Phase–coherence Effects in Antidot Lattices:
A Semiclassical Approach to Bulk Conductivity

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Abstract

We derive semiclassical expressions for the Kubo conductivity tensor. Within our approach the oscillatory parts of the diagonal and Hall conductivity are given as sums over contributions from classical periodic orbits in close relation to Gutzwiller’s trace formula for the density of states. Taking into account the effects of weak disorder and temperature we reproduce recently observed anomalous phase coherence oscillations in the conductivity of large antidot arrays.

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Interference phenomena in quantum electron transport through small microstructures are usually interpreted within two complementary frameworks: The Landauer–Büttiker formalism commonly describes transmission through single phase coherent devices [1]. The current is expressed in terms of (a sum over) conductance coefficients between channels in different leads attached. On the other hand linear response theory (Kubo formalism) has proved useful to treat bulk transport properties of samples with a size exceeding the phase breaking length. Besides coherence effects related to the presence of disorder (e.g., universal conductance fluctuations, weak localization) the development of high mobility devices has opened experimental access to the ballistic limit where the elastic mean free path is considerably larger than the system size and the conductance reflects the geometry or potential landscape of the microstructures. This has especially oriented interest to questions how classically regular or chaotic electron dynamics manifests itself on the level of quantum transport [2–4]. In this spirit a semiclassical approach to conductance within the Landauer–Büttiker framework has already been successfully performed expressing the conductance coefficients in terms of interfering electron paths [4].

Recent experiments on magnetotransport in antidot structures unveiled the lack of a corresponding semiclassical approach to Kubo bulk conductivity [3,5,6]. Antidot superlattices consist of arrays of periodically arranged holes "drilled" through a two dimensional electron gas (2DEG). Since the lattice constants $a$ (of typically 200–300 nm) are significantly larger than the Fermi wavelength $\lambda_F \sim 50$ nm the dynamics of the electrons moving in between the repulsive antidots can be considered to be of semiclassical nature. The combined potential of the superlattice and a perpendicular magnetic field gives rise to a variety of peculiar effects: The diagonal magnetoresistivity $\rho_{xx}$ exhibits pronounced peaks due to trapping of electrons encompassing a particular number of antidots at magnetic field strengths related to specific values of the normalized cyclotron radius $R_c/a$ [7]. Superimposed upon these resistivity peaks (reflecting the classical chaotic electron dynamics of the antidot geometry [8]) additional quantum resistivity oscillations of anomalous periodicity had been observed at sufficiently low temperature indicating phase coherence phenomena [3,8]. They cannot
be attributed to interfering electron waves traversing the whole device (as in the case of single junctions) since the antidot arrays are too large to maintain phase coherence. However, assuming that $\rho_{xx}$ reflects density of state oscillations we were able to describe the periodicity of the modulations observed in terms of quantized periodic orbits in the antidot array. 

Nevertheless, a complete direct semiclassical approach to the conductivity tensor was still missing in spite of important work by Wilkinson providing a semiclassical evaluation of the diagonal conductivity in a somewhat different context. Such an approach is also desirable since the antidot measurements have not yet been completely reproduced by quantum mechanical calculations which turn out to be rather involved.

In this letter we derive semiclassical Kubo–type transport formulas by stationary phase evaluation of the disorder averaged two–particle Green functions. We obtain diagonal and Hall conductivity oscillations in terms of sums over periodic orbit contributions with the classical actions of the orbits determining the periodicities. Using a model antidot potential and working at finite temperature we are able to reproduce the amplitudes and periodicities of measured quantum oscillations in antidot superlattices.

Within the Kubo formalism the static conductivity tensor at temperature $T$ is given by

$$\sigma_{ij}(T) = \frac{g_s}{V} \int \left( -\frac{df}{dE} \right) < \sigma_{ij}(E) > dE$$

where $V$ is the total area, $g_s$ accounts for the spin degeneracy, $f(E) = 1/[1+ \exp((E-E_F)/\beta)]$ is the Fermi function ($\beta = 1/kT$) and $<>$ denotes an average over weak disorder. The diagonal and Hall conductivities $\sigma_{ij} \equiv \sigma_{ij}(E)$ can be written as

$$\sigma_{xx} = \pi e^2 \hbar \text{Tr} \left\{ \hat{v}_x \hat{\delta}(E - \hat{H}) \hat{v}_x \hat{\delta}(E - \hat{H}) \right\}$$

$$\sigma_{xy} = e \frac{\partial N(\epsilon, B)}{\partial B} + \frac{i}{2} e^2 \hbar \text{Tr} \left\{ \hat{v}_x G^+(E) \hat{v}_y \hat{\delta}(E - \hat{H}) - \hat{v}_x \hat{\delta}(E - \hat{H}) \hat{v}_y G^-(E) \right\} .$$

Here, the $\hat{v}_i$ are the operators of the velocity components, $G^+(E)$ ($G^-(E)$) is the advanced (retarded) Green function, $N(E) = \int^E \text{Tr} \hat{\delta}(E' - \hat{H}) dE'$ the number of states below $E$ and $B$ is the magnetic field.

For the semiclassical evaluation of Eq. (2) it is convenient to use $\hat{\delta}(E - \hat{H}) = -[G^+(E) -
$G^{-}(E)/2\pi i$ and to work within position representation. Semiclassically, the operators $\hat{v}_i$ act as classical quantities and with $G^{-}_{E}(\mathbf{r},\mathbf{r'}) = G^{+\ast}_{E}(\mathbf{r'},\mathbf{r})$ we can reduce Eq. (2) to

$$\sigma_{xx} = \frac{e^2\hbar}{2\pi} \text{Re} \left\{ \int d\mathbf{r} \int d\mathbf{r}' v_x G^{+}_{E}(\mathbf{r},\mathbf{r'}) v'_x \left[ G^{+\ast}_{E}(\mathbf{r},\mathbf{r'}) - G^{+}\mathbf{(r'},\mathbf{r}) \right] \right\} , \quad (3a)$$

$$\sigma_{xy} = e \frac{\partial N(E)}{\partial B} + \frac{e^2\hbar}{2\pi} \text{Re} \left\{ \int d\mathbf{r} \int d\mathbf{r}' v_x G^{+}_{E}(\mathbf{r},\mathbf{r'}) v'_y \left[ G^{+\ast}_{E}(\mathbf{r},\mathbf{r'}) - G^{+}\mathbf{(r'},\mathbf{r}) \right] \right\} . \quad (3b)$$

We write the Green function as the Laplace transform of the Feynman propagator which is semiclassically given in terms of a sum over all classical paths $\alpha$ from $\mathbf{r}'$ at time $t' = 0$ to $\mathbf{r}$ at time $t$ [14]:

$$G^{+}_{E}(\mathbf{r},\mathbf{r'}) = -\frac{1}{2\pi\hbar^2} \int_{0}^{\infty} dt \ e^{E t/\hbar} \sum_{\alpha} D_{\alpha}(\mathbf{r}',\mathbf{r}) \exp \left[ \frac{i}{\hbar} W_{\alpha}(\mathbf{r}',0;\mathbf{r},t) + m_{\alpha} \frac{\pi t}{2} \right] e^{-t/2\tau_{s}} . \quad (4)$$

$W_{\alpha} = \int_{t}^{t'} \mathcal{L} dt$ is the Hamilton principal function $D_{\alpha}(\mathbf{r}',\mathbf{r}) = |\text{det}_{ij}(-\partial p_{i}^{\alpha}(\mathbf{r}',0;\mathbf{r},t)/\partial r_{j})|^{1/2}$ contains information of the phase space in the vicinity of the trajectory $\alpha$ and $m_{\alpha}$ is a topological phase. The factor $\exp(-t/2\tau_{s})$ ($\tau_{s}$ being the elastic scattering time) results from calculating the disorder averaged Green functions within Born approximation [15].

Inserting the representation Eq. (4) of $G^{+}_{E}$ and $G^{+\ast}_{E}$ into Eq. (3) leads to double sums $\sum_{\alpha\bar{\alpha}}$ of products of path contributions. We begin with the semiclassical evaluation of the traces over the terms $v_{i}G^{+}_{E}(\mathbf{r},\mathbf{r'})v'_{j}G^{+\ast}_{E}(\mathbf{r},\mathbf{r'})$ in Eq. (4). The phases of the diagonal parts ($\alpha = \bar{\alpha}$) cancel out and we obtain the classical contribution to the conductivity in two dimensions after one time integration and a transformation of the integral over the final coordinate into an integral over initial momenta (by means of $D_{\alpha}$ which acts as a Jacobian), i.e.,

$$\sigma_{ij}^{cl} = e^2/\hbar^2 \int_{0}^{\infty} dt < v_{i}(t)v_{j}(0) >_{pq} \exp(-t/\tau_{s}) .$$

Here, $< >_{pq}$ denotes a classical phase space average over the energy shell. Such a Kubo formula had been used in Ref. [8] to calculate numerically the classical part of the conductivity for antidot arrays.

In order to take care of quantum phase coherence phenomena we have to take into account non–diagonal ($\alpha \neq \bar{\alpha}$) parts in the sum $\sum_{\alpha\bar{\alpha}}$. Consider, e.g., the contribution of Green function products of direct paths $\alpha$ (from $\mathbf{r}'$ to $\mathbf{r}$) and paths $\bar{\alpha}$ with at least one selfcrossing as depicted in Fig. 1(a). We will compute the trace integrals — as usual for a semiclassical approach — by stationary phase approximation. The stationary phase condition for the $\mathbf{r}$
integral requires for the final momenta \( p_\alpha^f = p_\alpha^\tilde{\alpha} \) from which follows that the paths \( \alpha \) and \( \tilde{\alpha} \) must coincide between \( r' \) and \( r \) (Fig. 1(b)). Stationary phase approximation for the trace integral over \( r' \) selects all pairs of paths with the same initial momenta, i.e. \( p_\alpha^i = p_\tilde{\alpha}^i \). Both conditions are fulfilled for all pairs of orbits with initial and final phase space points lying on a periodic orbit (Fig. 1(c)). Besides the example shown in Fig. 1(c) we must include all pairs of orbits with the shorter one showing an arbitrary number of full traversals before reaching the final point \( r \) and the longer one having \( r \) additional repetitions along the periodic orbit.

The semiclassical evaluation of the trace integrals and one time integral follows similar lines as Gutzwiller’s derivation of the periodic orbit trace formula for the density of states [14,16,17]. After performing finally the convolution (Eq. (1)) with the Fermi function we obtain from the \( \sigma_{xx}^{osc} \) and \( \sigma_{xy}^{osc} \) terms oscillating parts of the diagonal and Hall conductivity as sums over contributions from all primitive periodic orbits (po) of the classical system and their repetitions \( r \):

\[
\sigma_{xx}^{osc}(E_F, B; T) = \frac{2g_s e^2}{V} \sum_{po} \sum_{r=1}^{\infty} \frac{R_r(\beta) e^{-r T_{po}/(2\tau_s)}}{|\det(M_{po}^r - 1)|^{1/2}} \cos \left[ r \left( S_{po}/\hbar - \mu_{po}\pi/2 \right) \right],
\]

\[
\sigma_{xy}^{osc}(E_F, B; T) = \frac{2g_s e^2}{V} \sum_{po} \sum_{r=1}^{\infty} \left( \frac{r}{e} \frac{\partial S_{po}}{\partial B} + C_{po}^{xy} \right) \frac{R_r(\beta) e^{-r T_{po}/(2\tau_s)}}{|\det(M_{po}^r - 1)|^{1/2}} \cos \left[ r \left( S_{po}/\hbar - \mu_{po}\pi/2 \right) \right].
\]

In Eq. (5) \( S_{po}(E, B) = \oint_{po} p\,dq \) is the classical action, \( T_{po} \) the period and \( \mu_{po} \) the Morse index of a periodic orbit. The monodromy matrix \( M_{po}^r \) measures its classical stability [10].

\[
C_{ij}^{po} = \int_0^\infty dt e^{-t/\tau_s} \int_0^{T_{po}} d\tau v_i(\tau) v_j(t + \tau)
\]

are velocity–correlation functions for motion along the periodic orbits. The function

\[
R_r(\beta) = \frac{r T_{po}/\tau_\beta}{\sinh(r T_{po}/\tau_\beta)} \quad ; \quad \tau_\beta = \frac{\hbar \beta}{\pi}
\]

gives rise to temperature damping which is exponential for orbits with \( T_{po} \gg \tau_\beta \).

Stationary phase evaluation of the trace integrals in Eq. (2) for the terms \( v_i G_E^+(r, r') v_j G_E^+(r', r) \) representing recurring paths from \( r \) via \( r' \) leads also to periodic orbits (see Fig. 1(d–f)). However, the corresponding velocity correlation functions vanish and therefore \( v_i G^+ v_j G^+ \) terms do not contribute to \( \sigma_{ij} \) semiclassically.
Up to the correlation functions $C_{xx}^{po}$ the trace formula Eq. (5a) for $\sigma_{xx}$ is exactly the same as Gutzwiller’s trace formula for the density of states. $\sigma_{ij}$ quantum oscillations are semiclassically related to interference (due to the phase differences $\sim r S_{po}/\hbar$) between pairs of paths along a periodic orbit differing by $r$ in their number of full traversals. This approach therefore requires only phase coherence on the length scale of a periodic orbit and not throughout the entire system.

In the following we will apply our results to magnetotransport in 2DEG’s. In the unmodulated case the electrons follow cyclotron orbits with action $S_{cyc} = 2\pi E_F/\omega$ and frequency $\omega = eB/m^*$. Then the classical amplitudes [18] and velocity correlation functions in the trace formulas (5) can be calculated analytically. For the diagonal conductivity we obtain, e.g.,

$$\sigma_{xx} = \frac{n_s e^2 \tau_s}{m^*} \frac{1}{1 + (\omega \tau_s)^2} \left[ 1 + 2 \sum_{r=1}^{\infty} (-1)^r R_r(\beta) \cos \left( r \frac{2\pi E_F}{\hbar \omega} \right) \exp \left( -\frac{r \pi}{\omega \tau_s} \right) \right]$$

(8)

($n_s$ being the carrier density) which represents a semiclassical approximation of the Shubnikov de Haas oscillations and coincides with the quantum mechanical result for a constant scattering time $\tau_s$ [19]. In the case of a high mobility 2DEG ($\omega \tau_s \gg 1$) with a distinct Landau level structure the use of a density of state dependent scattering time is usually required in order to obtain the correct conductivity amplitudes. However, in the antidot arrays which we consider in the following the periodic superlattice potential strongly mixes the Landau levels [11] and therefore justifies the use of an energy independent $\tau_s$. The inset of Fig. 2(a) depicts the measured magnetoresistivity $\rho_{xx}(B)$ of an antidot array for two temperatures $T=4.7$ K and 0.4 K. While the gross structure of the broad (classical) maximum at $2R_c(B) = a$ persists up to temperatures of 60 K the (quantum) oscillations at $T=0.4$ K on top of the maximum disappear with increasing temperature (at $T=4.7$ K).

In order to show that the quantum oscillations at $T=0.4$ K are related to $\sigma_{xx}^{osc}(B)$ we compare the experimental difference signal $\Delta \sigma_{xx} = \sigma_{xx}(T=0.4K) - \sigma_{xx}(T=4.7K)$ shown in Fig. 2(a) with our semiclassical predictions for $\sigma_{xx}^{osc}(B)$. As a model of the antidot lattice we use the potential $V(x, y) = V_0 |\sin(\pi x/a) \sin(\pi y/a)|^\beta$ which has already proved useful to
describe magnetotransport in antidot arrays [3,8]. \( V_0 \) is determined through the normalized width \( d/a \) of the antidots at the Fermi energy and \( \beta \) (governing the steepness of the antidots) remains as the only free parameter. Here we use \( d/a = 0.5 \) and \( \beta = 2.3 \).

In order to calculate numerically \( \sigma_{xx}^{osc}(B) \) it is convenient [20] to expand the prefactors in Eq. (5a) into geometrical series and to perform the sum over \( r \) to get the following form

\[
\sigma_{xx}^{osc}(E_F, B; T) = \frac{4g_s e^2}{V} \hbar \text{Re} \left\{ \sum_{p_o} \sigma_{xx}^{p_o} \frac{T^{p_o}}{\tau_\beta} \sum_{k,l=0}^{\infty} \frac{i^{(k,l)}_{p_o}}{(1 - i^{(k,l)}_{p_o})^2} \right\}
\]

with

\[
t^{(k,l)}_{p_o} = (\pm 1)^k \exp \left[ i \left( \frac{S^{p_o}}{\hbar} - \frac{\pi}{2} \mu^{p_o} \right) - \left( k + \frac{1}{2} \right) \lambda^{p_o} - (2l + 1) \frac{T^{p_o}}{\tau_\beta} - \frac{T^{p_o}}{2\tau_s} \right]
\]

Here, \( \lambda^{p_o} = i\gamma^{p_o}, \gamma^{p_o} \) (real) being the winding number, \( k \) a semiclassical quantum number for a stable periodic orbit and \( \lambda^{p_o} > 0 \) (real) being the Liapunov exponent in case of an unstable periodic orbit [20]. The “−” sign in Eq. (10) applies to unstable inverse hyperbolic orbits; otherwise the “+” sign holds. A correct application of Eq. (9) requires a detailed knowledge of the phase space structure of the underlying classical motion in the potential of the antidots and the magnetic field. It turns out that the major part of the classical phase space is chaotic with a few islands of stable motion imbedded which vanish with decreasing magnetic field [21]. Under the experimental conditions (\( T = 0.4 \) K and \( \omega\tau_s \approx 2 \) at \( 2R_c = a \) [22]) only the shortest periodic orbits contribute significantly to \( \sigma_{xx}^{osc} \) since the terms from longer orbits (\( T^{p_o} > \tau_s \) or \( T^{p_o} > \tau_\beta \)) are exponentially small. For our calculations we take into account the seven fundamental periodic orbits shown in Fig. 2(d).

Our result for \( \sigma_{xx}^{osc} \) (at \( T = 0.4 \) K) is shown as the full line in Fig. 2(b): \( \sigma_{xx}^{osc}(B) \) oscillates with the same frequency as the measured conductivity. The period of the oscillations is nearly constant with respect to \( B \) in contrast to the \( 1/B \) periodic behaviour of ordinary Shubnikov de Haas oscillations (Eq. (8)) which are shown in Fig. 2(c) for an unmodulated 2DEG under the same conditions. The B periodic behaviour of quantum oscillations in certain antidot arrays can be related to the mechanism that flux enclosing periodic orbits between antidots cannot expand with decreasing \( B \) as in the case of free cyclotron motion.
Having in mind that the antidot potentials are not precisely known also the semiclassical amplitudes are on the whole in agreement with the measured curve of $\Delta \sigma_{xx}$. They show — as in the experiment — an irregular behaviour resulting from interference effects between different periodic orbits and from the magnetic field dependence of the classical orbit parameter entering Eq. (9). The semiclassical curves show also the correct temperature dependence: Due to the temperature damping $R_r(\beta)$ (Eq. (7)) the periodic orbit oscillations decrease for $T = 2.5$ K (dotted line in Fig. 2(b)) and nearly disappear at $T = 4.7$ K (dashed curve) as in the experiment (dashed curve in the inset of Fig. 2(a)). Fig. 3(e) illustrates the $\omega \tau_s$ dependence of $\sigma_{xx}^{osc}(B)$ for three values $\omega \tau_s = 1, 2$ and 5 showing that the result does not strongly depend on the $\tau_s$ chosen.

In summary we derived semiclassical formulas for the magnetoconductivity tensor within the Kubo approach and applied them to quantum transport in antidot lattices. However, it remains to understand the semiclassical relation between the Kubo formalism leading to periodic orbit contributions and the semiclassical Landauer Büttiker approach based on interference effects due to non–closed classical trajectories since the two corresponding quantum mechanical approaches are known to be equivalent under certain conditions [23].

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FIGURES

FIG. 1. Typical semiclassical paths $\alpha, \bar{\alpha}$ contributing to (a) $v_i G_E^+(r, r') v'_j G_{E}^{+*}(r, r')$ and (d) $v_i G_E^+(r, r') v'_j G_{E}^{+*}(r', r)$. The stationary phase condition at $r$ selects paths with $p_\alpha(r) = p_{\bar{\alpha}}(r)$ (b,e). Paths along periodic orbits result from the stationary phase condition $p_\alpha(r') = p_{\bar{\alpha}}(r')$ at $r'$ (c,f).

FIG. 2. (a) Oscillatory part $\Delta \sigma_{xx} = \sigma_{xx}(0.4K) - \sigma_{xx}(4.7K)$ of the experimental diagonal conductivity ($\sigma_{xx} = \rho_{xx}/(\rho_{xx}^2 + \rho_{xy}^2)$) of an antidot array as a function of an applied magnetic field. Inset: Measured resistivity $\rho_{xx}$ at $T = 0.4$ K (full line) and $T = 4.7$ K (dashed line). (b) Semiclassically calculated oscillatory part $\sigma_{xx}^{osc}$ (from Eq. 9) for three different temperatures $T = 0.4$ K (full line), $T = 2.5$ K (dotted line) and $T = 4.7$ K (dashed line). (c) Semiclassical Shubnikov de Haas oscillations (Eq. 8) for an unmodulated 2DEG under the same conditions as in (b). (d) fundamental periodic orbits in a model antidot potential which enter the semiclassical calculation. (e) $\sigma_{xx}^{osc}$ at $T = 0.4$ K for $\omega \tau_s = 5$ (dotted line), 2 (full line) and 1 (dashed line).