ON RECOVERING THE SHAPE OF A DOMAIN FROM THE TRACE OF THE HEAT KERNEL

Z. Schuss¹

Department of Mathematics, Tel-Aviv University Ramat-Aviv, Tel-Aviv 69978, Israel

A. Spivak

Department of Sciences, Academic Institute of Technology, POB 305, Holon 58102, Israel

ABSTRACT

The problem of recovering geometric properties of a domain from the trace of the heat kernel for an initial-boundary value problem arises in NMR microscopy and other applications. It is similar to the problem of "hearing the shape of a drum", for which a Poisson type summation formula relates geometric properties of the domain to the eigenvalues of the Dirichlet or Neumann problem for the Laplace equation. It is well known that the area, circumference, and the number of holes in a planar domain can be recovered from the short time asymptotics of the solution of the initial-boundary value problem for the heat equation. It is also known that the length spectrum of closed billiard ball trajectories in the domain can be recovered from the eigenvalues or from the solution of the wave equation. This spectrum can also be recovered from the heat kernel for a compact manifold without boundary. We show that for a planar domain with boundary, the length spectrum can be recovered directly from the short time expansion of the trace of the heat kernel. The results can be extended to higher dimensions in a straightforward manner.

¹Partially supported by a research grant from the Foundation for Basic Research administered by the Israel Academy of Science and by a research grant from the US-Israel Binational Science Foundation.

1. Introduction

The problem of recovering geometric properties of a domain from NMR measurements arises in oil explorations and in non-invasive microscopy of cell structure [1]. In these measurements the trace of the heat kernel for the initial value problem with reflecting (Neumann) boundary conditions is measured directly. The problem is analogous to "hearing the shape of a drum", where the solution of the wave equation in the domain is measured directly (it is "heard").

The problem of recovering geometrical properties of a domain from the eigenvalues of the Dirichlet or Neumann problem for the Laplace equation in a domain has attracted much attention in the literature (see [2]-[7] for some history and early results; for more recent work see [8], [9] an references therein).

The mathematical statement of the problem is as follows. Green's function for the heat equation in a smooth planar domain Ω , with homogeneous Dirichlet boundary conditions, satisfies

$$\frac{\partial G(\boldsymbol{y}, \boldsymbol{x}, t)}{\partial t} = D\Delta \boldsymbol{y} G(\boldsymbol{y}, \boldsymbol{x}, t) \text{ for } \boldsymbol{y}, \boldsymbol{x} \in \Omega, \ t > 0$$
(1.1)

$$G(\boldsymbol{y}, \boldsymbol{x}, 0) = \delta(\boldsymbol{y} - \boldsymbol{x})$$
(1.2)

$$G(\boldsymbol{y}, \boldsymbol{x}, t) = 0 \qquad \text{for } \boldsymbol{y} \in \partial\Omega, \ \boldsymbol{x} \in \Omega, \ t > 0. \tag{1.3}$$

The function $G(\boldsymbol{x}, \boldsymbol{x}, t) d\boldsymbol{x}$ is the probability of return to $\boldsymbol{x} d\boldsymbol{x}$ at time t of a free Brownian particle that starts at the point \boldsymbol{x} at time t = 0 and diffuses in Ω with diffusion coefficient 1, with absorption at the boundary $\partial \Omega$. If it is reflected at $\partial \Omega$, rather than absorbed, the Dirichlet boundary condition (1.3) is replaced with the Neumann condition [10]

$$\frac{\partial G(\boldsymbol{y}, \boldsymbol{x}, t)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} = 0 \qquad \text{for } \boldsymbol{y} \in \partial \Omega, \ \boldsymbol{x} \in \Omega, \ t > 0, \qquad (1.4)$$

where $\boldsymbol{\nu}(\boldsymbol{y})$ is the unit outer normal at the boundary point \boldsymbol{y} . The trace of the heat kernel is defined as

$$P(t) = \int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}, t) \, d\boldsymbol{x}$$
(1.5)

and can be represented by the Dirichlet series

$$P(t) = \sum_{n=1}^{\infty} e^{-\lambda_n t},$$
(1.6)

where λ_n are the eigenvalues of Laplace equation with the Dirichlet or Neumann boundary conditions (1.3) or (1.4), respectively.

It has been shown by Kac [2] that for a domain Ω with smooth boundary $\partial\Omega$, the leading terms in the expansion of P(t) in powers of \sqrt{t} are

$$P_{\text{Kac}}(t) \sim \frac{|\Omega|}{4\pi t} - \frac{|\partial\Omega|}{8\sqrt{\pi t}} + \frac{1}{6}(1-r) + O\left(\sqrt{t}\right), \quad \text{for } t \to 0,$$

where $|\Omega|$ denotes the area of Ω , $|\partial \Omega|$ denotes the arc-length of $\partial \Omega$, and r is the number of holes in Ω . The full short time asymptotic power series expansion of P(t) in the form

$$P(t) \sim \sum_{n=0}^{\infty} a_n t^{n/2-1},$$

can be deduced from the large s expansion of the Laplace transform

$$g(s) = \int_0^\infty \exp\{-s^2t\} \left(P(t) - \frac{a_0}{t}\right) dt, \quad \left(a_0 = \frac{|\Omega|}{4\pi}\right)$$

in inverse powers of s. Such an expansion was given by Stewartson and Waechter [3] in the form

$$\hat{g}(s) \sim \sum_{n=1}^{\infty} \frac{c_n}{s^n},$$

where

$$c_n = a_n \Gamma\left(\frac{n}{2}\right).$$

The constants c_n are computable functionals of the curvature of the boundary. The full expansion is denoted

$$P_{\rm SW}(t) \sim \frac{|\Omega|}{4\pi t} - \frac{|\partial\Omega|}{8\sqrt{\pi t}} + \frac{1}{6}(1-r) + \sum_{n=3}^{\infty} a_n t^{n/2-1}, \quad \text{for } t \to 0.$$
(1.7)

If the boundary is not smooth, but has cusps and corners, the expansion contains a term of the order $t^{-\nu}$, where ν is a number between 0 and 1/2.

The Stewartson-Waechter expansion was used in [8] to deduce further geometric properties of Ω by extending g(s) into the complex plane. Examples were given in [8] of the resurgence of the length spectrum of closed billiard ball trajectories in the domain.

The full length spectrum of closed geodesics on a compact Riemannian manifold without boundary Ω appeared in the short time asymptotic expansion given in [6],

$$P(t) \sim \frac{1}{\sqrt{\pi t}} \sum_{n=0}^{\infty} P_n(\sqrt{t}) e^{-\delta_n^2/t}, \text{ for } t \to 0,$$
 (1.8)

where δ_n are the lengths of closed geodesics on Ω and $P_n(x)$ are power series in x.

In this paper, we construct an expansion of the form (1.8) for the trace of the heat kernel for the initial-boundary value problem (1.1)-(1.3) or (1.4) in a smooth bounded

domain Ω in \mathbb{R}^2 . The results can be generalized to higher dimensions in a straightforward manner.

The point of departure for our analysis is the observation that transcendentally small terms are not included in the expansion (1.7). These terms have been neglected in [3] and [8] even in the case of a circular domain, where the Laplace transform of $G(\boldsymbol{y}, \boldsymbol{x}, t)$ can be expressed explicitly in terms of modified Bessel functions. In [8] this Laplace transform is expanded in inverse powers of s and the coefficients c_n are evaluated asymptotically for large n.

A generalization of the asymptotic expansion "beyond all orders" (1.8) has the form

$$P(t) \sim P_{\text{SW}}(t) + \frac{1}{\sqrt{\pi t}} \sum_{n=1}^{\infty} P_n(\sqrt{t}) e^{-\delta_n^2/t}, \text{ for } t \to 0,$$
 (1.9)

where δ_n , ordered by magnitude, are constants to be determined, and $P_n(x)$ are power series in x. Transcendentally small terms may be, in fact, quite large and make a finite contribution to the expansion (1.9) [11].

To recover the geometrical information from the expansion (1.9), given the (measured) function P(t), we note that

$$|\Omega| = \lim_{t \to 0} 4\pi t P(t), \quad |\partial \Omega| = -\lim_{t \to 0} 8\sqrt{\pi t} \left[P(t) - \frac{|\Omega|}{4\pi t} \right], \tag{1.10}$$

and so on. This way the entire expansion (1.7) can be determined.

Once the coefficients of the expansion (1.7) have been determined, the exponent of the dominant term of the transcendentally small part, δ_1 , is found as

$$\delta_1 = -\lim_{t \to 0} t \log \left[P(t) - P_{\text{SW}}(t) \right].$$

Proceeding this way, we can recover the entire expansion (1.9) if P(t) is known (e.g., from measurements).

In this paper, we use the "ray method", as developed in [12]-[15], to construct a short time asymptotic expansion of the heat kernel. We use it to expand the trace asymptotically beyond all orders (the so called "hyperasymptotic expansion") and show that the exponents δ_i are the squares of half the lengths of the periodic orbits in the domain. The exponentially small terms in the expansion (1.9) are due to rays reflected in the boundary, much like in the geometric theory of diffraction [16]-[18]. This recovers the length spectrum of closed billiard ball trajectories in the domain. In particular, the smallest exponent δ_1 is the width of the narrowest bottleneck in the domain.

2. The one-dimensional case

The solution of the heat equation in an interval can be constructed by the method of images. Specifically, the Green function of the problem satisfies

$$\frac{\partial G(y, x, t)}{\partial t} = \frac{\partial^2 G(y, x, t)}{\partial y^2} \quad \text{for } 0 < x, y < a, \ t > 0$$
(2.1)

$$G(y, x, 0) = \delta(y - x)$$
 for $0 < x, y < a$ (2.2)

$$\left(\frac{\partial}{\partial y}\right)^k G(0, x, t) = \left(\frac{\partial}{\partial y}\right)^k G(a, x, t) = 0 \quad \text{for } 0 < x < a, \ t > 0, \ k = 0, 1.$$
(2.3)

The method of images gives the representation

$$G(y, x, t) =$$

$$\frac{1}{2\sqrt{\pi t}} \sum_{n=-\infty}^{\infty} \left[\exp\left\{ -\frac{(y-x+2na)^2}{4t} \right\} - (-1)^k \exp\left\{ -\frac{(y+x+2na)^2}{4t} \right\} \right], \quad (k = 0, 1).$$
(2.4)

Note that if the infinite series is truncated after a finite number of terms, the boundary conditions are satisfied only in an asymptotic sense as $t \to 0$. That is, the boundary values of the truncated solution decay exponentially fast in t^{-1} as $t \to 0$ and the exponential rate increases together with the number of retained terms.

The trace is given by

$$\int_{0}^{a} G(x, x, t) dx = \frac{1}{2\sqrt{\pi t}} \int_{0}^{a} \sum_{n=-\infty}^{\infty} \left[\exp\left\{-\frac{(na)^{2}}{t}\right\} + (-1)^{k} \exp\left\{-\frac{(x+na)^{2}}{t}\right\} \right] dx$$

$$= \frac{1}{2\sqrt{\pi t}} \sum_{n=-\infty}^{\infty} \left[a \exp\left\{-\frac{(na)^{2}}{t}\right\} + (-1)^{k} \int_{0}^{a} \exp\left\{-\frac{(x+na)^{2}}{t}\right\} dx \right]$$

$$= \frac{a}{2\sqrt{\pi t}} \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{(na)^{2}}{t}\right\} + \frac{(-1)^{k}}{2}$$

$$= \frac{a}{2\sqrt{\pi t}} + \frac{(-1)^{k}}{2} + \frac{a}{2\sqrt{\pi t}} \sum_{n\neq 0}^{\infty} \exp\left\{-\frac{(na)^{2}}{t}\right\}, \quad (k = 0, 1). \quad (2.5)$$

On the other hand,

$$\int_{0}^{a} G(x, x, t) \, dx = \sum_{n=1}^{\infty} e^{-\lambda_n t}, \tag{2.6}$$

where $\{\lambda_n\}$ are the eigenvalues of the homogeneous Dirichlet or Neumann problem for the operator d^2/dx^2 in the interval [0, a]. Thus

$$\sum_{n=1}^{\infty} e^{-\lambda_n t} = \frac{a}{2\sqrt{\pi t}} + \frac{(-1)^k}{2} + \frac{a}{2\sqrt{\pi t}} \sum_{n \neq 0} \exp\left\{-\frac{(na)^2}{t}\right\}, \quad (k = 0, 1).$$
(2.7)

If instead of a single interval of length a, we consider the heat equation in a set Ω consisting of K disjoint intervals of lengths l_j , (j = 1, ..., K), respectively, the resulting expansion is

$$\sum_{n=1}^{\infty} e^{-\lambda_n t} = \frac{\sum_{j=1}^{K} l_j}{2\sqrt{\pi t}} + (-1)^k \frac{2K}{4} + \sum_{j=1}^{K} \frac{l_j}{2\sqrt{\pi t}} \sum_{n \neq 0} \exp\left\{-\frac{(nl_j)^2}{t}\right\}, \quad (k = 0, 1).$$
(2.8)

The numerator in the first term on the right hand side of eq.(2.8) can be interpreted as the "area" of Ω , so we denote it $\sum_{j=1}^{K} l_j = |\Omega|$. The number 2K is the number of boundary points of Ω , which can be interpreted as the "circumference" of the boundary, so we denote it $|\partial \Omega| = 2K$. The exponents in the sum on the right hand side of eq.(2.8) can be interpreted as the "widths" of the components of Ω . Clearly, for small t, the term containing the smallest width, $r = \min_{1 \le j \le K} l_j$, will dominate the sum. Thus we can rewrite eq.(2.8) as

$$\sum_{n=1}^{\infty} e^{-\lambda_n t} = \frac{|\Omega|}{2\sqrt{\pi t}} - \frac{|\partial\Omega|}{4} + \frac{mr}{\sqrt{\pi t}} \exp\left\{-\frac{r^2}{t}\right\} + \sum_{l_j > r} \frac{l_j}{2\sqrt{\pi t}} \sum_{n \neq 0} \exp\left\{-\frac{(nl_j)^2}{t}\right\}, \quad (2.9)$$

where m is the number of the shortest intervals in Ω .

Equation (2.9) can be viewed as the short time asymptotic expansion of the sum on the left hand side of the equation. The algebraic part of the expansion consists of the first two terms and all other terms are transcendentally small. The geometric information in the various terms of the expansion consists of the "area" of Ω and the "circumference" $|\partial \Omega|$ in the algebraic part of the expansion. The transcendental part of the expansion is dominated by the term containing the smallest "width" of the domain, r.

The geometric information about Ω contained in the algebraic part is the information given in the "Can one hear the shape of a drum" expansions [2], [3]. The geometric information contained in the transcendentally small terms in (2.9) can be understood as follows. The terms nl_j in the exponents are the lengths of closed trajectories of billiard balls in Ω , or the lengths of closed rays reflected at the boundaries, as in [5].

The representation (2.4) can be constructed as a short time approximation to the solution of the heat equation (2.1)-(2.3) by the *ray method* [12]. In this method the solution is constructed in the form

$$G(y, x, t) = e^{-S^2(y, x)/4t} \sum_{n=0}^{\infty} Z_n(y, x) t^{n-1/2}.$$
(2.10)

Substituting the expansion (2.10) into the heat equation (2.1) and ordering terms by orders of magnitude for small t, we obtain at the leading order the *ray equation*, also called the *eikonal equation*,

$$\left|\frac{\partial S(y,x)}{\partial y}\right|^2 = 1, \qquad (2.11)$$

and at the next orders the transport equations

$$2\frac{\partial S(y,x)}{\partial y}\frac{\partial Z_n(y,x)}{\partial y} + Z_n(y,x)\left(\frac{\partial^2 S(y,x)}{\partial y^2} + \frac{2n}{S(y,x)}\right)$$
$$\frac{2}{S(y,x)}\frac{\partial^2 Z_{n-1}(y,x)}{\partial y^2}, \quad n = 0, 1, \dots.$$
(2.12)

Denoting

$$p(y,x) = \frac{\partial S(y,x)}{\partial y},$$

we write the equations of the *characteristics*, or rays of the eikonal equation (2.11) as [13]

$$\frac{\partial y(\tau, x)}{\partial t} = 2p, \quad \frac{dp(\tau)}{dt} = 0, \quad \frac{dS(\tau)}{d\tau} = 2p^2(\tau)$$
(2.13)

with the initial conditions

$$y(0, x) = x$$
, $p(0) = \pm 1$, $S(0) = 0$

The condition S(0) = 0 is implied by the initial condition $G(x, y, 0) = \delta(x - y)$. The solutions are given by

$$y(\tau, x) = x + 2p\tau, \quad p(\tau) = \pm 1, \quad S(\tau) = 2\tau = \pm (y - x).$$
 (2.14)

Thus S(y, x) is the length of the ray from y to x. We denote this solution by $S_0(y, x)$. It is easy to see that the solution of the transport equations corresponding to $S_0(y, x)$ is given by $Z_0(y, x) = const$, and $Z_n(y, x) = 0$ for all $n \ge 1$. The initial condition (2.2) implies that

$$Z_0(y,x) = \frac{1}{2\sqrt{\pi}}.$$

Combined in eq.(2.10) this solution gives Green's function for the heat equation on the entire line,

$$G_0(y, x, t) = \frac{1}{2\sqrt{\pi t}} \exp\left\{-\frac{(y-x)^2}{4t}\right\},$$

which is the positive term corresponding to n = 0 in the expansion (2.4).

The ray from x to y is not the only one emanating from x. There are rays emanating from x that end at y after reflection in the boundary. Thus the ray from x that reaches y after it is reflected at the boundary 0 has length y+x. Therefore there is another solution of the eikonal equation, $S_1(y, x)$, which is the length of the reflected ray, given by

$$S_1(y,x) = y + x.$$

The ray from x that reaches y after it is reflected at the boundary a has length 2a - x - y. The ray from x to 0, then to a, and then to y has length 2a + x - y. Thus the lengths of all rays that reach y from x after any number of reflections in the boundary generate solutions of the eikonal equation, which are the lengths of the rays, which in turn generate solutions of the heat equation. We denote them by $S_k(y, x)$ with some ordering. The corresponding solutions of the transport equation are

$$Z_{0,k}(y,x) = \frac{C_k}{2\sqrt{\pi}},$$

where C_k are constant. They are chosen so that the sum of all the ray solutions,

$$G_k(y, x, t) = \frac{Z_{0,k}(y, x)}{\sqrt{t}} e^{-S_k^2(y, x)/4t},$$

satisfies the boundary conditions (2.3). Note that for all $k \neq 0$

$$G_k(y, x, t) \to 0$$
 as $t \to 0$.

This construction recovers the solution (2.4).

3. The ray method for short time asymptotics of Green's function

The ray method consists in the construction of Green's function $G(\boldsymbol{y}, \boldsymbol{x}, t)$ in the asymptotic form

$$G(\boldsymbol{y}, \boldsymbol{x}, t) \sim e^{-S^2(\boldsymbol{y}, \boldsymbol{x})/4t} \sum_{n=0}^{\infty} Z_n(\boldsymbol{y}, \boldsymbol{x}) t^{n-1}.$$
(3.1)

The function $S(\boldsymbol{y}, \boldsymbol{x})$ is the solution of the *eikonal equation*

$$\left|\nabla \boldsymbol{y} S(\boldsymbol{y}, \boldsymbol{x})\right|^2 = 1$$
 (3.2)

and the functions $Z_n(\boldsymbol{y}, \boldsymbol{x})$ solve the transport equations

$$2\nabla \boldsymbol{y} S(\boldsymbol{y}, \boldsymbol{x}) \cdot \nabla \boldsymbol{y} Z_n(\boldsymbol{y}, \boldsymbol{x}) + Z_n(\boldsymbol{y}, \boldsymbol{x}) \left[\Delta \boldsymbol{y} S(\boldsymbol{y}, \boldsymbol{x}) + \frac{2n-1}{S(\boldsymbol{y}, \boldsymbol{x})} \right] = \frac{2}{S(\boldsymbol{y}, \boldsymbol{x})} \Delta \boldsymbol{y} Z_{n-1}(\boldsymbol{y}, \boldsymbol{x}), \quad \text{for } n = 0, 1, 2, \dots$$
(3.3)

The eikonal equation (3.2) is solved by the *method of characteristics* [13]. The characteristics, called *rays*, satisfy the differential equations

$$\frac{d\boldsymbol{y}(\tau,\boldsymbol{x})}{d\tau} = 2\nabla \boldsymbol{y} S(\boldsymbol{y}(\tau,\boldsymbol{x}),\boldsymbol{x}), \quad \frac{d\nabla \boldsymbol{y} S(\boldsymbol{y}(\tau,\boldsymbol{x}),\boldsymbol{x})}{d\tau} = 0, \quad \frac{dS(\boldsymbol{y}(\tau,\boldsymbol{x}),\boldsymbol{x})}{d\tau} = 2. \quad (3.4)$$

The initial condition (1.2) implies that the rays emanate from the point \boldsymbol{x} . Thus we choose the initial conditions

$$\boldsymbol{y}(0,\boldsymbol{x}) = \boldsymbol{x}, \quad \nabla \boldsymbol{y} S(\boldsymbol{y}(0,\boldsymbol{x}),\boldsymbol{x}) = \boldsymbol{\nu}, \quad S(\boldsymbol{y}(0,\boldsymbol{x}),\boldsymbol{x}) = 0,$$
 (3.5)

where $\boldsymbol{\nu}$ is a constant vector of unit length. The solution is given by

$$\boldsymbol{y}(\tau, \boldsymbol{x}) = \boldsymbol{x} + 2\boldsymbol{\nu}\tau, \quad S(\boldsymbol{y}, \boldsymbol{x}) = |\boldsymbol{y} - \boldsymbol{x}| = 2\tau, \quad \nabla \boldsymbol{y}S(\boldsymbol{y}, \boldsymbol{x}) = \boldsymbol{\nu}.$$
 (3.6)

The pair $(\tau, \boldsymbol{\nu})$ determines uniquely the point $\boldsymbol{y} = \boldsymbol{y}(\tau, \boldsymbol{x})$ and the value of $S(\boldsymbol{y}, \boldsymbol{x})$ at the point. The parameter τ is half the distance from \boldsymbol{y} to \boldsymbol{x} or half the length of the ray from \boldsymbol{x} to \boldsymbol{y} . The vector $\boldsymbol{\nu}$ is the unit vector in the direction from \boldsymbol{x} to \boldsymbol{y} .

The function $Z_0(\boldsymbol{y}, \boldsymbol{x})$ is easily seen to be a constant, $1/4\pi$, and $Z_n(\boldsymbol{y}, \boldsymbol{x}) = 0$ for all n > 0. This construction recovers the solution of the heat equation in the entire plane and disregards the boundary $\partial\Omega$, because in the plane every point can be seen from every other point by a straight ray. Note that to calculate the function P(t) in eq.(1.5) only the values of $S(\boldsymbol{x}, \boldsymbol{x})$ and $Z_0(\boldsymbol{x}, \boldsymbol{x})$ are needed. Thus $S(\boldsymbol{x}, \boldsymbol{x}) = 0$ and the first approximation to $G(\boldsymbol{x}, \boldsymbol{x}, t)$ is

$$G(\boldsymbol{x}, \boldsymbol{x}, t) = \frac{1}{4\pi t},$$

hence the first approximation to P(t) is

$$P_0(t) = \frac{|\Omega|}{4\pi t}.$$

There is another solution of the eikonal equation (3.2) constructed along rays that emanate from \boldsymbol{x} , but reach \boldsymbol{y} after they are reflected in $\partial\Omega$ [12]. The law of reflection is determined from the boundary conditions. Dirichlet and Neumann boundary conditions imply that the angle of incidence equals that of reflection [12]. Similarly, there are solutions of the eikonal equation that are the lengths of rays that emanate from \boldsymbol{x} and reach \boldsymbol{y} after any number of reflections in $\partial\Omega$. We denote these solutions $S_k(\boldsymbol{y}, \boldsymbol{x})$ with some ordering. Thus the full ray expansion of Green's function has the form

$$G(\boldsymbol{y}, \boldsymbol{x}, t) \sim \sum_{k=1}^{\infty} e^{-S_k^2(\boldsymbol{y}, \boldsymbol{x})/4t} Z_k(\boldsymbol{y}, \boldsymbol{x}, t), \qquad (3.7)$$

where

$$Z_k(\boldsymbol{y}, \boldsymbol{x}, t) = \sum_{n=0}^{\infty} Z_{n,k}(\boldsymbol{y}, \boldsymbol{x}) t^{n-1}.$$

As above, each one of the series

$$e^{-S_k^2(\boldsymbol{y}, \boldsymbol{x})/4t}Z_k(\boldsymbol{y}, \boldsymbol{x}, t)$$

is called a *ray solution* of the diffusion equation. The boundary values of $Z_k(\boldsymbol{y}, \boldsymbol{x}, t)$ are chosen so that $G(\boldsymbol{y}, \boldsymbol{x}, t)$ in eq.(3.7) satisfies the imposed boundary condition. In particular, the values of $S_k(\boldsymbol{x}, \boldsymbol{x})$ are the lengths of all rays that emanate from \boldsymbol{x} and are reflected from the boundary back to \boldsymbol{x} . Note that sums of ray solutions satisfy boundary conditions only at certain points.

To fix the ideas, we consider first simply connected domains. We denote

$$S_0(\boldsymbol{y}, \boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{y}|$$

and

$$G_0({m y},{m x},t) = rac{1}{4\pi t} e^{-S_0^2({m y},{m x})/4t}.$$

We consider first solutions corresponding to rays that are reflected only once at the boundary, and in particular, rays that are reflected back from the boundary to the points of their origin. Such rays hit the boundary at right angles (see Fig. 1 and [12]). If there is only one minimal eikonal $S_1(\boldsymbol{x}, \boldsymbol{x}) > 0$, we say that \boldsymbol{x} is a *regular* point of Ω . If there is more than one minimal eikonal $S_1(\boldsymbol{x}, \boldsymbol{x})$, we say that \boldsymbol{x} is a *critical* point of Ω . We denote by Γ the locus of critical points in Ω . The eikonal $S_1(\boldsymbol{y}, \boldsymbol{x})$ is the length of the shortest ray from \boldsymbol{x} to \boldsymbol{y} with one reflection in the boundary such that the ray from \boldsymbol{x} to the boundary does not intersect Γ . For $\boldsymbol{x} = \boldsymbol{y}$ the eikonal $S_1(\boldsymbol{x}, \boldsymbol{x})$ is twice the distance of \boldsymbol{x} to the boundary. We denote by \boldsymbol{x}' the orthogonal projection of \boldsymbol{x} on the boundary along the shortest normal from \boldsymbol{x} to the boundary. When $\boldsymbol{y} = \boldsymbol{x}'$

$$S_1(x', x) = S_0(x', x) = |x - x'|.$$
 (3.8)

The function

$$G_1(\boldsymbol{y}, \boldsymbol{x}, t) = e^{-S_1^2(\boldsymbol{y}, \boldsymbol{x})/4t} Z_1(\boldsymbol{y}, \boldsymbol{x}, t)$$

has to be chosen so that $G_0(\mathbf{x}', \mathbf{x}, t) - G_1(\mathbf{x}', \mathbf{x}, t) = 0$. In view of (3.8), we have to choose

$$Z_1\left(\boldsymbol{x}',\boldsymbol{x},t\right) = \frac{1}{4\pi t}$$

When y'' is the other boundary point on the normal from x' to x, we have

$$G_0(\boldsymbol{y}'', \boldsymbol{x}, t) - G_1(\boldsymbol{y}'', \boldsymbol{x}, t) = \frac{1}{4\pi t} e^{-|\boldsymbol{x} - \boldsymbol{y}''|^2/t} - e^{-(|\boldsymbol{x}' - \boldsymbol{x}| + |\boldsymbol{y}'' - \boldsymbol{x}'|)^2/t} Z_1(\boldsymbol{y}'', \boldsymbol{x}, t). \quad (3.9)$$

Next, we consider in $\Omega - \Gamma$ the minimal among the remaining eikonals $S_k(\boldsymbol{x}, \boldsymbol{x}) > S_1(\boldsymbol{x}, \boldsymbol{x})$ and denote it $S_2(\boldsymbol{x}, \boldsymbol{x})$. This eikonal is twice the length of a ray that emanates from \boldsymbol{x} , intersects Γ once, and intersects the boundary $\partial\Omega$ at right angles at a point, denoted \boldsymbol{x}'' . The eikonal $S_2(\boldsymbol{y}, \boldsymbol{x})$ is the length of the ray from \boldsymbol{x} to \boldsymbol{y} with one reflection in the boundary such that the ray from \boldsymbol{x} to the boundary intersects Γ once. When $\boldsymbol{y} = \boldsymbol{x}''$

$$S_2(\mathbf{x}'', \mathbf{x}) = S_0(\mathbf{x}'', \mathbf{x}) = |\mathbf{x} - \mathbf{x}''|.$$
 (3.10)

When y' is the other boundary point on the normal that emanates from x'' (see Fig.2), we have

$$S_2(oldsymbol{y}',oldsymbol{x}) = |oldsymbol{x}-oldsymbol{x}''| + |oldsymbol{y}'-oldsymbol{x}''|$$
 .

In general $x' \neq y'$ and $x'' \neq y''$. However, if the ray is a 2-periodic orbit (that hits the boundary at only 2 points), x' = y' and x'' = y'' so that

$$S_2(m{y}'',m{x}) = S_0(m{y}'',m{x}) = |m{x}-m{y}''|$$

and

$$S_2(y', x) = |x - x''| + |y'' - x'|.$$



Figure 1. The locus of critical points, Γ , is the segment AB. The first eikonal is $S_1(\boldsymbol{y}, \boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{c}| + |\boldsymbol{c} - \boldsymbol{y}|$. It is defined as the shortest reflected ray from \boldsymbol{x} to \boldsymbol{y} , such that $\boldsymbol{x} - \boldsymbol{c}$ does not intersect Γ . For $\boldsymbol{x} = \boldsymbol{y}$ the diagonal values are $S_1(\boldsymbol{x}, \boldsymbol{x}) = 2|\boldsymbol{x} - \boldsymbol{x}'|$. The diagonal values of the second eikonal are $S_2(\boldsymbol{x}, \boldsymbol{x}) = 2|\boldsymbol{x} - \boldsymbol{x}''|$. The vectors $\boldsymbol{x} - \boldsymbol{x}'$ and $\boldsymbol{x} - \boldsymbol{x}''$ are orthogonal to the boundary. For $\boldsymbol{x}_1 \in \Gamma$ the two eikonals are equal.

Since

$$|m{x}-m{y}''| < |m{x}-m{x}'| + |m{y}''-m{x}'| < |m{x}-m{x}''| + |m{y}''-m{x}'|$$

for all regular points \boldsymbol{x} , the order of magnitude of the boundary error (3.9) decreases if we use the approximation

$$G_0(\boldsymbol{y}, \boldsymbol{x}, t) \sim G_0(\boldsymbol{y}, \boldsymbol{x}, t) - G_1(\boldsymbol{y}, \boldsymbol{x}, t) - G_2(\boldsymbol{y}, \boldsymbol{x}, t)$$
(3.11)

with

$$Z_2(y'', x, t) = Z_1(y'', x, t) = Z_0(t).$$



Figure 2. The second eikonal $S_2(\boldsymbol{y}, \boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{d}| + |\boldsymbol{d} - \boldsymbol{y}|$. It is defined as the shortest reflected ray such that $\boldsymbol{x} - \boldsymbol{d}$ intersects Γ . The eikonals $S_3(\boldsymbol{x}, \boldsymbol{x})$ and $S_4(\boldsymbol{x}, \boldsymbol{x})$ are ordered according to magnitude.

4. The trace

To find the short time asymptotics of the Dirichlet series (1.6), as given in eq.(1.5),

$$P(t) = \int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}, t) \, d\boldsymbol{x},$$

we use the ray expansion (3.7) for the evaluation of the integral. We retain in the resulting expansion only terms that are transcendentally small, since all algebraic terms are contained in the expansion (1.7).

4.1 Simply connected domains

We note that according to Sard's theorem, Γ is a set of measure zero and that all points in the domain $\Omega - \Gamma$ are regular. For any point $\boldsymbol{x} \in \Omega$, we denote by $r_1(\boldsymbol{x})$ its distance to the boundary and note that $S_1(\boldsymbol{x}, \boldsymbol{x}) = 2r_1(\boldsymbol{x})$. We also denote by $s_1(\boldsymbol{x})$ the arclength at the boundary point \boldsymbol{x}' (the orthogonal projection of \boldsymbol{x} on $\partial\Omega$ along the shortest normal from \boldsymbol{x} to $\partial\Omega$), measured from a boundary point where the arclength is set to 0 (see Figure 3).



Figure 3. The arclength $s_1(\mathbf{x})$ is measured from the point E. Both transformations $\mathbf{x} \to (r_1(\mathbf{x}), s_1(\mathbf{x}))$ and $\mathbf{x} \to (r_2(\mathbf{x}), s_1(\mathbf{x}))$ are one to one mappings of $\Omega - \Gamma$. The images are given in Figure 4.

It follows that the change of variables in $\Omega - \Gamma$, given by

$$\boldsymbol{x} \to (r_1(\boldsymbol{x}), s_1(\boldsymbol{x})),$$
 (4.1)

is a one-to-one mapping of $\Omega - \Gamma$ onto a strip $0 \le r_1 \le r_1(s_1)$, $0 \le s_1 \le L$, where $r_1(s_1)$ is the distance from the boundary point corresponding to arclength s_1 to Γ .



Figure 4. The domain Ω is the ellipse $\frac{x^2}{a^2} + \frac{y^2}{b^2} \leq 1$. The domain enclosed between the s_1 -axis and the lower curve is the image of the ellipse under the transformation (4.1) and the domain enclosed between the upper and the lower curves is its image under (4.3).

We evaluate the integral over Ω separately for each summand k in the expansion (3.7). In this notation, we can write

$$\int_{\Omega} G_1(\boldsymbol{x}, \boldsymbol{x}, t) d\boldsymbol{x} =$$

$$\int_{\Omega} e^{-\left[S_1(\boldsymbol{x}, \boldsymbol{x})\right]^2/4t} \sum_{n=0}^{\infty} Z_{n,1}(\boldsymbol{x}, \boldsymbol{x}) t^{n-1} d\boldsymbol{x} = \int_0^L ds \int_0^{r_1(s_1)} e^{-r_1^2/t} J_1(r_1, s_1) Z_1(r_1, s_1, t) dr_1,$$
(4.2)

where $J_1(r_1, s_1)$ is the Jacobian of the transformation and

n=0

$$Z_1(r_1, s_1, t) = \sum_{n=0}^{\infty} Z_{n,1}(\boldsymbol{x}, \boldsymbol{x}) t^{n-1}.$$

Note that the Jacobian vanishes neither inside $\Omega - \Gamma$ nor at $r_1 = 0$, because the transformation is one-to-one in $\Omega - \Gamma$, however, it does on Γ .

We set $S_2(\boldsymbol{x}, \boldsymbol{x}) = 2r_2(\boldsymbol{x})$ and use it as a coordinate. We use $s_1(\boldsymbol{x})$ as the other coordinate of the point $\boldsymbol{x} \in \Omega - \Gamma$. Note that while $r_2(\boldsymbol{x})$ is the length of the longer normal from \boldsymbol{x} to $\partial\Omega$ (the one that intersects Γ), the other coordinate is the arclength corresponding to the shorter normal from \boldsymbol{x} to $\partial\Omega$ (the one that does not intersect Γ). The transformation

$$\boldsymbol{x} \to (r_2(\boldsymbol{x}), s_1(\boldsymbol{x}))$$
 (4.3)

maps $\Omega - \Gamma$ onto the strip $r(s_1) \leq r_2 \leq l(s_1)$, $0 \leq s_1 \leq L$, where $l(s_1)$ is the length of the segment of the normal that starts at the boundary point $r_1 = 0, s_1$ and ends at its other intersection point with the boundary. This mapping is one-to-one as well. It follows that

$$\int_{\Omega} G_2(\boldsymbol{x}, \boldsymbol{x}, t) \, d\boldsymbol{x} =$$
(4.4)

$$\int_{\Omega} e^{-\left[S_2(\boldsymbol{x}, \boldsymbol{x})\right]^2/4t} \sum_{n=0}^{\infty} Z_{n,2}(\boldsymbol{x}, \boldsymbol{x}) t^{n-1} d\boldsymbol{x} = \int_0^L ds_1 \int_{r(s_1)}^{l(s_1)} e^{-r_2^2/t} J_2(r_2, s_1) Z_2(r_2, s_1, t) dr_2,$$

where

$$Z_2(r_2, s_1, t) = \sum_{n=0}^{\infty} Z_{n,2}(\boldsymbol{x}, \boldsymbol{x}) t^{n-1}$$

Note that for \boldsymbol{x} on Γ both transformations (4.1) and (4.3) are identical and

$$J_2(r_2, s_1)Z_2(r_2, s_1, t) = J_1(r_1, s_1)Z_1(r_1, s_1, t).$$

It follows that the two equations (4.2) and (4.4) combine together to give

$$\int_{\Omega} [G_1(\boldsymbol{x}, \boldsymbol{x}, t) + G_2(\boldsymbol{x}, \boldsymbol{x}, t)] d\boldsymbol{x} =$$

$$\int_{0}^{L} \int_{0}^{l(s)} e^{-r^2/t} J(r, s) Z(r, s, t) dr ds,$$
(4.5)

where $s = s_1$, $r = r_1$, $J = J_1$, and $Z = Z_1$ for $0 < r < r_1(s_1)$, and $s = s_1$, $r = r_2$, $J = J_2$, and $Z = Z_2$ for $r_2(s_1) < r < l(s_1)$. Thus the domain of integration of the function $e^{-r^2/t}J(r,s)Z(r,s,t)$ in eq.(4.5) is the domain enclosed by the s_1 -axis and the upper curve in Figure 4. Now, for $t \ll 1$, we write the inner integral on the right hand side of eq.(4.5) as

$$\begin{split} \int_0^{l(s)} e^{-r^2/t} J(r,s) Z(r,s,t) \, dr &= \sqrt{\frac{\pi t}{2}} \mathrm{erf}\left(\frac{l(s)}{\sqrt{t}}\right) J(0,s) Z(0,s,t) \left(1 + O\left(\sqrt{t}\right)\right) = \\ \sqrt{\frac{\pi t}{2}} \left(1 - \frac{\exp\left\{-\frac{l^2(s)}{t}\right\} \sqrt{t}}{l(s)}\right) J(0,s) Z(0,s,t) \left(1 + O\left(\sqrt{t}\right)\right). \end{split}$$

Recall that $J(0, s)Z(0, s, t) \neq 0$. Only the exponentially small terms have to be considered, because the algebraic terms are included in the SW expansion. Thus

$$\int_{0}^{L} \int_{0}^{l(s)} e^{-r^{2}/t} J(r,s) Z(r,s,t) \, dr \, ds - \int_{0}^{L} \sqrt{\frac{\pi t}{2}} (0,s) Z(0,s,t) \left(1 + O\left(\sqrt{t}\right)\right) \, ds = -\int_{0}^{L} \exp\left\{-\frac{l^{2}(s)}{t}\right\} \frac{J(0,s) Z(0,s,t)}{l(s)} O(t) \, ds \quad \text{for } t \ll 1.$$

Evaluating the last integral by the Laplace method, we find that each point s_i that is an extremum point of l(s) contributes and exponential term of the form

$$\exp\left\{-\frac{l^2(s_i)}{t}\right\}\frac{J(0,s_i)Z(0,s_i,t)}{l(s_i)}O(t^{\nu}).$$
(4.6)

The expression (4.6) means that some of the δ_n -s in the expansion eq.(1.9) are the extremal values $l(s_i)$ and their multiples. These are half the lengths of the 2-periodic orbits of a billiard ball in Ω (see Figure 5). The 2-periodic orbits of the ellipse are the major axes, which correspond to the lowest and highest points of the top curve in Figure 4. There are other exponents as well, as discussed below.



Figure 5. The rays emanating from the boundary points s_1 and s_2 are orthogonal the boundary at both ends. They are 2-periodic orbits.

The pre-exponential terms in the expression (4.6) influence the factors $P_n(\sqrt{t})$ in

eq.(1.9). For example, if $l'(s_i) = 0$, $l''(s_i) \neq 0$, then $\nu = 3/2$. If the boundary is flatter, then $1 \leq \nu < 3/2$.

In addition to the 2-periodic orbits, there are ray solutions corresponding to rays from \boldsymbol{x} to \boldsymbol{y} that are reflected any number of times in the boundary. There are eikonals from \boldsymbol{x} to \boldsymbol{y} in Ω with N-1 different vertices on the boundary, which have N vertices on $\partial\Omega$ if $\boldsymbol{x} = \boldsymbol{y}$ and $\boldsymbol{x} \in \partial\Omega$ (this is a periodic orbit with N-1 reflections). Among these periodic orbits there are eikonals $S_N(\boldsymbol{x}, \boldsymbol{x})$ with extremal length, denoted $S_{N,j}$, (j = 1, ...). At points $\boldsymbol{x} \in \Omega$ on a 2-periodic orbit the eikonal $S_N(\boldsymbol{x}, \boldsymbol{x})$, which now has N-1 vertices on the boundary, may reduce to the 2-periodic orbit with N reflections. Therefore the change of variables $\boldsymbol{x} \to (S_N(\boldsymbol{x}, \boldsymbol{x}), \boldsymbol{s}(\boldsymbol{x}))$ will map the domain into a strip with extremal widths that are the differences between the lengths $S_{N,j}$ and the length of a 2-periodic orbit with N reflections. It follows that the evaluation of the trace by the Laplace method leads to exponents which are the extremal lengths of periodic orbits with any number of reflections.

For example, there is an eikonal in a circle (centered at the origin) that is the ray from \boldsymbol{x} to \boldsymbol{y} with 2 reflections in the boundary (see Figure 6).



Figure 6. The eikonal $S_3(\boldsymbol{y}, \boldsymbol{x})$ with two reflections in the circle.

For $\boldsymbol{x} = \boldsymbol{y}$ it is the equilateral triangle (see Figure 7) with circumference

$$S(\boldsymbol{x}, \boldsymbol{x}) = R\left(2\frac{\sqrt{2|\boldsymbol{x}|^2 + 1 + \sqrt{8|\boldsymbol{x}|^2 + 1}}}{\sqrt{4|\boldsymbol{x}|^2 + 1 + \sqrt{8|\boldsymbol{x}|^2 + 1}}} + \sqrt{4|\boldsymbol{x}|^2 + 2 + 2\sqrt{8|\boldsymbol{x}|^2 + 1}}\right)$$



Figure 7. The eikonal $S_3(\boldsymbol{x}, \boldsymbol{x})$ with two reflections, where $|\boldsymbol{x}| = OC$.

The eikonal $S_3(\boldsymbol{x}, \boldsymbol{y})$ reduces to a 2-periodic orbit with two reflections if $\boldsymbol{x} = \boldsymbol{y} = 0$ (the center of the circle). If \boldsymbol{x} is on the circumference, the eikonal becomes the isosceles triangle with one vertex at \boldsymbol{x} . To evaluate the contribution of the corresponding ray solution to the trace, we use this eikonal as a coordinate that varies between 4R, the length of the 2-periodic orbit with two reflections, and $3\sqrt{3}R$, the circumference of the inscribed isosceles triangle. The contribution of this integral to the exponential sum in eq.(1.9) contains exponents that are both lengths.

Similarly, the 2-periodic orbit with 3 reflections has length 6R while the periodic orbit with 3 reflections at 3 different points has length $4\sqrt{2}R < 6R$.

4.2 Multiply connected domains

Once again, we consider first rays from \boldsymbol{x} to \boldsymbol{y} that are reflected only once in the boundary. For every connected component of $\partial\Omega$, denoted $\partial\Omega_i$ (i = 1, ..., I), a point \boldsymbol{x}

in Ω is regular with respect to $\partial \Omega_i$ if there is only one minimal eikonal $S_{i,1}(\boldsymbol{x}, \boldsymbol{x}) > 0$ with one reflection at $\partial \Omega_i$. We denote by Γ_i the locus of the irregular points of Ω with respect to $\partial \Omega_i$.

As above, we define in $\Omega - \Gamma_i$ the minimal eikonal with one reflection in $\partial \Omega_i$ such that $S_{i,2}(\boldsymbol{x}, \boldsymbol{x}) > S_{i,1}(\boldsymbol{x}, \boldsymbol{x})$. We construct an approximation

$$G(\boldsymbol{y}, \boldsymbol{x}, t) \sim G_0(\boldsymbol{y}, \boldsymbol{x}, t) + \sum_{k=1}^2 \sum_{i=1}^I G_{i,k}(\boldsymbol{y}, \boldsymbol{x}, t)$$

where $G_{i,k}(\boldsymbol{y}, \boldsymbol{x}, t)$ are ray solutions with eikonals $S_{i,k}(\boldsymbol{y}, \boldsymbol{x})$ and $Z_{i,k}(\boldsymbol{y}, \boldsymbol{x})$ chosen so as to minimize the boundary values of the sum at the boundary points of rays orthogonal to the boundary, as above. The trace of the double sum is calculated by introducing the change of variables $2r_{i,k}(\boldsymbol{x}) = S_{i,k}(\boldsymbol{x}, \boldsymbol{x})$ and arclength $s_i(\boldsymbol{x})$ in $\partial\Omega_i$, as above. The Laplace evaluation of the integrals produces exponents that are the 2-periodic orbits in Ω .

Eikonals with two or more reflections contribute exponents that are lengths of extremal closed orbits with any number of reflections in the boundary, as in the case of simply connected domains. Thus the exponents δ_n in (1.9) consist of half the lengths of 2-periodic orbits in Ω and their multiples, and extremal lengths of closed periodic orbits with any number of reflections in the boundary and their multiples.

5. Discussion

First, we compare our result to that conjectured in [8]. The leading exponent in the remainder of the short time expansion of P(t) in an asymptotic power series and that in the large s expansion of its Laplace transform are related by the well known formula [19]

$$\mathcal{L}\left[\operatorname{erfc}\left(\frac{k}{2\sqrt{t}}\right)\right](s) = \frac{1}{s}e^{-k\sqrt{s}},$$

where

$$\operatorname{erfc}(z) \sim \frac{e^{-z^2}}{\sqrt{\pi z}} \quad \text{for } z \gg 1.$$

Thus the exponential rate of blowup of the Laplace transform on a Stokes line is twice the square root of the exponential decay rate of the remainder term in the expansion of the trace. It follows from our result that the exponential blowup rate of the Laplace transform is twice the square root of the exponential rate of decay in the time domain.

We illustrate our expansion for a disk, whose boundary has only one connected component and a single critical point. We consider points $\boldsymbol{x} = (x_1, y_1)$ and $\boldsymbol{y} = (x_2, y_2)$ inside a circle of radius R centered at the origin. The leading order eikonal is

$$S_0(\boldsymbol{y}, \boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{y}|.$$

When both \boldsymbol{x} and \boldsymbol{y} are on the x-axis, we have $y_1 = y_2 = 0$ and $S_0(\boldsymbol{y}, \boldsymbol{x}) = |x_1 - x_2|$. Denoting $\boldsymbol{x}_1 = (x_1, 0)$ and $\boldsymbol{x}_2 = (x_2, 0)$, we see that the values of the eikonal on the x-axis are $S_0(\boldsymbol{x}_1, \boldsymbol{x}_2) = |x_1 - x_2|$. We assume that $x_1 > 0$. The boundary values of the eikonal are

$$S_0(\boldsymbol{x}_1, \boldsymbol{x}_2) = R - x_1$$
 at $\boldsymbol{x}_2 = (R, 0)$

and

$$S_0(\boldsymbol{x}_1, \boldsymbol{x}_2) = R + x_1$$
 at $\boldsymbol{x}_2 = (-R, 0).$

Thus the leading order ray approximation to Green's function $G(\boldsymbol{y}, \boldsymbol{x}, t)$,

$$G_0(\boldsymbol{y}, \boldsymbol{x}, t) = \frac{1}{4\pi t} e^{-S_0^2(\boldsymbol{y}, \boldsymbol{x})/4t},$$

misses the boundary conditions when x and y are on the x-axis, giving

$$G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \frac{1}{4\pi t} e^{-(R-x_1)^2/4t}$$
 at $\boldsymbol{x}_2 = (R, 0)$

and

$$G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \frac{1}{4\pi t} e^{-(R+x_1)^2/4t} \quad \text{at } \boldsymbol{x}_2 = (-R, 0).$$
(5.1)

The next eikonal, denoted $S_1(\boldsymbol{y}, \boldsymbol{x})$, is given on the *x*-axis by $S_1(\boldsymbol{x}_1, \boldsymbol{x}_2) = 2R - x_1 - x_2$, and its boundary values are

$$S_1(\boldsymbol{x}_1, \boldsymbol{x}_2) = R - x_1$$
 at $\boldsymbol{x}_2 = (R, 0)$

and

$$S_1(\boldsymbol{x}_1, \boldsymbol{x}_2) = 3R - x_1$$
 at $\boldsymbol{x}_2 = (-R, 0).$

Thus the approximation of Green's function $G(\boldsymbol{y}, \boldsymbol{x}, t)$,

$$G(\boldsymbol{y}, \boldsymbol{x}, t) \sim G_0(\boldsymbol{y}, \boldsymbol{x}, t) - G_1(\boldsymbol{y}, \boldsymbol{x}, t),$$

corresponding to the ray solutions $G_0(\boldsymbol{y}, \boldsymbol{x}, t)$ and

$$G_1(\boldsymbol{x}, \boldsymbol{y}, t) = Z_1(\boldsymbol{x}, \boldsymbol{y}, t) e^{-S_1^2(\boldsymbol{y}, \boldsymbol{x})/4t},$$

will satisfy the boundary condition at (x_1, R) if $Z_1(\boldsymbol{y}, \boldsymbol{x}, t)$ is chosen so that

$$Z_1(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \frac{1}{4\pi t}$$
 at $\boldsymbol{x}_2 = (R, 0).$

However, this approximation does not satisfy the boundary condition at $\mathbf{x}_2 = (-R, 0)$. The error in the boundary values at $\mathbf{x}_2 = (-R, 0)$ is

$$G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, t) - G_1(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \frac{1}{4\pi t} e^{-(R+x_1)^2/4t} - Z_1(\boldsymbol{x}_1, \boldsymbol{x}_2, t) e^{-4(R-x_1)^2/4t}, \quad \text{at } \boldsymbol{x}_2 = (-R, 0)$$

and is of the same order of magnitude as that of the leading order approximation (5.1). To make up for the missed boundary condition the further approximation

$$G(\boldsymbol{y}, \boldsymbol{x}, t) \sim G_0(\boldsymbol{y}, \boldsymbol{x}, t) - G_1(\boldsymbol{y}, \boldsymbol{x}, t) - G_2(\boldsymbol{y}, \boldsymbol{x}, t)$$
(5.2)

can be used, with

$$G_{2}(\boldsymbol{y},\boldsymbol{x},t) = Z_{2}(\boldsymbol{y},\boldsymbol{x},t) e^{-S_{1}^{2}(\boldsymbol{y},\boldsymbol{x})/4t},$$

where on the x-axis

$$s_1(\boldsymbol{x}_1, \boldsymbol{x}_2) = 2R + x_1 + x_2$$

and

$$Z_2(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \frac{1}{4\pi t}$$
 at $\boldsymbol{x}_2 = (-R, 0).$

This eikonal corresponds to rays with two reflections in the boundary. The approximation (5.2) decreases the error in the boundary condition at $\boldsymbol{x}_2 = (-R, 0)$ to

$$-Z_1(\boldsymbol{x}_1, \boldsymbol{x}_2, t) e^{-4(R-x_1)^2/4t},$$

but misses the boundary condition at $\boldsymbol{x}_2 = (R, 0)$ with error

$$G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, t) - G_1(\boldsymbol{x}_1, \boldsymbol{x}_2, t) - G_2(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = -Z_2(\boldsymbol{x}_1, \boldsymbol{x}_2, t) e^{-(3R+x_1)^2/4t}$$
 at $\boldsymbol{x}_2 = (R, 0).$

This process gives successive approximations to Green's function with errors that decrease at transcendental rather than algebraic rates.

The approximation to the trace produced by $G_0(\boldsymbol{y}, \boldsymbol{x}, t)$ is the first algebraic term in the expansion (1.7). The contributions of the terms $-G_1(\boldsymbol{y}, \boldsymbol{x}, t)$ and $-G_2(\boldsymbol{y}, \boldsymbol{x}, t)$ in the approximation (5.2) of terms that are $O\left(\sqrt{t}e^{-R^2/t}\right)$ are identical, but with opposite signs and thus they cancel each other. The second term contributes a negative term that is $O\left(\sqrt{t}e^{-4R^2/t}\right)$. The term $O\left(\sqrt{t}e^{-R^2/t}\right)$ for small t corresponds to $O\left(\frac{1}{s}e^{-2R\sqrt{s}}\right)$ for large positive s in the Laplace plane. The number 2R is the length of the periodic orbit of a billiard ball bouncing inside a circle with the center removed, that is, inside the domain $\Omega - \Gamma$, where the set of critical points Γ consists of the center. Similarly, the term $O\left(\sqrt{t}e^{-4R^2/t}\right)$ for small t corresponds to $O\left(\frac{1}{s}e^{-4R\sqrt{s}}\right)$ for large positive s in the Laplace plane. The number 4R is the length of the minimal periodic orbit of a billiard ball bouncing inside a disk. We conclude that the conjecture of [8] should be supplemented with the orbit of length 2R.

If Ω is an annulus between two concentric circles, of radii a and b, respectively, (a > b), the two connected components of the boundary are the two circles and there are no critical points in the domain relative to either one of them. In this case $\delta_1 = (a - b)$.

If Ω is the ellipse

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} < 1$$

with a > b, the locus of critical points relative to the boundary is the segment

$$\Gamma = \left[-\frac{a^2 - b^2}{a}, \frac{a^2 - b^2}{a} \right]$$

on the x-axis. The segment Γ is the short diagonal of the evolute of the ellipse (the asteroid $(ax)^{2/3} + (by)^{2/3} = (a^2 - b^2)^{2/3}$). For the ellipse there are exponents in eq.(1.9) which are $\delta_1 = 2b$ and its multiples and $\delta_2 = 2a$ and its multiples, as well as extremal periodic orbits with any number of reflections in the boundary.

Finally, we observe that if the boundary is reflecting (i.e., a homogeneous Neumann boundary condition), the exponential decay rate of the transcendental terms in the expansion of the trace is the same as in the case of absorbing boundary (homogeneous Dirichlet boundary condition). In this case the second term in the expansion (1.9) changes sign.

Obviously, rays that are reflected from the boundary more than once also give rise to ray solutions. The number of ray solutions needed in the expansion (3.7) is determined by the required degree of asymptotic approximation of the boundary conditions. If only a finite sum of ray solutions satisfies the boundary conditions, the sum (3.7) is finite. Otherwise, additional ray solutions improve the degree of approximation of the boundary conditions, as described in the one-dimensional ray expansion in Section 2.

Finally, the asymptotic convergence of the ray expansion follows from the maximum principle for the heat equation in a straightforward manner.

References

- P.T. CALLAGHAN, Principles of Nuclear Magnetic Resonance Microscopy, Oxford University Press, NY 1991.
- [2] M. KAC, Can one hear the shape of a drum? Amer. Math. Monthly, 73 (4) (1966), part II, pp.1-23.
- [3] K. STEWARTSON AND R.T. WAECHTER, On hearing the shape of a drum: further results, Proc. Cambridge Philosophical Society, **69** (1971), pp.353-363.
- [4] P. GREINER, An asymptotic expansion for the heat equation, Arch. Rat. Mech. Anal. 41 (3), pp.163-218 (1971).
- [5] R. BALIAN AND C. BLOCH, Distribution of eigenfrequencies for the wave equation in a finite domain: III. eigenfrequency density oscillations, Ann. Phys. 69, pp.76-160 (1972).
- [6] Y. COLIN DE VERDIÈRE, Spectre du Laplacien et longueurs des géodésiques périodiques I, Composito Mathematica 27 (1), pp.83-106 (1973), Spectre du Laplacien et longueurs des géodésiques périodiques II, Composito Mathematica 27 (2), pp.159-184 (1973).

- [7] V. GUILLEMIN AND R. MELROSE, The Poisson summation formula for manifolds with boundar, Adv. in Math. **32**, pp.204-232 (1979).
- [8] M.V. BERRY AND C.J. HOWLS, High orders of the Weyl expansion for quantum billiards: resurgence of periodic orbits, and the Stokes phenomenon, Proc. R. Soc. Lond. A 447, pp.525-555 (1994)
- [9] S. ZELDITCH, Spectral determination of analytic bi-axisymmetric plane domains, Geometric and Functional Analysis, **10**, pp.628-677 (2000).
- [10] Z. SCHUSS, Theory and Applications of Stochastic Differential Equations, Wiley Series in Probability and Statistics John Wiley Sons, Inc., New York, 1980.
- [11] R.E. MEYER, *Exponential asymptotics*, SIAM Rev. **22** (2) (1980), pp.213-224
- [12] J. COHEN AND R. LEWIS, Ray Method for the asymptotic solution of the diffusion equation, J. Inst. Maths. Applies, 3 (1967), pp. 266-290.
- [13] R. COURANT AND D. HILBERT, Methods of Mathematical Physics, Wiley, NY 1989.
- [14] J.K. COHEN, F. HAGIN, AND J.B. KELLER, Short time asymptotic expansion of solutions of parabolic equations, Journal of Math. Analysis and Applications, 38 (1972), pp.82-91.
- [15] C. TIER AND J.B. KELLER, Asymptotic analysis of diffusion equations in population genetics, SIAM J. Appl. Math. 34 (3) (1978), pp.549-576.
- [16] B.D. SECKLER AND J.B. KELLER, Geometrical theory of diffraction in inhomogeneous media J. Accoust. Soc. Amer. 31, (1959), pp.192-205
- [17] J.B. KELLER, Geometrical theory of diffraction, J. Optical Soc. Amer. 52, (1962), pp.116-130.
- [18] R.M. LEWIS AND J.B. KELLER, Asymptotic methods for partial differential equations: the reduced wave equation and Maxwell's equations, NYU Research Report no. EM-194, NYU 1964.
- [19] M. ABRAMOWITZ AND I.A. STEGUN, Handbook of Mathematical Functions, Dover, NY 1970.
- [20] E. ZAUDERER, Partial Differential Equations of Applied Mathematics, 2-nd edition, Wiley-Interscience, NY 1989.