Pairing and persistent currents - the role of the far levels

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Abstract

We calculate the orbital magnetic response to Aharonov Bohm flux of disordered metallic rings with attractive pairing interaction. We consider the reduced BCS model, and obtain the result as an expansion of its exact solution to first order in the interaction. We emphasize the connection between the large magnetic response and the finite occupation of high energy levels in the many-body ground state of the ring.

I. INTRODUCTION

One of the remarkable phenomena of mesoscopic physics is the existence of equilibrium persistent currents in small normal metal rings, in the regime where the elastic mean free path l is much smaller than the ring's circumference L. This was both predicted theoretically [1] and observed experimentally. [2,3,4,5,6,7] For the ensemble-averaged persistent current, the experimental results [2,5,6,7] are much larger than the value obtained using the model of noninteracting electrons, [8,9] and show predominantly diamagnetic response at zero flux. In an attempt to resolve this discrepancy, the contribution of electron-electron

("e-e") interactions was calculated [10] and it was later suggested that the diamagnetic response is due to effective attractive e-e interactions. [11] Though indeed the inclusion of e-e interactions increased the theoretical value, it was still smaller by a factor of about 5 than the experimental results, for both repulsive and attractive interactions. [11]

In a recent work |13| we suggested that the contribution of high energy levels (denoted "far levels"), further than the Thouless energy $E_{\rm Th}$ from the Fermi energy $E_{\rm F}$, results in an enhanced orbital magnetic response (the derivative of the persistent current at zero flux). This was shown for the model of attractive pairing interactions described by the reduced BCS Hamiltonian, by doing perturbation theory in both the magnetic field and the e-e interaction. In this paper we repeat the calculation for the same model, doing perturbation theory in the magnetic field only, using the exact many-body states of the system with e-e interactions. In this way we can treat on the same footing different regimes of the strength of the interaction. We consider briefly the limits of zero interaction and the opposite limit where the interaction is strong enough and the system is superconducting. We then treat in more detail the case of weak e-e interaction, using Richardson's exact solution for the reduced BCS Hamiltonian. [14,15] In this way we obtain [see Eq. (18)] the result of Ref. [II] as a leading order expansion of an exact solution, instead of first order perturbation theory in the interaction. Furthermore, the present derivation has the merit of emphasizing the connection between the enhanced magnetic response and the pairing correlations of all the levels up to the high energy cutoff at the Debye frequency $\omega_{\rm D}$. These correlations exist in the exact many-body ground state (g.s.) of the ring [see Eqs. (14),(15) and discussion after Eq. (16)]. The contribution of the pairing correlations of the far levels was first realized in connection to superconductivity in small grains. [16] There it was shown that this contribution results in a much larger condensation energy than that given by the BCS theory in a large regime in which superconducting correlations are well developed, as well as in a correction to the spin magnetization and susceptibility as function of magnetic field H that persists up to $H = \omega_{\rm D}/\mu_{\rm B}$.

II. MAGNETIC RESPONSE

We consider a quasi one dimensional disordered ring with a finite number of electrons $N_{\rm e}$, penetrated by a constant Aharonov Bohm (AB) flux in its middle. We take the case of zero temperature, and the average spacing between noninteracting energy levels is d. The Hamiltonian is given by

$$H = \sum_{\alpha} \int dr \, \psi_{\alpha}^{\dagger}(r) \left[\frac{1}{2m} (\vec{P} - \frac{e}{c} \vec{A})^2 + U(r) \right] \psi_{\alpha}(r) + H_{ee}$$
 (1)

where U(r) is the external potential which includes the disorder, and $H_{\rm ee}$ represents the e-e interactions. The vector potential corresponding to the AB flux Φ in the middle of the ring is given in the London gauge by $\vec{A} = \Phi/(2\pi\rho)\hat{\phi}$, where ρ is the distance from the origin and the angle $\hat{\phi}$ is in the clockwise direction of the ring. The ground state energy of the system is flux dependent, and can be written for small flux as

$$E(\Phi) = E_0 - \frac{1}{2}E_2\Phi^2 + \dots$$
 (2)

The persistent current is given by $I = -dE/d\Phi$. [17] Since, due to time reversal symmetry there is no linear term of the energy as function of flux, hence I(0) = 0 and $dI/d\Phi \mid_{\Phi=0} = E_2$.

Since we are interested in E_2 , we calculate the ground state energy of the system to second order in the flux. We take as the unperturbed Hamiltonian

$$H_0 = \sum_{\alpha} \int dr \, \psi_{\alpha}^{\dagger}(r) \left[\frac{P^2}{2m} + U(r) \right] \psi_{\alpha}(r) + H_{ee}$$
 (3)

and the magnetic field represented by the vector potential as perturbation

$$H_I = \sum_{\alpha} \int dr \, \psi_{\alpha}^{\dagger}(r) \left[-\frac{e}{2mc} (\vec{P} \cdot \vec{A} + \vec{A} \cdot \vec{P}) + \frac{e^2}{2mc^2} A^2 \right] \psi_{\alpha}(r) \,. \tag{4}$$

We assume that the width of the ring is much smaller than its circumference L. [18] Then the A^2 term gives the "diamagnetic" contribution,

$$\frac{1}{2} \left(\frac{e\Phi}{mcL} \right)^2 \hat{N} , \qquad (5)$$

which is independent of the e-e interactions and results in

$$E_2^{\text{dia}} = -\left(\frac{e\Phi}{mcL}\right)^2 N_{\text{e}} \,. \tag{6}$$

We denote by $|i\rangle$ the eigenstates of the noninteracting electrons in the disordered ring without magnetic field. In this basis the first and relevant term of H_I is

$$H_{\rm I}^1 = -\sum_{ij\alpha} \frac{e\Phi}{mcL} P_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} . \tag{7}$$

Here c_i destroys an electron in the state $|i\rangle$ with wavefunction $\chi_i(r)$ and $P_{ij} = \langle i|P_{\parallel}|j\rangle$ is the matrix element of the momentum parallel to the ring's direction. We choose the χ_i 's to be real, and then P_{ij} is pure imaginary and $P_{ii} = 0$. Using second order perturbation theory in H_I^1 we write the paramagnetic part of E_2 as

$$E_2^{\text{par}} = -2\left(\frac{e}{mcL}\right)^2 \sum_{I} \sum_{ijkl,\alpha\alpha'} \frac{\left\langle \text{g.s.} | P_{ij}c_{i\alpha}^{\dagger}c_{j\alpha}|I\right\rangle \left\langle I | P_{kl}c_{k\alpha'}^{\dagger}c_{l\alpha'}|\text{g.s.}\right\rangle}{E_{\text{g.s.}} - E_I}$$
(8)

where E_I are the energies of the intermediate states $|I\rangle$. We model the e-e interactions by the reduced BCS interaction

$$H_{\rm ee} = -\lambda d \sum_{ij} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{j\downarrow} c_{j\uparrow} , \qquad (9)$$

where λ is the dimensionless pairing parameter and the sum is over all levels with energies between $E_{\rm F} - \omega_{\rm D}$ and $E_{\rm F} + \omega_{\rm D}$. This interaction Hamiltonian is the usual one used when discussing superconducting grains, both in the perturbative and nonperturbative regimes [19] and its validity is discussed in, e.g. Refs. [II,II,II]. (In particular, for the model to be valid the grain's dimensionless conductance g must be much larger than one.) In this model the ground state has no singly occupied noninteracting states [14,15] (we assume, for simplicity, that the number of electrons in the ring is even). Therefore, $|I\rangle$ has two singly occupied states, with opposite spins. We denote by I_{mn} the set of many-body states where state m(n) in occupied with one electron with spin up (down). Eq. (8) can then be written as

$$E_2^{\text{par}} = -2\left(\frac{e}{mcL}\right)^2 \sum_{mn} \sum_{I \in I_{mn}} |P_{mn}|^2 \frac{\left|\left\langle I | c_{m\uparrow}^{\dagger} c_{n\uparrow} - c_{n\downarrow}^{\dagger} c_{m\downarrow} | \text{g.s.}\right\rangle\right|^2}{E_{\text{g.s.}} - E_I} . \tag{10}$$

We now analyze this equation for the cases of $\lambda=0$ (normal metal), $\lambda>1/\ln N$ (superconductor, see Ref. [II]), and $0<\lambda\ll 1/\ln N$ (weak attractive interactions). Here $N\equiv\omega_{\rm D}/d$.

For $\lambda = 0$ the ground state is the noninteracting Fermi state, and the only relevant intermediate states are those with one electron-hole pair (the lowest energy states within each subspace I_{mn}). A straightforward calculation results in

$$E_2^{\text{par(n)}} = \left(\frac{2e}{mcL}\right)^2 \sum_{m>0, n<0} \frac{|P_{mn}|^2}{\omega_{mn}} \tag{11}$$

where m > 0 denotes states with energies larger than $E_{\rm F}$ and $\omega_{mn} = \epsilon_m - \epsilon_n$, the difference between the energies of the single particle states m and n. For a diffusive ring this paramagnetic term is of the same order as the diamagnetic term in Eq. (6). The difference between these terms is of the order of the contribution of the last level (and can therefore have either sign) and constitutes the noninteracting sample specific result for the magnetic response. [17]

The opposite limit is the superconducting regime. In this regime one can use the BCS approximation for the ground and excited states of the system, and the Bogoliubov transformation for the creation and annihilation operators. Eq. (10) is then reduced to

$$E_2^{\text{par(BCS)}} = 2\left(\frac{e}{mcL}\right)^2 \sum_{m,n} \frac{|P_{mn}|^2 (u_m v_n - u_n v_m)^2}{E_m + E_n} . \tag{12}$$

Here u_m, v_m are the coherence factors, and E_m is the energy of the electron-hole quasiparticle of state m. In the ballistic case, $P_{mn} = P_m \delta_{mn}$ and therefore the paramagnetic term is zero. This results in the well known perfect diamagnetism of a superconductor. For the diffusive case the ensemble-averaged momentum matrix elements are given by [13]

$$\left\langle |P_{mn}|^2 \right\rangle = \frac{p_F^2 \tau d}{\pi (1 + \omega_{mn}^2 \tau^2) s} \tag{13}$$

which is roughly constant for $\omega_{mn} < 1/\tau$ and zero for $\omega_{mn} > 1/\tau$ (τ is the elastic mean free time and s = 1, 2, 3 is the effective dimension of the ring for diffusive motion). The total response in this case (sum of diamagnetic and paramagnetic terms) is diamagnetic, with an approximate magnitude of $(l/\xi)E_2^{\text{dia}}$, where ξ is the (ballistic) superconducting coherence length.

We now turn to the calculation of $E_2^{\rm par}$ for the case of weak attractive interaction ($\lambda < 1/\ln N$). We calculate the interaction correction to E_2 to first order in λ . Using Richardson's exact solution [15] one finds that to first order in λ the ground state can be written as

$$\Psi_{\text{g.s.}} = \sum_{\{f_1...f_N\}} \phi(f_1...f_N) b_{f_N}^{\dagger} ... b_{f_1}^{\dagger} |vac\rangle$$

$$\tag{14}$$

with

$$\phi(1...N) = 1$$

$$\phi(1...N; \neq j, k) = \frac{\lambda d}{2(\epsilon_k - \epsilon_j)}.$$
(15)

Here $(f_1...f_N)$ denotes a set of N out of the 2N noninteracting eigenstates between $E_F - \omega_D$ and $E_F + \omega_D$, $b_{f_1}^{\dagger} \equiv c_{f_1\uparrow}^{\dagger} c_{f_1\downarrow}^{\dagger}$ and $\phi(1...N; \neq j, k)$ is the amplitude of the many-body state with a filled Fermi sea except a pair excitation from state j below E_F to state k above E_F . To first order in λ , the amplitude of all the other possible configurations is zero for the ground state. The finite amplitude to occupy noninteracting states with energies larger than E_F is a result of the interaction. For any small λ the system gains energy by having a different ground state than the Fermi state. Note that the amplitudes of all the different configurations come with the same sign. Similar analysis of the intermediate states shows that the only intermediate states that contribute to E_2 in first order in λ are I_{mn}^1 , the lowest energy states of each subspace I_{mn} , with m and n on opposite sides and within ω_D of the Fermi surface. Then

$$\left\langle I_{mn}^{1} | c_{m\uparrow}^{\dagger} c_{n\uparrow} - c_{n\downarrow}^{\dagger} c_{m\downarrow} | g.s. \right\rangle = 1 - \frac{\lambda d}{2\omega_{mn}} \tag{16}$$

and $E_{g.s.}-E_I=\omega_{mn}+\lambda d$. Thus, the pairing interaction contributes to the magnetic response in two ways. First, due to the finite occupancy of levels above $E_{\rm F}$ the matrix element in Eq. (16) has a contribution not only from the annihilation of an electron in state n below $E_{\rm F}$ and the creation of an electron in state m above $E_{\rm F}$. Since in the ground state there is a finite amplitude for state m to be doubly occupied and state n to be empty, there is a finite contribution to the matrix element from annihilating and electron in state m above $E_{\rm F}$ and creating it in state n below $E_{\rm F}$ [second term in Eq. (16)]. Second, it adds a term λd to the energy of the excited states due to the excess pairing energy of a doubly occupied state. The latter term is a Hartree-like contribution, coming from the diagonal part of the pairing interaction, while the former is due to pairing correlations of pairs in different single-particle states [offdiagonal part of the Hamiltonian in Eq. (9)]. Both of these contributions suppress the paramagnetic term in the case of attractive interaction, and as a result, to first order in λ ,

$$E_2^{\text{par(fo)}} = E_2^{\text{par(n)}} - \lambda d \left(\frac{2e}{mcL}\right)^2 \sum_{m>0, n<0} \frac{|P_{mn}|^2}{\omega_{mn}^2} . \tag{17}$$

Using Eq. (13) we find that the derivative of the persistent current at zero flux, to first order in the interaction, is given by

$$\left\langle E_2^{\text{fo}} \right\rangle = \frac{8\pi\lambda E_{\text{Th}}}{\Phi_0^2} \ln \frac{\omega_{\text{D}}}{d} \,.$$
 (18)

In comparison with the known result for the first order interaction correction to the magnetic response [10], our result has a much larger logarithmic cutoff, $\omega_{\rm D}$ compared with $E_{\rm Th}$. This enhancement is irrespective of the higher order correction, which for attractive interaction further increases the first order result. [11] The large logarithm we obtain is a result of enhanced pairing correlations of all the states within $1/\tau$ from $E_{\rm F}$. We expect that semiclassically this term necessitates only one circulation of the ring, and will therefore affect the magnitude of the persistent current as well (see discussion in Ref. [II]). This may lead to a resolution of the discrepancy between the experimental results and theory of persistent currents in diffusive normal rings.

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