Semiclassical Theory of Chaotic Quantum Transport

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(Received 8 May 2002; published 24 October 2002)

We present a refined semiclassical approach to the Landauer conductance and Kubo conductivity of clean chaotic mesoscopic systems. We demonstrate for systems with uniformly hyperbolic dynamics that including off-diagonal contributions to double sums over classical paths gives a weak-localization correction in quantitative agreement with results from random matrix theory. We further discuss the magnetic-field dependence. This semiclassical treatment accounts for current conservation.

DOI: 10.1103/PhysRevLett.89.206801 PACS numbers: 73.23.-b, 03.65.Sq, 05.45.Mt, 73.20.Fz

Among the prominent wave phenomena which constitute mesoscopic behavior of small phase-coherent conductors, weak localization (WL) represents one key mechanism. This quantum effect shows up as a decrease in the average conductivity with respect to the classical one. WL, originally observed for light [1] and electron waves [2] in disordered samples, has been extensively studied during the last decade for electrons in ballistic conductors, i.e., mesoscopic cavities or quantum dots where the elastic mean free path is considerably larger than the system size. WL is attributed to constructive interference of electron waves which are either coherently backscattered from impurities in disordered systems or multiply reflected at the boundaries of ballistic devices.

In describing ballistic transport semiclassical methods have attracted much interest, since they establish a direct link between quantum transport and features of the corresponding classical dynamics, e.g., chaotic, integrable, or mixed behavior [3,4]. This was demonstrated for clean microstructures in a seminal semiclassical approach [5] to the average reflection in the Landauer framework: the WL peak profile (as a function of a magnetic field) was shown to be Lorentzian for chaotic systems while being linear for integrable geometries, probing in an impressive way the imprint of the classical dynamics on a measured quantum effect [6]. However, while the line shape of the WL peak agreed with results from random matrix theory (RMT), the approach turned out to be inadequate to give the correct WL magnitude for ballistic systems, contrary to the diffusive case [2]. This long-lasting problem to semiclassically obtain the correct leading-order quantum correction to the conductance is related to the so-called *diagonal approximation* used. It is based on the consideration of a restricted class of pairs of paths built from each backscattered orbit and its time-reversed partner, which moreover violates current conservation [7]. Similarly, WL is not captured in a related semiclassical approach to the Kubo conductivity of ballistic systems [8].

The possible relevance of pairs of nonidentical backscattered paths, differing slightly in their initial directions, was first pointed out by Argaman [9], who found agreement with RMT results by introducing a self-consistently chosen electric field within the Kubo formalism. Aleiner and Larkin [10] approached the problem of ballistic WL using both perturbation theory and supersymmetrical methods to derive a RMT result for the conductance. However, their techniques still rely on the presence of quantum scatterers (to regularize the Liouville operator) and strictly speaking do not treat the case of a clean, disorder-free, system. Their approach was semiclassically interpreted in Ref. [11] arguing that diffraction effects are relevant for ballistic WL.

We present an adequate, current-conserving semiclassical treatment of the problem to quantitatively describe the average quantum conductance in *clean* chaotic systems without relying on any diffraction or impurity scattering effects. We consider the leading-order off-diagonal contribution in a semiclassical loop expansion of the Landauer conductance. The relevant terms consist of pairs of orbits which are very close almost everywhere (in configuration space), and differ only in whether they undergo or avoid a self-intersection with a small crossing angle. Analogous pairs of periodic orbits have recently been used to derive the τ^2 term in the spectral form factor of RMT [12]. They are ballistic analogs of corresponding objects in the diffusive regime [13]. Our results for transport are strictly derived for chaotic systems with uniformly hyperbolic dynamics, but related results for ballistic cavities show [14] that they apply to general chaotic systems.

We first compute semiclassical conductance contributions beyond the diagonal approximation in the Landauer framework and later return to the corresponding problem in the Kubo formalism. Consider a two-dimensional, classically chaotic clean cavity with two leads of width $w(w')$ attached that support $N(N')$ open channels. The Landauer formula for the conductance G then reads [15]

$$G(E,B) = 2\frac{e^2}{h}\mathcal{T} = 2\frac{e^2}{h}\sum_{n=1}^{N'}\sum_{m=1}^{N}|t_{nm}|^2. \qquad (1)$$

$t_{nm}(E,B)$ is the transition amplitude between incoming and outgoing channels m and n at energy E in the presence of a magnetic field B, and $\mathcal{T}(\mathcal{R})$ is the transmission (reflection), $\mathcal{T} + \mathcal{R} = N$. We first consider the case of time-reversal symmetry, $B = 0$, and return to the B dependence of WL later. We assume that the ergodic time is much smaller than the escape time τ of the cavity and that contributions from direct, lead-connecting processes are negligible. Then the following RMT results for the averages of the transmission and reflection probabilities hold which we give for later reference [16,17]:

$$\langle |t_{nm}|^2 \rangle = \frac{1}{N + N' + 1} = \frac{1}{N + N'} \sum_{k=0}^{\infty} \left[\frac{-1}{N + N'} \right]^k, \quad (2)$$

$$\langle |r_{nm}|^2 \rangle = \frac{1 + \delta_{nm}}{N + N' + 1} = \frac{1 + \delta_{nm}}{N + N'} \sum_{k=0}^{\infty} \left[\frac{-1}{N + N'} \right]^k. \quad (3)$$

Our conductance calculation is based on the semiclassical representation of transmission amplitudes [18],

$$t_{nm} \simeq -\sqrt{\frac{\pi\hbar}{2ww'}} \sum_{\gamma(\bar{n},\bar{m})} \frac{\Phi_\gamma \exp[(i/\hbar)S_\gamma]}{|\cos\theta'_{\bar{n}} \cos\theta_{\bar{m}} M_{21}^{\gamma}|^{1/2}}. \quad (4)$$

The sum runs over all lead-connecting trajectories γ which enter into the cavity at (x, y) with an angle $\sin\Theta_{\bar{m}} = \bar{m}\pi/(kw)$ and exit the cavity at (x', y') with angle $\sin\Theta_{\bar{n}} = \bar{n}\pi/(kw')$, where $\bar{n} = \pm n$, and $p = \hbar k$ is the momentum; see Fig. 1(a). In Eq. (4), S_γ is the classical action, M_{21}^{γ} an element of the stability matrix, and $\Phi_\gamma = \mathrm{sgn}(\bar{n})\mathrm{sgn}(\bar{m}) \exp[i\pi(\bar{m}y/w - \bar{n}y'/w' - \mu_\gamma/2 + 1/4)]$ is a phase factor where μ_γ contains the Morse index. An expression corresponding to Eq. (4) holds true for r_{nm} in terms of paths reflected back.

The Landauer Eq. (1) contains products $t_{nm}t_{nm}^*$ which semiclassically amounts to evaluate double sums over an infinite number of trajectory pairs. In a treatment of the energy-averaged conductance most pairs, consisting of orbits with uncorrelated actions, will cancel each other upon summation. The existing semiclassical approach [5] is based on the diagonal approximation, where only pairs of identical orbits or orbits related to each other by time inversion are taken into account. Then the phase factors from Eq. (4) cancel, and one has $|t_{nm}|^2_{\mathrm{diag}} = \pi\hbar/(2ww') \sum_{\gamma(\bar{n},\bar{m})} |\cos\theta'_{\bar{n}} \cos\theta_{\bar{m}} M_{21}^{\gamma}|^{-1}$.

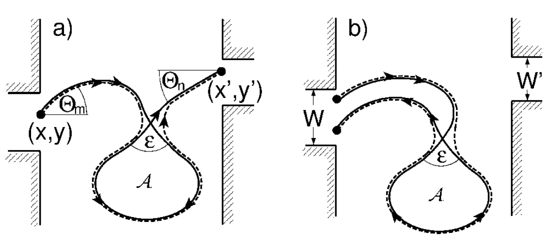

FIG. 1. Sketch of an off-diagonal trajectory pair formed by a self-intersecting classical orbit (solid line) with small crossing angle ε and a neighboring orbit (dashed) differing mainly in the region around the self-intersection. The paths represent orbits with many reflections at the system boundaries. They contribute to the quantum transmission (a) and reflection (b).

First we give an alternative further evaluation of this expression employing the sum rule [19]

$$\sum_{\gamma(y',\theta'_n;y,\theta_m)} \frac{\delta(T - T_\gamma)}{|M_{21}^{\gamma}|} \simeq \frac{\cos\theta'_n \cos\theta_m}{\Sigma(E)} dy dy' \rho(T) \quad (5)$$

for ergodic dynamics. The sum runs over all orbits with periods T_γ, which begin and end in intervals dy' and dy around y' and y with fixed orientations of the initial and final velocities. $\Sigma(E) = 2\pi m A$ is the energy surface in phase space for billiards of area A. The survival probability $\rho(T) \sim \exp(-T/\tau)$ (for $T \to \infty$) represents the exponential loss of particles with velocity v which escape through the openings characterized by the escape rate

$$\frac{1}{\tau} = \frac{v(w + w')}{A\pi} = \frac{\hbar}{mA}(N + N'). \quad (6)$$

By applying the sum rule (5) to the diagonal contribution, integrating over the lead cross sections, and including a factor of 4 for each tupel $(\bar{n}, \bar{m})$ one finds for the average of the transmission coefficient of an ergodic system

$$|t_{nm}|^2_{\mathrm{diag}} = 4\frac{\pi\hbar/2}{2\pi m A} \int dT e^{-T/\tau} = \frac{1}{N + N'}. \quad (7)$$

Correspondingly, the average of a quantum reflection coefficient reads in the diagonal approximation

$$|r_{nm}|^2_{\mathrm{diag}} = \frac{1}{N + N'} + \frac{\delta_{nm}}{N + N'}. \quad (8)$$

The semiclassical evaluation at this level yields the $(k = 0)$ term of the RMT result (2) and (3). Note that the sum rule (5) allows us to compute *individual* transmission and reflection coefficients, while Ref. [5] gives results only for the entire classical transmission and reflection.

Summing the first term in Eq. (8) over all channels yields the classical reflection $\mathcal{R}_{\mathrm{cl}} = N^2/(N + N')$. The second term in Eq. (8) arises from contributions to $|r_{nn}|^2$ from backscattered orbits paired with their time-reversed partners (elastic enhancement). This gives rise to the diagonal contribution to WL, $\delta\mathcal{R}_{\mathrm{diag}} = N/(N + N')$ [5]. For $N = N' \to \infty$ one has $\delta\mathcal{R}_{\mathrm{diag}} = 1/2$, deviating from the RMT result $\delta\mathcal{R}_{\mathrm{RMT}} = 1/4$.

In the following we go beyond the diagonal approximation and consider pairs of different trajectories as sketched in Fig. 1 in coordinate space. They consist of a long, self-intersecting orbit [solid line in Figs. 1(a) and 1(b)] with small crossing angle ε forming a closed loop and a second orbit in its close vicinity (dashed line). The two orbits are traversed along the two open trajectory segments, beginning and ending at (exponentially) close points at the lead mouths, in the same direction but along the loop in opposite directions. Given a self-intersecting orbit with small ε we showed that the neighboring orbit, indeed, exists by linearizing the motion in its vicinity

[20]. The action difference $\Delta S(\varepsilon)$ of the two orbits is computed by expanding the action around the self-intersecting orbit up to second order. The resulting formula for ΔS, expressed through the elements of the stability matrices for the loop and the two open segments, is rather involved. Hence, we will focus from now on onto chaotic systems with uniformly hyperbolic dynamics characterized by a single Lyapunov exponent λ and no conjugate points. One then finds [20]

$$\Delta S(\varepsilon) \approx \frac{p^2\varepsilon^2}{2m\lambda}. \tag{9}$$

Since a partner orbit is associated with each self-intersection with small crossing angle, we compute the conductance contribution from all such orbit pairs by first summing for each orbit $\gamma(\bar{n}, \bar{m})$ over all ε self-intersections and finally by integrating over ε. Using Eq. (9) for the action differences occurring in $t_{nm}t^*_{nm}$ [with t_{nm} from Eq. (4)] and the sum rule (5) one finds for this "loop" contribution

$$\begin{aligned} |t_{nm}|^2_{\rm loop} &\simeq \frac{\pi\hbar}{ww'} \sum_{\gamma(\bar{n},\bar{m})} \frac{\delta(T - T_\gamma)}{|\cos\theta'_{\bar{n}} \cos\theta_{\bar{m}} M^\gamma_{21}|} I(T) \\ &\simeq \frac{2\hbar}{mA} \int dT e^{-T/\tau} I(T) \end{aligned} \tag{10}$$

with

$$I(T) = \mathrm{Re} \int_0^\pi d\varepsilon P(\varepsilon; T) \exp\left(\frac{ip^2\varepsilon^2}{2\hbar m\lambda}\right). \tag{11}$$

In the semiclassical limit ($\hbar \to 0$) the contribution from small angles is dominant. In Eq. (11), the density $P(\varepsilon; T)$ of self-crossings with angle ε for a long orbit of time T can be expressed as an integral over all loops, associated with the self-crossings, with times $T_{\rm min}(\varepsilon) < t < T$:

$$P(\varepsilon; T) \simeq 2mv^2 \int_{T_{\rm min}(\varepsilon)}^T dt (T - t) \sin(\varepsilon)\, p_{\rm erg}, \tag{12}$$

where $p_{\rm erg} = 1/(2\pi mA)$ is the ergodic classical return probability. The lower cutoff accounts for the fact that a minimum time $T_{\rm min}(\varepsilon)$ is required to form a closed loop from two trajectories starting at the crossing with initial angular difference ε. Because of the exponential divergence of neighboring orbits in a hyperbolic system, $T_{\rm min}(\varepsilon)$ can be estimated from $c \simeq \varepsilon \exp[\lambda T_{\rm min}(\varepsilon)/2]$ with c of order π. Detailed numerical and analytical studies [12] have shown that this, indeed, holds true and that the number of crossings for $T \to \infty$ is given by

$$P(\varepsilon; T) d\varepsilon \sim \frac{T^2 v^2}{\pi A} \frac{\sin\varepsilon}{2} \left[1 - 2\frac{T_{\rm min}(\varepsilon)}{T}\right] d\varepsilon \tag{13}$$

with $T_{\rm min}(\varepsilon) = -(2/\lambda)\ln(\varepsilon/c)$. The integral (11) over the leading-order T^2 term in Eq. (13) is purely imaginary, and thus its contribution vanishes. However, the contribution to $I(\varepsilon, T)$ of the second, logarithmic term in Eq. (13) is finite and gives $-(\hbar/2mA)T$, independent of λ. We then obtain from Eq. (10)

$$|t_{nm}|^2_{\rm loop} \simeq -\left[\frac{\hbar}{mA}\right]^2 \int dT T e^{-T/\tau} = \frac{-1}{(N + N')^2}. \tag{14}$$

Hence, the lack of short loops with $t < T_{\rm min}(\varepsilon)$ gives rise to a negative quantum correction to the transmission.

Correspondingly, we find for the loop correction to the average of the reflection coefficient

$$|r_{nm}|^2_{\rm loop} = -\frac{1 + \delta_{nm}}{(N + N')^2}. \tag{15}$$

Here, as for the diagonal contribution (8), backscattering into the same channel is twice as probable.

Summing over all initial and final channels we obtain for the leading-order quantum transmission and reflection $\delta\mathcal{T}_{\rm loop} = -NN'/(N + N')^2$ and $\delta\mathcal{R}_{\rm loop} = -N(N + 1)/(N + N')^2$. For $N, N' \gg 1$ we have $\delta\mathcal{R}_{\rm diag} + \delta\mathcal{R}_{\rm loop} \simeq NN'/(N + N')^2 = -\delta\mathcal{T}_{\rm loop}$. This implies conservation of the average current in the semiclassical limit. *Considering off-diagonal terms allows us to semiclassically compute WL corrections consistently in either transmission or reflection.* They precisely coincide with the RMT result $\delta\mathcal{T}_{\rm RMT} = -1/4$ for $N = N' \to \infty$. Comparison with RMT for finite N, N' suggests that the kth order terms in Eqs. (2) and (3) correspond to semiclassical k-loop contributions; the diagonal terms are considered as 0-loop and the orbits in Fig. 1 as 1-loop terms.

Since the closed loops formed by the off-diagonal orbit pairs are traversed in opposite directions (see Fig. 1), these orbits acquire an additional action or phase difference in the presence of a weak magnetic field B due to the flux enclosed. For a uniform perpendicular field the action difference is $4\pi\mathcal{A}B/\phi_0$, where $\mathcal{A}$ is the area of the loops and ϕ_0 the flux quantum. We assume that the distribution $p(t; \mathcal{A})$ of enclosed areas for trajectories of time t is Gaussian with a system specific parameter β,

$$p(t; \mathcal{A}) \simeq \frac{1}{\sqrt{2\pi t\beta}} \exp\left(-\frac{\mathcal{A}}{2t\beta}\right). \tag{16}$$

This is usually well fulfilled for chaotic systems [3–5]. For finite B fields we have to perform an additional integration of the field-induced phase differences over the area distribution: $\int_{-\infty}^{\infty} d\mathcal{A}\, p(t; \mathcal{A}) \times \cos(4\pi\mathcal{A}B/\phi_0) = \exp(-t/t_B)$, with the magnetic time $t_B = \phi_0^2/(8\pi^2\beta B^2)$. Up to time scales $T_{\rm min}(\varepsilon)$ a negligible flux is enclosed by loops with small crossing angles. We consider this by a respective time shift when inserting $\exp(-t/t_B)$ into the integral (12) over loop lengths:

$$\begin{aligned} P_B(\varepsilon; T) &\simeq \frac{v^2}{\pi A} \sin\varepsilon \int_{T_{\rm min}(\varepsilon)}^T dt (T - t) e^{-[t - T_{\rm min}(\varepsilon)]/t_B} \\ &\sim \frac{v^2 t_B^2}{\pi A} \sin\varepsilon \left[\frac{T}{t_B} + (e^{-T/t_B} - 1)\left(1 + \frac{T_{\rm min}(\varepsilon)}{t_B}\right)\right]. \end{aligned} \tag{17}$$

In Eq. (17) we used $T_{\rm min}(\varepsilon) \ll t_B$. This corresponds to the original assumption, $T_{\rm min}(\varepsilon) \ll \tau$, in the range of interest, $\tau \sim t_B$. Only the term linear in $T_{\min}(\varepsilon)$ contributes to the integral (11), and we obtain from Eq. (10) a Lorentzian field dependence of the transmission coefficient: $|t_{nm}(B)|^2_{\text{loop}} \simeq |t_{nm}(0)|^2_{\text{loop}}/(1 + \tau/t_B)$. A corresponding result applies to $|r_{nm}(B)|^2_{\text{loop}}$. This coincides with the WL line shape obtained in the diagonal approximation [5], making clear why the diagonal terms already qualitatively account for the WL peak profile. The entire WL correction from the diagonal and off-diagonal (1-loop) contribution then reads, in terms of the classical reflection and transmission coefficients r_{cl} and t_{cl},

$$\delta\mathcal{R}(B) \simeq \frac{t_{\text{cl}} r_{\text{cl}}}{1 + \tau/t_B}. \tag{18}$$

Our refined semiclassical approach to the Landauer conductance yields the correct WL magnitude *and* line shape.

For the *Kubo conductivity* the trace integral in the Kubo formula is semiclassically evaluated by approximating the products of Green functions involved through double sums over classical paths. Pairing identical orbits (diagonal approximation) leads to the classical conductivity [4,8,9]; off-diagonal terms are again required to compute WL. Consider a two-dimensional Lorentz gas as a prototype of an extended clean chaotic system. It has been experimentally realized by ensembles of antidots in semiconductor heterostructures [21]. The antidots act as classical scatterers leading to diffusive motion on long time scales, while the dynamics for intermediate times is governed by chaotic scattering.

Our semiclassical treatment of WL is based on orbit pairs similar to the orbits discussed [Fig. 1(b)]: they consist of a long self-intersecting path being backscattered after multiple bounces with antidots with nearly opposite momentum and a neighboring orbit following the loop formed by the first in opposite direction. The evaluation of the trace integral for such paths (involving again cutoff times logarithmic in the crossing angle) yields a negative quantum contribution $\delta\sigma$ at $B = 0$ [20]. This WL correction for chaotic systems with classical scatterers turns out to coincide with that from disordered systems with quantum impurity scattering. We find

$$\delta\sigma \simeq -(e^2/\pi h)\ln(t_\phi/t_{\text{el}}), \tag{19}$$

where t_ϕ is the phase-coherence time and t_{el} the elastic scattering time due to reflections at the antidots. Diffusive motion, accounted for in a sum rule similar to Eq. (5), is reflected in the logarithm. Equation (19) coincides with the result of Ref. [10] for antidot systems when t_ϕ is large compared to the Ehrenfest time.

To conclude, a semiclassical treatment beyond the diagonal approximation is appropriate to compute quantum corrections to the average conductance in clean chaotic conductors. Chaotic classical dynamics is responsible for a logarithmic angular dependence of the classical return probability or the loops involved, respectively, which turns out to be crucial for computing WL. This behavior holds true also for nonuniformly hyperbolic systems [14] indicating that the mechanism presented here is rather general. While higher-order loop corrections are not negligible for the spectral form factor, the one-loop corrections considered here play the dominant role for quantum transport in the mesoscopic regime.

This work was supported by the Deutsche Forschungsgemeinschaft under Contract No. Ri-681/5-1.

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