Semiclassical Analysis of
the Conductance of Mesoscopic Systems

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(February 16, 1995)

Abstract

The Kubo formula for the conductance of classically chaotic systems is
analyzed semiclassically, yielding simple expressions for the mean and the
variance of the quantum interference terms. In contrast to earlier work, here
times longer than $O(\log \hbar^{-1})$ give the dominant contributions, i.e. the limit
$\hbar \to 0$ is not implied. For example, the result for the weak localization
correction to the dimensionless conductance of a chain of $k$ classically ergodic
scatterers connected in series is $-\frac{1}{4} \left[1 - (k+1)^{-2}\right]$, interpolating between the
ergodic ($k = 1$) and the diffusive ($k \to \infty$) limits.

73.20.Fz, 03.65.Sq
When a micron–sized conducting sample is cooled to sub–Kelvin temperatures, the electrons’ coherence length increases beyond the system size, and classical dynamics no longer applies. The conductance through the sample becomes sensitive to very small magnetic fields, of the order of a flux quantum through the sample. Interest in these well–known mesoscopic effects, known as Weak Localization [1] (WL) and Universal Conductance Fluctuations [2] (UCF), has recently intensified, notably due to experiments on samples so clean that impurity scattering is no longer important [3]. Originally WL and UCF were observed in disordered conductors with diffusive dynamics, which are described well by diagrammatic perturbation theory with respect to the impurity potential [1,2]. The recent clean systems require different theoretical tools, and calculations using Random Matrix Theory [4] (RMT) and the Nonlinear $\sigma$–Model [5] (NL$\sigma$M) have appeared. These assume ergodic dynamics, meaning that all states at the Fermi energy are accessible “with equal probability”. A semiclassical theory for these effects should allow for any dynamics, not limited to diffusive or ergodic behavior.

Although the relevance and importance of semiclassical concepts was recognized from the outset [6,7], they were used at first only for interpretation, and explicit calculations based on the Semiclassical Approximation (SCA) appeared only later [8–10]. These calculations are, in a sense, beset by difficulties. For example, although the dependence on a magnetic field was obtained, the absolute magnitude of the interference effects had to be calibrated to either diagrammatic theory [7] or RMT [9,10]. The reason for this difficulty is obvious: both the mean (WL) and the standard deviation (UCF) of the quantum interference corrections to the conductance are smaller in powers of $\hbar$ than the leading, classical term. Such corrections to semiclassical propagators in chaotic systems are only very recently being studied [11]. In the perturbative theory, such corrections may be obtained by using diagrammatic elements called Hikami boxes [12]. They are known to give a vanishing contribution to the conductance, if it is expressed through the Kubo formula rather than the Landauer formula [13] (the latter served as the starting point for Refs. [8–10]).

Mesoscopic systems typically have non–separable Hamiltonians with chaotic classical
dynamics (integrable or intermediate systems require separate consideration). The SCA for the Kubo conductivity in such chaotic systems has been developed by Wilkinson [14]. He was interested in the genuine semiclassical limit, \( \hbar \to 0 \), and emphasized that his expressions fail for orbits longer than the Ehrenfest time \( t_E \), i.e. those which are long enough for an initially minimal wavepacket to spread due to classical chaos (Lyapunov exponents) and lose its correspondence to a point in classical phase–space. However, often (e.g. for the system of Ref. [3]) the lengths of the relevant orbits, or the escape time \( t_{esc} \), is much longer than \( t_E \), because \( t_E \to \infty \) only logarithmically as \( \hbar \to 0 \). The fact that the SCA can give accurate results also in this “mixing” regime, was clearly demonstrated [15] only after the work of Wilkinson had been published.

An application of the SCA to WL in the mixing regime will be described here. Some of the details, and a similar treatment of UCF are given elsewhere [16]. The conducting system, connected to two particle reservoirs through ideal leads, is described by a degenerate Fermi distribution of noninteracting electrons (quasiparticles) moving in an effective potential with completely chaotic (i.e. hyperbolic) classical dynamics. In order for the SCA to apply, we assume that all the features of the potential are smooth on the scale of the Fermi wavelength [17], and that the spectrum is essentially continuous, i.e. that the level spacing is much smaller than \( \hbar / t_{esc} \). For simplicity, we describe here only the zero temperature DC conductance, and ignore dephasing. Spin degeneracy, time reversal symmetry, and the absence of additional symmetries are assumed. We concentrate on the magnitude of the WL correction at zero magnetic field — for the semiclassical description of the field dependence see Refs. [3–10].

The relationship \( j(r') = \int d\mathbf{r} \ \underline{\sigma}(\mathbf{r}, \mathbf{r'}) \mathbf{E}(\mathbf{r}) \), where \( j(\mathbf{r}) \) and \( \mathbf{E}(\mathbf{r}) \) are the current density and the electric field in the sample, defines the space–dependent conductivity \( \underline{\sigma}(\mathbf{r}, \mathbf{r'}) \). The conductance \( G \) of a finite system is given in terms of \( \underline{\sigma}(\mathbf{r}, \mathbf{r'}) \) by dividing the dissipated power, \( \int d\mathbf{r'} \ \mathbf{E}(\mathbf{r'}) \cdot j(\mathbf{r'}) \), by the voltage \( V \) squared:

\[
G = \frac{1}{V^2} \int d\mathbf{r} \ d\mathbf{r}' \ \mathbf{E}(\mathbf{r'}) \underline{\sigma}(\mathbf{r}, \mathbf{r'}) \mathbf{E}(\mathbf{r}) . \quad (1)
\]
A straightforward derivation, starting from the Kubo formula and using the SCA, gives a result of the type

$$\sigma(r, r') \propto \sum_{\alpha, \beta \in \{r, r', E_F\}} A_\alpha A_\beta^* e^{i(S_\alpha - S_\beta)/\hbar} \ldots ,$$  

(2)

where $\alpha$ and $\beta$ label the classical trajectories starting at $r$, ending at $r'$, and propagating at the Fermi energy $E_F$. The amplitudes and actions corresponding to these orbits are denoted by $A_\alpha$ and $S_\alpha$ etc., and the dots represent further factors which depend, e.g., on the momenta of the orbits $\alpha$ and $\beta$. The derivatives of the action $S_\alpha = \int_{\alpha} p \cdot dr$ are given by $\frac{\partial S_\alpha}{\partial r} = -p_\alpha$, $\frac{\partial S_\alpha}{\partial r'} = p'_\alpha$ and $\frac{\partial S_\alpha}{\partial E} = t_\alpha$, where $p_\alpha$, $p'_\alpha$ and $t_\alpha$ are respectively the initial momentum, final momentum and duration of the corresponding orbit.

The classical conductivity is obtained by removing all the interference terms, i.e. retaining only terms with $\alpha = \beta$. The resulting sum, $\sum_\alpha |A_\alpha|^2 \ldots$, may be replaced by a mathematically equivalent integration over $\delta$ functions [16], as follows. Any given classical initial conditions, $r$ and $p$, and propagation time $t$, imply a unique final point in phase space, which we denote by $r_t$ and $p_t$. The distribution of classical paths is thus $f(r', p', t; r, p) = \delta(r' - r_t)\delta(p' - p_t)$. It is convenient to factor out a $\delta$ function due to conservation of energy, defining the distribution $f_E$ on the energy hypersurface through $f_E(r', p', t; r, p) \delta(H(r, p) - H(r', p')) = f(r', p', t; r, p)$ where $H(r, p)$ is the classical Hamiltonian for the system (for an ergodic system $f_E$ approaches a constant at long times). In terms of this distribution, the classical conductivity becomes [16]

$$\sigma^{cl}(r, r') = \frac{2e^2}{m^2 h^d} \int_0^\infty dt \int dp_E dp'_E f_E(r', p', t; r, p) p' p,$$  

(3)

where $e$ is the charge of the electron, $m$ is its (effective) mass, $h$ is Planck’s constant, $d$ is the dimensionality of the system (2 for a two-dimensional electron gas, 3 for a bulk sample), and the momentum integrals are restricted to the Fermi surface, $\int dp_E \ldots = \int dp \ \delta(H(r, p) - E_F) \ldots$. For a uniform system this expression can be integrated over $r'$ and averaged over $r$, giving a more familiar form: $\sigma^{cl} = \frac{e^2}{m^2} \nu \int_0^\infty dt \langle p(0)p(t) \rangle$. Here $\nu = \frac{2}{h^d \text{Vol}} \int dr dp_E$ is the density of states (the factor of 2 accounts for the spin degeneracy),
and the angular brackets denote averaging over all \((r, p)\) points on the Fermi surface \(p(0) = p\) and \(p(t) = p_t\).

The WL correction to the conductance is given by averaging the interference terms in Eq. (2). We assume that in the mixing regime \(S_\alpha\) and \(S_\beta\) are uncorrelated, except when \(\alpha\) and \(\beta\) are related by symmetry, i.e. \(\beta = \alpha^T\) where \(\alpha^T\) is the time-reversed partner of \(\alpha\) (\(\alpha\) and \(\alpha^T\) have the same action and amplitude). The possibility of \(\beta = \alpha^T\) occurs only if \(r = r'\) because \(\beta \in \{r, r', E_F\}\) and \(\alpha^T \in \{r', r, E_F\}\). Clearly, the ratio between the average conductivity and the classical conductivity increases gradually from 1 to 2 as \(r'\) approaches \(r\), and we therefore consider all contributions for which \(\beta\) approaches \(\alpha^T\) when \(r'\) approaches \(r\). For \(r' \simeq r\), the phase follows from the derivatives of the actions mentioned above. Using \(p'_\beta = -p_\alpha\) for \(\beta = \alpha^T\), we find that for the average conductivity a term

\[
\Delta \sigma^{WL}(r, r') \simeq \frac{2e^2}{m^2 h^d} \int_0^\infty dt \int d\mathbf{p}_E d\mathbf{p}'_E f_E(r', p', t; r, p) \mathbf{p}' \mathbf{p} e^{i(p + p')(r' - r)/\hbar}
\]

should be added to the classical term of Eq. (3).

The phase factor may be used to perform some of the \(dr\) and/or \(dp_E\) integrations in the stationary phase approximation. However, the sharp \(\delta\)-function nature of \(f_E\) leads to difficulties: in the standard SCA the integrations in Eq. (3) are performed first, giving back \(\Delta \sigma^{WL}(r, r') \simeq \sum_{\alpha \in \{r, r', E_F\}} |A_\alpha|^2 \exp \left( i(p_\alpha + p'_\alpha)(r' - r)/\hbar \right) \ldots \). When the \(dr'\) integration is then performed, the phase is only stationary if \(\alpha\) is a self-retracing orbit \((\alpha = \alpha^T)\), and these contributions have already been included in \(\sigma^{cl}(r, r')\). There are thus no stationary phase contributions to WL in the strict \((\hbar \to 0)\) sense \([18]\). In the mixing regime there are many orbits with \(p_\alpha + p'_\alpha\) different from 0 but so small that the phase \(\left( S_\alpha(r, r', E_F) - S_{\alpha^T}(r, r', E_F) \right)/\hbar\) is negligible throughout the relevant \(dr'\) integration region, and it is unclear how their contribution is to be accounted for. An alternative is to replace \(f_E\) by a smooth function \(f_E(r', p', t; r, p)\) describing the density of classical orbits, which is obtained from the original \(f_E\) by averaging over small ranges in initial and/or final conditions. These ranges are taken small enough (compared to the Fermi wavelength in \(r\), and \(\hbar\) over the size of the integration region in \(p\)), so as not to affect Eq. (3). For times \(t\) significantly
longer than the Ehrenfest time $t_E$, $f_E$ is a smooth function \[1\].

The integration over the components of $\mathbf{r}'$ and $\mathbf{p}'$ transverse to the direction of $\mathbf{p}$ can then easily be performed \[2\]: the stationary phase condition identifies $\mathbf{p}'$ with $-\mathbf{p}$ and the transverse components of $\mathbf{r}'$ with those of $\mathbf{r}$, and the integral gives a factor of $h^{d-1}$. The integration over the longitudinal component of $\mathbf{p}'$ gives a factor of $1/v_F$, where $v_F$ is the Fermi velocity. The phase is independent of the component of $\mathbf{r}'$ parallel to $\mathbf{p}$ (for $d=2$ and a specific orbit $\alpha$, this component can in fact be defined by the condition $S_{\alpha} = S_{\alpha^e}$). We therefore label the effective length of this integration region by $l(\mathbf{r}, \mathbf{p})$, leading to our main result \[21\]:

$$\Delta G^{WL} \simeq -\frac{2e^2}{h} \int_0^\infty dt \int d\mathbf{r} d\mathbf{p} f_E(\mathbf{r}, -\mathbf{p}, t; \mathbf{r}, \mathbf{p}) \frac{(\mathbf{p} \cdot \mathbf{E})^2}{m^2 V^2} \frac{l(\mathbf{r}, \mathbf{p})}{v_F} \tag{5}$$

(the minus sign is due to the identification of $\mathbf{p}'$ with $-\mathbf{p}$). The precise definition of $l(\mathbf{r}, \mathbf{p})$ becomes apparent if one notices that the component of $\mathbf{r}$ parallel to $\mathbf{p}$ should also be integrated along the same segment $l(\mathbf{r}, \mathbf{p})$, and that due to the $(\mathbf{p} \cdot \mathbf{E})/mv_F$ factors, each of these integrals gives the voltage difference between the two ends of the integration range, $\Delta V(\mathbf{r}, \mathbf{p})$. The integration range can be curved and should extend beyond the next or previous scattering event in the $\pm \mathbf{p}$ direction \[22\], but it is effectively limited by the “Ehrenfest length” $v_F t_E$, because of the averaging in $l(\mathbf{r}, \mathbf{p}) = \Delta V(\mathbf{r}, \mathbf{p})/(\mathbf{p} \cdot \mathbf{E})$. Note also that the classical results for $\mathbf{E}(\mathbf{r})$ may be used in Eq. (5), and higher order corrections to $\mathbf{E}(\mathbf{r})$ may be ignored.

Applications of Eq. (5) require a detailed knowledge of the classical distribution of orbits $f_E(\mathbf{r}', \mathbf{p}', t; \mathbf{r}, \mathbf{p})$ and voltage drops $V(\mathbf{r}, \mathbf{p})$. For some systems this information is readily available — for example in a diffusive system $f_E$ is known from the diffusion equation, and $l(\mathbf{r}, \mathbf{p})$ fluctuates within the system, but is known to be equal to twice the transport mean free path, on the average (because both forward and backward propagation are included). Eq. (5) then reproduces the result of Ref. \[7\]. A more interesting application is to a chain of $k$ ergodic cavities, connected in series and to the two particle reservoirs through $k+1$ ideal leads of equal widths. The assumption of ergodicity within each cavity, meaning that
$t_{\text{esc}}$ is long compared to the ergodic time for that cavity, implies that $f_E(r',p',t;r,p)$ is independent of the fine details of the initial and final positions for long times. It also implies that the electrostatic potential within each cavity is a constant $23$, with a potential drop of $V/(k+1)$ across each lead, i.e. $\Delta V(r,p) = \pm V/(k+1)$ for all points $r$ within any one of the leads. It is convenient to define a classical dynamic probability $p_{l,m}(n)$, equal to the probability that an electron will be in the $m$th cavity, having started from the $l$th cavity and having traversed through a lead $n$ times. The sum $\sum_{n=0}^{\infty} p_{l,m}(n)$ represents the total number of times that an electron originating in cavity $l$ will be found leaving cavity $m$, and is obviously related to integrals over $f_E$ similar to those of Eq. (5). Only the special case $l=m$ is relevant to Eq. (5), because if $p' = -p$, and $r' = r$ is a position within one of the leads (the only place where $E(r)$ does not vanish) then the conditions $(r,p)$ are directed into the same cavity that $(r',p')$ is directed out of. In terms of $p_{l,m}(n)$, Eq. (5) is

$$\Delta G^{WL} = -\frac{2e^2}{h} \frac{1}{(k+1)^2} \sum_{l=1}^{k} \sum_{n=0}^{\infty} p_{l,l}(n) ,$$

which can easily be generalized to any configuration of ergodic cavities connected by leads of various widths.

A dynamic equation, similar to the diffusion equation, may be written for $p_{l,m}(n)$:

$$p_{l,m}(n+1) = \frac{1}{2} [p_{l,m-1}(n) + p_{l,m+1}(n)] ,$$

with the initial condition $p_{l,m}(0) = \delta_{l,m}$ and the boundary conditions $p_{l,0}(n) = 0$ and $p_{l,k+1}(n) = 0$. It is easily solved: $p_{l,m}(n) = \sum_{i=1}^{k} \beta_{i,l} \alpha_i^n \beta_{i,m}$, where $\alpha_i = \cos \frac{i}{k+1} \pi$, and $\beta_{i,l} = \sqrt{\frac{2}{k+1}} \sin \frac{i}{k+1} \pi$. As in other evaluations of WL and UCF, only the eigenvalues $-1 < \alpha_i < 1$ play a role, and the necessary summation can be done: $\sum_{i=1}^{k} \frac{1}{1-\alpha_i} = k(k+2)/3$. The final result for this system is thus

$$\Delta G^{WL} = -\frac{2e^2}{h} \frac{1}{3} \left( 1 - \frac{1}{(k+1)^2} \right) .$$

The result for UCF, which is obtained through a similar but more lengthy calculation in Ref. [16], turns out to involve the 4th rather than the 2nd inverse power of $k+1$. Both
results reproduce those of RMT [4] for a single ergodic cavity, \( k = 1 \) (\( k = 0 \) describes an ideal wire), and approach the known results for a one-dimensional diffusive wire [24] when \( k \to \infty \). A similar system has been studied in Ref. [25], using the NL\( \sigma \)M, and giving a set of more complicated results for the \( k = 1 \) to \( k \to \infty \) crossover. In that study adjacent ergodic cavities were connected to each other through matrix elements in the Hamiltonian, rather than through ideal leads.

The failure of the SCA for the Landauer formula [15], compared to its success for the Kubo formula, can be traced to the fact that semiclassical evolution is not unitary, and the SCA for \( g(r, r') \) (like the Chambers formula for \( g^{cl}(r, r') \) in diffusive systems) does not conserve current. It is somewhat surprising that current conservation is not obeyed order by order in \( \hbar \). The issue can be clarified with a more fully understood calculation, using the random scattering matrices of the Circular Orthogonal Ensemble [4] (COE). The Landauer formula for the dimensionless conductance of a system connected to two reservoirs through ideal leads with \( N \) propagating modes in each lead is

\[
g = \sum_{i=1}^{N} \sum_{j=N+1}^{2N} |S_{i,j}|^2.
\]

For ergodic cavities, the scattering matrix \( S_{i,j} \) can be taken as a random member of the COE of \( 2N \times 2N \) matrices. Using the unitarity of scattering matrices (current conservation), \( \sum_{j=1}^{2N} |S_{i,j}|^2 = 1 \) for each row or column, one may re-express sums over transmission coefficients in terms of sums over reflection coefficients. Use of the “actual electric field” in the sample, i.e. taking the potential within the cavity to be appropriately intermediate between the potential in the reservoirs, corresponds to making this replacement with a weight of \( \frac{1}{2} \) for each row and each column and gives the “Kubo formula”:

\[
g = \frac{N}{2} - \sum_{i,j=1}^{2N} E_i E_j |S_{i,j}|^2,
\]

where the “classical electric field” factors are \( E_i = \frac{1}{2} \) for \( 1 \leq i \leq N \) and \( E_i = -\frac{1}{2} \) for \( N+1 \leq i \leq 2N \). The average conductance can be obtained from either the Landauer or the Kubo formula by using the known result \( \langle |S_{i,j}|^2 \rangle = (1+\delta_{i,j})/(2N+1) \) (the \( \delta_{i,j} \) term represents coherent backscattering), and gives \( g = N^2/(2N+1) \). The “semiclassical” or large \( N \) approximation violates unitarity: \( \langle |S_{i,j}|^2 \rangle \simeq (1+\delta_{i,j})/2N \). However, it still gives the correct
results to order $O(N^0)$ if the “Kubo formula”, Eq. (9), rather than the Landauer formula is used: $\langle g \rangle = \frac{N}{2} - \frac{1}{4} + O(N^{-1})$ [while only the $O(N)$ classical term is reproduced correctly in the Landauer formula]. Here, as in the diagrammatic calculation, higher order corrections to the “propagators” or the $\langle |S_{i,j}|^2 \rangle$ could in principle give contributions comparable to the WL effect being calculated, but when their contribution is integrated with the classical electric field $E(r)$, it vanishes. Unfortunately, a general proof of this is still lacking, and we are forced to conjecture that it holds in the SCA as well. It is expected that this “classical electric field” could be very useful in other calculation schemes too, e.g., that of Ref. [5].

The appearance of new, “non–strictly semiclassical”, contributions to physical quantities such as the Kubo conductance in the mixing regime was not emphasized earlier, apparently because in most applications of the SCA the density of states was considered, and only periodic orbits were involved. For periodic orbits the necessity of replacing $f_E$ by $\overline{f_E}$ does not arise, as exemplified by the UCF calculation [16], where there are two contributions — one involving periodic orbits and corresponding to Wilkinson’s results [14], and the other appearing only in the mixing regime. It is suggested that in the mixing regime these novel terms may dominate the strictly $\hbar \to 0$ corrections studied in Ref. [11].

The important task of demonstrating the SCA results for a given potential, rather than assuming a known distribution $\overline{f_E}$, is left for future research. It is emphasized that as only the statistical distribution of classical paths is necessary, the required numerical computation is not as demanding as, e.g., that of Ref. [15]. It would also be interesting to evaluate SCA corrections to the conductivity, e.g. due to caustics, and to contrast them with the higher order corrections which can be obtained diagrammatically.

The author wishes to thank H. U. Baranger, Y. Imry, R. A. Jalabert, A. Kamenev, U. Smilansky, A. D. Stone, and D. Ullmo for helpful discussions. This work was supported by the German Israel Foundation (GIF) Jerusalem and the Minerva Foundation (Munich, Germany).
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