Correlations and fluctuations of a confined electron gas

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Abstract

The grand potential $\Omega$ and the response $R = -\partial \Omega / \partial x$ of a phase-coherent confined noninteracting electron gas depend sensitively on chemical potential $\mu$ or external parameter $x$. We compute their autocorrelation as a function of $\mu$, $x$ and temperature. The result is related to the short-time dynamics of the corresponding classical system, implying in general the absence of a universal regime. Chaotic, diffusive and integrable motions are investigated, and illustrated numerically. The autocorrelation of the persistent current of a disordered mesoscopic ring is also computed.

PACS numbers: 73.23.-b, 73.20.Dx, 05.45.Mt

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A major advance in mesoscopic physics has been the observation of single-electron interference or more generally of quantum mechanical effects in mesoscopic objects. Among these we can mention the supershell structure in atomic clusters, the persistent currents in mesoscopic rings, or the quantization of the longitudinal conductance in microjunctions [1].

In all these experiments the spatial confinement of the electron gas plays a significant role. When a parameter controlling the system is varied – like the chemical potential, a magnetic field, or the shape of the confining potential – the response of the gas shows irregular fluctuations as a function of the parameter. While the average value of the variation is related to a macroscopic property of the system (like its volume), the wild fluctuations are the imprint of quantum mechanical interference.

Neglecting the interactions between the electrons, our purpose is to provide a general description of the fluctuating properties of the many-particle ground state electron gas when different parameters – like temperature $T$, chemical potential $\mu$, or external parameter $x$ – are varied. Taking as reference parameters $(x_0, \mu_0, T_0)$, the system is described in the grand-canonical ensemble by the grand potential

$$\Omega(x_0, \mu_0, T_0) = -\int dE \mathcal{N}(E, x_0) f(E, \mu_0, T_0) ,$$

with $\mathcal{N}(E, x_0) = g_s \sum_k \Theta(E - E_k(x_0))$ the counting function of the single particle states $E_k(x_0)$, $\Theta$ the Heavyside step function, $f(E, \mu_0, T_0) = 1/[1 + \exp((E - \mu_0)/kT_0)]$ the Fermi distribution and $g_s = 2$ for spin degeneracy.

The reaction of the system to a variation of the external parameter is characterized by the response function

$$R(x_0, \mu_0, T_0) = -\partial\Omega/\partial x_0|_{\mu_0, T_0} .$$

The physical interpretation of $R$ depends on the geometry of the sample and the nature of the parameter $x$. It is a magnetic moment if $x$ is a magnetic field, a persistent current when the sample geometry is annular and $x$ is an Aharonov-Bohm flux, or a force when $x$ controls the shape of the confining potential (like when deforming a metallic cluster for example).
We characterize the fluctuating properties of the electron gas by computing the autocorrelation function

\[ C_{\Omega}(x, \mu, T) = \left\langle \tilde{\Omega}(\mathbf{q}_-) \, \tilde{\Omega}(\mathbf{q}_+) \right\rangle_{x_0, \mu_0}, \]  

(2)

with \( \mathbf{q}_\pm = (x_0 \pm x/2, \mu_0 \pm \mu/2, T_0 \pm T/2) \). An analogous definition holds for \( C_R(x, \mu, T) \).

We denote the fluctuating part by an upper tilde symbol (see below). The brackets denote some energy and parameter averages.

Parametric correlations like \( C_{\Omega} \) or \( C_R \) have been studied in the past for chaotic and disordered systems for “individual” (single-particle) levels, rather than for a many-body ground state. The single-particle analog of \( C_R(x, 0, 0) \) is the velocity-velocity correlation \[2\]. Although for the latter no global expression is known, its tail \( x \to \infty \) has been shown to be universal \[2,4\]. In contrast to this, we will see below that for a Fermi gas the parametric correlators are explicitly computable and are expressed semiclassically, even at zero temperature, in terms of the classical short time dynamics of the system. Because the latter is system-specific, the correlators are in general system-dependent with no universal regime whatsoever. This difference with the universal local properties occurs mainly because the typical time scale of a perturbed ground state Fermi gas is \( h/\mu_0 \), which is much smaller than the Heisenberg time.

We express the counting function in Eq.(1) as a sum of smooth plus oscillatory terms \( \mathcal{N} = \mathcal{N} + \mathcal{N} \). The smooth part is given by the usual Weyl or Thomas-Fermi approximation. Semiclassically, the oscillatory part is \( \mathcal{N} = 2\hbar g_s \sum_p (A_p/\tau_p) \sin(S_p/\hbar) \). The sum is over the periodic orbits \( p \) with action \( S_p \) (including the Maslov index), period \( \tau_p = \partial S_p/\partial E \), and stability amplitude \( A_p \) \[3\]. This sum is inserted in Eq.(1) to compute the oscillatory part of the grand potential. To leading order in \( \hbar \) and for \( kT_0 \ll \mu_0 \) \[3,7\],

\[ \tilde{\Omega}(x_0, \mu_0, T_0) \approx 2\hbar^2 g_s \sum_p \tilde{A}_p \cos(S_p/\hbar), \]  

(3)

with \( \tilde{A}_p = A_p \kappa(\tau_p, T_0)/\tau_p^2 \). The factor \( \kappa(\tau_p, T_0) = \frac{\tau_p/\tau_c}{\sinh(\tau_p/\tau_c)} \), with \( \tau_c = h/\pi kT_0 \) takes into account finite temperature effects and acts as an exponential cut off for long periodic
orbits. All the classical quantities entering this expression are evaluated at \((x_0, \mu_0)\). The main dependence on \(x\) comes from the oscillatory terms via the dependence of the actions, \(S_p = S_p(x_0, \mu_0)\). Taking this into account, the oscillating part of the response function
\[
\tilde{R} = -\frac{\partial \tilde{\Omega}}{\partial x_0}|_{\mu_0, T_0}
\]
is
\[
\tilde{R}(x_0, \mu_0, T_0) \approx 2\hbar g_s \sum_p \tilde{A}_p \frac{\partial S_p}{\partial x_0}|_{\mu_0, T_0} \sin\left(\frac{S_p}{\hbar}\right),
\]
(4)
with \(Q_p = \frac{\partial S_p}{\partial x_0}|_{\mu_0, T_0}\).

Replacing Eq.(3) in (2) we obtain a double sum over periodic orbits with oscillations depending on the difference of their actions. The averages in Eq.(3) are done over some range \(\Delta \mu\) and \(\Delta x\) which contain several oscillations of \(\tilde{\Omega}\) but are on the other hand small in comparison to the scale over which the classical functions vary. As mentioned before, the main dependence on \((x, \mu)\) comes from the actions, which may be linearized with respect to these parameters. The average restricts the sum to orbits having approximately the same \(Q_p\) and \(\tau_p\). Ordering the orbits by their period, taking into account these restrictions and using the semiclassical definition of the parametric form factor \(K(\tau, x)\) (i.e., the Fourier transform of the two-point correlation function \([3]\)) we obtain
\[
C_\Omega = \frac{\hbar^2 g_s^2}{2\pi^2} \int_0^\infty d\frac{\tau}{\Delta^4} \chi(\tau, T) \cos(\mu \tau / \hbar) K(\tau, x),
\]
(5)
with \(\chi(\tau, T) = \kappa(\tau, T_0 - T/2) \kappa(\tau, T_0 + T/2)\). The autocorrelation of the response function follows from Eq.(3) by derivation with respect to the external parameter.

Due to the factor \(\tau^4\) in the denominator, the integral in (3) is dominated by the short-time dynamics of the system. For chaotic systems a naive replacement of the form factor \(K(\tau, x)\) by the random matrix result produces a divergence. In real systems, this divergence is avoided by the cut off introduced by the shortest periodic orbit of period \(\tau_{\text{min}}\) (the form factor vanishes for \(\tau < \tau_{\text{min}}\)). Then even at \(T_0 = T = 0\) (\(\chi = 1\)), the autocorrelation will be described with good accuracy by computing in Eq.(5) only the contribution of the shortest periodic orbits, the longer ones representing a small correction. Because this short-time dynamics is system-specific, then in general we do not expect any universality for \(C_\Omega\) and \(C_R\).
Eq. (5) may therefore be restricted to the diagonal approximation \( p = p' \) for the form factor, \( K_D(\tau) = h^2 \sum_p A_p^2 \delta(\tau - \tau_p) \), with the result

\[
C_\Omega = \frac{h^2 g_s^2}{2\pi^2} \int_0^\infty \frac{d\tau}{\tau^4} \chi \cos(\mu \tau/\hbar) \langle \cos(Qx/\hbar) \rangle K_D(\tau) .
\]  

(6)

Here the average is evaluated over the \( Q_p \)'s taken among all the periodic orbits having a period between \( \tau \) and \( \tau + d\tau \). The expression for the response function is

\[
C_R = \frac{g_s^2}{2\pi^2} \int_0^\infty \frac{d\tau}{\tau^4} \chi \cos(\mu \tau/\hbar) \langle Q^2 \cos(Qx/\hbar) \rangle K_D(\tau) .
\]

(7)

To leading order, Eq. (6) is also valid for systems with a fixed number of particles \( n \). The form factor is now evaluated at \( E = \bar{\mu}(n, x_0) \) obtained by inverting \( n = \bar{\mathcal{N}}(\bar{\mu}, x_0) \). On the other hand, Eq. (7) is modified according to \( Q^2 \rightarrow Q^2 + \tau^2 (\partial \bar{\mu}/\partial x_0)^2 \). The importance of this new term depends on the nature of the external parameter. If \( x \) is a flux in an Aharonov-Bohm geometry, \( \bar{\mathcal{N}} \) is independent of \( x \) and \( \partial \bar{\mu}/\partial x_0 = 0 \). On the other hand, if \( x \) is the deformation of a two dimensional billiard, we find that the contribution of this additional term is comparable to the \( Q^2 \) term if the area of the billiard varies, while it is smaller by a factor \( 1/n \) when the area is kept fixed.

Eqs. (6) and (7) are the basic results of this paper. We now proceed to analyze them for different physical situations. First we consider a ballistic motion in a regular cavity (the trajectories of the electrons occur on phase-space tori). As an example of regular dynamics we have studied a Fermi gas contained in a two dimensional rectangular box of fixed area \( \mathcal{A} \) and sides \( a \) and \( b \). We choose \( x = a/b \) as the external parameter. Exact expressions for \( A_p, \tau_p, S_p \) and \( Q_p \) are known in this case. We can therefore explicitly evaluate \( C_\Omega \) and \( C_R \) as a function of \( \mu \) or \( x \). In Fig. 1 we show the numerical results for \( x_0 \approx 1.3 \) compared to the theoretical curves using only the first 10 orbits as a function of the rescaled variable \( \xi = \sqrt{\mu_0} x/x_0^{3/2} \). We observe erratic long-range oscillations accurately described by our formulas.

We now turn our attention to chaotic systems. Considering that the form factor is strictly zero for \( \tau < \tau_{\text{min}} \), the simplest approximation one can made for these systems is to assume a random matrix theory [9] behavior for \( K_D(\tau) \) starting at \( \tau = \tau_{\text{min}} \).
\[ K_D(\tau) = \begin{cases} 0, & \tau < \tau_{\text{min}} \\ 2\tau/\beta, & \tau_{\text{min}} < \tau << \tau_H \end{cases} \]  

where \( \beta = 1(2) \) for systems with (without) time-reversal symmetry. Because the short-time dynamics usually dominates the correlation functions, this oversimplified approximation that doesn’t consider individually the contribution of other short trajectories is not expected to be very precise in general. However, what is interesting about Eq.(8) is that it leads to universal expressions for \( C_\Omega \) and \( C_R \), since as we will now see the system-dependent features may be re-absorb by a rescaling of the parameters. These universal results then serve as a guide (in particular in experimental situations where the shape of the potential is not well known), and are useful to obtain simple qualitative estimates of the different characteristic scales involved.

Let’s evaluate using (8) the variance of the fluctuations of the grand potential and of the response function. Restricting to zero temperature, we obtain from Eq.(6)

\[ C^0_\Omega = C_\Omega(0, 0, 0) = \frac{g_s^2}{2\beta \pi^2} \frac{\hbar^2}{\tau_{\text{min}}^2}, \]  

where \( \tau_{\text{min}} \) is computed at \((x_0, \mu_0)\). This simple expression relates the typical fluctuations to the period of the shortest orbit. For a billiard, \( \tau_{\text{min}} = (m/2\mu_0)^{1/2}L_{\text{min}} \), with \( L_{\text{min}} \) the length of the orbit. Weyl’s law allows to express \( \mu_0 \) in terms of the average number of particles in the gas \( n = N(\mu_0, x_0) \). We find \( C^0_\Omega \sim n^{2/d} \), with \( d \) the space dimensionality. This may be compared to the variance of the sum of \( m \) energy levels located in a small energy window around \( \mu_0 \), which is universal and proportional to \( m^2 \log m \) [10]. If a finite temperature is considered, we find that \( C^0_\Omega \) is damped by a factor \( 4(\tau_{\text{min}}/\tau_c) \exp(-\tau_{\text{min}}/\tau_c) \) when \( \tau_c << \tau_{\text{min}} \).

For the variance of the response function we must compute the variance of the distribution of the \( Q_p \)’s. We assume for chaotic systems a Gaussian distribution [11,12]. The variance is \( \langle Q^2 \rangle = \alpha \tau \). Explicit expressions for \( \alpha \) valid for chaotic billiards were given in [13]. Its value depends on energy, with a dependence \( \sim E^{3/2} \). These results as well as the approximation (8) in Eq.(7) lead to
\[ C^0_R = C_R(0,0,0) = \frac{g_s^2}{\beta \pi^2} \frac{\alpha}{\tau_{\text{min}}}. \]  

It is interesting to compare \( C^0_R \) to the “local” variance of the response of the individual single-particle levels \( E_k \) located in a small energy window around \((x_0, \mu_0)\), \( \langle v^2 \rangle = \langle (\partial E_k/\partial x)^2 \rangle = 2\alpha g_s^2/\beta \tau_H \) \( (\tau_H = \hbar \bar{\rho} \text{ is the Heisenberg time, conjugate to the mean level spacing}). \)

We have
\[ C^0_R = \frac{1}{2\pi^2} (\tau_H/\tau_{\text{min}}) \langle v^2 \rangle. \tag{11} \]

Because \( \tau_H \gg \tau_{\text{min}} \), the electron gas amplifies the local fluctuations. For billiards the amplification factor is proportional to \( n^{(d-1)/d} \), while the overall dependence on \( n \) is \( C^0_R \sim n^{4/d} \).

The autocorrelation functions are now evaluated in the approximation (8). Setting \( \mu = T = T_0 = 0 \) in (9) and using \( \langle \cos(Qx/\hbar) \rangle = \exp(-\alpha \tau x^2/2\hbar^2) \) by the Gaussian assumption we get
\[ \frac{C_\Omega(\xi,0,0)}{C^0_\Omega} = (1 - \xi^2/2) e^{-\xi^2/2} + \xi^4 \Gamma(0, \xi^2/2)/4, \tag{12} \]

where \( \Gamma(a,z) = \int_z^{\infty} t^{a-1} e^{-t} \, dt \). We have rescaled the parameter according to
\[ \xi = \sqrt{\alpha \tau_{\text{min}}} x/\hbar = \sqrt{C^0_R/2C^0_\Omega} \, x, \tag{13} \]

which makes, at this level of approximation, \( C_\Omega/C^0_\Omega \) a universal rapidly-decreasing function. The typical parameter scale over which \( C_\Omega \) decorrelates is \( \delta x = \hbar/\sqrt{\alpha \tau_{\text{min}}} \). This is consistent with the previous assumptions made, e.g., \( \delta x \) is small in the semiclassical \( \hbar \to 0 \) limit.

It is interesting to compare \( \delta x \) to the analogous local scale for a single-particle level \( \delta x_L = 1/\bar{\rho} \sqrt{\langle v^2 \rangle} \).

Since \( \delta x = g_s \sqrt{\tau_H/2\beta \pi^2 \tau_{\text{min}}} \delta x_L \), the scale of the Fermi gas is larger by a factor \( \sim n^{(d-1)/2d} \).

Expressed in terms of the same rescaled variable, the autocorrelation function of the response is
\[ \frac{C_R(\xi,0,0)}{C^0_R} = e^{-\xi^2/2} - 3 \xi^4 \Gamma(0, \xi^2/2)/2. \tag{14} \]
Analogous results are obtained when computing the autocorrelation in energy, \( C_\Omega(0, \epsilon, 0) \) and \( C_R(0, \epsilon, 0) \), were the rescaled parameter is \( \epsilon = \mu \tau_{\text{min}} / \hbar \).

In order to test numerically the goodness of these approximations we have considered an electron gas in a chaotic cavity. The cavity is the two-dimensional Limaçon billiard \([15]\), whose shape is defined by the conformal transformation \( w = z + b z^2 + c e^{i\delta} z^3 \). For parameter values around \( b = c = 0.2 \) it was numerically shown that the dynamics is dominated by chaotic trajectories \([15][16]\). We take \( x = \delta \) as the external parameter. Fig. 1 shows the numerical results compared to the theoretical curves. The approximation \( (8) \) provides a good qualitative description of the main features. The deviations observed may be due to contributions of periodic orbits other than the shortest one.

Analogous results may be obtained for diffusive systems by using the appropriate form factor in Eqs.\((3)\) and \((7)\). We concentrate on a particular example, the calculation of the autocorrelation of the persistent current of an electron gas in a disordered ring threaded by an Aharonov-Bohm flux \( \phi \).

The current at thermodynamic equilibrium is given by \( I = -c \frac{\partial \Omega}{\partial \phi} \). Only the fluctuating part of \( \Omega \) depends on \( \phi \). We replace \( S_p / \hbar \rightarrow S_p / \hbar + 2\pi w_p \phi / \phi_0 \) in Eq.\((3)\) to include the flux, with \( \phi_0 = h c / e \) the flux quantum and \( w_p \) the winding number of the periodic orbit \( p \) around the ring. The current in the ring is

\[
I(\lambda) = \frac{4\pi \hbar^2 c g_s}{\phi_0} \sum_p \tilde{A}_p w_p \sin \left( \frac{S_p}{\hbar} + 2\pi w_p \lambda \right),
\]

where we have introduced \( \lambda = \phi / \phi_0 \). The autocorrelation of the current \( C_I(\lambda, \lambda_R) = \langle I(\lambda_R + \lambda) I(\lambda_R) \rangle \) is computed in the diagonal approximation taking into account the contribution of the primitive orbits and of their time reversal partners. As before, it can be expressed in terms of the form factor, which now takes into account the diffusive motion of the particle \([17][18]\). For simplicity we restrict the calculation to a quasi one-dimensional ring and set the temperature to zero. At \( \phi = 0 \) we get the well known variance of the persistent current \( C_I^0 \) \([19][18]\). Normalizing \( C_I \) with this variance and averaging both with respect to the reference flux \( \lambda_R \), we arrive at
\[
\frac{C_I(\lambda)}{C^0_I} = \frac{1}{\zeta(3)} \sum_{w=1}^{\infty} \frac{\cos(2\pi w \lambda)}{w^3},
\] (16)

where \(\zeta(s)\) is the Riemann zeta function.

Eq. (16) is a universal function, independent of the specific aspects of the dynamics (i.e., independent of the elastic time between collisions or the diffusion constant), but depends on the dimensionality of the system. No rescaling of the parameter was needed. This interesting fact is due to the geometry of the sample and the physical quantity considered. Orbits with zero winding number do not contribute to the current because they have no flux dependence, while those with \(w \geq 1\) have a period \(\tau >> \tau_e\), the elastic time. As a consequence, all the non-universal shortest orbits gave no contribution, and the autocorrelation is a universal function (at fixed \(d\)).

In conclusion, we have studied the statistical properties of a phase-coherent non-interacting confined electron gas in response to a parameter. The results are applicable to any confined fermionic system. The autocorrelations \(C_\Pi\) and \(C_R\) were computed explicitly. Their behavior is described by the shortest classical periodic orbits, making them system-dependent within general no universal regime. When the form factor is simplified to take into account only the shortest orbit, it is possible to remove the dependence on specific properties of the system by a rescaling determined by \(\tau_{\text{min}}\). The typical fluctuations of the gas are also expressed by simple formulas in terms of \(\tau_{\text{min}}\). This is different from the rescaling of parametric correlations of single-particle levels, determined by \(\tau_H\). This latter time is of secondary importance in our context, and long orbits represent a small correction to our results. In the case of persistent currents in a diffusive Aharonov-Bohm geometry, the autocorrelation is independent of the parameters of the system, without any rescaling, due to the suppression by the geometry of the short-time orbits. The analytical results have been verified by numerical simulations on chaotic and regular cavities.

We are especially grateful to H. Bruus, C. H. Lewenkopf and E. R. Mucciolo for providing the program for the numerical simulation of the Limaçon billiard.
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FIG. 1. Normalized autocorrelation functions (points) compared to theoretical predictions (dashed lines): (a) $C_\Omega(\xi,0,0)/C_\Omega^0$ and (b) $C_R(\xi,0,0)/C_R^0$ for the (integrable) rectangular billiard; (c) $C_\Omega(0,\epsilon,0)/C_\Omega^0$ and (d) $C_R(0,\epsilon,0)/C_R^0$ for the chaotic Limaçon billiard