

Diffraction and boundary conditions in semiclassical open billiards

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The conductance through open quantum dots, or quantum billiards, shows fluctuations that can be explained as interference between waves following different paths between the leads of the billiard. We examine such systems by the use of a semiclassical Green's functions. In this paper we examine how the choice of boundary conditions at the lead mouths affects the diffraction. We derive a superior formula for the S -matrix element. Finally, we compare semiclassical simulations to quantum mechanical ones, and show that this formula yields superior results.

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Lateral quantum dots, also called quantum billiards serve as model systems in the study of the relation between quantum and classical physics. A very large number of experiments have been done on transport through open semiconductor quantum dot,¹⁻⁴ and also experiments on analog systems such as microwave billiards have been performed.⁵⁻⁸ These studies show rapid conductance oscillations as function of energy or of an applied magnetic field. To provide a quantitative description of these oscillations, several approaches have been adopted, such as random matrix theory,⁹ numerical solution of the Schrödinger equation,^{2,10-13} and semiclassical (SC) methods. In the SC view, the conductance oscillations arise due to interference between pairs of classical trajectories, carrying a quantum mechanical (QM) phase,¹⁴⁻¹⁶ between the leads of the billiard.¹⁷ The SC approach has been used to describe statistical properties of the conductance oscillations^{15,16} including weak-localization line shapes in chaotic and regular cavities, and fractal conductance in systems with mixed phase space. One should, however, be careful in relying on these results.¹⁸ The SC approach can also provide an interpretation of specific frequencies in the conductance oscillations, by relating them to specific classical trajectories in a billiard. In calculating conductance or transmission amplitudes of a system, a SC approximation of the systems Green's function is used. In relating this Green's function to the transmission amplitude between leads of the billiard, one has to take into account diffraction effects at the lead mouths. In this paper we study how the choice of boundary conditions (BC's) on the Green's function affect the diffraction and make comparison to QM calculations.

We study a billiard with hard walls and a zero inner potential. The Hamiltonian inside the billiard is

$$H = \frac{(-i\hbar\nabla + e\mathbf{A})^2}{2m^*}, \quad (1)$$

where \mathbf{A} is the vector potential of a magnetic field, e is the electron charge and m^* is the electron's effective mass. The dynamics is decided by the Schrödinger equation

$$(H - E)\psi = 0. \quad (2)$$

We define the Green's function

$$(H - E)G(\mathbf{q}, \mathbf{q}') = \delta(\mathbf{q}, \mathbf{q}'). \quad (3)$$

The SC approximation of the Green's function in two dimensions is¹⁷

$$G^{\text{SC}}(\mathbf{q}, \mathbf{q}', k_F) = \frac{2\pi}{(2\pi i\hbar)^{3/2}} \sum_p |D_p(\mathbf{q}, \mathbf{q}', k_F)|^{1/2} \times \exp\left[\frac{i}{\hbar} S_p(\mathbf{q}, \mathbf{q}', k_F) - \frac{i\pi}{2} \mu_p\right], \quad (4)$$

where the density of trajectories D_p (Ref. 17) is taken to vary slowly in comparison with the phase from the action S_p and μ_p is called the Maslov index.^{17,19}

To calculate the S matrix, we start by letting the Hamiltonian act on the wave function ψ and expand the expression to

$$H\psi = -\frac{\hbar^2}{2m^*} \nabla^2 \psi - \frac{i\hbar e}{2m^*} \nabla \cdot (\mathbf{A}\psi) - \frac{i\hbar e}{2m^*} \mathbf{A} \cdot \nabla \psi + \frac{e^2 \mathbf{A}^2}{2m^*} \psi. \quad (5)$$

The divergence theorem states

$$\int_S d\mathbf{q}'^2 \nabla \cdot \mathbf{F} = - \oint_C dl' \mathbf{F} \cdot \hat{\mathbf{n}}, \quad (6)$$

where C is the boundary to the area S and $\hat{\mathbf{n}}$ is an inward normal to the boundary C . Let

$$\mathbf{F} = -\frac{\hbar^2}{2m^*} \phi^* \nabla \psi, \quad (7)$$

and evaluate

$$\begin{aligned} \nabla \cdot \mathbf{F} &= -\frac{\hbar^2}{2m^*} \phi^* \nabla^2 \psi - \frac{\hbar^2}{2m^*} \nabla \phi^* \cdot \nabla \psi \\ &= \phi^* H \psi + \frac{i\hbar e}{2m^*} [\phi^* \nabla \cdot (\mathbf{A}\psi) + \phi^* \mathbf{A} \cdot \nabla \psi] \\ &\quad - \frac{e^2 \mathbf{A}^2}{2m^*} \phi^* \psi - \frac{\hbar^2}{2m^*} \nabla \phi^* \cdot \nabla \psi. \end{aligned} \quad (8)$$

We also get

$$\mathbf{F} \cdot \hat{\mathbf{n}}' = -\frac{\hbar^2}{2m^*} \phi^* \frac{\partial \psi}{\partial n'}. \quad (9)$$

Equations (6)–(9) results in an analog to Green's first identity

$$\begin{aligned} \int_S d\mathbf{q}'^2 \left[\phi^* H \psi + \frac{i\hbar e}{2m^*} [\phi^* \nabla \cdot (\mathbf{A} \psi) + \phi^* \mathbf{A} \cdot \nabla \psi] \right. \\ \left. - \frac{e^2 \mathbf{A}^2}{2m^*} \phi^* \psi - \frac{\hbar^2}{2m^*} \phi^* \nabla \psi \right] = \oint_C dl' \frac{\hbar^2}{2m^*} \phi^* \frac{\partial \psi}{\partial n'}. \end{aligned} \quad (10)$$

We take the complex conjugate of Eq. (10), interchanging ϕ and ψ , and subtracting it from Eq. (10), after some manipulations we get

$$\begin{aligned} \int_S d\mathbf{q}'^2 \left[\phi^* H \psi - \psi H \phi^* + \frac{i\hbar e}{m} (\psi \mathbf{A} \cdot \nabla \phi^* + \phi^* \mathbf{A} \cdot \nabla \psi) \right] \\ = -\frac{\hbar^2}{2m^*} \oint_C dl' \left[\psi \frac{\partial \phi^*}{\partial n'} - \phi^* \frac{\partial \psi}{\partial n'} \right]. \end{aligned} \quad (11)$$

We would, however, like to get rid of the magnetic terms on the left hand side, we now insert

$$\mathbf{F} = \frac{e\mathbf{A}}{m^*} \psi \phi^* \quad (12)$$

into the divergence theorem and choose a gauge such that $\nabla \cdot \mathbf{A} = 0$, resulting in

$$\begin{aligned} \int_S d\mathbf{q}'^2 \frac{i\hbar e}{m^*} [\psi \mathbf{A} \cdot \nabla \phi^* + \phi^* \mathbf{A} \cdot \nabla \psi] \\ = - \oint_C dl' \frac{i\hbar e}{m^*} \mathbf{A} \cdot \hat{\mathbf{n}}' \psi \phi^*. \end{aligned} \quad (13)$$

This allows us to rewrite Eq. (11), while replacing $\phi^*(\mathbf{q}') = G(\mathbf{q}, \mathbf{q}')$ as

$$\begin{aligned} \int_S d\mathbf{q}'^2 [G(\mathbf{q}, \mathbf{q}') H \psi - \psi H G(\mathbf{q}, \mathbf{q}')] \\ = - \oint_C dl' \left[\frac{\hbar^2}{2m^*} \left(\psi \frac{\partial G(\mathbf{q}, \mathbf{q}')}{\partial n'} - G(\mathbf{q}, \mathbf{q}') \frac{\partial \psi}{\partial n'} \right) \right. \\ \left. - \frac{i\hbar e}{m^*} \psi G(\mathbf{q}, \mathbf{q}') \mathbf{A} \cdot \hat{\mathbf{n}}' \right], \end{aligned} \quad (14)$$

a version of Green's theorem.

We now calculate the diffraction from a lead mouth, following in the steps of Kirchhoff.²² The area S is taken to be the half circle, see Fig. 1(a). The contour C is taken to be divided into two parts C_1 , the entrance lead mouth and C_0 , the rest of C . We make the requirement that $\psi = 0$ and $\partial \psi / \partial n' = 0$ along the wall, this requirement is elaborated on

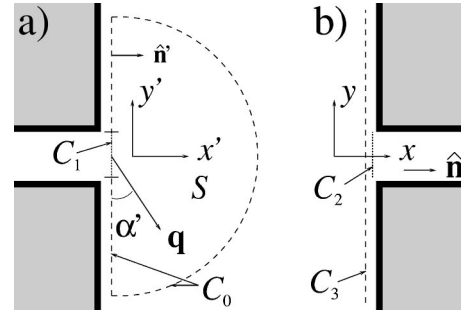


FIG. 1. (a) Geometry of the entrance lead, S is the half circle enclosed by $C = C_0 \cup C_1$, where C_1 across the entrance only, $\hat{\mathbf{n}}'$ is an inward normal to C , α' is an angle at the entrance, \mathbf{q} is a coordinate and x' and y' form a local coordinate system. (b) Geometry of the exit lead, $\hat{\mathbf{n}}$ is into the lead, x and y form a local coordinate system. Path C_2 is across the exit and C_3 is along the entire wall.

later in the text. With zero magnetic field, $G, \psi \sim r^{-1/2}$, and the integration along the half circle part of C tends to zero as the radius $r \rightarrow \infty$.²⁰ The motivation for letting $r \rightarrow \infty$ within a finite billiard is that in the SC theory the wave function along all classical trajectories is the free space wave function. The total wave function is then the superposition of all such trajectory wave functions. In nonzero magnetic field we are dealing with edge states, localized near the wall. If we assume that the current is going in the $-y$ direction, then $\psi(\mathbf{q}')$ will vanish everywhere on the half circle except near the wall in the lower half-plane ($y' < 0$). On the other hand the Green's function $G(\mathbf{q}, \mathbf{q}')$ is also localized to near the wall but for $G(y \gg y', y')$, i.e., the Green's function at the interior point \mathbf{q} will not see an excitation at a point \mathbf{q}' that is far enough downstream the wall. For an interior point \mathbf{q} either $\psi(\mathbf{q}')$ or $G(\mathbf{q}, \mathbf{q}')$ will go (exponentially) fast to zero on the half circle when $r \rightarrow \infty$. It is thus enough to integrate over C_1 instead of C in Eq. (14). Using Eqs. (2) and (3) in Eq. (14) we can obtain the wave function inside the billiard

$$\begin{aligned} \psi(\mathbf{q}) = \int_{C_1} dy' \left[\frac{\hbar^2}{2m^*} \left(\psi^0(\mathbf{q}') \frac{\partial G(\mathbf{q}, \mathbf{q}')}{\partial x'} \right. \right. \\ \left. \left. - G(\mathbf{q}, \mathbf{q}') \frac{\partial \psi^0(\mathbf{q}')}{\partial x'} \right) - \frac{i\hbar e}{m^*} \psi^0(\mathbf{q}') G(\mathbf{q}, \mathbf{q}') \mathbf{A} \cdot \hat{\mathbf{n}}' \right], \end{aligned} \quad (15)$$

where $dy' = -dl'$.

To calculate transmission amplitudes, we start from the definition of the current density operator²¹

$$\tilde{\mathcal{J}}(\mathbf{q}) = \frac{1}{2m^*} [\tilde{\mathcal{P}} \delta(\mathbf{q} - \mathbf{q}') + \delta(\mathbf{q} - \mathbf{q}') \tilde{\mathcal{P}}], \quad (16)$$

where $\tilde{\mathcal{P}} = -i\hbar \nabla + e\mathbf{A}$ is the momentum operator. We obtain an operator for the current into the exit lead by integrating across it

$$\mathcal{J} = \int_{C_2} dy \vec{\mathcal{J}}(y) \cdot \hat{\mathbf{n}}, \quad (17)$$

where C_2 is across the exit and y the transverse coordinate, see Fig. 1(b). The eigenmodes n in the entrance lead are taken to be

$$\psi_n^0(x', y') = \frac{1}{\sqrt{v_n}} \xi_n(y') e^{ik_n x'} = \sqrt{\frac{m^*}{\hbar k_n}} \xi_n(y') e^{ik_n x'}, \quad (18)$$

where v_n is the velocity in the lead, k_n the k -vector, and x' and y' are defined in Fig. 1. The eigenmode wave functions of the exit $\psi_m^0(x, y)$ are defined analogously. The continuation ψ_n of ψ_n^0 into the billiard is given by Eq. (15). The scattering matrix element is equal to the matrix element

$$S_{mn} = \langle \psi_m^0 | \mathcal{J} | \psi_n \rangle = \int dy \left[\frac{-i\hbar}{2m^*} \left(\psi_m^{0*} \frac{\partial \psi_n}{\partial x} - \psi_n \frac{\partial \psi_m^{0*}}{\partial x} \right) + \frac{e\mathbf{A} \cdot \hat{\mathbf{x}}}{m^*} \psi_m^{0*} \psi_n \right]. \quad (19)$$

By inserting Eqs. (15) and (18) we get

$$S_{mn} = -\frac{i\hbar^3}{4m^{*2}\sqrt{v_m v_n}} \int dy \int dy' \xi_m^*(y) \xi_n(y') \left[\frac{\partial^2 G}{\partial x \partial x'} - \frac{i}{\hbar} [m^* v_n + 2e\mathbf{A}(y') \cdot \hat{\mathbf{x}}'] \frac{\partial G}{\partial x} + \frac{i}{\hbar} [m^* v_m + 2e\mathbf{A}(y) \cdot \hat{\mathbf{x}}] \frac{\partial G}{\partial x'} + \frac{1}{\hbar^2} [m^* v_m + 2e\mathbf{A}(y) \cdot \hat{\mathbf{x}}] \times [m^* v_n + 2e\mathbf{A}(y') \cdot \hat{\mathbf{x}}'] G \right], \quad (20)$$

where primed coordinates relate to the entrance and unprimed to the exit.

Equation (20) is the transmission amplitude calculated using the Kirchhoff approximation, which to recall consists of the following assumptions: (1) ψ and $\partial\psi/\partial n$ vanish everywhere on C except on the lead mouth, (2) the values of ψ and $\partial\psi/\partial n$ on the lead mouth are equal to the values of the incident wave in the lead. For example, Schwieters *et al.*²⁰ use this approximation. There are however some inconsistencies in the Kirchhoff approximation.²² It can be shown for the Schrödinger equation that if $\psi=0$ and $\partial\psi/\partial n'=0$ on any finite surface, the only solution is $\psi=0$ everywhere. This inconsistency can be lifted by choosing Green's functions with appropriate BC, i.e., either Dirichlet or Neumann. We start with the Neumann Green's functions

$$\frac{\partial G_N}{\partial n'}(\mathbf{q}, \mathbf{q}') = 0 \quad \text{for } \mathbf{q}' \text{ on } C. \quad (21)$$

If the contour C is an infinite line across the entrance and S all space to the right, the Neumann Green's function can be obtained by the method of images

$$G_N(\mathbf{q}, \mathbf{q}') = G(\mathbf{q}, \mathbf{q}') + G(\mathbf{q}, \mathbf{q}''), \quad (22)$$

where \mathbf{q}'' is the mirror image of \mathbf{q}' , reflected in C . In the case where \mathbf{q}' lies on C , the Neumann Green's function reduces to

$$G_N(\mathbf{q}, \mathbf{q}') = 2G(\mathbf{q}, \mathbf{q}'). \quad (23)$$

We then get the wave function in the billiard to be

$$\psi = - \int_{C_1} dl' G_N(\mathbf{q}, \mathbf{q}') \left[\frac{\hbar^2}{2m^*} \frac{\partial \psi^0}{\partial n'} + \frac{i\hbar e}{m} \psi^0 \mathbf{A} \cdot \hat{\mathbf{n}}' \right]. \quad (24)$$

The coupling to the exit lead should be handled in a way, analog to the coupling to the entrance lead. The equation for the scattering matrix element should be symmetric with respect to the direction, renaming the entrance and exit leads should make no difference. We therefore need to make the same restriction as on the entrance lead, i.e., we make a demand on the Green's function on a boundary C_3 crossing the exit

$$\frac{\partial G_N}{\partial n}(\mathbf{q}, \mathbf{q}') = 0 \quad \text{for } \mathbf{q} \text{ on } C_3. \quad (25)$$

This is again done by the method of images

$$G_{N2}(\mathbf{q}, \mathbf{q}') = G_N(\mathbf{q}, \mathbf{q}') + G_N(\mathbf{q}'', \mathbf{q}'), \quad (26)$$

where \mathbf{q}'' is a mirror image of \mathbf{q} , reflected in C_3 . For $\mathbf{q}' \in C$ and $\mathbf{q} \in C_3$, we get

$$G_{N2}(\mathbf{q}, \mathbf{q}') = 4G(\mathbf{q}, \mathbf{q}'). \quad (27)$$

Using this Green's function and Eq. (24) in Eq. (19), we obtain

$$S_{mn} = -\frac{i\hbar}{m^{*2}\sqrt{v_m v_n}} \int dy \int dy' \xi_m^*(y) \xi_n(y') [m^* v_m + 2e\mathbf{A}(y) \cdot \hat{\mathbf{x}}] [m^* v_n + 2e\mathbf{A}(y') \cdot \hat{\mathbf{x}}'] G, \quad (28)$$

which in case of zero magnetic field or if gauge can be chosen such that $\mathbf{A} \cdot \hat{\mathbf{n}} = 0$ and $\mathbf{A} \cdot \hat{\mathbf{n}}' = 0$, reduces to

$$S_{mn} = -i\hbar \sqrt{v_m v_n} \int dy \int dy' \xi_m^*(y) \xi_n(y') G, \quad (29)$$

which we recognize as the QM expression for the S matrix. This expression is also most commonly used for SC calculations. However, in QM calculations the Green's function is derived in a way that includes the effects of the leads. This expression is exact when using a QM Green's function. This is not true for the SC Green's function which totally ignores the eigenmodes of the leads. Given that the wave function ψ must be zero on the billiard walls, the choice of Neumann BC is obviously wrong, since C partially coincides with the

billiard wall. We conclude that this commonly used expression does not use the correct BC.

The correct BC to use with the SC Green's function is Dirichlet

$$G_D(\mathbf{q}, \mathbf{q}') = 0 \text{ for } \mathbf{q}' \text{ on } C. \quad (30)$$

The Dirichlet Green's function can also be obtained by the method of images

$$G_D(\mathbf{q}, \mathbf{q}') = G(\mathbf{q}, \mathbf{q}') - G(\mathbf{q}, \mathbf{q}''). \quad (31)$$

The normal derivative of the Green's function on C can be computed to

$$\frac{\partial G_D(\mathbf{q}, \mathbf{q}')}{\partial n'} = 2 \frac{\partial G(\mathbf{q}, \mathbf{q}')}{\partial n'}, \quad (32)$$

for \mathbf{q}' on C . The wave function in the billiard is in this case

$$\psi = \frac{\hbar^2}{2m^*} \int_{C_1} dy' \psi^0 \frac{\partial G_D(\mathbf{q}, \mathbf{q}')}{\partial x'}. \quad (33)$$

Following the path of derivation for the Neumann Green's function we arrive at

$$S_{mn} = - \frac{i\hbar^2}{m\sqrt{k_m k_n}} \int dy \int dy' \xi_m^*(y) \xi_n(y') \frac{\partial^2 G}{\partial x \partial x'}, \quad (34)$$

which is our new formula for calculating S -matrix elements.

Details on calculating trajectories for the SC Green's function can be found in Ref. 18. We need, however, to take the derivative of the Green's function too. We will here restrict our self to zero or weak magnetic field, because the derivatives of the semiclassical Green's function in magnetic field are very complicated to compute. In zero magnetic field the action only depends on the length of the trajectory and it is enough to only look at the ends of the trajectory to calculate a derivative of the action. In nonzero magnetic field the action will depend on the total geometry of the trajectory and thus also the derivative. In the following derivation we assume zero magnetic field, and in the end of this article we show that the resulting formula still yield very good correspondence to QM, even in finite magnetic field. The density of trajectories D_p in Eq. (4) is considered to vary slowly in comparison to the phase given by the exponential function. The contribution of one trajectory to the Green's function is considered to be a plane wave in the vicinity of the trajectory. The $\partial/\partial x'$ derivative then reduces to taking the derivative along the trajectory and projecting on the $\hat{\mathbf{x}}'$ direction, i.e., multiplying with $\sin \alpha'_s$, where the angle α'_s of the trajectory is defined in Fig. 1(a).

$$\begin{aligned} \frac{\partial G^{\text{SC}}(\mathbf{q}, \mathbf{q}', k_F)}{\partial x'} &= \frac{2\pi}{(2\pi i \hbar)^{3/2}} \sum_p |D_p(\mathbf{q}, \mathbf{q}', k_F)|^{1/2} \\ &\times \sin \alpha'_s \frac{i}{\hbar} \frac{S_p(\mathbf{q}, \mathbf{q}', k_F)}{\partial q'_\parallel} \\ &\times \exp \left[\frac{i}{\hbar} S_p(\mathbf{q}, \mathbf{q}', k_F) - \frac{i\pi}{2} \mu_p \right], \end{aligned} \quad (35)$$

where q'_\parallel is a coordinate along the trajectory. The action can be written as

$$S_p = \hbar k_F l_p, \quad (36)$$

where l_p is the length of the trajectory. We can then calculate a derivative as

$$\frac{\partial S_p}{\partial q'_\parallel} = -\hbar k_F, \quad (37)$$

and the Green's function derivative

$$\begin{aligned} \frac{\partial G^{\text{SC}}(\mathbf{q}, \mathbf{q}', k_F)}{\partial x'} &= \frac{-2\pi i k_F}{(2\pi i \hbar)^{3/2}} \sum_p |D_p(\mathbf{q}, \mathbf{q}', k_F)|^{1/2} \\ &\times \sin \alpha'_s \exp \left[\frac{i}{\hbar} S_p(\mathbf{q}, \mathbf{q}', k_F) - \frac{i\pi}{2} \mu_p \right]. \end{aligned} \quad (38)$$

The above expression for the Green's function derivative and the corresponding derivative of x have been used in the following transmission computations. We have, as mentioned above, used Eq. (38) and the corresponding x derivative as approximations in weak magnetic fields, we have although inserted the exact expression for the action S_p into these derivative approximations. This results in an exact phase but approximate amplitude for the contribution of a trajectory. The resulting good agreement with QM, as will be seen below, justifies this approximation.

Calculations were made on more than ten different billiards (triangles and rectangles with different aspect ratio and different lead positions) of which two are included in this

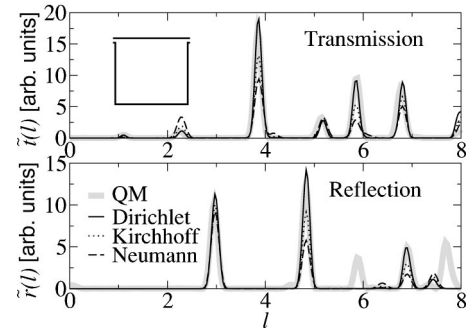


FIG. 2. The transmission and reflection length spectrum for S_{11} calculated QM and SC using Kirchhoff approximation [Eq. (20)], Neumann BC [Eq. (28)], and Dirichlet BC [Eq. (34)] for a rectangle, see inset, in zero magnetic field.

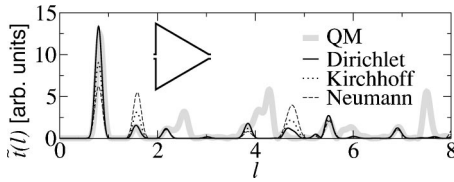


FIG. 3. The transmission length spectrum for S_{11} calculated QM and SC using Kirchhoff approximation [Eq. (20)], Neumann BC [Eq. (28)], and Dirichlet BC [Eq. (34)] for a triangle, see inset, in a magnetic field with cyclotron radius $r_c = 0.6L$, where L is side of triangle.

article, see insets in Figs. 2 and 3. The computations have been made both using QM for comparison and using SC theory with the three different equations (20), (28), and (34). Details on QM calculations can be found in Ref. 23. The conductance through the two billiards have been analyzed in terms of their length spectrum of the transmission/reflection amplitude defined as

$$\tilde{t}(l) = \int dk_F t(k_F, B = \hbar k_F / (e r_c)) e^{-i l k_F}, \quad (39)$$

where $r_c = \hbar k_F / (e B)$ is the cyclotron radius, and t is the transmission amplitude, i.e., an S -matrix element. The length spectrum is thus in magnetic field calculated at constant cyclotron radius, so the geometry of the trajectories stays constant. The action along a trajectory in a magnetic field can be written as

$$S_p(\mathbf{q}, \mathbf{q}', k_F) = \hbar k_F (l_p + A_p r_c^{-1}), \quad (40)$$

where A_p is an area related to the trajectory. With the density of trajectories varying slowly with respect to k_F we can see that the length spectrum of the transmission amplitude will be strongly peaked at $l = l_p + A_p r_c^{-1}$, or in zero magnetic field $l = l_p$ which makes the name “length spectrum” obvious.

The two analyzed billiards included in this paper, see insets in Figs. 2 and 3, are a rectangle, with sides of length L and $1.1L$ in zero magnetic field and a triangle in magnetic field with $r_c = 0.6L$, where L is the side of the triangle. The leads have a width $w = L/15$, and the transmission and reflection amplitudes has been calculated in the regime of one conducting mode in the leads. There is a good correspondence between the positions of the peaks in QM and SC calculations. The peaks that are missing in SC calculations are due to “ghost” trajectories, which bounce diffractively against the lead mouths. These trajectories are not included in this SC model.^{18,20} The included billiard geometries have been specially chosen to avoid that “ghost” trajectories coincide in length with normal trajectories which otherwise makes comparison with QM computations difficult.

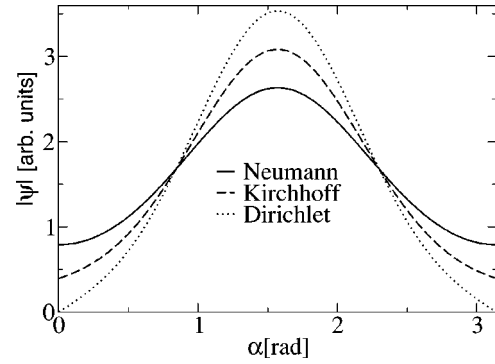


FIG. 4. The Fraunhofer diffraction pattern from a single lead for $k_F = 1.5\pi/w$, where w is the width of the lead. The plot shows the amplitude of the wave functions in the far-field as function of entrance angle α , with the three different boundary conditions.

There is a very good correspondence between SC calculations using Dirichlet BC [Eq. (34)] and the QM calculations. The Neumann BC [Eq. (28)] still gets the peaks in the right positions but can not reproduce the correct amplitude. The Kirchhoff approximation [Eq. (20)] can be seen as a mean value between Neumann and Dirichlet BC and produce peak amplitudes between the Neumann and Dirichlet amplitudes. It is interesting to note that even in the case of the triangle where the geometry near one of the leads differs from the case in the derivation and we are using an only approximate expression for the Green's function derivative, the Dirichlet BC still gives superior results (there is no derivative in the expression for the Neumann BC transmission amplitude, so it is not affected by the approximation). The actual difference between the usage of the three different BC is, at least in zero magnetic field, in the diffraction from the leads. The different BC yield different diffraction patterns, see Fig. 4.

To conclude, we have studied the effect of the choice of boundary conditions at the lead mouths. We find that in contrast to prior practise of using an expression from QM that agrees with Neumann BC, or using the Kirchhoff approximation, one should use Dirichlet BC. This is not in disagreement with QM because the QM Green's function differs from its SC counterpart in that it includes the effect of the eigenmodes in the leads, while the SC Green's function does not. The SC Green's function is only an approximation of the QM Green's function and because of its ignorance of the wave function outside of the billiard it should be treated differently from the QM Green's function. We therefore propose an expression for the scattering matrix, Eq. (34). By comparison to QM calculations, we show this expression to yield superior results.

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