Interacting Electrons in Disordered Potentials: Conductance versus Persistent Currents

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An expression for the conductance of interacting electrons in the diffusive regime as a function of the ensemble averaged persistent current and the compressibility of the system is presented. This expression involves only ground-state properties of the system. The different dependencies of the conductance and persistent current on the electron-electron interaction strength becomes apparent. The conductance and persistent current of a small system of interacting electrons are calculated numerically and their variation with the strength of the interaction is compared. It is found that while the persistent current is enhanced by interactions, the conductance is suppressed.

There has been much recent interest in the physics of interacting electrons in disordered systems [1–19]. Part of this attention is motivated by the large amplitudes of persistent currents observed in mesoscopic metallic rings [20,21]. These values are larger by up to 2 orders of magnitude than theoretical predictions based on the single electron picture using the value of the mean free path as measured by transport experiments. Another motivation has to do with the rich physics contained therein. The metal-insulator transition can be triggered by two different physical mechanisms: electron-electron (*e-e*) interactions (generally referred to as the Mott-Hubbard transition) and disorder (known as the Anderson transition). Although much effort has been devoted to the investigation of the interplay between the two, the problem of metal-insulator transition in the presence of disorder and interactions is not yet completely settled [22,23].

Theoretically, it has been established that due to *e-e* interactions the amplitude of the persistent current (at zero temperature) may be enhanced compared to its non-interacting value. The precise nature of this interaction induced modification depends on the model used and on the specific domains in parameter space. For spinless electrons in one-dimensional (1D) continuum models the amplitude can reach its disorder-free value for strong interactions [8]. On the other hand, for spinless electrons in 1D lattice models a negligible enhancement of the amplitude occurs and that happens only for weak interactions in the localized regime [9,12,14]. When spin is taken into account, a sizable enhancement of the amplitude is found [17,18]. Large enhancements occur also for 2D and 3D spinless electrons in lattice models for weak and medium ranges of interaction strengths [16,19].

Thus one may conclude that it is conceivable that significant enhancement of persistent currents may result in calculations for realistic 3D lattice models which take spin into account. Nevertheless, there still remain several important questions which have not yet been fully answered. The first, and perhaps the most interesting one from a general point of view, is why does *e-e* interaction play such an important role in the determination of the persistent current while it is believed to play no important role in determining the value of the conductance. Or, to pose the question in another way, it is conceivable that for the models considered, *e-e* interactions enhance also the conductance and therefore do not explain the discrepancy between theory and experiment. Other questions are connected with the precise origin and nature of the enhancement.

In this Letter we shall concentrate on the first question. A new expression for the calculation of the dissipative conductance for a system of interacting electrons is presented. It can be written as the derivative of the persistent current at zero flux multiplied by the compressibility of the system. It is argued that in the diffusive regime the derivative of the current is of the same order of magnitude as its amplitude, (which is enhanced by *e-e* interaction), while the compressibility is suppressed. Therefore, in the same regime of disorder and interaction strength for which the persistent current is enhanced, the conductance might behave in quite a different way. The new formulation is then applied in the numerical evaluation of the conductance for 2D spinless electrons on a lattice which is known to exhibit large enhancement of the persistent current. The results are compared with the conductance as calculated via the Kubo-Greenwood formula (suitably adopted for interacting systems). For both methods of calculations, the conductance of the system is suppressed by the interactions, thus supporting the suggestion that *e-e* interactions might explain the discrepancy between theory and experiment.

As the starting point we shall use the Akkermans-Montambaux [24] definition of the conductance which is based on the response of a system to a change in its boundary condition

$$g_d(\mu) = -\frac{1}{4} \frac{\partial^2}{\partial\Phi^2} \langle \delta N^2(\mu, \Phi) \rangle_{\Phi=0}, \qquad (1)$$

where the boundary condition on the wave function of the system is given by $\psi(x_1, y_1, z_1; \ldots; x_j, y_j, z_j; \ldots) = \psi(x_1, y_1, z_1; \ldots; x_j + L, y_j, z_j; \ldots)e^{i\Phi}$. This form of

boundary condition is similar to the one arising in a ring encompassing a magnetic flux ϕ. In that case $\Phi = 2\pi\phi/\phi_0$, where ϕ_0 is the quantum flux unit. $N(\mu, \Phi)$ is the number of particles for a given realization of the disorder, with specific values of the chemical potential μ and Φ. Here $\langle\delta N^2(\mu, \Phi)\rangle = \langle N^2(\mu, \Phi)\rangle - \langle N(\mu, \Phi)\rangle^2$, and $\langle\cdots\rangle$ represents an average over disorder realizations. Since this expression describes the conductance at a fixed chemical potential, it is especially appropriate for a system coupled with the external world, for example, by leads. It is applicable in the metallic regime in which the usual diagrammatic expansion is valid. In the mesoscopic regime, it is the case for which the level broadening γ is larger than the averaged single-particle level spacing Δ [25], which is compatible with the experimental situation. Thus, one must be careful in applying expression (1) in the deep quantum limit in which the level broadening is smaller than the level separation (see Ref. [26]). The above definition remains valid also for interacting particles described by a Fermi liquid picture. A connection between the relation (1) for the conductance and the Thouless formula $g_c = \langle|\partial^2 E_n/\partial\Phi^2|\rangle_{\Phi=0}/\Delta$ (where E_n is the energy of a single electron level in the vicinity of the Fermi energy) in the absence of e-e interaction was established analytically [24]. From numerical studies [26] it seems that $g_d \propto g_c$ holds (for varying disorder strength) even in the deep quantum limit although the proportionality factor changes.

We would like to express g_d in terms of the persistent current. Altshuler, Gefen, and Imry [27] have shown that the fluctuations in the number of particles in the grand canonical ensemble is connected to the disordered-averaged persistent current in the canonical ensemble (i.e., an average over different realizations of disorder with a fixed number of electrons N_0) in the following way [28]:

$$\langle I(\Phi)\rangle_{N_0} = \frac{\pi}{\phi_0}\left[\left\langle\frac{\partial N}{\partial\mu}\right\rangle^{-1}\frac{\partial}{\partial\Phi}\langle\delta N^2(\mu, \Phi)\rangle\right]_{\mu=\langle\mu\rangle}, \quad (2)$$

where $\langle\partial N/\partial\mu\rangle$ is the averaged compressibility and $\langle\mu\rangle$ is the averaged chemical potential for which $N(\mu = \langle\mu\rangle) = N_0$. This connection is general and valid for interacting systems as well.

Combining Eqs. (1) and (2) one obtains

$$g_d(\mu) = \frac{\phi_0}{4\pi}\left\langle\frac{\partial N}{\partial\mu}\right\rangle_{\mu=\langle\mu\rangle}\frac{\partial}{\partial\Phi}\langle I(\Phi)\rangle_{N_0,\Phi=0}. \quad (3)$$

Thus, in the metallic regime where the usual diagrammatic expansion is valid ($\gamma \gtrsim \Delta$) one can relate the derivative of the averaged persistent current at zero flux

for a canonical ensemble to the dissipative conductance at a given chemical potential. This connection remains valid also for interacting systems under the previously mentioned restrictions. Expression (3) is extremely useful for numerical calculations of the dissipative conductance at zero temperature for such systems since it involves only the ground-state properties (energy and compressibility) of a system with fixed number of particles.

The definition [Eq. (3)] agrees with our physical concept of the conductance especially for systems in interaction. As pointed out by Lee [29], the conductivity for the interacting case can be written as $\sigma = (\partial N/\partial\mu)D/L^d$, (where D is the diffusion constant and d is the dimensionality of the system) which is simply the Einstein relation. Thus the conductance is $g = L^{d-2}\sigma = (\partial N/\partial\mu)D/L^2$, which is exactly the content of Eq. (3). This is easily verified in the noninteracting limit where the derivative of the averaged persistent current was calculated by Altshuler, Gefen, and Imry [27], and was shown to be $\phi_0\langle\partial I(\Phi)/\partial\Phi\rangle_{N_0,\Phi=0} = (D/L^2)\Delta/\gamma$. For $\gamma = \Delta$ the continuous spectrum conductance is recovered, and for $\gamma > \Delta$ the Drude formula for conductance with inelastic scattering is obtained.

It is also possible to directly connect g_d to the amplitude of the persistent current for the interacting case. In the diffusive regime, the average persistent current is determined by the first few harmonics of the current [2,27,30]. The situation changes in the presence of interactions where it was shown analytically that the first harmonic describes very well the current for any value of the flux [1]. Later on it has also been confirmed numerically [8,16]. Thus, for interacting electrons $\langle I(\Phi)\rangle_{N_0} \sim \langle I(\Phi = \pi/2)\rangle_{N_0}\sin(\Phi)$, which results in $\langle\partial I(\Phi)/\partial\Phi\rangle_{N_0,\Phi=0} \sim \langle I(\Phi = \pi/2)\rangle_{N_0}$. Inserting this relation into Eq. (3) one obtains $g_d \sim (\langle\partial N/\partial\mu\rangle)\langle I(\Phi = \pi/2)\rangle_{N_0}$. Therefore, the conductance is proportional to the persistent current multiplied by the compressibility. This implies that strong correlations might influence persistent currents and conductance in an opposite way. While persistent currents are enhanced by e-e interactions, the conductance which is the persistent current multiplied by the compressibility (a decreasing function of interaction) might be suppressed at higher values of interactions.

We shall now illustrate our arguments by calculating the conductance for a system of interacting electrons on a 2D cylinder of circumference L_x and height L_y. In this model large enhancement of the persistent current in the diffusive regime has been found [16]. The model Hamiltonian is given by

$$H = \sum_{k,j}\epsilon_{k,j}a_{k,j}^\dagger a_{k,j} - V\sum_{k,j}[\exp(i\Phi s/L_x)a_{k,j+1}^\dagger a_{k,j} + \text{H.c.}] - V\sum_{k,j}(a_{k+1,j}^\dagger a_{k,j} + \text{H.c.}) + \varepsilon_c\sum_{k,j>l,p}\frac{a_{k,j}^\dagger a_{k,j}a_{l,p}^\dagger a_{l,p}}{|\vec{r}_{k,j} - \vec{r}_{l,p}|/s}, \quad (4)$$

where $a_{k,j}^\dagger$ is the fermionic creation operator, $\epsilon_{k,j}$ is the energy of a site (k, j), which is chosen randomly between $-W/2$ and $W/2$ with uniform probability, V is a constant hopping matrix element, and s is the lattice constant. The

interaction term represents a Coulomb interaction between electrons confined to a 2D cylinder embedded in a 3D space with $\varepsilon_c = e^2/s$.

Let us start by presenting numerical results for g_d. Since we are concerned with an exact diagonalization of the Hamiltonian for interacting electrons, the size of the system is naturally limited. We consider a 4×4 lattice with $m = 16$ sites which in the half-filled case ($N_0 = 8$) corresponds to a $12\,870 \times 12\,870$ matrix. As previously mentioned, the main interest lies in the diffusive regime. Therefore we must chose the disorder strength W accordingly, i.e., $\xi > L_x, L_y \gg \ell$, where ξ is the localization length and ℓ is the mean free path. We take $W = 8V$ for which $\xi = 8.4s$ (estimated using the participation ratio) and $\ell = 0.97s$ (estimated from the Thouless conductance g_c). We also checked that the single-electron level spacing distribution is close to the Gaussian ensemble prediction, thus confirming that the system is in the metallic regime [31].

For systems with interacting electrons it is not possible to calculate directly the Thouless conductance, since the single electron energy levels are not defined. On the other hand, the basic ingredients needed for the calculation of g_d are easily available once the ground-state energy of the many-particle system as a function of flux is obtained by diagonalizing the Hamiltonian (4). The persistent current can be calculated via the well-known relation $\langle I(\Phi) \rangle_{N_0} = -(2\pi/\phi_0)\langle \partial E(\Phi)_{\text{g.s.},N_0}/\partial\Phi \rangle$ [where $E(\Phi)_{\text{g.s.},N_0}$ is the ground-state energy of an interacting system of N_0 particles] and $\langle \partial\mu/\partial N \rangle = \langle E_{\text{g.s.},N_0+1} - 2E_{\text{g.s.},N_0} + E_{\text{g.s.},N_0-1} \rangle$. Thus, once the ground-state energies for systems with $N_0 \pm 1$ particles are known, the conductance g_d can be immediately calculated.

The derivative of the persistent current at zero flux for $N_0 = 8$ averaged over 4500 realizations is presented in Fig. 1. It can be seen that an enhancement of the derivative as function of the interaction strength ε_c is obtained. This is similar to the enhancement of the current at $\Phi = \pi/2$ shown in the inset. Thus our assumption $\langle \partial I(\Phi)/\partial\Phi \rangle_{N_0,\Phi=0} \sim \langle I(\Phi = \pi/2) \rangle_{N_0}$ is validated.

The inverse of the compressibility at $N_0 = 8$ averaged over 500 samples is shown in the inset of Fig. 2. It can be seen that, for $\varepsilon_c > 2V$, $\langle \partial\mu/\partial N \rangle \sim \varepsilon_c^{4/3}$. The dissipative conductance is presented in Fig. 2. For small values of ε_c, g_d shows a substantial decrease since the derivative of the current is only weakly enhanced and the main influence on the conductance comes from the compressibility. For larger values of interactions ($\varepsilon_c > 2V$), the enhancement of the current is compensated by the compressibility and the conductance slowly decreases. Thus, for all values of ε_c the conductance is not enhanced by the interactions. This strongly points toward e-e interactions as a possible explanation for the large amplitudes of persistent current measured in experiments [20,21].

A useful check of our formalism is to compare the values of g_d to the values obtained from a many-particle formulation of the Kubo-Greenwood conductance g_k for
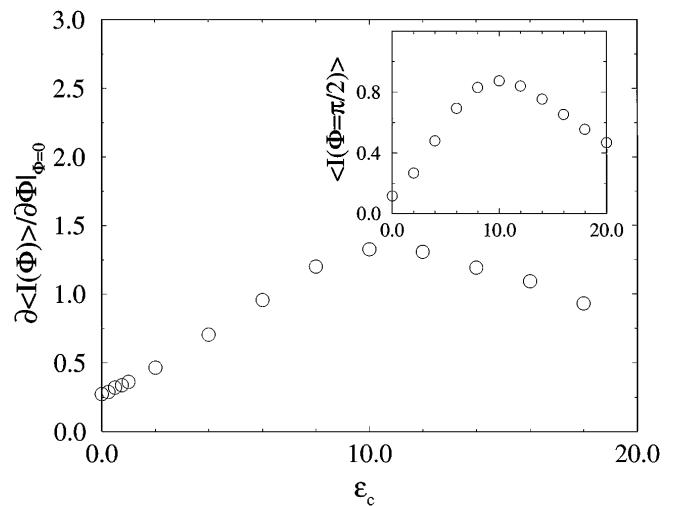

FIG. 1. The derivative of the averaged persistent current at zero flux for a fixed number of particles as a function of the interaction strength (in units of V). The derivatives were averaged over 4500 realizations. In the inset the averaged persistent current at a given flux for the same system is presented.

the same system. Following Kohn [32,33] the real part of the conductance may be written as $g_k = (8\pi h/L^2 e^2) \times \sum_\alpha' |\langle \alpha|J_x|0 \rangle|^2 \varepsilon_{\alpha,0} \gamma (\varepsilon_{\alpha,0}^2 + \gamma^2)^{-2}$, where $|0\rangle$ is the many-particle ground state, J_x is the current operator, and $\varepsilon_{\alpha,0} = \varepsilon_\alpha - \varepsilon_0$. This is a very cumbersome calculation since it involves calculating the many-particle low-lying eigenvalues and eigenvectors for each realization of disorder. We chose the inelastic broadening to be of the same order as the single-electron level separation, i.e., $\gamma = 0.7V$. The results for g_k averaged over 180 realizations are plotted in the inset of Fig. 3. As in the relationship between g_c and g_d [24,26], g_k is an order of magnitude larger than g_d. g_k seems to follow g_d for $\varepsilon_c > 2V$ (for which
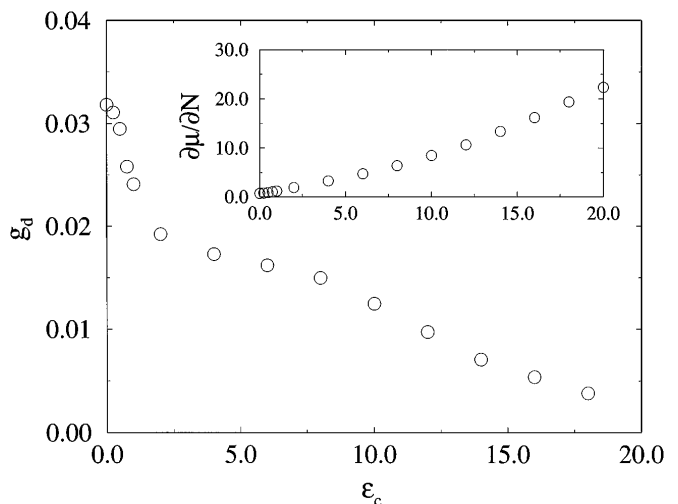

FIG. 2. The dissipative conductance g_d as a function of the interaction strength. In the inset the inverse of the averaged compressibility as a function of the interaction strength for the same system is presented.
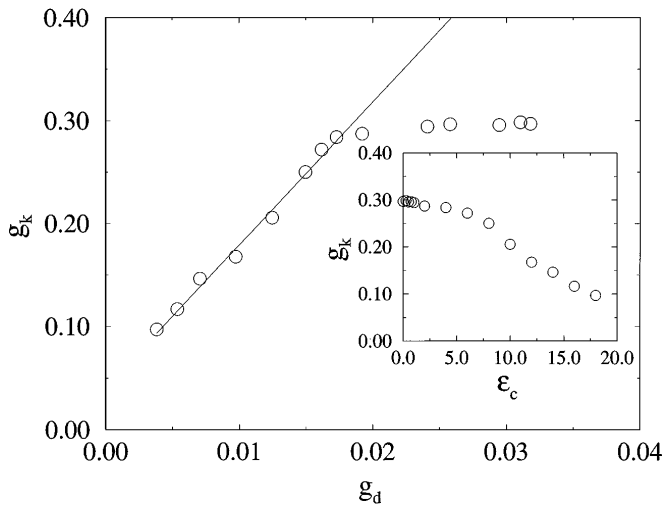
FIG. 3. The correspondence between the Kubo conductance g_k and the dissipative conductance g_d. For strong interactions ($\varepsilon_c > 2V, g_d < 0.015$) a good fit with a linear relation $g_k = 13.9 g_d + 0.04$ is obtained. In the inset g_k as a function of the interaction strength is presented.

the excitation separation is much bigger than γ), while there is no sharp decrease for small values of interactions. This may be clearly seen in Fig. 3 where g_k is plotted as a function of g_d. For $\varepsilon_c > 2V$ a clear linear relation $g_k = 13.9 g_d + 0.04$ is obtained, which can be compared to the noninteracting relation $g_k = 8.9 g_d + 0.04$. For $\varepsilon_c < 2V$ g_k is almost constant while g_d decreases. This might be connected to the transition of the statistical properties of the many-particle energy levels for weak interactions [34] and to the influence of interactions on the inelastic broadening γ currently under investigation. Nevertheless, in both methods of calculation the conductance never increases as function of interaction strength.

In conclusion, we have presented a new method for calculating the conductance of an interacting electronic system in the presence of static disorder. This formulation clarifies the difference in the interaction dependence between the persistent current and the conductance. Since the compressibility decreases as a function of the e-e interaction, the conductance is always less enhanced (or probably suppressed) compared with the persistent current. Thus, e-e interactions are a probable candidate for explaining the discrepancy between theory and experiment. This method has also the advantage of being dependent only on ground-state energies of neighboring systems, which are much easier to calculate numerically than the full spectrum of eigenvalues and eigenvectors.

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