## Temperature enhanced persistent currents and " $\phi_0/2$ periodicity"

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We predict a non-monotonous temperature dependence of the persistent currents in a ballistic ring coupled strongly to a stub in the grand canonical as well as in the canonical case. We also show that such a non-monotonous temperature dependence can naturally lead to a  $\phi_0/2$  periodicity of the persistent currents, where  $\phi_0$ =h/e. There is a crossover temperature  $T^*$ , below which persistent currents increase in amplitude with temperature while they decrease above this temperature. This is in contrast to persistent currents in rings being monotonously affected by temperature.  $T^*$  is parameter-dependent but of the order of  $\Delta_u/\pi^2k_B$ , where  $\Delta_u$  is the level spacing of the isolated ring. For the grand-canonical case  $T^*$  is half of that for the canonical case.

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### I. INTRODUCTION

Although the magnitude of persistent current amplitudes in metallic and semiconductor mesoscopic rings [1] has received experimental attention [2], much attention has not been given to qualitative features of the persistent current. Qualitative features reflect the underlying phenomena, and are more important than the order of magnitude. Incidentally, the order of magnitude and sign of the persistent currents in metallic rings is still not understood.

With this background in mind, we study the temperature dependence of persistent currents in a ring strongly coupled to a stub [3]. We predict a non-monotonous temperature dependence of the amplitude of persistent currents in this geometry both for the grand-canonical as well as for the canonical case. We show that there is a crossover temperature  $(T^*)$  above which it decreases with temperature and below which it increases with temperature, and energy scales determining this crossover temperature are quantified. This is in contrast to the fact that in the ring, temperature monotonously affects the amplitude of persistent currents. However, so does dephasing and impurity scattering, which are again directly or indirectly temperature dependent [1,4], except perhaps in very restrictive parameter regimes where it is possible to realize a Luttinger liquid in the ring in the presence of a potential barrier [5]. Recent study, however, shows that in the framework of a Luttinger liquid, a single potential barrier leads to a monotonous temperature dependence of the persistent currents for non-interacting as well as for interacting electrons [6]. We also show a temperature-induced switch over from  $\phi_0$  periodicity to  $\phi_0/2$  periodicity. This is a very non-trivial temperature dependence of the fundamental periodicity that cannot be obtained in the ring geometry.

There is also another motivation behind studying the temperature dependence of persistent currents in this ring-stub system. In the ring, the monotonous behavior of the persistent current amplitude with temperature stems from the fact that the states in a ring pierced by a magnetic flux exhibit a strong parity effect [4]. There are two ways of defining this parity effect in the single channel ring (multichannel rings can be generalized using the same concepts and mentioned briefly at the end of this paragraph). In the single-particle picture (possible only in the absence of electron-electron interaction), it can be defined as follows: states with an even number of nodes in the wave function carry diamagnetic currents (positive slope of the eigenenergy versus flux) while states with an odd number of nodes in the wave function carry paramagnetic currents (negative slope of the eigenenergy versus flux) [4]. In the many-body picture (without any electron-electron interaction), it can be defined as follows: if N is the number of electrons (spinless) in the ring, the persistent current carried by the N-body state is diamagnetic if N is odd and paramagnetic if N is even [4]. Leggett conjectured [7] that this parity effect remains unchanged in the presence of electron-electron interaction and impurity scattering of any form. His arguments can be simplified to say that when electrons move in the ring, they pick up three different kinds of phases: 1) the Aharonov-Bohm phase due to the flux through the ring, 2) the statistical phase due to electrons being Fermions and 3) the phase due to the wave-like motion of electrons depending on their wave vector. The parity effect is due to competition between these three phases along with the constraint that the many-body wave function satisfy the periodic boundary condition (which means if one electron is taken around the ring with the other electrons fixed, the many-body wave function should pick up a phase of  $2\pi$  in all). Electron-electron interaction or simple potential scattering cannot introduce any additional phase, although it can change the kinetic energy or the wave vector and hence modify the third phase. Simple variational calculations showed that the parity effect still holds [7]. Multichannel rings can be understood by treating impurities as perturbations to decoupled multiple channels, which means small impurities just open up small gaps at level crossings within the Brillouin zone and keep all qualitative features of the parity effect unchanged. Strong impurity scattering in the multichannel ring can, however, introduce strong level correlations,

which is an additional phenomenon. Whether and how the parity effect gets modified by these correlations is an interesting problem.

In a one-dimensional (1D) system where we have a stub of length v strongly coupled to a ring of length u (see the left bottom corner in Fig. 1), we can have a bunching of levels with the same sign of persistent currents, [8] i.e., many consecutive levels carry persistent currents of the same sign. This is essentially a breakdown of the parity effect. The parity effect breaks down in this single channel system because there is a new phase that does not belong to any of the three phases discussed by Leggett and mentioned in the preceding paragraph. This new phase cancels the statistical phase and so the N-body state and the (N+1)-body state behave in similar ways or carry persistent currents of the same sign [9,10]. When the Fermi energy is above the value where we have a node at the foot of the stub (that results in a transmission zero in transport across the stub), there is an additional phase of  $\pi$  arising due to a slip in the Bloch phase [9] (the Bloch phase is the third kind of phase discussed above, but the extra phase  $\pi$  due to slips in the Bloch phase is completely different from any of the three phases discussed above because this phase change of the wave function is not associated with a change in the group velocity or kinetic energy or the wave vector of the electron [9,10]). The origin of this phase slip can be understood by studying the scattering properties of the stub structure. One can map the stub into a  $\delta$ -function potential of the form  $k \cot(kv)\delta(x-x_0)$  [9]. So one can see that the strength of the effective potential is  $k \cot(kv)$  and is energy dependent. Also the strength of the effective potential is discontinuous at  $kv = n\pi$ . Infinitesimally above  $\pi$  an electron faces a positive potential while infinitesimally below it faces a negative potential. As the effective potential is discontinuous as a function of energy, the scattering phase, which is otherwise a continuous function of energy, in this case turns out to be discontinuous as the Fermi energy sweeps across the point  $kv = \pi$ . As the scattering phase of the stub is discontinuous, the Bloch phase of the electron in the ring-stub system is also discontinuous. This is pictorially demonstrated in Figs. 2 and 3 of Ref. [9]. In an energy scale  $\Delta_u \propto 1/u$  (typical level spacing for the isolated ring of length u) if there are  $n_b \sim \Delta_u/\Delta_v$  (where  $\Delta_v \propto 1/v$ , the typical level spacing of the isolated stub) such phase slips, then each phase slip gives rise to an additional state with the same slope and there are  $n_b$  states of the same slope or ithe same parity bunching together with a phase slip of  $\pi$  between each of them [9]. The fact that there is a phase slip of  $\pi$  between two states of the same parity was generalized later, arguing from the oscillation theorem, which is equivalent to Leggett's conjecture for the parity effect [11]. Transmission zeros are an inherent property of Fano resonance generically occurring in mesoscopic systems and this phase slip is believed to be observed [12] in a transport measurement [13]. For an elaborate discussion on this, see Ref. [14]. A similar case was studied in Ref. [15], where they show the transmission zeros and abrupt phase changes arise due to degeneracy of "dot states" with states of the "complementary part" and hence these are also Fano-type resonances.

The purpose of this work is to show a very non-trivial temperature dependence of persistent currents due to the breakdown of the parity effect. The temperature effects predicted here, if observed experimentally, will further confirm the existence of parity-violating states, which is a consequence of this new phase. To be precise, the new phase is the key source of the results discussed in this work.

#### II. THEORETICAL TREATMENT

We concentrate on the single channel system to bring out the essential physics. The multichannel ring also shows a very strong bunching of levels even though the rotational symmetry is completely broken by the strongly coupled stub and wide gaps open up at the level crossings [10] within the Brillouin zone. Hence let us consider a one-dimensional loop of circumference u with a onedimensional stub of length v, which contain noninteracting spinless electrons. The quantum-mechanical potential is zero everywhere. A magnetic flux  $\phi$  penetrates the ring (see the left bottom corner in Fig. 1). In this paper we consider both the grand-canonical case (when the particle exchange with a reservoir at temperature T is present and the reservoir fixes the chemical potential  $\mu$ ; in this case we will denote the persistent current as  $I_{\mu}$ ) and the canonical case (when the number N of particles in the ring-stub system is conserved; in this case we will denote the persistent current as  $I_N$ ). For the grand canonical case we suppose that the coupling to a reservoir is weak enough and the eigenvalues of electron wave number k are not affected by the reservoir [4]. They are defined by the following equation [8].

$$\cos(\alpha) = 0.5\sin(ku)\cot(kv) + \cos(ku),\tag{1}$$

where  $\alpha=2\pi\phi/\phi_0$ , with  $\phi_0=h/e$  being the flux quantum. Note that Eq. (1) is obtained under the Griffith boundary conditions, [16] which take into account both the continuity of an electron wave function and the conservation of current at the junction of the ring and the stub; and the hard-wall boundary condition at the dead end of the stub. Each of the roots  $k_n$  of Eq.(1) determines the one-electron eigenstate with an energy  $\epsilon_n=\hbar^2k_n^2/(2m)$  as a function of the magnetic flux  $\phi$ . Further we calculate the persistent current  $I_{N/\mu}=-\partial F_{N/\mu}/\partial \phi$  [17], where  $F_N$  is the free energy for the regime N=const and  $F_\mu$  is the thermodynamic potential for the regime  $\mu=const$ . In the latter case for the system of noninteracting electrons the problem is greatly simplified as we can use the Fermi distribution function

 $f_0(\epsilon) = (1 + \exp[(\epsilon - \mu)/T])^{-1}$  when we fill up the energy levels in the ring-stub system and we can write the persistent current as follows [4].

$$I_{\mu} = \sum_{n} I_{n} f_{0}(\epsilon_{n}), \tag{2}$$

where  $I_n$  is a quantum-mechanical current carried by the nth level and is given by [8]

$$\frac{\hbar I_n}{e} = \frac{2k_n \sin(\alpha)}{\frac{u}{2}\cos(k_n u)\cot(k_n v) - \left[\frac{v}{2}\csc^2(k_n v) + u\right]\sin(k_n u)}.$$
(3)

For the case of N = const we must calculate the partition function Z, which determines the free energy  $F_N = -T \ln(Z)$  [18],

$$Z = \sum_{m} \exp\left(-\frac{E_m}{T}\right),\tag{4}$$

where  $E_m$  is the energy of a many-electron level. For the system of N spinless noninteracting electrons  $E_m$  is a sum over N different (pursuant to the Pauli principle) one-electron energies  $E_m = \sum_{i=1}^N \epsilon_{n_i}$ , where the index m numbers the different series  $\{\epsilon_{n_1}, ..., \epsilon_{n_N}\}_m$ . For instance, the ground-state energy is  $E_0 = \sum_{n=1}^N \epsilon_n$ .

#### III. RESULTS AND DISCUSSIONS

First we consider the peculiarities of the persistent current  $I_{\mu}$ , i.e., for the regime  $\mu = const.$  In this case the persistent current is determined by Eqs.(1)-(3). Our calculations show that the character of the temperature dependence of the persistent currents is essentially dependent on the position of the Fermi level  $\mu$  relative to the groups of levels with similar currents. If the Fermi level lies symmetrically between two groups (which occurs if  $u/\lambda_F = n$  or n + 0.5, where n is an integer and  $\lambda_F$  is the Fermi wavelength), then the current changes monotonously with the temperature that is depicted in Fig. 1 (the dashed curve). In this case the low-lying excited levels carry a current which is opposite to that of the ground-state; the line shape of the curve is similar to that of the ring [4]. On the other hand, if the Fermi level lies within a group  $(u/\lambda_F \sim n + 0.25)$  then lowlying excited states carry persistent currents with the same sign. In that case there is an increase of a current at low temperatures as shown in Fig. 1 (the dotted curve). At low temperatures the currents carried by the low-lying excited states add up with the ground-state current. However, these excited states are only populated at the cost of the ground state population. Although in the clean ring higher levels carry larger persistent currents, this is not true for the ring-stub system. This is because the scattering properties of the stub are energy-dependent and at a higher energy the stub can scatter more strongly. Hence a lot of energy scales such as temperature, Fermi energy and number of levels populated compete with each other to determine the temperature dependence. A considerable amount of enhancement in persistent current amplitudes as obtained in our calculations appears for all choices of parameters whenever the Fermi energy is approximately at the middle of a group of levels that have the same slope. At higher temperatures when a large number of states get populated, the current decreases exponentially. So in this case the current amplitude has a maximum as a function of the temperature and we can define the temperature corresponding to the maximum as the crossover temperature  $T^{*}$ .

It is worth mentioning that in the ring system, although there is no enhancement of persistent currents due to temperature, one can define a crossover temperature below which persistent currents decrease less rapidly with temperature. Essentially this is because at low temperatures thermal excitations are not possible because of the large single-particle level spacings. Hence this crossover temperature is the same as the energy scale that separates two single-particle levels, *i.e.*, the crossover temperature is proportional to the level spacing  $\Delta = hv_F/L$  in the ideal ring at the Fermi surface, where  $v_F$  is the Fermi velocity and L is the length of the ring. The crossover temperature obtained by us in the ring-stub system is of the same order of magnitude, *i.e.*,  $\Delta_u = hv_F/u$ , although different in meaning.

In the case of  $u/\lambda_F = n + 0.25$  at low temperatures we show the possibility of obtaining  $\phi_0/2$  periodicity, although the parity effect is absent in this system. This is shown in Fig. 2, where we plot  $I_{\mu}/I_0$  versus  $\phi/\phi_0$  at a temperature  $k_BT/\Delta_u$ =0.01 in solid lines, which clearly show a  $\phi_0/2$  periodicity. Previously two mechanisms are known that can give rise to  $\phi_0/2$  periodicity of persistent currents. The first is due to the parity effect [19], which does not exist in our system, and the second is due to the destructive interference of the first harmonic that can only appear in a system coupled to a reservoir so that the Fermi energy is an externally adjustable parameter. The later mechanism can be understood by putting  $k_F L = (2n\pi + \pi/2)$  in eq. 2.11 in Ref. [4]. If this later case is the case in our situation, then the periodicity should remain unaffected by temperature and for fixed N we should only get  $\phi_0$  periodicity [4], because then the Fermi energy is not an externally adjustable parameter but is determined by N. We show in Fig. 2 (dashed curve) that the periodicity changes with temperature and in the next two paragraphs we will also show that one can obtain  $\phi_0/2$  periodicity for fixed N. The dashed curve in Fig. 2 is obtained at a temperature  $k_BT/\Delta_u=0.15$  and it shows a  $\phi_0$  periodicity. As it is known, the crossover temperature depends on the harmonic number m:  $T_m^* = T^*/m$ [4], in this case a particular harmonic can actually increase with temperature initially and decrease later, different harmonics reaching their peaks at different temperatures. Therefore, the second harmonic that peaks at a lower temperature than the first harmonic can exceed the first harmonic in certain temperature regimes. At higher temperatures it decreases with the temperature faster than the first harmonic and so at higher temperature  $\phi_0$  periodicity is recovered.

In view of a strong dependence of the considered features on the chemical potential, we consider further the persistent current  $I_N$  in the ring-stub system with a fixed number of particles N = const. In this case we calculate the persistent current using the partition function (Eq.(4)).

The numerical calculations show that in this case there is also a non-monotonous temperature dependence of the persistent current amplitude in the canonical case as in the grand-canonical case. This is shown in Fig. 1 by the solid curve. The maximum of  $I_N(T)$  is more pronounced if v/u is large and the number of electrons (N) is small. Besides, if the number of electrons is more than  $n_b/2$ , then the maximum does not exist. The crossover temperature is higher by a factor 2 as compared to that in  $I_{\mu}$ . This was also found for the 1D ring [4,20], where, as mentioned before, the crossover temperature has a different meaning. To show that one can have  $\phi_0/2$  periodicity for fixed N, we plot in the inset of Fig. 2 the first harmonic  $I_1/I_0$  (solid curve) and the second harmonic  $I_2/I_0$ (dotted curve) of  $I_N$  for N=5,  $v=7k_F$  and  $u=2.5k_F$ . At low temperature the second harmonic exceeds the first harmonic because the stub reduces the level spacing and in a sense can adjust the Fermi energy in the ring to create partial but not exact destruction of the first harmonic. There are distinct temperature regimes where  $I_1$ exceeds  $I_2$  and vice versa and the two curves peak in completely different temperatures.  $I_2$  also exhibits more than one maxima. Experimentally different harmonics can be measured separately and the first harmonic as shown in Fig. 2 can show tremendous enhancement with temperature.

An important conclusion that can be made from Fig. 2 is that observation of  $\phi_0/2$  periodicity as well as  $\phi_0$  is possible even in the absence of the parity effect quite naturally because the absence of the parity effect also means one can obtain an enhancement of the persistent current amplitude with temperature, and as a result an enhancement of a particular harmonic with temperature, resulting in different harmonics peaking at different temperatures.

#### IV. CONCLUSIONS

In summary, we would like to state that the temperature dependence of persistent currents in a ring strongly coupled to a stub exhibits very nontrivial features. Namely, at small temperatures it can show an enhancement of the amplitude of persistent currents in the grand-canonical as well as in the canonical case. The

fundamental periodicity of the persistent currents can change with temperature. If detected experimentally, these can lead to a better understanding of the qualitative features of persistent currents. It will also confirm the existence of parity-violating states that is only possible if there is a new phase apart from the three phases considered by Leggett [7] while generalizing the parity effect. This new phase is the sole cause of the nontrivial temperature dependence. There is a crossover temperature  $T^*$  above which the amplitude of persistent currents decreases with temperature. How the crossover temperature is affected by electron correlation effects and dephasing should lead to interesting theoretical and experimental explorations in the future.

Finally, with the large discrepancies between theory and experiments for the persistent currents in disordered rings, one cannot completely rule out the possibility of parity violation in the ring system as well. The stub is not the only way to produce this new phase that leads to a violation of the parity effect. There can be more general ways of getting transmission zeros [11] that may also be parity violation. In that case, the ring-stub system may prove useful as a theoretical model to understand the consequences of parity violation. Its consequences on the temperature dependence shown here may motivate future works in this direction.

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# Figure captions

Fig. 1. The ring of length u with a stub (resonant cavity) of length v threaded by a magnetic flux  $\phi$  (left bottom corner). The dependence of the current amplitude  $I_{\mu}$  in units of  $I_0 = ev_F/u$  on the temperature T in units of  $\Delta_u/2\pi^2k_B$  for the regime  $\mu = const$  with  $v = 15\lambda_F$  and  $u = (5+x)\lambda_F$  at x = 0 (dashed curve) and x = 0.25 (dotted curve); and  $I_N/I_0$  for the isolated ring-stub system with v/u = 10, and N = 3 (solid curve). For the appropriate scale the curves 2 and 3 are multiplied by factors of 3 and 15, respectively.

Fig. 2. The dependence of the persistent current  $I_{\mu}$  in units of  $I_0 = ev_F/u$  on the magnetic flux  $\phi$  in units of  $\phi_0$  for the regime  $\mu = const$  with  $v = 15\lambda_F$  and  $u = 5.25\lambda_F$  for  $T/\Delta_u = 0.01$  (dashed curve) and  $T/\Delta_u = 0.15$  (solid curve). The curve 2 is multiplied by a factor of 5 for the appropriate scale. The inset shows the first harmonic  $I_1$  (solid curve) and second harmonic  $I_2$  (dotted curve) of  $I_N$  in units of  $I_0$  for N fixed at 5,  $v = 7k_F$  and  $u = 2.5k_F$  versus temperature in units of  $\Delta_u/2\pi^2k_B$ .



