 - \frac{\operatorname{arccot} a}{\pi}\Big)\Big). \qquad \square$$

Proof of Theorem 1.2. This follows immediately from Proposition 3.1 and Proposition 1.1. □

Remark 3.4. The second term of the expansion in [6, Theorem 1.1] is obtained by computing

$$(2\pi h)^{1-d} \int_{-\infty}^{1} (1-\sigma) \int e^{i(x'-y')\cdot\xi'}\, dE_{T_a}(\sigma - |\xi'|^2)(x_1, y_1)\, d\xi'\, d\sigma \tag{3.19}$$

instead of (3.6).

4. Relation to Dirichlet boundary condition

In this section we observe that the limit $a \to -\infty$ corresponds to the Dirichlet boundary condition. More precisely, we have

Proposition 4.1. *Let* $\mathsf{N}_h^-(-\infty)$ *denote the limit*

$$\mathsf{N}_h^-(-\infty) := \lim_{a\to-\infty} \mathsf{N}_h^-(a),$$

where $\mathsf{N}_h^-(a)$ *is given by* (1.18). *Then we have*

$$\mathsf{N}_h^-(-\infty) = \#\{\lambda_j \le h^{-1} \mid \lambda_j^2 \textit{ is a Dirichlet eigenvalue of } \Delta\}. \tag{4.1}$$

Remark 4.2. Because the quadratic form (1.16) is monotone in a, the counting function $\mathsf{N}_h^-(a)$ is monotone in a. Hence the limit above exists.

Proof. We use the min-max characterisation of eigenvalues. Let $\tilde{\mathsf{N}}_D(\lambda)$ denote the number of Dirichlet eigenvalues (counted with multiplicity) less than or equal to $\lambda = h^{-1}$. This is equal to the maximal dimension of a subspace of $H_0^1(M)$ on which the quadratic form Q_D, given by

$$Q_D(u,u) = h^2\|\nabla u\|_2^2 - \|u\|_2^2 \tag{4.2}$$

is negative semidefinite. On the other hand, $\tilde{\mathsf{N}}_h^-(a)$ is equal to the maximal dimension of a subspace of $H^1(M)$ on which the quadratic form Q_a given by (1.16) is (strictly) negative definite.

We first show that $\tilde{N}_D(h^{-1}) \le \tilde{N}_h^-(-\infty)$. Let V be the vector space spanned by Dirichlet eigenfunctions with eigenvalue $\le \lambda^2$. Clearly, the quadratic form Q_a is negative *semi*definite on V, and if λ^2 is not a Dirichlet eigenvalue, then it is negative definite, proving the assertion. In the case that λ^2 is a Dirichlet eigenvalue, we perturb V to V_ϵ, a vector space of $H^1(M)$ of the same dimension as V, so that, for for ϵ sufficiently small depending on a, Q_a is negative definite on V_ϵ. For simplicity we only do this in the case that the λ^2-eigenspace is one dimensional, leaving the general case to the reader. To do this, we choose an orthonormal basis of V (with respect to the L^2 inner product) of Dirichlet eigenfunctions $v_1, \dots, v_k$ with eigenvalues $\lambda_1^2 \dots \lambda_k^2$, where $\lambda_k = \lambda$. Then we perturb only v_k, leaving the others fixed. We choose $s \in H_0^1(M)^\perp$, the orthogonal complement of $H_0^1(M)$ in $H^1(M)$ (with respect to the inner product in $H^1(M)$), so that

$$Q_a(v_i, s) = 0, \quad i < k \text{ and } Q_a(v_k, s) > 0. \tag{4.3}$$

We check that this is possible. Notice that $s \in H_0^1(M)^\perp$ implies that $(\Delta + 1)s = 0$ in M. Then as v_i has zero boundary data, we have

$$(\lambda_i^2 + 1)(v_i, s)_M = (\Delta v_i, s)_M - (v_i, \Delta s)_M = \langle \partial_\nu v_i, s\rangle_{\partial M}. \tag{4.4}$$

We choose s so that $\langle \partial_\nu v_i, s\rangle_{\partial M}$ vanishes for $i < k$ and is positive for $i = k$. This is possible: in fact, due to the unique solvability of the boundary value problem

$$(\Delta + 1)s = 0, \quad s|_{\partial M} = f \in H^{1/2}(M), \tag{4.5}$$

for $s \in H^1(M)$, we see that s can have any boundary value in $H^{1/2}(\partial M)$ which is dense in $L^2(\partial M)$. Then using (4.4) we see that $\langle \partial_\nu v_k, s\rangle_{\partial M} > 0$ implies that $(v_k, s)_M > 0$.

We now define V_ϵ to be the span of $v_1, \dots, v_{k-1}$ and $v_k + \epsilon s$. Then we have

$$Q_a(v_i, v_k + \epsilon s) = 0, \; i < k \tag{4.6}$$

and

$$\begin{aligned} Q_a(v_k + \epsilon s, v_k + \epsilon s) &= Q_a(v_k, v_k) + 2\epsilon Q_a(v_k, s) + \epsilon^2 Q_a(s, s) \\ &= 2\epsilon Q_a(v_i, s_i) + \epsilon^2 Q_a(s_i, s_i) \\ &= -2\epsilon(h^2 + 1)(v_i, s_i)_M + O(\epsilon^2 a^2), \end{aligned} \tag{4.7}$$

which is strictly negative for ϵa^2 small enough. It follows that Q_a is negative definite on V_k when ϵa^2 is small enough. A similar construction can be made when λ^2 has multiplicity greater than 1.

We next show that $\tilde{\mathrm{N}}_D(h^{-1}) \geq \mathrm{N}_h^-(-\infty)$. We argue by contradiction: if not, then for any a, there is a vector space W of dimension $\geq k+1$ on which Q_a is negative definite. Then there is a nonzero vector $w \in W$ orthogonal (in the $H^1(M)$ inner product) to V. We can write $w = w' + s$ where $w' \in H_0^1(M)$ and $s \in H_0^1(M)^\perp$. Then w' is a linear combination of Dirichlet eigenfunctions with eigenvalue $\geq \lambda' > \lambda$, where λ' is the smallest eigenvalue larger than λ. We then have

$$\begin{aligned} 0 &> Q_a(w'+s, w'+s) \\ &= Q_a(w', w') + 2Q_a(w', s) + Q_a(s,s) \\ &\geq (\lambda' - \lambda)\|w'\|_2^2 - 2(h^2+1)\|w'\|_2\|s\|_{L^2(M)} - ha\|s\|^2_{L^2(\partial M)}. \end{aligned} \tag{4.8}$$

However, some standard potential theory shows that $\|s\|_{L^2(M)}$ is bounded by a constant times $\|s\|_{L^2(\partial M)}$. To see this, extend M to a larger manifold $\tilde{M}$ of the same dimension, and let $G(x,y)$ be the Schwartz kernel of the inverse of $(\Delta_{\tilde{M}} + 1)^{-1}$ on $L^2(\tilde{M})$, with Dirichlet boundary conditions at $\partial\tilde{M}$. We can write s as $\int_{\partial M} d_{\nu_y} G(x,y)h(y)\,dy$ where $(1/2 + D)h = s|_{\partial M}$ and D is the double layer operator on ∂M determined by G. Standard arguments show that $(1/2 + D)$ has a bounded inverse on $L^2(\partial M)$ and $d_{\nu_y}G(x,y)$ is a bounded integral operator from $L^2(\partial M)$ to $L^2(M)$. So we can write, for $a < 0$,

$$\begin{aligned} 0 &> Q_a(w'+s, w'+s) \\ &\geq (\lambda' - \lambda)\|w'\|_2^2 - 2C(h^2+1)\|w'\|_2\|s\|_{L^2(\partial M)} + h|a|\|s\|^2_{L^2(\partial M)^2} \end{aligned}$$

and the RHS is clearly positive for $|a|$ large enough, giving us the desired contradiction. □

Appendix A. Standard semiclassical asymptotics

The proof of the standard semiclassical asymptotics (i.e. asymptotics of the number of negative eigenvalues of $H_a := h^2\Delta - 1$ with the boundary condition $(h\partial_{x_1} + a)u|_{\partial M} = 0$) is in [14], Section 8.3 and also in [13], Section 5.3, but we describe a simplified albeit less general proof. Basically it is a simplified proof of [11], used also in [10], Section 29.3.

A.1. Tauberian theorem. We use the following 'semiclassical' version of the Tauberian theorem in [11].

Proposition A.1. *Let* $e_h(\lambda)$ *be an nondecreasing function of* λ*, depending on the parameter* $h > 0$*, equal to zero for* $\lambda \le \lambda_0$*. Let* $\beta \in C_c^\infty(\mathbb{R})$ *be a cutoff function with* $\beta(t) = 1$*,* $|t| \le 1/2$*,* $\beta(t) = 0$*,* $|t| \ge 1$*, and* $\hat\beta(\lambda) > 0$*. Let* $\beta_T(t) = \beta(t/T)$*. Assume that for all* λ*, we have*

$$|e_h(\lambda)| \le C'(1 + |\lambda|)^M h^{-d} \tag{A.1}$$

and, for all $\lambda \in [\lambda_0, \lambda_1]$ *we have*

$$\frac{1}{h}\int_{-\infty}^{\infty} \hat\beta_T\Big(\frac{\lambda-\mu}{h}\Big) de_h(\mu) = A_0(\lambda)h^{-d} + A_1(\lambda)h^{1-d} + o(h^{1-d}), \quad h \to 0.$$

Then for all $\lambda \in [\lambda_0, \lambda_1 - \epsilon]$ *we have*

$$|e_h(\lambda) - B_0(\lambda)h^{-d} - B_1(\lambda)h^{1-d}| \le \frac{C\|A_0\|_{L^\infty([\lambda_0,\lambda_1])}}{T} h^{1-d} + o(h^{1-d}),$$

where

$$B_i(\lambda) = \int_{-\lambda_0}^{\lambda} A_i(\mu)\, d\mu$$

and C *depends only on* ϵ*,* λ_1*,* C' *and* β*.*

This is proved by modifying the proof of the corresponding proposition in [16, pp. 152-3].

A.2. Propagator. We now fix $a \in \mathbb{R}$ and let $e_h(\lambda)$ be the number of eigenvalues, counting multiplicity, of the operator $P_{a,h}$ that are less than λ, or equivalently, the trace of the spectral projection $E_{a,h}(\lambda)$ for $P_{a,h}$. According to Proposition A.1, it suffices to consider the smoothed spectral projector,

$$\operatorname{Tr} \frac{1}{h}\int_{-\infty}^{\infty} \hat\beta\Big(\frac{\lambda-\mu}{h}\Big) dE_{a,h}(\mu),$$

since it is straightforward to show that the estimate (A.1) holds with $M = d$. By the spectral theorem, this is precisely the trace of the operator

$$\operatorname{Tr} \hat\beta\Big(\frac{\lambda - P_{a,h}}{h}\Big).$$

If we are only interested in this for λ in some interval $[\lambda, \lambda_1]$, then, up to $O(h^\infty)$ errors we can compose with a smooth function $\phi(P_{a,h})$ where $\phi \in C_c^\infty(\mathbb{R})$, and $\phi = 1$ on $[\lambda - \epsilon, \lambda_1 + \epsilon]$. Then, using the Fourier transform we can express this operator in terms of the propagator $e^{itP_{a,h}/h}$:

$$\int_{-\infty}^{\infty} e^{-it\lambda/h} \beta(t)\phi(P_{a,h}) e^{itP_{a,h}/h}\, dt.$$

Since $(hD_t - P_{a,h})e^{itP_{a,h}/h} = 0$, this is the same as

$$\int_{-\infty}^{\infty} e^{-it\lambda/h}\beta(t)\phi(hD_t)e^{itP_{a,h}/h}\,dt. \tag{A.2}$$

The advantage of the spectral cutoff $\phi(hD_t)$ is that the operator $\phi(hD_t)e^{itP_{a,h}/h}$ has finite speed of propagation.

A.3. Propagation of singularities. Let $u_h(x,y,t)$ be the Schwartz kernel of $e^{ih^{-1}tP_{a,h}}$; then $u_h(x,y,t) = u_h^0(x,y,t) + u_h^1(x,y,t)$ where $u_h^0(x,y,t)$ is a free space solution and $u_h^1(x,y,t)$ satisfies

$$(hD_t - P_{a,h})u^1 = 0, \quad u^1|_{t=0} = 0, \quad (hD_{x_1} + a)(u^0 + u^1)|_{\partial M} = 0. \tag{A.3}$$

We define

$$\sigma_h^i(t) := \int_M \phi(hD_t)u^i(x,x,t)\,dx, \quad i = 0, 1.$$

We claim that, for suitable ϕ, $\sigma_h^i(t)$ has an isolated singularity (in the semiclassical sense of nontrivial behaviour as $h \to 0$) at $t = 0$. More precisely, we claim that if $\phi \in C^\infty$ and is supported in $(-\epsilon_0, \epsilon_0)$, then

$$\sigma_h^i(t) = O(h^\infty) \quad \text{for } \epsilon \le |t| \le \epsilon_0, \tag{A.4}$$

where ϵ_0 is a fixed, sufficiently small constant, and $0 < \epsilon < \epsilon_0$ is arbitrary.

This follows from propagation of singularities arguments. The bicharacteristic flow for $P_{a,h}$ is given by

$$\begin{aligned} \dot{t} &= 1, \\ \dot{\tau} &= 0 \\ \dot{x}^i &= 2g^{ij}(x)\xi_j \\ \dot{\xi}_j &= -2\frac{\partial g^{kl}}{\partial x^j}\xi_k\xi_l \end{aligned}$$

That is, with respect to the parameter t, (x,ξ) moves along a geodesic at speed $2|\xi|_g$, and τ is fixed. By standard propagation of singularities arguments, the (semiclassical) wavefront set of u^0 is contained in the conormal bundle of $\{t = 0, s = y\}$ together with the forward bicharacteristic flow from this conormal bundle intersected with the characteristic variety of $hD_t - P_{a,h}$, namely $\{\tau = |\xi|_g^2 - 1\}$. Composing with $\phi(hD_t)$ restricts this wavefront set to be contained in $\{\tau \in (-\epsilon_0, \epsilon_0)\}$. That implies that $|\,|\xi|_g - 1| \le 2\epsilon_0$. So for small time, the wavefront set of u_0 is restricted to the set where $|d(x,y) - 2t| \le 2\epsilon_0 t$. In particular, points with $x = y$ are not in the wavefront set for t in a deleted neighbourhood of 0. This proves (A.4) for $i = 0$.

A similar argument for u^1 shows that $\phi(hD_t)u^1(t,x,y)$ is $O(h^\infty)$ for $|t| \le \epsilon_0$ unless we have

$$\mathrm{dist}(x,\partial M) + \mathrm{dist}(y,\partial M) \le 2\epsilon_0(1+2\epsilon_0).$$

Thus, we can work in a collar neighbourhood of ∂M. We can choose coordinates $x = (x_1, x')$ so that the boundary is given by $x_1 = 0$, $x_1 \ge 0$ on M, and the metric takes the form $dx_1^2 + g'_{ij}(x_1,x')x'^i x'^j$, that is, Fermi coordinates near the boundary. Now we split the analysis of u^1 into two cases. We write the identity operator in the x' coordinates in the form $\mathrm{Id} = Q_{\mathrm{norm}} + Q_{\mathrm{tan}}$, where Q_* are pseudodifferential operators in the x' variables such that the symbol q_{norm} of Q_{norm} is supported in $\{|\xi'| \le 2\epsilon_1\}$ and q_{tan} is supported in $\{|\xi'| \ge \epsilon_1\}$. Correspondingly, write $\phi(hD_t)u^1 = \phi(hD_t)Q_{\mathrm{tan}}(x',hD_{x'})u^1 + \phi(hD_t)Q_{\mathrm{norm}}(x',hD_{x'})u^1$. For the first term, a standard positive commutator argument in the x' variables only shows that this term is $O(h^\infty)$ unless $\mathrm{dist}(x',y') \ge 2\epsilon_1 t - \epsilon'$ for arbitrary $\epsilon' > 0$; in particular, if $x' = y'$ then this is $O(h^\infty)$ for $t \ge \epsilon$, $\epsilon > 0$ arbitrary. On the other hand, for the Q_{norm} term, then we have $\xi_1^2 = 1 + O(\epsilon_0 + \epsilon_1)$. In particular, this means that $\dot{x}_1 = 1 + O(\epsilon_0+\epsilon_1)$, so the propagation is transverse (in fact, nearly normal) to ∂M. A standard propagation of singularities argument shows that the wavefront set of $\phi(hD_t)Q_{\mathrm{norm}}u^1$ for $\epsilon \le |t| \le \epsilon_0$ is contained in

$$\begin{aligned}&\mathrm{WF}_h(\phi(hD_t)Q_{\mathrm{norm}}u^1) \cap \{x = y,\ \epsilon \le |t| \le \epsilon_0\}\\ &\quad\subset \{(t,x,x;\tau,\xi,\eta) \mid \xi_1,\eta_1 = 1 + O(\epsilon_0+\epsilon_1)\},\end{aligned}$$

since the only way to have $x = y$ is to bounce off the boundary, in which case ξ_1, the momentum in the normal direction, changes from being approximately opposite to η_1 to being approximately equal. This wavefront set is killed under restriction to $x = y$ and then integration in x, showing that $\phi(hD_t)Q_{\mathrm{norm}}u^1$ is also $O(h^\infty)$ for $\epsilon \le |t| \le \epsilon_0$. This establishes (A.4).

A.4. Method of successive approximations. We now observe that (A.4) self-improves to the statement that

$$\sigma_h^i(t) = O(h^\infty) \quad \text{for } h^{1-\delta} \le |t| \le \epsilon_0,\ \delta > 0. \tag{A.5}$$

This follows from a simple scaling argument. Fix a base point $y \in \partial M$, and consider the scaled metric (following [15])

$$g_{T,y} = g_{ij}(TX+y)dX^i dX^j$$

where T is a small parameter. Let $u_{T,\hbar}(t,X)$ be given by

$$u_{T,\hbar}(t,X) = T^{d+1}(\phi(hD_t)u_{T\hbar})(Tt, y+TX, y);$$

then, with $\hbar := h/T$ we have

$$(\hbar D_t - \hbar^2 \Delta_{g_{T,y}}) u_{T,\hbar}(t, X) = T^{(d+1)}(hD_t - h^2 \Delta_g) u_h(Tt, y + TX, y)$$
$$= \phi(hD_t)\delta(t)\delta(X),$$

$$(\hbar \partial_{X_1} + a) u_{T,\hbar}(t, X) = 0, \quad X_1 = 0.$$

Using (A.4) we see that we have

$$\int_M \phi(\hbar D_t) u_{T,\hbar}(X, X, t)\, dX = O(T^{-(d+1)} h^\infty) \quad \text{for } \epsilon \le |t| \le \epsilon_0, \tag{A.6}$$

In particular, (A.6) is $O(h^\infty)$ provided that $T \ge h^{1-\delta}$ for arbitrary $\delta > 0$. Unravelling the scaling demonstrates (A.5).

Therefore if we want to construct $\sigma(t)$ for $|t| \le \epsilon_0$ it suffices to construct it for $|t| \le t_* = h^{1-\delta}$. However on this short interval we can construct it by the method of successive approximations. For each $y \in M$ we let P_y be the constant coefficient differential operator $P_{a,h}$ with coefficients frozen at y. Then we regard $P_{h,a}$ as a perturbation of P_y for x close to y. So $K = P_{h,a} - P_y$ is a second order differential operator with coefficients that are $O(x-y)$. The perturbation K is $O(t_*)$ due to finite speed of propagation and each successive term in the approximation acquires a factor not exceeding $Ct_* \cdot t_*/h = Ct_*^2 h$ due to Duhamel's principle. So the construction works for $t_* \le h^{\frac{1}{2}+\delta}$.

If we apply this to the u^0 term then the calculation proceeds as follows. We let $\overline{u^0}$ denote the propagator for the constant coefficient operator P_y with coefficients frozen at $y \in M$ (and taking only the second order derivatives). Then, with E the forward fundamental solution for P_y, we obtain a formula

$$u^0 = \overline{u^0} + EKu^0,$$

leading to a formal series

$$u^0 = \sum_{k=0}^{m} (EK)^k \overline{u^0} + (EK)^{m+1} u^0.$$

Applying the Fourier transform in x, we find that the first term is

$$\phi(hD_t)\overline{u^0} = (2\pi h)^{-d} \int e^{i(x-y)\cdot\xi/h} e^{it(|\xi|^2-1)/h} \phi(|\xi|^2 - 1)\, d\xi.$$

If we then plug this term into (A.2) then we find that this term is h^{-d} times a smooth function of λ and a. The method of successive approximations then generates a series of the form $\sum_{n=1}^{\infty} \kappa_n'(a,\lambda)h^{-d+n}$, and the terms corresponding to odd n are given by the integral in ξ of an odd function of ξ, hence vanish.

Using this expansion of u^0, we compute a series for u^1. In this case, the leading term $\overline{u^1}$ is given as follows:

$$\phi(hD_t)\overline{u^1} = (2\pi h)^{-d}\int e^{-i(x_1+y_1)\xi_1/h}e^{i(x'-y')\cdot\xi'/h}e^{it(|\xi|^2-1)/h}\phi(|\xi|^2-1)\,\frac{i\xi_1+a}{i\xi_1-a}d\xi.$$

We can form a similar formal series for u^1, which converges when $t \le h^{1/2+\delta}$. As with the case of u^0, we can check that the successive terms in the approximation for u^1, when plugged into (A.2), give a series with the contribution of $\phi(hD_t)\overline{u^1}$ at order h^{1-d} and with successive terms contributing at increasing integer powers of h.

Now, using this together with the Tauberian theorem, Proposition A.1, shows that we get a leading Weyl asymptotic with remainder term $O(h^{1-d})$, as in (1.19).

A.5. Two term expansion. If we assume that the measure of periodic generalized bicharacteristics is zero, then we can use the standard method to obtain a two-term expansion of the counting function. We briefly recall here the argument, following [11].

Let $\epsilon > 0$ be given. Then we decompose the identity operator on $L^2(M)$ as a sum of three terms. The first is multiplication by a cutoff function ζ identically 1 near ∂M and supported in a collar neighbourhood of ∂M, such that

$$\int_M \zeta^2 \le \epsilon.$$

The second and third are pseudodifferential operators chosen as follows. With $T > 1$ a large constant to be chosen later, we let λ_T denote the union of points in

$$\{(x,\xi) \in T^*M \mid |\xi|_g \in (1-\epsilon_0, 1+\epsilon_0)\}$$

which are either periodic with period $\le T$ under generalized bicharacteristic flow (for $P_{a,h}$), or for which the generalized bicharacteristic of length T in both directions are not transverse to the boundary. This is a closed set of measure zero so one can find two open sets U_1, U_2 such that $T^*M = U_1 \cup U_2$, $\lambda_T \subset U_1$, and the measure of U_1 is less than ϵ. Then we choose (semiclassical) pseudodifferential operators Q_1, Q_2 such that Q_i is microsupported in the conic set determined by U_i, and such that $\mathrm{Id} = \zeta^2 + Q_1^* Q_1 + Q_2^* Q_2$. We then define

$$e_h^0(\lambda) = \operatorname{Tr} \zeta^2 E_{h,a}(\lambda) = \operatorname{Tr} \zeta E_{h,a} \zeta,$$
$$e_h^i(\lambda) = \operatorname{Tr} Q_i^* Q_i E_{h,a}(\lambda) = \operatorname{Tr} Q_i E_{h,a}(\lambda) Q_i^*, \quad i = 1, 2;$$

notice that each of these is nondecreasing in λ, and the sum of the three terms is equal to the counting function for $P_{h,a}$. Correspondingly, we break (A.2) into a sum of three terms, with $i = 0, 1, 2$.

Using the series for u^0 and u^1 sketched above, we compute expansions for the three terms. Applying Proposition A.1 we find that

$$|e_h^0(\lambda) - A_0^0(\lambda) h^{-d} - A_1^0(\lambda) h^{1-d}\| = O(\epsilon h^{1-d}),$$

since in this case $A_0^0(\lambda)$ is $O(\epsilon)$, as it is proportional to $\int_M \zeta^2$. For the term $i = 1$ we similarly find that

$$|e_h^1(\lambda) - A_0^1(\lambda) h^{-d} - A_1^1(\lambda) h^{1-d}| = O(\epsilon h^{1-d}),$$

since $A_0^1(\lambda)$ is proportional to the integral of $|\sigma(Q_1)|^2$ which is also $O(\epsilon)$. For the third term, we scale β to β_T, exploiting the condition that on the microsupport of Q_2, there are no periodic bicharacteristics up to time T, hence the trace of $\phi(hD_t) e^{itP_{a,h}/h}$ has no singularities for $t \in [-T, T]$ except at $t = 0$. Hence this term also has an expansion in powers of h, and we find that

$$|e_h^2(\lambda) - A_0^2(\lambda) h^{-d} - A_1^2(\lambda) h^{1-d}| = O\Big(\frac{h^{1-d}}{T}\Big).$$

Choosing T sufficiently large, this is also $O(\epsilon h^{1-d})$, and we have shown the existence of a two-term expansion.

It only remains to identify the first two terms. But once we know that there *is* a two-term expansion, we can identify the coefficients from the first two terms in the expansion of $\operatorname{Tr} \phi(hD_t) e^{itP_{a,h}/h}$ at $t = 0$. From the method of successive approximations we see that these terms arise from the contribution of $\overline{u^0}$ and $\overline{u^1}$. We observe that $\overline{u^0} + \overline{u^1}$ gives precisely the propagator for the $h^2 \Delta_{\mathbb{R}^d_+}$, the flat Laplacian on the half-space $\mathbb{R}^d_+ = \{x_1 \geq 0\}$, with the boundary condition $(h\partial_{x_1} + a)\bar{u}(x, y, t) = 0$ at $x_1 = 0$. It follows that the local densities for each term of the two-term expansion is equal to the local density for the flat half-space model. This justifies the calculations in Section 3 based on this flat model.

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Andrew Hassell, Mathematical Sciences Institute, Australian National University, Canberra, ACT 0200, Australia

e-mail: Andrew.Hassell@anu.edu.au

Victor Ivrii, Department of Mathematics, University of Toronto, 40, St.George Str., Toronto, Ontario M5S 2E4, Canada

e-mail: ivrii@math.toronto.edu