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Persistent-current paramagnetism and spin-orbit interaction in mesoscopic rings

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The persistent currents in arrays of isolated mesoscopic metallic rings are shown by conventional diagrammatic analysis (within a noninteracting model) to retain their paramagnetic character even in the presence of strong spin-orbit interaction. It is also shown that this result is consistent with the nonperturbative one-dimensional results of Meir *et al.*, if these results are correctly applied to the canonical ensemble.

Recently, there has been considerable progress in our understanding of persistent currents[1] in arrays of isolated mesoscopic normal-metal rings penetrated by an Aharonov-Bohm (AB) flux. In such a system one measures the disorder-averaged current; this quantity was found theoretically to be exponentially small in the metallic limit when calculated at fixed chemical potential (i.e., in the grand canonical ensemble),[2] while neglecting electron-electron interactions. However, in an electrically isolated array the assumption of coupling to a particle bath is not realized, a point stressed by Bouchiat and Montambaux,[3] who argued for a nonvanishing *average* persistent current with flux period $h/2e$ in such fixed-number arrays. Subsequently, experimental work by Levy *et al.*[4] on such arrays *did* measure a persistent current with period $h/2e$. This stimulated several theoretical calculations which took into account both the effect of fixed particle number[5-7] and the effect of electron-electron interactions in the grand canonical ensemble.[8] Both sets of calculations find an average persistent current with period $h/2e$ which does not decay on the scale of the elastic mean free path. Although the magnitudes obtained due to the two effects differ, currently both calculations appear to predict magnitudes substantially smaller than that observed experimentally.[4]

One of the most striking results from the noninteracting calculation is that the low-field sign of the response is *paramagnetic* (in contrast to the bulk orbital magnetic response of a Fermi gas which is diamagnetic), signaling a qualitatively new magnetic phenomenon characteristic of *mesoscopic* metallic systems.[7] Levy *et al.*[4] tentatively attributed a diamagnetic sign to the experimentally measured effect (although they pointed out that this determination contained some ambiguity). They suggested that the diamagnetic sign was due to the influence of spin-orbit (SO) interaction (within the noninteracting theory). Their argument was based on an extension of the results of Meir *et al.*[9] who proved that for a strictly one-dimensional (1D) system in an AB geometry there exists a remarkable exact relationship between a problem with SO interaction and its "bare" version with no SO interaction. A naive application of this result predicts a sign reversal, as will be discussed below.

In the recent work by Altshuler, Gefen, and Imry[7] it was stated (but not shown) that for the many-channel case no sign reversal occurs due to SO interaction, but that the sign should change as the 1D limit is approached to be consistent with the results of Meir *et al.*[9] Such a nontrivial dependence on the channel number would be surprising and in contrast to other calculations (e.g., universal conductance fluctuations) in which the results of perturbation theory extrapolate smoothly to the 1D limit. Thus for several reasons it is particularly interesting to examine the effect of SO interaction on the average persistent current.

In this paper we first calculate the noninteracting average persistent current in the presence of SO interactions within the conventional diagrammatic approach and confirm the statement of Altshuler, Gefen, and Imry[7] that the sign remains paramagnetic. In the strong SO limit the magnitude is reduced by a factor of $\frac{1}{4}$, as are the universal conductance fluctuations and density of states fluctuations.[10] We then provide a brief rederivation of the results of Meir *et al.* and note that the simple relationship they derived between expectation values of a system with and without SO interaction only holds for certain *grand canonical* expectation values. We show that their approach leads to a more complicated relationship between the canonical persistent current with and without SO interaction. We then demonstrate that this relationship implies a paramagnetic persistent current in the metallic regime.

We begin by reviewing the calculation of the fixed number persistent current for noninteracting spinless electrons in a disordered ring at $T=0$ threaded by an AB flux. In a crucial advance, Imry[11] has shown that the expectation value at a fixed number can be related approximately to expectation values at fixed chemical potential, and this allows one to write[5,7] the leading contribution to the persistent current as

$$I_N(\phi)=\frac{-e}{4\pi\langle\rho(E_f)\rangle}\frac{\partial}{\partial\phi}\times\int_{-\infty}^{E_f}dE\int_{-\infty}^{E_f}dE'\langle\delta\rho_\phi(E)\delta\rho_\phi(E')\rangle\,, \qquad (1)$$

where $\langle\cdots\rangle$ denotes an average over disorder, $\rho_\phi(E)$ is the density of states (which is a function of flux), $\delta\rho_\phi(E)=\rho_\phi(E)-\langle\rho_\phi(E)\rangle$, and E_f is the disorder averaged chemical potential.

The leading contribution to the density-of-states correlation function in (1) comes from diagrams of the type shown in Fig. 1(a). We apply hard-wall boundary conditions in the transverse direction and periodic boundary

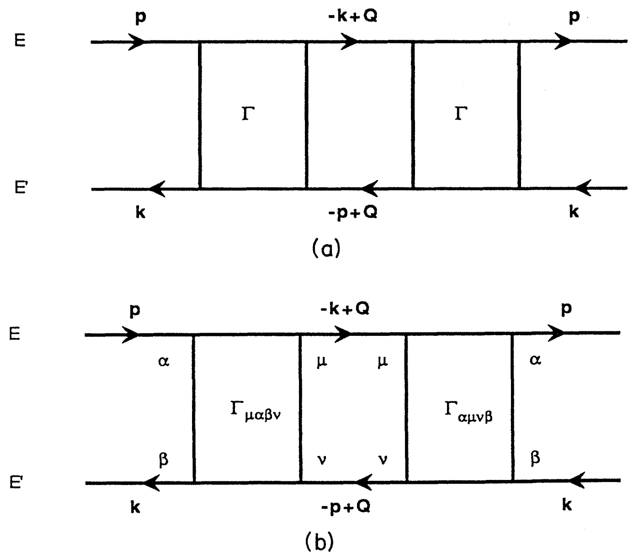

FIG. 1. Leading contribution to the density-of-states correlation. A summation over the external momenta and spin indices is implicit. $\Gamma(Q)$ denotes the cooperon.

conditions around the circumference of the ring. The presence of the AB flux through the loop is then incorporated into the longitudinal boundary conditions so that the momentum vectors **k** and **p** are vectors of the type $[2\pi(n_x-\phi)/L, \pi n_y/L_y, \pi n_z/L_z]$, where L denotes the circumference of the ring, L_y and L_z are the cross-section dimensions, n_x,n_y,n_z are integers, and ϕ is the flux in units of h/e. It follows from the fact that the Cooper pole involves the sum of the two external momenta that the longitudinal x component of **Q** is of the type $2\pi(m-2\phi)/L$, where m is an integer.

In evaluating the diagrams one can ignore the flux dependence of **k** and **p** and perform these sums by replacing them by integrals which yield

$$\langle\delta\rho_\phi(E)\delta\rho_\phi(E')\rangle \simeq \frac{1}{2\pi^2}\sum_Q \mathrm{Re}\{1/[i(E'-E)+\gamma+DQ^2]^2\}, \quad (2)$$

where $\gamma=1/\tau_{\rm in}$ is the inelastic-scattering rate. The entire flux dependence of the right-hand side is contained in **Q**, and period halving follows from $Q_x=2\pi(m-2\phi)/L$. One cannot replace the **Q** summation by an integration due to its singular nature, so further evaluation is facilitated by the identity

$$\frac{1}{L}\sum_{q\in 2\pi(m-2\phi)/L} A(q)=\sum_r\int\frac{dq}{2\pi}\exp(i4\pi r\phi)\times\exp(iqrL)A(q). \quad (3)$$

Inserting (2) in (1) and using (3), one obtains after some work

$$I_N(\phi)=\frac{ev_f}{L}\frac{1}{\pi M}\sum_{r>0}\sin(4\pi r\phi)\exp\left(-\frac{rL}{L_{\rm in}}\right). \quad (4)$$

Here M denotes k_f^2A/π, the number of transverse channels.

We now introduce SO interaction into the calculation. The leading contribution to $\langle\delta\rho_\phi^{\rm SO}(E)\delta\rho_\phi^{\rm SO}(E')\rangle$ comes from the diagrams in Fig. 1(b). As usual,[12] we introduce the total-spin-representation cooperon which is defined through

$$\Gamma_{\alpha\beta\gamma\delta}=\sum_{J,m}C_{\alpha\gamma}^{Jm*}C_{\beta\delta}^{Jm}\Gamma_{Jm}, \quad (5)$$

where $C_{\beta\delta}^{Jm}$ are the Clebsch-Gordan coefficients. Using the property

$$\sum_{\alpha,\rho}C_{\alpha\rho}^{Jm*}C_{\alpha\rho}^{J'm'}=\delta_{JJ'}\delta_{mm'} \quad (6)$$

we are able to decompose the contribution of Fig. 1(b) into a sum over the four total-spin channels.

We thus obtain

$$\langle\rho_\phi^{\rm SO}(E)\rho_\phi^{\rm SO}(E')\rangle \simeq \frac{1}{2\pi^2}\sum_Q \mathrm{Re}\{1/[i(E'-E)+\gamma+DQ^2]^2\} + \frac{3}{2\pi^2}\sum_Q \mathrm{Re}\{1/[i(E'-E)+\gamma+4/3\tau_{\rm SO}+DQ^2]^2\}. \quad (7)$$

The first term in (7) is due to the singlet channel, the second is due to the three triplet channels. Introduce the definition $L_{\rm SO}\equiv(3\tau_{\rm SO}D/4)^{1/2}$. Comparison of (7) and (2) shows that, as usual, SO interaction only introduces a modified cutoff in the triplet channel whose contribution can then be evaluated by simple transcription in Eq. (4). For the strong SO limit ($L_{\rm in}\gg L\gg L_{\rm SO}$) the cutoff length is $\approx L_{\rm SO}$ for the triplet channels and $L_{\rm in}$ for the singlet channel; hence we obtain

$$I_N^{\rm SO}(\phi)=\frac{ev_f}{L}\frac{1}{2\pi M}\sum_{r>0}\sin(4\pi r\phi)\exp\left(-\frac{rL}{L_{\rm in}}\right) + \frac{3ev_f}{L}\frac{1}{2\pi M}\sum_{r>0}\sin(4\pi r\phi)\exp\left(-\frac{rL}{L_{\rm SO}}\right). \quad (8)$$

Since in the strong SO limit the second term in (8) is exponentially smaller than the first, the presence of strong SO scattering is seen to reduce the persistent current magnitude by a factor of $\frac{1}{4}$, but does not change the sign.

We now discuss the relationship of these results to those of Meir *et al.* In this discussion we will only consider the same contribution to the persistent current as treated above, although other contributions may be important in an exactly 1D system. For a 1D (single-channel) system Meir *et al.* have shown rigorously that the energy eigenvalues of the system with SO at flux ϕ are the same as those of two spinless systems with the same spatial disorder and flux $\phi\pm\lambda$, where λ is a measure of the SO interaction. For completeness and clarity, we rederive this result in a way that exhibits more explicitly the relationship between the wave functions of the SO problem and its bare version.

Consider a single-orbital tight-binding model with two states at each site $|n,\sigma\rangle$, distinguished by their spin z eigenvalue $\sigma=\pm1$. Because we are dealing with an N-site ring threaded by an AB flux, the relationship between the states at sites 1 and $N+1$ is

$$|1,\sigma\rangle=\exp(-i2\pi\phi)|N+1,\sigma\rangle. \quad (9)$$

The Hamiltonian is

$$H=\sum_{n,\sigma}\varepsilon_n|n,\sigma\rangle\langle n,\sigma| + \sum_{n,\sigma,\sigma'} t_n(S_n)_{\sigma\sigma'}|n,\sigma\rangle\langle n+1,\sigma'|+\text{H.c.} \quad (10)$$

Here t_n is real and S_n is an SU(2) matrix.

It is useful to introduce new states $|n,\alpha\rangle$ ($\alpha=\pm 1$) at each site by performing site-dependent rotations in spin space:

$$|n,\sigma\rangle=\sum_{\alpha}|n,\alpha\rangle U^{(n)}_{\alpha\sigma}\,. \quad (11)$$

We choose

$$U^{(n)}=U^{(1)}S_1\cdots S_{n-1}\,, \quad (12)$$

which fixes all the U's in terms of an arbitrary $U^{(1)}$. The relation between the states at site 1 and site $N+1$ is

$$|1,\alpha\rangle=\sum_{\alpha'}|N+1,\alpha'\rangle\exp(-i2\pi\phi)(U^{(1)}S_1\cdots S_N U^{(1)\dagger})_{\alpha'\alpha}\,. \quad (13)$$

We may now choose $U^{(1)}$ to be the diagonalizing matrix for the product $S_1\cdots S_N$, which then yields

$$|1,\alpha\rangle=\exp[-i2\pi(\phi+\alpha\lambda)]|N+1,\alpha\rangle\,, \quad (14)$$

where $\exp(-i2\pi\alpha\lambda)$ are the eigenvalues of $S_1\cdots S_N$. This relation between the states at sites 1 and $N+1$ is exactly as would hold in the spinless case if our system were threaded by a flux $\phi\pm\lambda$ [remember that $\alpha=\pm 1$, cf. Eq. (9)].

Using Eqs. (11) and (12) we can rewrite the Hamiltonian (10) in terms of the new states as

$$H=\sum_{n,\alpha}\varepsilon_n|n,\alpha\rangle\langle n,\alpha|+\sum_{n,\alpha}t_n|n,\alpha\rangle\langle n+1,\alpha|+\text{H.c.}\,, \quad (15)$$

which is diagonal in spin. It follows that the energy eigenvalues are exactly those for the spinless system at $\phi\pm\lambda$. This completes the derivation.

The relationship between the wave functions of the bare and SO interacting problems is seen to be

$$\psi_\alpha(n)=\sum_{\sigma}U^{(n)}_{\alpha\sigma}\psi_\sigma(n)\,. \quad (16)$$

Generalized gauge transformations of this type often arise in problems treated in an adiabatic approximation.[13] Usually one finds a vector potential type interaction in the alternative gauge, which is expressed in this case through the spin-dependent effective flux λ; however, in this case the appearance of an effective gauge potential involves no approximation.

The above results imply

$$\rho^{\text{SO}}_\phi(E)=\rho_{\phi+\lambda}(E)+\rho_{\phi-\lambda}(E)\,, \quad (17)$$

where $\rho_\phi(E)$ is the spinless density of states. This has the obvious implication for the grand canonical average of spin-independent one-particle operators $Q(E)$ that

$$\overline{Q^{\text{SO}}(\phi)}\equiv\int_{-\infty}^{\infty}dE\,Q(E)f(E)\rho^{\text{SO}}_\phi(E) =\overline{Q(\phi+\lambda)}+\overline{Q(\phi-\lambda)}\,, \quad (18)$$

where $\overline{Q}$ denotes the grand canonical average for the bare spinless problem. A naive application of this result to the canonical persistent current would imply that the persistent current with SO interaction is given by Eq. (4) with an additional factor of $\langle\cos(4\pi r\lambda)\rangle_{\text{SO}}$ multiplying the summand. Here $\langle\cdots\rangle_{\text{SO}}$ denotes an appropriate average over the phase shift λ induced by the SO interaction; this average for the first harmonic in the strong SO limit is evaluated in Ref. 9, giving $\langle\cos(4\pi\lambda)\rangle_{\text{SO}}=-\frac{1}{2}$. Thus, as mentioned above, uncritical application of Eq. (18) would predict a diamagnetic persistent current in the stong SO limit. Note, however, that Eq. (18) does not hold for *two-body* operators and since the fixed number persistent current calculated in Refs. 5 and 7 depends on the density of states ρ^{SO}_ϕ quadratically, it need not satisfy Eq. (18). Hence the question of its sign remains to be determined in this approach.

This contribution to the persistent current is determined by the density-of-states correlation function defined in Eq. (1). Using Eq. (17) we now find

$$\langle\delta\rho^{\text{SO}}_\phi(E)\delta\rho^{\text{SO}}_\phi(E')\rangle=\langle\delta\rho_{\phi+\lambda}(E)\delta\rho_{\phi+\lambda}(E')\rangle+\langle\delta\rho_{\phi-\lambda}(E)\delta\rho_{\phi-\lambda}(E')\rangle+\langle\delta\rho_{\phi+\lambda}(E)\delta\rho_{\phi-\lambda}(E')\rangle+\langle\delta\rho_{\phi-\lambda}(E)\delta\rho_{\phi+\lambda}(E')\rangle\,, \quad (19)$$

where $\langle\cdots\rangle$ now denotes an average over spatial disorder only.

The first two terms are the sum of the spinless density-of-states correlations at flux $\phi+\lambda$ and $\phi-\lambda$ in accord with Eq. (18), however, the two additional cross terms are nonvanishing and we now show that these terms give rise to contributions whose flux dependence is not shifted by λ.

Using the harmonic expansion for the density of states $\delta\rho_\phi(E)=\sum_n a_n(E)\cos(2\pi n\phi)$,

$$\langle\delta\rho_{\phi+\lambda}(E)\delta\rho_{\phi-\lambda}(E')\rangle=\sum_{n,m}\langle a_n(E)a_m(E')\rangle\cos[(2\pi n)(\phi+\lambda)]\cos[(2\pi m)(\phi-\lambda)]\,. \quad (20)$$

We expect $\langle a_n(E)a_m(E')\rangle=\delta_{mn}C_n(E-E')$, since, e.g., semiclassically the amplitude $a_n(E)$ is determined by classical paths that wind around the ring n times and its disorder average must vanish due to the arbitrary relative phase of distinct classical paths.

Thus with some rearrangement

$$\langle\delta\rho_{\phi+\lambda}(E)\delta\rho_{\phi-\lambda}(E')\rangle=\sum_{n}\langle a_n(E)a_n(E')\rangle\left[\frac{\cos(4\pi n\lambda)}{2}+\frac{\cos(4\pi n\phi)}{2}\right]. \quad (21)$$

Thus the flux-dependent part of these terms is independent of λ. By comparison to Eq. (20) with $\lambda=0$ we see that it is identical to the flux-dependent part of the spinless $\langle\delta\rho_\phi(E)\delta\rho_\phi(E')\rangle$, and so must give the same contribution to the persistent current. Hence

$$I_{1D}^{SO}(\phi)=\tfrac{1}{2}[I_{1D}^{0}(\phi+\lambda)+I_{1D}^{0}(\phi-\lambda)+2I_{1D}^{0}(\phi)]\,, \qquad (22)$$

where the factor of $\frac{1}{2}$ arises because $\langle\rho^{SO}(E_f)\rangle=2\langle\rho(E_f)\rangle$, the subscript denotes that the relationship is only exact in 1D, and the superscript 0 denotes the spinless persistent current. Hence we see explicitly that the persistent current does not satisfy a relation of the form of Eq. (18).

We may confirm diagrammatically that the cross terms in Eq. (19) are independent of λ. In particular, for such terms the longitudinal component of **k** is of the type $2\pi(n_x-\phi-\lambda)/L$, the longitudinal component of **p** is of the type $2\pi(n_x-\phi+\lambda)/L$. Thus Q_x is of the type $2\pi(m-2\phi)/L$; i.e., the shift of the flux by the parameter λ has canceled in the cooperon just as we found in the more general argument above. Clearly then the third and fourth terms in Eq. (19) are equal and yield the persistent current at flux ϕ. Since perturbation theory is not valid in the exactly 1D case and other contributions may appear in this limit, we only use the diagrammatic argument in the 1D case as a consistency check of our general result in Eq. (22). The metal rings of experimental interest have 10^4–10^5 transverse channels and are far from the exactly 1D limit, so our earlier diagrammatic result should be quantitatively correct (within the models of Refs. 5–7).

From Eq. (22) it is straightforward to derive the factor of $\frac{1}{4}$ reduction of the 1D persistent current based on the approach of Meir *et al.* We know that the spinless persistent current is periodic with fundamental $h/2e$ so that $I_{1D}^{0}(\phi)=\sum_n i_n\cos(4\pi n\phi)$, hence

$$\begin{aligned}I_{1D}^{0}(\phi+\lambda)+I_{1D}^{0}(\phi-\lambda)&=\sum_n i_n\{\cos[(4\pi n)(\phi+\lambda)]+\cos[(4\pi m)(\phi-\lambda)]\}\\&=2\sum_n i_n\cos(4\pi n\phi)\cos(4\pi n\lambda)\,.\end{aligned} \qquad (23)$$

As noted above, in the strong SO limit the average over λ of the factor $\cos(4\pi\lambda)$ equals $-\frac{1}{2}$. Hence averaging over λ in Eq. (22) yields for the fundamental of the persistent current $I_{1D}^{SO}=\frac{1}{2}I_{1D}^{0}=\frac{1}{4}2I_{1D}^{0}$. Remembering that the persistent current with spin but without SO scattering is twice the spinless persistent current, we see that we have recovered from the approach of Meir *et al.* the factor of $\frac{1}{4}$ reduction due to strong SO scattering for the $h/2e$ periodic contribution. Since higher harmonics undergo different reduction factors in the approach of Meir *et al.* and not in the perturbative approach, there still remains a minor discrepancy between diagrammatic calculations and the results of Ref. 9. Nonetheless, we have shown that the 1D results of Meir *et al.* are consistent with the result derived above for the many-channel case that the mesoscopic orbital magnetic response is always paramagnetic, even in the presence of strong SO interaction.

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[1]M. Buttiker, Y. Imry, and R. Landauer, Phys. Lett. **96A**, 365 (1983).

[2]H.F. Cheung, E. K. Riedel, and Y. Gefen, Phys. Rev. Lett. **62**, 587 (1989).

[3]H. Bouchiat and G. Montambaux, J. Phys. (Paris) **50**, 2695 (1989).

[4]L. P. Levy, G. Dolan, J. Dunsmuir, and H. Bouchiat, Phys. Rev. Lett. **64**, 2094 (1990).

[5]A. Schmid, Phys. Rev. Lett. **66**, 80 (1991).

[6]F. von Oppen and E. Riedel, Phys. Rev. Lett. **66**, 84 (1991).

[7]B. L. Altshuler, Y. Gefen, and Y. Imry, Phys. Rev. Lett. **66**, 88 (1991).

[8]V. Ambegaokar and U. Eckern, Phys. Rev. Lett. **65**, 381 (1990).

[9]Y. Meir, Y. Gefen, and O. Entin-Wohlman, Phys. Rev. Lett. **63**, 798 (1989).

[10]B. L. Altshuler and B. I. Shklovskii, Zh. Eksp. Teor. Fiz. **91**, 220 (1986) [Sov. Phys. JETP **64**, 127 (1986)].

[11]Y. Imry, in *Quantum Coherence in Mesoscopic Systems*, edited by B. Kramer (Plenum, New York, in press).

[12]G. Bergmann, Phys. Rep. **107**, 1 (1984).

[13]M. V. Berry, Proc. R. Soc. London, Ser. A **392**, 45 (1984). For a possible mesoscopic application, see D. Loss, P. Goldbart, and A. V. Balatsky, Phys. Rev. Lett. **65**, 1655 (1990).