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Semiclassical diffractive scattering for transport through open rectangular microstructure

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Abstract. We study the transport through weakly open rectangular billiards by a new semiclassical approach within the framework of the Fraunhofer diffraction. Based on a Dyson equation for the semiclassical Green's function, the transmission amplitude can be expressed as the sum over all classical trajectories connecting the entrance and the exit leads. We find that the peak positions of the transmission power spectrum not only correspond to classical trajectories but associate with a lot of nonclassical trajectories and the contributions to the power spectrum of the transmission amplitude for the first mode are largely depending on the classical trajectories with small incident angles showing a good agreement with the diffracted angular distribution within the framework of the diffractive scattering effect at the lead openings.

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Key words: Semiclassical approach, Fraunhofer diffraction, transmission amplitude.

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1 Introduction

During the recent few decades, mesoscopic physics has evolved into a greatly progressing and fascinating field of physics [1, 2]. Remarkable advances in the fabrication of submicron semiconductor microstructures have made it possible to produce the mesoscopic devices in the experiment. Mesoscopic devices, whose dimensions are intermediate between microscopic and macroscopic systems, exhibit both classical and quantum signatures [3]. Two-dimensional open quantum billiards has extensively served as model systems to study the ballistic transport through the mesoscopic microstructures [4].

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Semiclassical theory is widely used to describe and analyze the quantum transport property in mesoscopic systems. Several semiclassical methods [5-11] to quantum transport have been proposed, which provide a link between the classical dynamics of the electron motion in the billiards and quantum transport. Semiclassical approximations provide a way to handle quantum mechanics problems by a simplified path integral formalism to bridge the gap between quantum mechanics and its classical limit in a very direct way: each classical trajectory carries an amplitude reflecting its geometric stability and a phase which contains the classical action and accounts for quantum interference effect [12-15]. Due to the fact that the width of the leads is comparable to de Broglie wavelength, several semiclassical approximations were presented on the basis of Kirchhoff diffraction [12], Fraunhofer diffraction [13-15], geometric theory of diffraction and uniform theory of diffraction [16-18].

In this paper, we use a semiclassical approximation within the framework of the Fraunhofer diffraction to study the transport through a weakly open rectangular microstructure as depicted in Fig. 1 (a). Starting from a Dyson equation for the semiclassical Green's function, we formulate the transmission amplitude between the two leads of the rectangular quantum billiards as for Fig. 1 (b). We investigate the correspondence between the peak positions of the transmission power spectrum and the classical trajectories according to classical dynamics, and we find that the transmission probability not only associate with classical trajectories but contain prominent contributions from a series of nonclassical trajectories due to the diffractive scatterings at the lead openings.

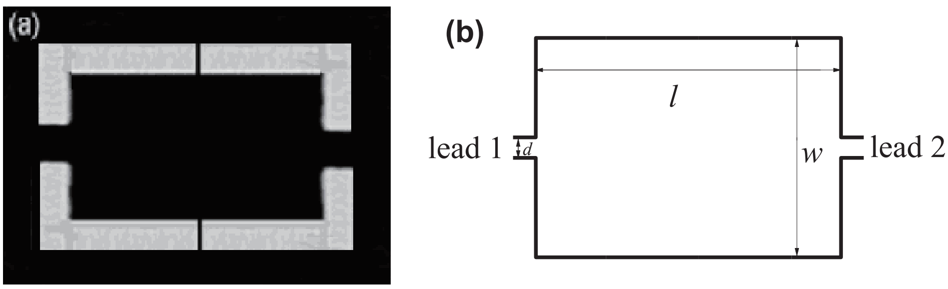

Figure 1: (a) Scanning electron micrograph of a rectangular device [19]. (b) Rectangular quantum billiards as the schematic of the rectangular device with length l=3.5, width w=2.0, and the width of the leads d=0.25. All dimensions are in μm.

The structure of this paper is arranged as follows. In Section 2 we introduce the theoretical approach in detail. In Section 3 we use the stationary-phase condition to calculate the classical trajectories according to the classical dynamics of the electron motion in the billiards. Numerical results and discussions are given in Section 4, followed by a short conclusion in the last section.

2 Transport according to Landauer formula

The conductance g for the transport through the billiards as depicted in Fig. 1(b) is given by Landauer formula [20] as a function of the electron's wave number k.

$$g(k)=\frac{2e^2}{h}\left(\sum_{m=1}^{M}\sum_{n=1}^{M}\left|t_{n,m}(k)\right|^2\right) \tag{1}$$

where $t_{n,m}(k)$ is the transmission amplitude from transverse mode m in the entrance lead 1 to mode n in the exit lead 2, and M is the number of total open modes in the leads.

The m th transverse wave function in the lead with infinitely high potential walls is

$$\phi_m(y)=\sqrt{\frac{2}{d}}\sin\left[\frac{m\pi}{d}(y+\frac{d}{2})\right]. \tag{2}$$

Due to the quantization of the transverse momentum in the leads, the electron enters the billiards with the discrete quantized angles

$$\theta_{1,m}=\pm\arcsin\frac{m\pi}{dk} \tag{3}$$

and exits the billiards with the discrete quantized angles

$$\theta_{2,n}=\pm\arcsin\frac{n\pi}{dk} \tag{4}$$

The transmission amplitude $t_{n,m}(k)$ is customarily expressed as the projection of the retarded Green's propagator $G(y_2,y_1,k)$ onto the transverse wave functions [21]

$$t_{n,m}(k)=-i\sqrt{k_{x_2,n}k_{x_1,m}}\int dy_2\int dy_1\phi_n^*(y_2)G(y_2,y_1,k)\phi_m(y_1) \tag{5}$$

where $k_{x_1,m}=\sqrt{k^2-|m\pi/d|^2}(k_{x_2,n}=\sqrt{k^2-|n\pi/d|^2})$ is the longitudinal component of the wave number of the incoming (outgoing) wave function. Here and in the following, atomic units $\hbar=|e|=m_e=1$ are used.

Considering the diffractive effect at the lead openings, the electron enters and exits the billiards no longer with the discrete quantized angles θ_m but with a continuous distribution of angles θ.

The transmission amplitudes is modified as

$$\begin{aligned} t_{n,m}(k)=&-i\sqrt{k_{x_2,n}k_{x_1,m}}\\ &\times\int dy_2\int dy_1\varphi_{2,n}^*(y_2,\theta_2)G^{SC}(y_2,y_1,k)\varphi_{1,m}(y_1,\theta_1) \end{aligned} \tag{6}$$

where $\varphi(y,\theta)$ are the diffraction transverse wave function describing the diffractive coupling from mode m in the entrance lead into the billiards and from the billiards into mode n in the exit lead.

3 Classical trajectories and semiclassical Green's function

The motion of the electron after it enters the billiards from the entrance lead and before it leave from the exit lead is described by classical dynamics.

The semiclassical Green's function in Eq. (6) is given by

$$G^{SC}(y_2,y_1,k)=\sum_{t:y_1\to y_2}\frac{|D_t(y_2,y_1,k)|^{1/2}}{(2\pi i)^{1/2}}\times\exp\left[\imath\left(S_t(y_2,y_1,k)-\frac{\pi}{2}\mu_t\right)\right] \tag{7}$$

where the summation extends over all classical trajectories t connecting y_1 in the entrance lead 1 with y_2 in the exit lead 2 at energy $E=\frac{1}{2}k^2$. $D_t(y_2,y_1,k)$ is the classical deflection factor (weighting factor) which is a measure for the divergence of nearby trajectories, $S_t(y_2,y_1,k)=kL_t(y_2,y_1)$ is the action of the trajectory t of length L_t, and μ_t denotes the Maslov index of the trajectory t.

The electron entering the billiards with an angle θ for an interval $(-\pi/2,\pi/2)$ from the entrance lead 1, moves freely within the billiards, along a straight line, until it encounters and bounce several times off the hard-wall boundary where it reflects specularly.

According a simple geometric continuation in the extended zone scheme of the rectangular period element as depicted in Fig. 2 (a), the length of the trajectory t connecting y_1 at the centre of the entrance lead 1 with y_2 at the centre of the exit lead 2 should satisfy

$$L_t(a,b)=al\cos\theta+bw\sin\theta \tag{8}$$

where a=1,3,5$\cdots$, and b=0,±1,±2,$\cdots$. Some of the classical trajectories noticed by (a,b) with the corresponding values a and b are shown in Fig. 2 (b).

Then the action of the trajectory t can be written as

$$S(\theta)=k(al\cos\theta+bw\sin\theta) \tag{9}$$

We obtain from the stationary phase condition by only considering the derivation of the classical action with respect to θ equals to zero

$$S(\theta)=k(-al\sin\theta+bw\cos\theta)=0. \tag{10}$$

The "stationary" angles of the trajectory t connecting y_1 at the centre of the entrance lead 1 with y_2 at the centre of the exit lead 2 is

$$\theta=\arctan\frac{bw}{al}. \tag{11}$$

The electron from a weakly open lead entering the inner of the billiards, makes the potential of the transverse direction changed. The change of the width of the potential can be considered as the perturbation at the lead opening approximatively.

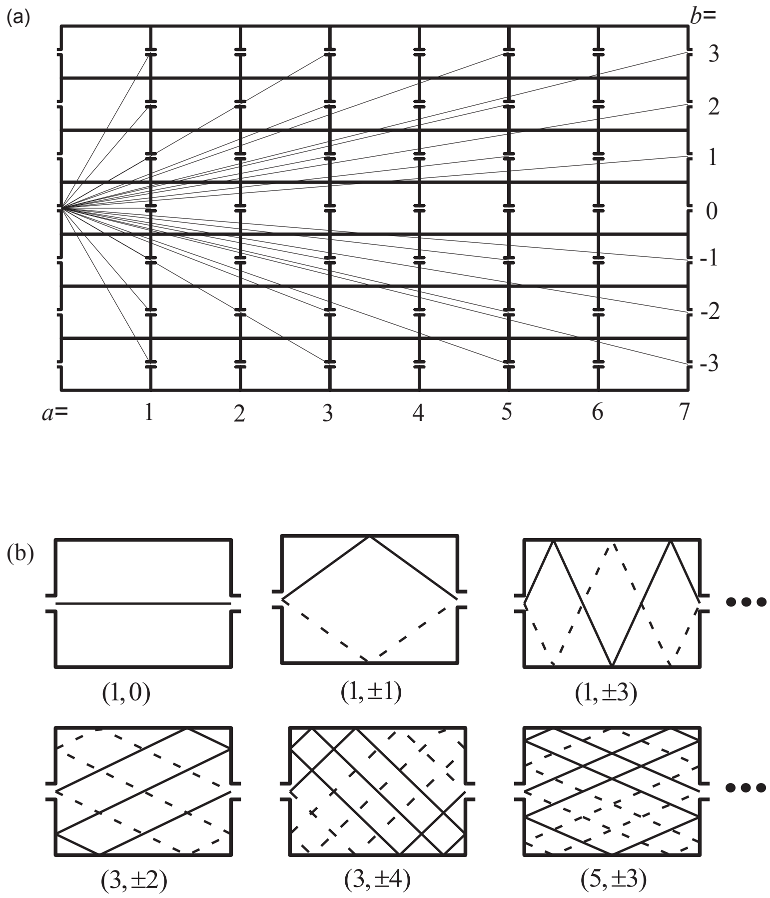

Figure 2: (a) The simple geometric continuation of the rectangular period element. (b) Simple schematic of some classical trajectories.

The classical action with a Taylor series expansion in the transverse coordinate y is expanded as [15]

$$L_1(y) = L_1 + \sin(\theta_1)y + \frac{\cos(\theta_1)}{L_1}y^2 + \cdots \tag{12}$$

where $L_1 = L_1(y=0)$ is the length of the trajectories starting from the centre of the entrance lead 1. Keeping the first two terms results in a Fraunhofer diffraction approximation. Within the framework of the Fraunhofer diffraction, the diffracted transverse wave function $\varphi(y,\theta)$ in lead 1 is expressed as [14, 15]

$$\varphi(y,\theta) = \sqrt{\frac{2}{d}}\sin\left[\frac{m\pi}{d}(y+\frac{d}{2})\right]\int_{-d/2}^{d/2} e^{ik\sin\theta y}dy. \tag{13}$$

Starting from a Dyson equation for the semiclassical (SC) Green's function, we get the new semiclassical (NSC) Green's function with the diffractive scatterings at the lead opening taken into account [15].

$$\begin{aligned} G^{NSC} &= G^{SC} + G^{SC} V G^{NSC} \\ &= \frac{G^{SC}}{1 - rG^{SC}}. \end{aligned} \tag{14}$$

In Eq. (13), the diffractive scatterings coefficient in lead 1 is given by [15]

$$r(\theta,\theta_m,k) = k\sqrt{\cos\theta\cos\theta_m}\int_{-d/2}^{d/2} e^{i(k\sin\theta_m + k\sin\theta)} \tag{15}$$

with $\theta = \arctan\frac{bW}{aL}$ being the "stationary" angles and $\theta_m = \pm\arcsin\frac{m\pi}{kd}$ being the discrete quantized angles of the trajectory t.

4 Numerical results and discussion

In the following, we present the numerical results for the transmission probability from the first mode of the entrance lead 1 to the first mode of the exit lead 2, and present a quantitative comparison between the result calculated by the new semiclassical approximation (NSCA) and that calculated by the standard semiclassical approximation (SSCA).

As depicted in Fig. 3, both results calculated by the new semiclassical approximation and by the standard semiclassical approximation display strong fluctuations in the transmission probability as a function of the wave number k, but the peak values to describe the contribution of the classical trajectories to the transmission probability are generally different.

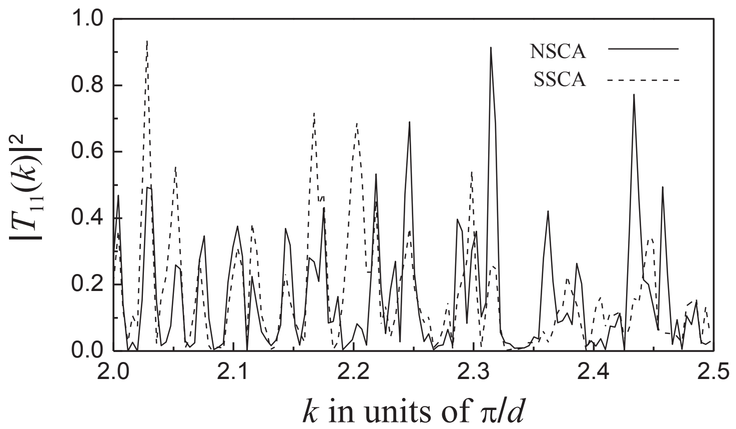

Figure 3: Square modulus of transmission amplitude $t_{11}(k)$, calculated by the new semiclassical approximation (solid curve) and by the standard semiclassical approximation (dashed curve), in a finite interval of k, $2.0 \leq k \leq 2.5$ in units of π/d.

Table 1: Comparison between the lengths of the classical trajectories and the corresponding peak positions.

Trajectory shape	(1,0)	(1,±1)	(3,0)	(3,±1)	(3,±2)
Incident angle	0	±0.52	0	±0.19	±0.36
Trajectory length	3.50	4.03	10.50	10.69	11.24
Peak position	3.5	4.1	10.5	10.7	11.2

Trajectory shape	(3,±3)	(5,±1)	(5,±2)	(5,±3)	(5,±4)
Incident angle	±0.52	±0.11	±0.22	±0.33	±0.43
Trajectory length	12.10	17.61	17.95	18.50	19.24
Peak position	12.1	17.6	17.9	18.5	19.2

In order to identify the classical trajectories, we define the length power spectrum as

$$P_{n,m}(L) = \int_{k_{min}}^{k_{max}} e^{-ikL} t_{n,m}(k) dk \tag{16}$$

which is a function of the variable L conjugate to wave number k as the Fourier transformation of the transmission amplitude $t_{n,m}(k)$ in a finite interval of $k_{min} \leq k \leq k_{max}$.

In Fig. 4 we present the length power spectrum of the transmission amplitude $t_{1,1}(k)$ in the finite number of trajectories with the lengths $L_t \leq 20$.

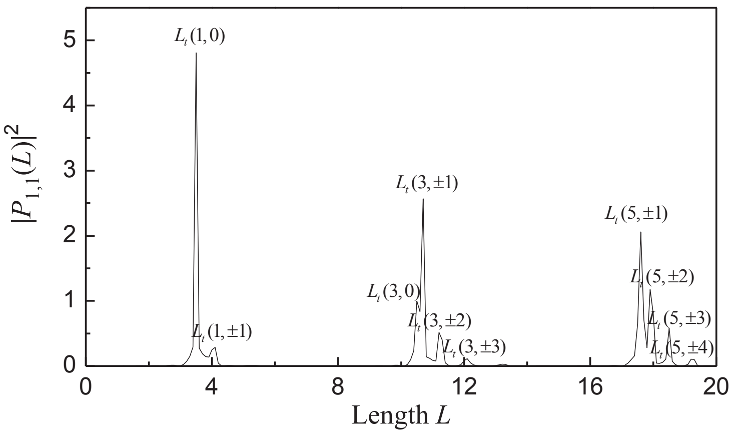

Figure 4: Transmission length power spectrum of the transmission amplitude $t_{1,1}(k)$ in a finite interval of k, $2.0 \leq k \leq 6.0$ in units of π/d. The scaled length L corresponds to a fixed area of the billiards region $A = lw$.

In the following, we present the comparison between the peaks positions of the transmission power spectrum obtained from the new semiclassical approximation and the corresponding lengths of the classical trajectories connecting y_1 at the centre of the entrance lead 1 with y_2 at the centre of the exit lead 2 according to classical dynamics in Tab. 1.

Fig. 4 and Tab. 1 display a good correspondence between the lengths of the classical trajectories and the peaks positions of the transmission length power spectrum. Each peak in the power spectrum is accurately identified with a family of classical trajectories, and the peak height can be used to describe the probability of the classical trajectories that the electron walks along. And the power spectrum contains prominent contributions from a series of nonclassical trajectories which are directly reflected back into the billiards instead of exiting the lead openings due to the diffraction scatterings effect. For example, the third peak with the length $L^{(3)}(3,0)$=10.50 and the sixth peak with the length $L^{(6)}(3,\pm 3)$=12.10, are caused by the diffraction scattering effect at the lead openings. These are so-called "ghost paths" [12] or "pseudo paths"[15] which can be automatically attributed to the nonclassical trajectories due to the diffraction scatterings at the lead openings based on a Dyson equation for the semiclassical Green's function in our calculation.

In Fig. 4, the peaks correspond to only a few of classical trajectories with small incident angles, while there is no peak emerging at classical trajectories with large incident angles. In order to investigate the reason, on the basis of Fraunhofer diffraction theory, we present a quantitative description for the angular distribution of the electron injected from the entrance lead 1 into the billiards by the absolute square of the diffracted angular distribution function

$$I(k,\theta) = \sqrt{k\cos\theta}\int_{-d/2}^{d/2}\varphi(y,\theta)dy \tag{17}$$

as a function of θ at a fixed wave number k for the first mode.

Fig. 5 displays that an electron at a fixed wave number $k = 4\pi/d$ enter the billiards classical trajectories with the incident angles in a small window of [-0.25π,0.25π] for the first mode. Hence, there are the classical trajectories with small incident angles largely contributing to the length power spectrum of the transmission amplitude $t_{1,1}(k)$.

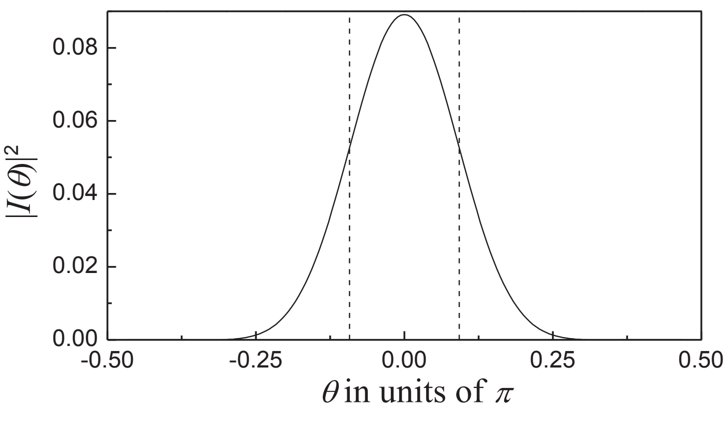

Figure 5: Angular distribution of the electron injected from the entrance lead 1 into the billiards. Solid line: $|I(\theta)|^2$ at $k = 4\pi/d$ for the first mode. Dashed line: the discrete quantized angle $\theta_1 = \pm\arcsin\frac{\pi}{kd}$ for the first mode in the standard semiclassical approximation.

5 Conclusion

Within a new semiclassical approximation on the basis of the Fraunhofer diffraction, we have analyzed the power spectrum of the transmission amplitude for the first mode. We find there is an excellent numerical agreement between the peaks positions of the power spectrum and the corresponding lengths of the classical trajectories, and find that the peak positions of the transmission power spectrum not only correspond to classical trajectories but associate with a lot of nonclassical trajectories due to the diffractive scatterings at the lead openings. The contributions to the length power spectrum of the transmission amplitude for the first mode are largely depending on the classical trajectories with small incident angles, which shows a good agreement with the diffracted angular distribution of the electron injected from the entrance lead 1 into the billiards.

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