SPECTRAL CORRELATIONS IN DISORDERED MESOSCOPIC METALS
AND THEIR RELEVANCE FOR PERSISTENT CURRENTS

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Received

We use the Lanczos method to calculate the variance \( \sigma^2(E, \phi) \) of the number of energy levels in an energy window of width \( E \) below the Fermi energy for non-interacting disordered electrons on a thin three-dimensional ring threaded by an Aharonov-Bohm flux \( \phi \). We confirm numerically that for small \( E \) the flux-dependent part of \( \sigma^2(E, \phi) \) is well described by the Altshuler-Shklovskii-diagram involving two Cooperons. However, in the absence of electron-electron interactions this result cannot be extrapolated to energies \( E \) where the energy-dependence of the average density of states becomes significant. We discuss consequences for persistent currents and argue that for the calculation of the difference between the canonical- and grand canonical current it is crucial to take the electron-electron interaction into account.

The mesoscopic persistent current in a small metal ring threaded by an Aharonov-Bohm flux \( \phi \) has been predicted long time ago by Hund. However, the role of disorder and electron-electron interactions has only been addressed quite recently, and is not completely understood. The experiment by Levy et al. and the subsequent experiments by other groups have motivated many recent theoretical works. There exists now general agreement that the surprisingly large experimentally observed persistent currents can only be explained by taking the electron-electron interaction into account. Nevertheless, the calculations within models of non-interacting electrons have lead to new insights into the nature of mesoscopic disordered systems. In particular, in a seminal paper Altshuler, Gefen and Imry have shown that for non-interacting electrons in the diffusive regime the dominant contribution to the average persistent current arises from striking differences between the canonical and grand-canonical ensembles. Because experimentally no external leads were attached to the rings, one should calculate the canonical persistent current

\[
I(N, \varphi) = \frac{-e}{\hbar} \left( \frac{\partial F(N, \varphi)}{\partial \varphi} \right)_N,
\]

where \( F(N, \varphi) \) is the canonical free energy, the flux \( \varphi = \phi/\phi_0 \) is measured in units of the flux quantum \( \phi_0 = hc/e \), and \(-e\) is the charge of the electron. Unfortunately, the usual methods of quantum statistical mechanics are based on the grand canonical formalism, where the chemical potential \( \mu \) is held constant. In Ref. the disorder
averaged canonical current $\overline{I(N, \varphi)}$ was therefore related to the variance
\[
\Sigma^2(\mu^*, \varphi) = N^2(\mu^*, \varphi) - \left[ \overline{N(\mu^*, \varphi)} \right]^2 \tag{2}
\]
of the particle number $N(\mu, \varphi)$ in a corresponding grand-canonical ensemble at a
certain value $\mu^*$ of the chemical potential. Here and below the overbar denotes
averaging over the disorder. $\mu^*$ should be chosen such that the disorder- and flux-
averaged particle number in the corresponding grand-canonical ensemble agrees
with the given particle number $N$ in the original canonical ensemble, i.e.
\[
\int_0^1 d\varphi \overline{N(\mu^*, \varphi)} = N . \tag{3}
\]
The expression derived in Ref.\textsuperscript{10} can be written as\textsuperscript{11}
\[
\overline{I(N, \varphi)} - \overline{I_{gc}(\mu^*, \varphi)} \approx -\frac{e}{\hbar} \frac{1}{2\kappa(\mu^*, \varphi)} \frac{\partial}{\partial \varphi} \Sigma^2(\mu^*, \varphi) , \tag{4}
\]
where $\overline{I_{gc}(\mu^*, \varphi)}$ is the average grand-canonical current, and
$\kappa(\mu, \varphi) = \left( \partial \overline{N(\mu, \varphi)} / \partial \mu \right)_\varphi$ is the average compressibility. For non-interacting electrons in the diffusive regime
$\overline{I_{gc}(\mu^*, \varphi)}$ is exponentially small; the leading interaction contribution to $\overline{I_{gc}(\mu^*, \varphi)}$ is not negligible and has been calculated by Ambegaokar and Eckern.\textsuperscript{3}

Note that Eq.\textsuperscript{3} defines $\mu^*$ as function of $N$, so that the right-hand side of Eq.\textsuperscript{4}
is indeed a function of $N$ and $\varphi$. As it stands, Eq.\textsuperscript{4} is valid even for interacting
systems, and can be used to take the effect of electron-electron interactions on the
canonical current in a simple but non-perturbative way into account.\textsuperscript{12} In this
work we would like to restrict ourselves to non-interacting electrons in the diffusive
regime. Then $\kappa^{-1}(\mu^*, \varphi)$ can be approximated by a flux-independent constant $\Delta$, the
average level spacing at the Fermi energy $\mu^*$. In this way the calculation of the
average canonical persistent current is reduced to the problem of calculating the
flux-dependent part of the variance $\Sigma^2(\mu, \varphi)$ of the particle number in a grand
canonical ensemble. To calculate this quantity, let us write
\[
\Sigma^2(\mu, \varphi) = \lim_{E \to \infty} \sigma^2(E, \mu, \varphi) , \tag{5}
\]
with
\[
\sigma^2(E, \mu, \varphi) = \int_{\mu - E}^\mu d\epsilon \int_{\mu - E}^\mu d\epsilon' K_2(\epsilon, \epsilon', \varphi) , \tag{6}
\]
\[
K_2(\epsilon, \epsilon', \varphi) = \rho(\epsilon, \varphi) \rho(\epsilon', \varphi) - \rho(\epsilon, \varphi) \rho(\epsilon', \varphi) . \tag{7}
\]
Here $\rho(\epsilon, \varphi) = \sum_\alpha \delta(\epsilon - \epsilon_\alpha(\varphi))$ is the density of states for a given realization of
the disorder. (The $\epsilon_\alpha(\varphi)$ are the exact solutions of the Schrödinger equation for
fixed random potential.) Note that $\sigma^2(E, \mu, \varphi)$ is the variance of the number of
energy levels in an interval of width $E$ below the Fermi energy. Combining Eqs.\textsuperscript{4},\textsuperscript{5},\textsuperscript{6},\textsuperscript{7},
we obtain for the average canonical persistent current of non-interacting electrons
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(ignoring the contribution \( I_{gc}(\mu^*, \varphi) \), which is exponentially small in the diffusive regime)

\[
I(N, \varphi) \approx -\frac{e}{2} \frac{\Delta}{\hbar} \lim_{E \to \infty} \int_{\mu^*-E}^{\mu^*} d\epsilon \int_{\mu^*-E}^{\mu^*} d\epsilon' K_2(\epsilon, \epsilon', \varphi). \tag{8}
\]

This expression has been used in Refs. 10, 14, 15 to calculate the average persistent current. For the covariance function \( K_2(\epsilon, \epsilon', \varphi) \) these authors have substituted a perturbative approximation due to Altshuler and Shklovskii 16, which for a thin quasi one-dimensional ring (where diffusion is only possible along the circumference) is given by

\[
K_2(\epsilon, \epsilon', \varphi) \approx \frac{1}{2\pi^2} \sum_{k=-\infty}^{\infty} \frac{1}{[4\pi^2 E_c(k + 2\varphi)^2 - i(\epsilon - \epsilon') + \Gamma]^2} + \frac{1}{[4\pi^2 E_c k^2 - i(\epsilon - \epsilon') + \Gamma]^2}. \tag{9}
\]

The first term in the curly braces is due to the two-Cooperon diagram, while the second term is due to the two-Diffuson diagram 16. Here \( E_c \) is the Thouless energy 10, and \( \Gamma \) is a cutoff energy that has been introduced by hand into the non-interacting model. For non-interacting electrons non-perturbative effects due to higher-order terms give rise to contributions to \( \Gamma \) of the order of the average level spacing 17, 18.

In the presence of electron-electron interactions, \( \Gamma \) should take inelastic processes approximately into account 14. Eq. 9 is believed to be the dominant contribution to \( K_2 \) in the regime \( \Delta \lesssim |\epsilon - \epsilon'| \lesssim \hbar/\tau \), where \( \tau \) is the elastic lifetime.

It is tempting to substitute Eq. 9 into Eq. 8 and obtain in this way a simple analytic result for the average canonical persistent current 10, 14, 15. However, such a procedure is based on a hidden assumption, which apparently has not been noticed in the recent literature on persistent currents: In the derivation of Eq. 9 it is implicitly assumed that in the energy window of interest the energy-dependence of the average density of states can be neglected. On the other hand, according to Eq. 8 the limit \( E \to \infty \) has to be taken in order to obtain the physical persistent current, so that we need to know the function \( K_2(\epsilon, \epsilon', \varphi) \) for all energies \( \epsilon \) and \( \epsilon' \) below the Fermi energy. Obviously, in this regime the energy-dependence of the average density of states \( \rho(\epsilon, \varphi) \) cannot be ignored. Of course, if we proceed by performing the above substitution anyway, it is easy to show that (see Eq. 10 below)

\[
\frac{\partial}{\partial \varphi} \Sigma^2(\mu, \varphi) = \frac{\partial}{\partial \varphi} \sigma^2(E, \mu, \varphi), \quad \text{for all } E \gtrless E_c. \tag{10}
\]

Thus, at the first sight it seems that the limit \( E \to \infty \) in Eq. 8 is trivial and the above substitution is justified. However, this way of reasoning is clearly not self-consistent, because the result 10 depends via Eq. 9 on the assumption of a constant density of states. In this work we shall carefully examine this point numerically. Our main result is that for non-interacting electrons Eq. 10 is not correct, so that
the physical persistent current cannot be calculated by simply substituting the Altshuler-Shklovskii result into Eq.8. We also present a numerical test of Eq.9. In a three-dimensional system Altshuler-Shklovskii scaling has recently been reproduced numerically by Braun and Montambaux, but these authors examined only the flux-independent part of \( \sigma^2(E, \mu, \varphi) \).

Using the Lanczos method, we have numerically calculated the exact energy levels \( e_\alpha(\varphi) \) of the spinless nearest-neighbor tight-binding Anderson Hamiltonian with diagonal disorder. The site-diagonal random potentials are assumed to be box-distributed in the interval \([-w/2, w/2]\). The Aharonov-Bohm flux is taken into account by choosing flux-dependent hopping energies in the \( \pm x \)-directions, \( t_{\pm x} = t e^{\pm 2\pi i \varphi/N_x} \), where \( N_x \) is the number of lattice sites in the direction \( x \). For convenience, all energies will be measured in units of the hopping energy \( t \), i.e. we formally set \( t = 1 \). For a quasi one-dimensional ring with \( N_x = 20, N_y = N_z = 5 \) we found diffusive behavior for \( w = 2.5 \). However, in order to reduce the statistical errors so that even the flux-dependent part of \( \sigma^2(E, \mu, \varphi) \) can be resolved, it is necessary to average over an extremely large number (typically 20000) of statistically independent realizations of the random potential. Our calculations were performed with the help of a parallel code on a cluster of up to 30 work-stations.

Because the Altshuler-Shklovskii result is based on the assumption that in the energy window of interest the average density of states \( \rho(\epsilon, \varphi) \) can be approximated by a constant, it is important to choose the chemical potential \( \mu \) properly. In Fig.1 we show the numerical result for the average density of states for a typical set of parameters. Obviously \( \mu = -0.8 \) is a good choice, because then the Fermi energy

![Fig. 1. Average density of states for a 20 \times 5 \times 5 lattice. We used \( w = 2.5 \) and averaged over 20000 realizations of the disorder. Thick line: \( \varphi = 0 \); thin line: \( \varphi = 1/4 \). The inset shows part of the central regime on a larger scale, together with our choice of the chemical potential \( \mu = -0.8 \).]
lies on the right-hand side of a broad maximum, so that the width of the interval \([\mu - E, \mu]\) where \(p(\epsilon, \phi)\) can be approximated by a constant is as large as possible.

Next, let us test the Altshuler-Shklovskii prediction for the variance \(\sigma^2(E, \mu, \varphi)\) of the number of energy levels in an energy window of width \(E\) below the Fermi energy. For better comparison with the numerical results, it is convenient to expand the theoretical prediction for \(\sigma^2(E, \mu, \varphi)\) into a Fourier series. Substituting Eq. 9 into Eq. 6, we obtain

\[
\sigma^2(E, \mu, \varphi) = \sigma_0^2(\tilde{E}) + \sum_{m=1}^{\infty} \sigma_{2m}^2(\tilde{E}) \cos(4\pi m \varphi) ,
\]

where for \(m \geq 1\)

\[
\sigma_{2m}^2(\tilde{E}) = \frac{2}{\pi^2 m} \left\{ \exp \left[ -m \tilde{\Gamma}^{1/2} \right] - \exp \left[ - \frac{m}{\sqrt{2}} \left( \sqrt{E^2 + \tilde{\Gamma}^2} + \tilde{\Gamma} \right)^{1/2} \right] \times \cos \left[ \frac{m}{\sqrt{2}} \left( \sqrt{E^2 + \tilde{\Gamma}^2} - \tilde{\Gamma} \right)^{1/2} \right] \right\} ,
\]

and the flux average is

\[
\sigma_0^2(\tilde{E}) = \frac{2}{\pi^2} \left[ \frac{1}{\sqrt{2}} \left( \sqrt{E^2 + \tilde{\Gamma} + \tilde{\Gamma}} \right)^{1/2} - \tilde{\Gamma}^{1/2} \right] + \sum_{m=1}^{\infty} \sigma_{2m}^2(\tilde{E}) .
\]

Here \(\tilde{E} = E/E_c\), and \(\tilde{\Gamma} = \Gamma/E_c\). Note that \(E_c\) (and hence \(\tilde{E}\)) implicitly depends on \(\mu\). For \(\tilde{E} \gg 1\) \(\gg \tilde{\Gamma}\), Eqs. 12 and 13 reduce to

\[
\sigma_{2m}^2(\tilde{E}) \sim \frac{2}{\pi^2 m} \exp \left[ -m \tilde{\Gamma}^{1/2} \right] , \quad m = 1, 2, \ldots
\]

\[
\sigma_0^2(\tilde{E}) \sim \frac{\sqrt{2}}{\pi^2} \tilde{E}^{1/2} + \frac{2}{\pi^2} \ln[\tilde{\Gamma}^{-1/2}] .
\]

Hence, the higher harmonics \(\sigma_{2m}^2(\tilde{E})\) become independent of \(\tilde{E}\) as soon as \(\tilde{E} \gtrsim 1\), implying the validity of Eq. 14. Physically this means that the dominant contribution to the flux-dependent part of \(\sigma^2(E, \mu, \varphi)\) is due to states with energies in an interval of width \(E_c\) below the Fermi level. In Fig. 2 we show our numerical results for the flux-dependent part of \(\sigma^2(E, \mu, \varphi)\) for different values of \(\tilde{E} = E/E_c\). The flux-oscillations with a fundamental period of \(\phi_0/2\) are clearly visible, and the amplitude is in perfect agreement with the diagrammatic calculation based on the two-Cooperon diagram of Altshuler and Shklovskii. Note also that the amplitude of the flux modulation does not change when the energy \(E\) is increased beyond the Thouless energy. To the best of our knowledge, this is the first numerical confirmation that the flux-dependence of \(\sigma^2(E, \mu, \varphi)\) is indeed correctly described by the two-Cooperon diagram given in Ref. 14. Our numerical data for the flux-independent part \(\sigma^2(E, \mu, \varphi)\) is shown in Fig. 3. Although the overall quantitative
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Fig. 2. The variance $\sigma^2(E, \mu, \varphi)$ as function of $\varphi$ for different values of $\tilde{E} = E/E_c$ for $\mu = -0.8$ and $E_c = 0.01$. From bottom to top: $\tilde{E} = 1$; $\tilde{E} = 5$; $\tilde{E} = 15$; $\tilde{E} = 60$. The solid lines are theoretical curves according to Eq.12 with $\tilde{\Gamma} = 0$.55. We have chosen the flux-average $\sigma^2_0(\tilde{E})$ as a fitting parameter. See Fig.3 for a numerical calculation of $\sigma^2_0(\tilde{E})$.

Fig. 3. Flux average $\sigma^2_0$ of $\sigma^2(E, \mu, \varphi)$ as function of $\tilde{E} = E/E_c$. The parameters are chosen as in Figs.2 and 2. The solid line is the theoretical prediction 13 with $\tilde{\Gamma} = 0.55$. The
agreement is not as good as in the case of the flux-dependent part, the quasi-one-dimensional $\sqrt{E}$-behavior is clearly visible. It should be kept in mind, however, that the Altshuler-Shklovskii calculation is only valid for energies $E \lesssim \hbar/\tau$. Using simple second order perturbation theory, we estimate $\hbar/\tau \approx 0.5$ in the parameter regime relevant to the figures. With $E_c \approx 0.01$, the theoretical curve in Fig. 3 should be quantitatively accurate for $\tilde{E} \lesssim 50$.

The theoretical results [12, 15] have been derived under the assumption that in the energy interval of interest the average density of states can be approximated by a constant. The important question is now whether it is allowed to use the small-$E$ regime as a basis for the extrapolation of the flux-dependent part of $\sigma^2(E, \mu, \varphi)$ to $E \to \infty$. According to Eq. 8 this extrapolation is necessary to obtain the persistent current. Note that in Refs. 10, 14, 15 such a procedure is adopted without further comment. In Fig. 4 we have plotted our numerical result for the second harmonic $\sigma^2_2(\tilde{E})$ as function of energy. Although for sufficiently small $\tilde{E}$ we obtain excellent agreement with the theoretical result [12], at $\tilde{E} \approx 150$ the numerical data begin to deviate strongly from the theoretical curve. Note that this energy cannot be identified with $\hbar/(\tau E_c) \approx 50$ – instead, it is the energy scale where the average density of states (shown as dashed line in Fig. 3) starts to deviate significantly from its value at the Fermi energy. In contrast, according to the theoretical prediction [14] the non-zero harmonics $\sigma^2_{2m}(\tilde{E})$ should saturate for $\tilde{E} \gtrsim 1$, and nothing special should happen at $\tilde{E} = \hbar/(\tau E_c) \approx 50$. Indeed, at $\tilde{E} \approx 50$ our numerical result for $\sigma^2_2(\tilde{E})$ still agrees well with the theoretical prediction. However, as soon as the

![Fig. 4. Second Fourier component $\sigma^2_2$ of $\sigma^2(E, \mu, \varphi)$ as function of $\tilde{E}$. The parameters are chosen as in Figs. 1 and 2. The solid line is the theoretical prediction [12] with $\tilde{\Gamma} = 0.55$. The upper labels on the horizontal axis and the right vertical scale refer to the corresponding average density of states $\rho_\epsilon(\varphi)$ at $\varphi = 0$ (dashed line).](image-url)
average density of states deviates from its value at the Fermi energy, our numerical data in Fig.4 clearly disagree with the theoretical curve. We therefore conclude that the extrapolation of Eq.12 to $E \to \infty$ is not possible. Hence, at least for non-interacting electrons, the average persistent current cannot be calculated by simply substituting the Altshuler-Shklovskii result for $\sigma^2(E, \mu, \varphi)$ into the formula 8 and taking the limit $E \to \infty$ to obtain the variance $\Sigma^2(\mu, \varphi)$ of the total particle number. The physical reason is that $\Sigma^2(\mu, \varphi)$ depends on all energies $\epsilon_\alpha(\varphi) \leq \mu$. Because in the diffusive regime energy levels tend to repel each other, the fluctuations of energy levels $\epsilon_\alpha(\varphi)$ deep inside the Fermi sea induce also changes in the energy levels in the vicinity of the Fermi energy. Thus, the variance of the total particle number depends on the statistical properties of the entire spectrum below the Fermi energy, so that the energy-dependence of the density of states cannot be ignored.

Realistic models of non-interacting electrons certainly should have energy-dependent densities of states, so that for non-interacting electrons the flux-dependent part of the variance $\Sigma^2(\mu, \varphi)$ of the total particle number cannot be calculated from the Altshuler-Shklovskii diagram. In other words, in the absence of electron-electron interactions the second term in Eq.4 is not determined by the statistical properties of the spectrum in the vicinity of the Fermi energy. On the other hand, in the presence of electron-electron interactions we expect a completely different scenario: in this case Eq.11 should be at least qualitatively correct, because in an interacting many-body system weakly damped propagating quasi-particles exist only in the vicinity of the Fermi energy. But only quasi-particles that can propagate coherently around the ring can probe the sensitivity to twists in the boundary conditions (and thus contribute to the flux-dependence of the particle number variance), so that we expect that electron-electron interactions will eliminate the contribution from many-body states with energies deep inside the Fermi sea. In other words the difference $\overline{I(N, \varphi)} - I_{gc}(\mu^*, \varphi)$ in Eq.4 should be extremely sensitive to electron-electron interactions in the sense that only if the damping of the quasi-particles is taken into account, the flux-dependent part of $\Sigma^2(\mu^*, \varphi)$ is determined by the spectrum close to the Fermi energy (see Eq.10). In this sense the procedure adopted in Refs.10,14 was physically correct, although within a model of non-interacting electrons it cannot be justified. Note, however, in the presence of electron-electron interactions the contribution $\overline{I_{gc}(\mu^*, \varphi)}$ in Eq.4 is not negligible, and it is not clear whether the persistent current is still dominated by the difference between the canonical and the grand-canonical current.

We would like to emphasize that at this point the above scenario should be considered as a plausible hypothesis, which implicitly has also been made in Refs.14,15,15. We suspect that in an interacting many-body system the microscopic mechanism which eliminates contributions from states deep inside the Fermi sea is closely related to the phenomenological cutoff parameter $\Gamma$ in Eq.9. A perturbative calculation of $\Gamma$ in an interacting mesoscopic conductor has recently been reported by Blanter, but in the present context more accurate calculations are needed, which take also the energy-dependence of $\Gamma$ into account. Although we have
started from a model of non-interacting electrons, we have arrived at the problem of electron-electron interactions. We believe that a satisfactory and generally accepted solution of the long-standing persistent current problem will only be obtained if the role of electron-electron interactions in mesoscopic disordered conductors is more thoroughly understood.

To conclude, let us briefly summarize our main results: First of all, we have numerically confirmed that for a thin three-dimensional ring in the diffusive regime the variance \( \sigma^2(E, \mu, \varphi) \) of the number of energy levels in a small interval of width \( E \) can indeed be described by the perturbative expression derived by Altshuler and Shklovskii. Our second important result is the observation that for non-interacting electrons the flux-derivative \( \partial \Sigma^2(\mu, \varphi) / \partial \varphi \) of the variance of the total number of energy levels below the Fermi energy cannot be obtained from the Altshuler-Shklovskii expression for \( \sigma^2(E, \mu, \varphi) \). We have argued that electron-electron interaction should modify this result, but a microscopic proof of this conjecture requires a better understanding of dephasing in disordered mesoscopic conductors. We hope to come back to this point in a future publication.

Acknowledgements

This work was financially supported by the Deutsche Forschungsgemeinschaft (SFB 345). We would like to thank J. A. Holm for providing us with his “Master-Slave Implementation for Parallel Virtual Machines”, which was crucial to run our numerical simulation efficiently on a work-station cluster.

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\[
\left( \frac{\partial \varphi}{\partial N} \right)_\mu \approx \frac{\delta \varphi}{\delta N} \quad \text{and cancel the } \delta \varphi, \text{ we obtain } \delta N \approx -\left( \frac{\partial N}{\partial \mu} \right)_\varphi \delta \mu. \text{ The minus-sign is missed if one naively treats } \delta N \text{ and } \delta \mu \text{ as conventional differentials.}
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