Does the persistent current in a quantum loop depend on an electron–electron interaction?

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The mechanism for the "exclusion" of the Coulomb interaction from the expression for the persistent current is clarified in the limit of a strong correlation of the electrons forming a Wigner molecule in a 1D loop. The cases in which theories with and without the interaction lead to different results are identified. © *1994 American Institute of Physics.*

Persistent currents in quasi-1D loop structures have been discussed in the literature for quite a long time now.[1,2] Interest in this topic recently revived in connection with progress in submicron technology which has made possible experiments with ensembles of loops[3,4] and also with single loops.[5] Mailly *et al.*[5] measured the magnetization of a single loop of 2D electrons in a GaAs–GaAlAs heterostructure. They showed that the experimental results are (unexpectedly) described well by the theory of free, i.e., noninteracting, electrons. Significantly, the mean free path of the electrons in the original material was four or five times the diameter of the loops; i.e., the experiments were carried out in the ballistic regime.

The experiments of Ref. 5 stimulated several theoretical papers, in which authors demonstrated, with various degrees of generality, that the persistent current was independent of an electron–electron interaction. For example, Müller-Groeling *et al.* asserted that an electron–electron interaction W does not affect persistent currents if the commutation relation $[\hat{L}_z W]=0$ holds, where $\hat{L}_z$ is the projection of the resultant orbital angular momentum of the system onto the magnetic field. The field was directed perpendicular to the plane of the loop. It is easy to see that this assertion is too strong. The condition offered is satisfied by any interaction which depends on only pairs of differences between the coordinates of the electrons.

Let us assume that there are only two electrons, which interact with each other not by a simple Coulomb mechanism but by some "molecular" mechanism (e.g., a Lennard–Jones mechanism). The electrons then form a pair, and the equilibrium distance between the electrons is determined by the parameters of the potential. This distance may be much smaller than the radius of the loop. In this case, the oscillations of the persistent current as a function of the magnetic flux will clearly occur with a period $\Phi_0/2$ ($\Phi_0=hc/e$) which is by no means the same as in the case of noninteracting electrons, in which the period is Φ_0.

Krive *et al.*[7] studied a 1D loop Wigner crystal, using as a model Hamiltonian a continuous string, which is valid in the long-wave approximation. They derived correct expressions for the ballistic persistent current, but their associated comments give the impression that there is agreement with the free-electron theory in the high-temperature limit, also. However, a simple comparison with that theory[8] reveals a substantial difference (the argument of an exponential function!) between these two expressions at $T \gtrsim NB$, where N is the number of electrons in the loop, and B is the rotational quantum.

In the present letter we consider a discrete model: an N-electron molecule that forms, quite naturally, at a sufficiently low density of particles, at which the correlation energy is much larger than the Fermi energy. A corresponding estimate is found by comparing the kinetic energy $N^2\hbar^2/(ma^2)$ with the potential energy $N\tilde{e}^2/a$, where a is the radius of the loop, m is the effective mass, and $\tilde{e}$ is the effective charge, i.e., the charge incorporating the dielectric constant. We see that Coulomb effects are predominant under the condition $a > Na^*$, where a^* is the effective first Bohr radius.

A loop molecule has a single rotational degree of freedom and $N-1$ vibrational degrees of freedom (the ballistic regime, without pinning). It is easy to show that the latter degrees of freedom do not affect the total persistent current. To show this, we start from the original Hamiltonian of the model in a magnetic field H:

$$\hat{\mathcal{H}} = \sum_{k=1}^{N} \frac{1}{2m}\left(\hat{P}_k - \frac{e}{c}A_k\right)^2 + W. \tag{1}$$

In this Hamiltonian we transform to Jacobi variables:

$$\varphi_0 = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}\varphi_k, \quad \theta_1 = \frac{\varphi_1 - \varphi_2}{\sqrt{1\times 2}}, \quad \theta_2 = \frac{\varphi_1 + \varphi_2 - 2\varphi_3}{\sqrt{2\times 3}}, \ldots . \tag{2}$$

Here φ_k are azimuthal angles which specify the positions of the particles on a circle; we have $\hat{P}_k = -i(\hbar/a)\partial/\partial_{\varphi k}$; and we also have $A_k = Ha/2$ (A_k is independent of k). In these new variables, and for the new unknown function

$$\chi = \exp(-i\varphi_0\lambda\sqrt{N})\psi(\varphi_0; \quad \theta_1, \ldots, \theta_{N-1}), \quad \lambda \equiv \Phi/\Phi_0,$$

we find an equation which does not contain the magnetic field:

$$-B\left(\frac{\partial^2}{\partial\varphi_0^2} + \sum_{k=1}^{N-1}\frac{\partial^2}{\partial\theta_k^2}\right)\chi + W\chi = E\chi, \quad B \equiv \frac{\hbar^2}{2ma^2}. \tag{3}$$

The obvious solution is $\chi = f(\theta_k)\exp(i\kappa\varphi_0)$, and the energy is $E = E_{\text{int}} + B\kappa^2$, where E_{int} is the purely vibrational energy corresponding to the internal degrees of freedom θ_k. This vibrational energy does not depend on the magnetic flux Φ. The condition for periodicity under rotation of the entire system as a whole through an angle 2π ($\varphi_0 \to \sqrt{N}\times 2\pi$, $\theta_k \to \theta_k$) yields an expression from which we can determine κ:

$$(\lambda\sqrt{N} + \kappa)\frac{2\pi}{\sqrt{N}} = 2\pi J,$$

where J is an integer. Hence the rotational energy is

$$E_{\text{rot}}=E-E_{\text{int}}=\frac{B}{N}(J-N\lambda)^2. \tag{4}$$

Expression (4) corresponds to the energy of a plane rotator with a radius a , a mass Nm, and a charge Ne in a magnetic field H. In general, this expression yields a persistent current which oscillates with a period Φ_0/N as a function of H. However, the symmetry of the Wigner molecule and the Pauli principle impose restrictions on the values of the rotational quantum number J. For a two-electron "molecule," we thus have the familiar problem of ortho and para states: $J=0, \pm 2, \pm 4, \ldots$, if the total spin is $S=0$; or $J=\pm 1, \pm 3, \ldots$, for $S=1$. In the case of three electrons, the situation is analogous to the NH_3 molecule.[9] In the superortho state ($S=3/2$), the symmetry of the term is A_2, and the possible values are $J=0, \pm 3, \pm 6, \ldots$. In the ortho–para state ($S=1/2$), the symmetry is E, and we have $J=\pm 1, \pm 2, \pm 4, \pm 5, \ldots$.

We consider an N-electron loop molecule in the superortho state $S=N/2$. By virtue of the symmetry of the equilibrium positions of the particles, a rotation through an angle $2\pi/N$, which contributes a factor $\exp(i2\pi J/N)$ to the wave function, is equivalent to a cyclic permutation of N identical fermions. This situation introduces a factor $(-1)^{N-1}$. We can thus find the possible values of J:

$$J=nN+N(N-1)2, \tag{5}$$

where n is an arbitrary temperature. For odd N we find $J=N\times$ (an integer); for even N we should have $J=N\times$ (a half-integer). Other values of J are possible only if $S<N/2$.

We would also point out the substantial dependence of the properties of a 1D system of fermions on the parity of the number of particles—a dependence which is well known from other examples.

To find the current it is sufficient to calculate the rotational part of the partition function of the system. Since we are dealing with a single molecule (a single loop) at thermal equilibrium with its surroundings (a heterostructure plus a substrate, etc.), we should use a Gibbs distribution for the subsystem. For odd N we have

$$Z_N=\sum_{k=-\infty}^{+\infty}\exp[-\beta BN(k-\lambda)^2], \quad \beta=1/T, \tag{6a}$$

and for even N we have

$$Z_N=\sum_{k=-\infty}^{+\infty}\exp[-\beta BN(k-\lambda-1/2)^2]. \tag{6b}$$

At low temperatures ($T\ll NB$), only a single term is important in series (6a) and (6b); for the persistent current we find the expression

$$I=cT\frac{\partial \ln Z}{\partial \Phi}=(-1)^N\frac{2eBN}{h}\left[\frac{\Phi}{\Phi_0}-I_n t\left(\frac{\Phi}{\Phi_0}+\frac{1}{2}\right)\right], \tag{7}$$

which is indeed the same as the result for noninteracting electrons. Under the condition $T \gtrsim NB$, however, we find the following from (6a) and (6b):

$$I=(-1)^N \frac{4\pi cT}{\Phi_0} \exp\left(-\frac{\pi^2 T}{NB}\right) \sin \frac{2\pi\Phi}{\Phi_0}. \tag{8}$$

Here we have written only the leading term of the Fourier series of I in Φ/Φ_0, which follows from (6a) and (6b) after we apply the Poisson summation formula. Expression (8) is the same as that derived by Krive *et al.*,[7] who examined a system of "spinless" fermions. In other words, they actually considered the case of a total spin polarization ($S=N/2$). However, that expression differs from the high-temperature limit for free electrons (see Ref. 8; in the expression in that paper, we need to make the obvious transformation from a thin cylinder to a 1D loop),

$$I_f=-\frac{4\pi cT}{\Phi_0} N \exp\left(-\frac{\pi^2 T}{B}\right) \sin \frac{2\pi\Phi}{\Phi_0}, \tag{9}$$

in both the T dependence and the N dependence. This situation is completely natural, since expression (8) corresponds to high temperatures, but still to a molecule which has not dissociated into free particles.

We see from the discussion above that the results for highly correlated electrons are by no means always the same as the results for free electrons. They are the same only at a sufficiently low temperature, in connection with the high-symmetry equilibrium configuration of the particles, itself a consequence of the strong repulsion of the particles. Furthermore, as can easily be verified in the cases of two- and three-electron systems, the persistent current depends on the total spin in the case $T=0$, changing sign as we go from $S=1$ to $S=0$ or from $S=3/2$ to $S=1/2$. These points must be kept in mind in a discussion of the problem in the model of spinless fermions, which is frequently used.

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