

Persistent current in isolated mesoscopic rings

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The persistent current in isolated mesoscopic rings is studied using the continuum and tight-binding models of independent electrons. The calculation is performed with disorder and also at finite temperature. In the absence of disorder and at zero temperature agreement is obtained with earlier results by Loss and Goldbart in that there is half-quantum flux periodicity for a large and odd number of electrons, but full-quantum periodicity for any even number of electrons in the ring. Strong disorder converts the period into full-quantum periodicity. Finite temperature reduces the magnitude of the current, but preserves the quantum flux periodicity at zero temperature. However, the sign of the current may change as disorder or temperature is increased. A generalization of the parity effect, previously discussed by Leggett, Loss, and Kusmartsev is described for the case where there are electrons with spin, influenced by finite temperature and disorder.

I. INTRODUCTION

Since the early work by Byers and Yang,¹ Kohn,² Bloch,³ Gunther and Imry,⁴ Kulik,⁵ Büttiker and co-workers,^{6,7} and Refs. 8–12, it has been realized that spinless electrons do not lead to the same current as electrons with spin, due to Fermi statistics. In reality the results that were originally obtained, presumably for any number of electrons, apply only to the cases of even number of electrons; or to the case of a single electron. It was realized that there are four separate cases to be analyzed, in which the number N of electrons on the ring can take the values $N=4n$, $4n+1$, $4n+2$, and $4n+3$, where $n=0,1,2,3,\dots$. This situation was discussed by Kusmartsev¹³ and calculations of the current are found in Loss and Goldbart.¹⁴ Based on this information, a more modern treatment of the current in rings requires adding disorder or using finite temperature. In particular it was realized by Loss and Goldbart¹⁴ that in an ordered ring with a large enough odd number of electrons, the persistent current shows almost perfect half-quantum flux periodicity rather than the full-quantum flux periodicity of spinless electrons. This result follows simply from the Fermi statistics for electrons with spin.

The behavior of rings can be studied either for isolated rings or for rings with leads. In the first case the number of electrons must be a constant, while in the second case electrons may be lost or gained through the leads. In the first case the chemical potential is a function of flux, cal-

culated with $\sum_{n\alpha} f(E_{n\alpha})=N$ where the sum is over energy levels and spins. Since the energy levels depend on flux, so does the chemical potential. In the case of a ring with leads, the chemical potential is imposed from the outside, and must be considered a constant. Electrons are then lost or gained through the leads, as with the increase of the flux the appropriate levels cross the fixed chemical potential. Therefore, the kind of averaging that is required depends on the physical condition of the rings, whether they are isolated or not. This work deals with isolated rings, without inelastic scattering.

Investigation of the influence of the spin degrees of freedom on the Aharonov-Bohm effect is also especially important if spin-orbit interaction is taken into account.¹⁵ This creates extra quasi-half-quantum flux-periodicity effects. It is well known that such interaction plays a major role in semiconductors, when electrons or holes interact with a magnetic field. Instead of paramagnetic resonance, we have the so-called combined resonance (Rashba effect). The orbital moments or orbital currents on the ring, which change in the magnetic field, may also cause spin-flip processes,¹⁶ via the spin-orbit interaction. However, we do not carry out such spin-orbit calculations here, and neglect Zeeman splitting, which is a very small effect for the fields of interest.

II. METHODS OF CALCULATION

We consider a system of N noninteracting electrons of mass m on a one-dimensional ring of length L , threaded

by a magnetic flux ϕ . The Hamiltonian of the system is given as

$$H = \frac{1}{2m} \left[-i\hbar \frac{\partial}{\partial x} + eA \right]^2 \rightarrow \frac{\hbar^2}{2m} \sum_{\substack{\alpha=1 \\ \sigma=\pm}}^N \left[-i \frac{\partial}{\partial x_\alpha} - \frac{2\pi}{L} f \right]^2, \quad (1)$$

where x_α is the coordinate of the α th electron of spin σ along the ring, starting from some origin $f = \Phi/\Phi_0$, Φ_0 is the quantum flux h/e , and Φ is the total magnetic flux through the ring. Using the wave function

$$\psi(x) = A e^{ikx} e^{i(x/L)2\pi f},$$

and the boundary condition coming from the uniqueness of the wave function, $\psi(x) = \psi(x+L)$, one obtains the single-particle energy levels,

$$E_{n\sigma} = \frac{\hbar^2}{L^2} \frac{4\pi^2}{2m} [n+f]^2, \quad (2)$$

where $n = 0, \pm 1, \pm 2, \dots$.

Since these levels are periodic in flux, with period Φ_0 , the early presumption was that current, magnetization, and other properties necessarily be periodic functions with period Φ_0 . While this is true, one cannot exclude the possibility of periodicities with smaller period due to other reasons, for example, electron-electron interaction.

For more than one electron there may be a redistribution of electrons in the energy levels, to gain the lowest ground-state energy, when there are degenerate level crossings. For example, one can place two electrons in the state $n=0$. If there is a total of three electrons, the third electron, for $f \sim 0$, can be placed in either the $n=1$ state or the $n=-1$ state, depending on whether f is infinitesimally negative or positive. These rearrangements, when permitted by Fermi statistics, lead to discontinuous jumps in the current, with changes of sign. Repeating the analysis for the cases $N=4n, 4n+1, 4n+2, 4n+3$ leads to the results given in Ref. 14.

For odd numbers of electrons it is seen that there is an approximate half-quantum flux periodicity, which however improves as the number of electrons increases. For even number of electrons there is full-quantum flux periodicity. These two cases taken along reproduce the original results obtained for spinless electrons.

The total current from all occupied levels at $T=0$ is given by $I = \sum_n I_n$, where the sum is over occupied levels of spin states. Note that the main contribution to the sum is always from an electron located in the uppermost level. If $T \neq 0$ it is first necessary to calculate the chemical potential at each flux value, as described in the Introduction. Thereafter the $T \neq 0$ result can be found from

$$I = \sum_{\alpha} I_{n\sigma} f(E_{n\alpha}),$$

where $I_{n\sigma}$ are the different current contributions and $f(E_{n\sigma})$ is the Fermi function, which is determined after the chemical potential is calculated. The sum over states is taken until there is a negligible remaining contribution. For the excited states there is greater freedom of redistri-

buting electrons among levels. Since higher levels contribute to opposite signs of the current one can ask whether there are possible changes of sign. The periodicity of the chemical potential, which is that of one flux quantum, also influences the results.

Disorder is introduced in the tight-binding formulation in the form of the usual Anderson-type model, for single-site energies along the rings, with hopping parameter t . Thus there is disorder taken from uniform distribution of energies in $[-W/2, W/2]$. Flux is introduced in the usual way by multiplying the hopping parameters by a phase factor $e^{i\phi}$ for anticlockwise motion or by $e^{-i\phi}$ for clockwise motion along the ring, where $\phi = (2\pi/N)f$.

Current can be calculated either from the slope of the eigenvalues as a function of flux, in the usual way; or from (see Refs. 17,18).

$$I_m = \left[\frac{2ae}{\hbar} \right] \text{Im}(C_{n,\sigma}^{*(m)} C_{n-1,\sigma}^{(m)} H_{n,n-1}) \\ = \frac{2ae}{\hbar} \text{Im}(C_{n,\sigma}^* C_{n-1,\sigma} t e^{-i\phi}), \quad (3)$$

where $a = L/N$ is the lattice constant.

This expression is actually independent of site number n . The $C_{n,\sigma}^{(m)}$ are the normalized eigenvectors of the diagonalized Hermitian matrix representing the Hamiltonian for the m th state and n th site and spin σ .

Both methods are equivalent, but the slope method is more commonly used, since eigenvalues are determined more accurately. For the zero-temperature calculation, at each separate flux the energy levels must be filled with a fixed number of electrons, starting from the bottom, according to Fermi statistics, to get the total current from the individual currents of the separate levels. This procedure guarantees that the ground state is always achieved, with readjustments in the level filling at degeneracies described earlier, thus avoiding a common mistake.

It has been shown that the half-quantum flux period arises by averaging over many rings in situations in which there is only single-quantum flux periodicity for single rings. Montambaux and co-workers^{19,20} average over an ensemble of rings having different numbers of electrons to get the half-quantum flux period. We also find that this is a good method to obtain half-flux-quantum periodicity. Averaging over the four separate cases $N=4n, 4n+1, 4n+2, 4n+3$ is one way to accomplish this periodicity, even without disorder. The most realistic way to average is, however, to keep the number of electrons constant. For strong disorder the sign of the current is sample dependent and cannot be predicted for a single ring, but will have a period of just one flux quantum. The emergence of the half flux quantum on averaging is due to the random phase ($N \gg \Delta N$, where ΔN is the width of the distribution.)

III. RESULTS AND DISCUSSION

For both disorder and finite temperature one finds that regions near $f=0$ and $f=\frac{1}{2}$ have degenerate level crossings. The latter are very sensitive to various physical

effects. In these regions, instead of sudden jumps, the current will become a continuous function of flux, passing through zero, as soon as there is finite disorder or temperature.

We have noted earlier that for a small odd number of electrons the current is only a quasi-half-periodic function of flux, with a slightly asymmetric shape. For five electrons the current vanishes at $f=0.2$ instead of $f=0.25$, for example.

When the ring is disordered, the current changes to a full-quantum flux periodicity Φ_0 as shown in Fig. 1. For a small number of odd electrons the phase of the Φ_0 period has a definite sign, to accommodate the direction of the largest current that one obtains in the ordered case. For a larger odd number of electrons one cannot predict *a priori* the phase of the cycle. Note that the quasi-half-quantum flux period has disappeared when disorder is added, for individual rings. This behavior is similar to that found in simulations on rings with or without leads,¹⁻¹² with independent electrons.

Let us note that on a single ring, at fixed value of flux, the direction of the current changes upon adding one

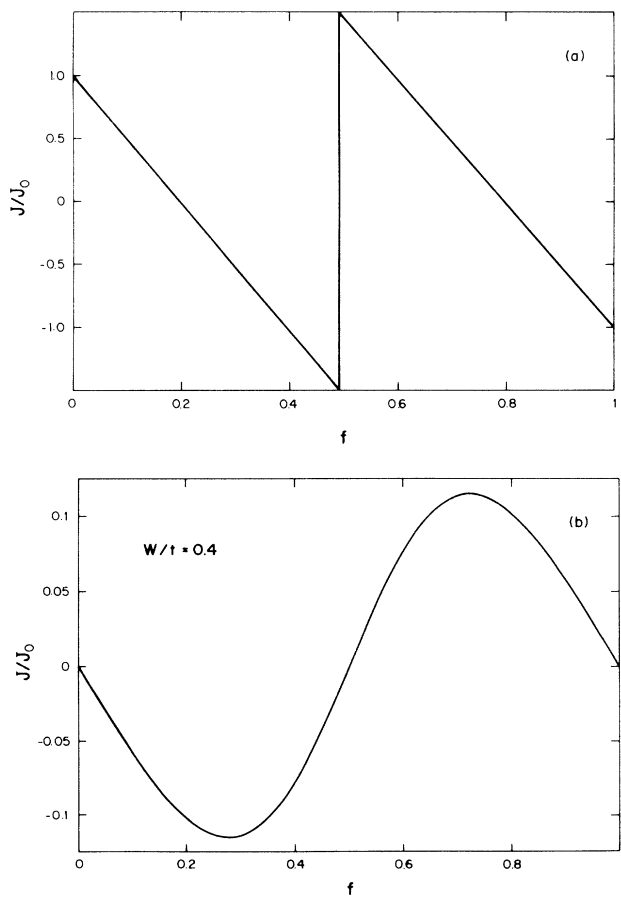


FIG. 1. Persistent current for (a) ordered and (b) disordered rings with five electrons and 40 sites. In the ordered case, the current vanishes at $f=0.20$ rather than $f=0.25$. For the disordered case, a parameter $W=0.4t$ was used, with the Anderson model. Note the change in sign of the current for some values of flux. With disorder the quasi-half-quantum-flux period has disappeared.

electron. The uppermost level plays the main role in determining the direction and sign of the current. Therefore one expects that processes which move an electron from one level to another can change the sign of the current. Such situations may arise with finite temperature, or disorder. For finite temperature there will be an activation energy $\Delta E \sim T$ for the process. The upper level has less occupation, but if the difference of current for a single electron transferred is large enough, there will be changes of sign. Similarly, it is clear that disorder may play a similar role, where one has fluctuations in the internal potential instead of temperature fluctuations.

The finite-temperature results are shown in Figs. 2(a) and 2(b), both as a function of flux f (for a fixed temperature) and as a function of βt for a particular value of f . The results show how the current changes, but the shape is preserved, and how there is a change of sign as the temperature is increased. This change of sign occurs

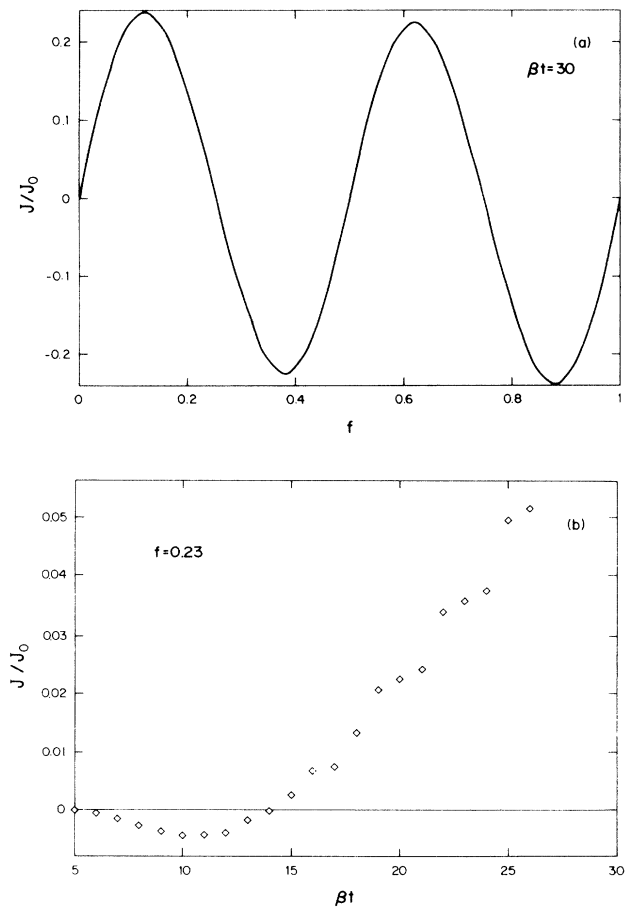


FIG. 2. (a) Current at a fixed finite temperature ($\beta t = 30$) as a function of flux, for an isolated ring of 41 electrons and 40 sites. The current is zero at degenerate level-crossing points $f=0$ and $f=\frac{1}{2}$. Additionally, the periodicity of $\frac{1}{2}$ flux quantum for the zero-temperature ordered chain is maintained. (b) Current as a function of temperature (βt variable) for a fixed value of flux ($f=0.23$). A change of sign is seen at high temperature, in the region in which the current is small. The change in sign is due to excitation to higher levels, which carry current of the opposite sign. Additional structure due to the discreteness of levels is also seen, which is smoothed out at higher temperature.

when the current is already rather small. Also, we neglect inelastic events in the calculation. However, this change of sign may perhaps be subject to experimental observation; detailed temperature studies for isolated individual rings are still lacking. In the limit of low temperature, Fig. 2(b) shows a fine step structure. We believe that this structure reflects the discreteness of the energy levels for these small systems. The structure disappears at higher temperatures.

Let us now see how we can reconcile some of the results with experiment. Recent experiments²¹ have detected only the full-quantum period in the case of individual rings.

The easiest way to understand this is either

- (a) that only individual independent single electrons (i.e., the one-electron case) contribute to the result; or
- (b) that the individual rings are sufficiently disordered to show only the full-quantum periodicity.

Averaging over the four cases indicated immediately gives the $\Phi_0/2$ period. This interpretation is then natural for the experimental results concerning many rings.²² It is interesting to note also that in the ordered limit the cases with even numbers of electrons carry a greater current than cases with odd numbers of electrons. Where the original problem had been to explain $\Phi_0/2$ periodicity, it seems that now there are too many ways to get it. The problem now seems to be why the Φ_0 period is seen in individual rings.

Recently it has been argued that correlations, being important, cannot be ignored. Note that for the spinless fermions the correlations do not destroy the parity effect, as was shown by Kuzmartsev,^{23,24} with the aid of the Bethe ansatz for the limit of strong interactions. This was generalized by Leggett²⁵ and proved by Loss²⁶ with the aid of the bosonisation method for arbitrary coupling.

For the case of electrons with spin, the problem is that these correlations easily destroy the parity effect and create the half-quantum period,^{27,28} or more generally the fractional Φ_0/N periodicity for N electrons as shown in Ref. 29 and confirmed in other studies.³⁰ Recently, we have found that this fractional Aharonov-Bohm effect may exist for any coupling in dilute systems.³¹ Why these effects are not yet seen in individual rings remains an open problem. Correlations are just one extra factor to be considered, but so is the problem of multiple channels expected for rings of finite cross section.

However, for a ring of noninteracting electrons with spin, in the presence of just weak disorder, parity effects may exist for a small number of electrons and have the characteristics which we describe. This effect is relevant to the phenomenon of directional changes of the persistent current with temperature. For strong disorder the direction of the current cannot be predicted and is essentially random and sample dependent for individual rings. Parity effects are then seemingly inconsequential in this limit, but the situation is further discussed in detail below.

IV. DOUBLE-PARITY EFFECT

The essence of the parity effect for spinless interacting fermions lies in the Fermi statistics.²³⁻²⁶ When the num-

ber of spinless fermions on the ring changes from odd to even, there is a statistical half flux quantum which shifts the energy-flux dependence by exactly half of the fundamental flux quantum. Therefore, for small values of the flux and at odd number of spinless fermions, the ring behaves as a diamagnet. When there is an even number of particles it behaves as a paramagnet. Kuzmartsev obtained this result by exact solution with the aid of the Bethe ansatz, in a model of interacting spinless fermions on the ring.^{23,24} This was also independently discussed qualitatively by Leggett for the general case (called the Leggett conjecture)²⁵ and was proved by Loss,²⁶ with the aid of the bosonisation method in the framework of the same model,^{23,24} but for arbitrary coupling. Thus, the difference between paramagnetic and diamagnetic responses is related to the statistical flux on the ring.

The parity effect also occurs because the energy position of the uppermost filled level has the most importance. With a new incoming electron, a new level is occupied and the persistent current changes direction. However at finite temperature and/or with finite disorder there occurs an intermixing between levels and it seems that the parity effect disappears. In fact this is not quite correct; the parity effect does not disappear. The temperature as well as disorder makes the single-flux-periodic energy-flux dependence smoother. That is, with temperature or with disorder the persistent current-flux dependence takes a form similar to a $\sim \sin(2\pi f)$ curve. The parity effect shows up as a shift of this curve by π with a change in the number of spinless fermions. In other words, the half-quantum flux shift of the energy-flux dependence with the change from even to odd or from odd to even number of spinless fermions does not disappear.

To take a specific example, with finite temperature and an odd number of fermions on the ring, the persistent current first decreases from zero and then increases to zero when the flux changes from zero to $\frac{1}{2}$ of the fundamental flux quantum. For the next $\frac{1}{2}$ flux quantum $\frac{1}{2} < f < 1$, the current first increases from zero and then decreases to zero. On the other hand, for an even number of fermions on the ring, for the first $\frac{1}{2}$ flux quantum $0 < f < \frac{1}{2}$, the current first increases from zero and then decreases to zero, and for the next $\frac{1}{2}$ flux quantum $\frac{1}{2} < f < 1$, the persistent current first decreases from zero and then increases to zero. This is an example of the appearance of the parity effect for the ring with spinless fermions at nonzero temperature or with the presence of disorder.

Let us now take the case of electrons with spin. As discussed above, due to Fermi statistics and due to the intersection of four levels at zero flux (for spinless fermions there was an intersection of two levels) there occur four cases, associated with numbers of electrons $N = 4n - 1, 4n, 4n + 1, 4n + 2$, where the behavior of the persistent current is distinct. The cases with $N = 4n - 1$ and $N = 4n + 1$ resemble the case of spinless fermions. For these cases the ground-state energy-flux dependence is shifted by half a flux quantum. The same situation occurs for the other two cases of $N = 4n$ and $4n + 2$ elec-

trons on the ring.

That is, for the single ring with free electrons we have two parity effects which occur when the number of electrons changes by 2. When the number of electrons changes from $N=4n-1$ to $N=4n$, the shape of the ground-state energy-flux dependence changes gradually, becoming a quasi-half-flux-periodic function. The dependence of the persistent current on the flux f ($0 < f < \frac{1}{2}$) in this case consists of two nonequivalent half periods. One is much smaller than the other. This nonequivalence for the small-amplitude half period which occurs at small flux arises in the case when three of four intersecting levels are filled by electrons, that is, when $N=4n+1$. It is important to note that in all cases here except when all intersecting levels are filled the paramagnetic response occurs. For the cases $N=4n+2$ the response will have diamagnetic character. The same occurs when the number of electrons changes from $N=4n-1$ to $N=4n$, where behavior similar to that discussed above occurs, but with a shift by $\frac{1}{2}$ flux quantum. The reason for such behavior is that the addition of the new electron creates the statistical $\frac{1}{2}$ flux quantum.

To conclude with the case of electrons with spin, the parity effect also exists, but takes a new form: instead of two types of ground-state energy-flux dependence for spinless fermions, which are related to even and odd numbers of particles, there are four different types of ground-state energy-flux dependence. However with finite disorder or finite temperature the discussed parity effect changes character. With finite temperature the intersecting levels become equally populated. Let us consider each of the four cases independently. When there are only one or two electrons in the four intersecting levels, then with a slight increase of the temperature all four levels will be populated and the current will be changed only in the flux region where these levels are near each other. The absolute value of that current strongly decreases, resulting in a smooth behavior. With the flux increase f , the distance between levels $\Delta(f)$ increases, the temperature T is switched off, if approximately $T < \Delta(f)$, and will be switched on only in the flux region of the next four intersecting levels, where $\Delta(f) < T$.

Now let us consider the case when there are three electrons in four intersecting levels. In that case, a small-amplitude half period occurs in the flux dependence of the persistent current (in the flux region $0 < f < 0.2$). At finite temperature all these four levels will be equally populated, with vanishing resulting current. As a result the original single-quantum flux periodicity will appear. Thus, in fact, the reason why the single-quantum flux periodicity occurs with finite temperature or with disorder is the intersection of levels and the parity effect, originating in the Fermi statistics.

Let us discuss what kind of parity effect we have at finite temperature. As we have discussed above, the cases

with $N=4n-1$ and $N=4n$ electrons behave similarly to each other. In both of these cases the response is paramagnetic. The other two self-similar cases are associated with $N=4n+1$ and $4n+2$ electrons on the ring, but the response in the latter two cases has a diamagnetic character. The dependence of the persistent current on the flux for the first group may be obtained from the second one with a shift of $\frac{1}{2}$ flux quantum. Thus the parity effect might be seen by comparing these two different types of flux-current dependence.

Note, however, that a Hubbard-like interaction may destroy the parity effect with the creation of the fractional Aharonov-Bohm effect.²⁹⁻³¹ As described by Haldane, fractional statistics or statistical flux may appear with this interaction.³² In this case the interaction creates the needed $\frac{1}{2}$ flux quantum to compensate the statistical flux which occurs due to the parity effect.

V. RECENT EXPERIMENT

Recently, an experiment on a semiconductor single loop in the GaAs/Ga_{1-x}Al_xAs system was reported, for which single-quantum flux periodicity has been detected.³³ After an analysis of the experimental data it was strongly concluded²¹ that in current theories the disorder is not correctly taken into account. Since the loop has only a few electron channels (estimated as equal to 4), our theory may be applicable:

- (1) The single-quantum flux periodicity is due to disorder, as described in the text.
- (2) The persistent currents are sample specific. Note that, as we have shown, the persistent current may change even in sign, with change of the level of disorder.

To complete a confirmation of our predictions (to observe the temperature changes of the sign of the persistent current), one needs to measure the persistent current at distinct values of temperature and of flux. That such measurements are needed was also concluded in Ref. 33. It is worth noting that our findings are also applicable to description of the frequency changes of phonons on the ring in a magnetic field (see Ref. 13) with temperature.

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