Equilibrium currents in quantum double ring system: A non-trivial role of system-reservoir coupling.

Colin Benjamin and A. M. Jayannavar
Institute of Physics, Sachivalaya Marg, Bhubaneswar 751 005, Orissa, India
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Amperes law states that the magnetic moment of a ring is given by current times the area enclosed. Also from equilibrium statistical mechanics it is known that magnetic moment is the derivative of free energy with respect to magnetic field. In this work we analyze a quantum double ring system interacting with a reservoir. A simple S-Matrix model is used for system-reservoir coupling. We see complete agreement between the aforesaid two definitions when coupling between system and reservoir is weak, increasing the strength of coupling parameter however leads to disagreement between the two. Thereby signifying the important role played by the coupling parameter in mesoscopic systems.

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I. INTRODUCTION

Mesoscopics, a fertile branch of Physics deals with systems and phenomena in the scale of nano- to micrometers. The distinguishing feature of these systems is that at extremely low temperatures an electron retains it’s phase coherence throughout the sample. These systems have revealed a new range of unexpected quantum phenomena, often counter-intuitive. The notion of the usual ensemble averaged transport coefficients such as the conductivity, i.e., local and material specific, has to be replaced by that of conductance, i.e., global and operationally specific to the sample as well as the nature of probes of measurement. Some novel and hitherto unheard of features in classical physics, e.g., non-local current-voltage relationships, breakdown of Ohm’s law, absolute negative resistance (four probe), normal-state Aharonov-Bohm effects, quantization of point-contact conductance (Landauer formalism), universal conductance fluctuations (new form of ergodicity), persistent currents, spin-polarized transport, coulomb blockade and many novel effects arising due to electron correlations, have been observed in these systems. Interpretation of these require full recognition of the wave nature of quasi particles and keeping track of their phase coherence over the entire sample including the measurement leads and probes (quantum measurement process). Even the equilibrium properties, are very sensitive to the nature of statistical ensemble used. The results differ qualitatively from one ensemble to another.

II. MOTIVATION

Recently it has been proposed that these systems will provide a testing ground for verifying the violation in the basic laws of thermodynamics. This behavior has been explained by taking recourse to the effects of entanglement, through which the quantum system is so interlinked with the bath that the resulting behavior of the system alone cannot be treated within a conventional thermodynamic approach. Here the finite coupling between the bath and the system plays a crucial role. It should be noted that equilibrium thermodynamics of the super-system comprising of system (sub-system) plus bath, does not imply standard equilibrium thermodynamics for the sub-system alone. In-fact the thermodynamic equilibrium properties of the system depend on the coupling parameter, unlike equilibrium statistical mechanics. For example, it has been shown via an analytical treatment that the mean orbital magnetic moment, a thermodynamic property, is determined by the electrical resistivity (which is related to system-bath coupling parameter) of the material. What is crucial for dissipative diamagnetism is that system-bath interaction has to be treated exactly, there is no clear cut separation between what is the system and what is the bath - both are inexorably linked to one many-body system. In this work, motivated by the above results, we provide a simple example wherein the equilibrium properties are determined by the system-reservoir coupling parameter in a non-trivial manner. Our results follow from the consideration of the dephasing of a single particle quantum coherence while the earlier dynamical treatments required in addition to quantum coherence, entanglement between system and bath. It is in this spirit that we study the persistent current densities in a quantum double ring system coupled to a reservoir via a simple voltage probe method due to Büttiker. We explicitly show that when the coupling parameter is very small there is perfect agreement between the magnetic moments calculated from the local currents (via Amperes law) and that from the derivative of free energy with respect to magnetic field, increasing the strength of coupling parameter however leads to disagreement between the two.

III. BACKGROUND

It is well known that spontaneous currents which never decay can flow in super-conducting systems. In 1983,
Büttiker, Imry and Landauer first predicted that, a normal metal ring threaded by an Aharonov-Bohm flux \( \phi \), in the phase coherent domain carries persistent currents. These arise because the magnetic flux breaks the time reversal symmetry thus inducing currents. This is a quantum effect and the total current flowing in the ring is related to the derivative of free energy with respect to flux from. For clean rings it is periodic in flux with period of \( 2\pi\phi/\phi_0 \). The magnetic flux incidentally plays the same role as a periodic potential in the Bloch sense, and therefore one gets the band structure, elastic scattering if present in the loop induces gaps in the spectrum and reduces the magnitude of persistent currents. Later in 1985, Büttiker investigated the effect of a reservoir coupled to a ring. This simply means breaking the phase coherence. Electrons enter the reservoir lose their phase memory and are re-injected again from the reservoir with an uncorrelated phase. The S-Matrix for coupling between system and reservoir is given by:

\[
S_f = \begin{pmatrix} 
\frac{-a + b}{\sqrt{\epsilon}} & \frac{\sqrt{\epsilon}}{a} & \frac{\sqrt{\epsilon}}{b} & \frac{-a + b}{\sqrt{\epsilon}} \\
\frac{\sqrt{\epsilon}}{a} & \frac{\sqrt{\epsilon}}{a} & \frac{-a + b}{\sqrt{\epsilon}} & \frac{\sqrt{\epsilon}}{b} \\
\frac{\sqrt{\epsilon}}{b} & \frac{-a + b}{\sqrt{\epsilon}} & \frac{\sqrt{\epsilon}}{b} & \frac{\sqrt{\epsilon}}{a} \\
\frac{\sqrt{\epsilon}}{b} & \frac{\sqrt{\epsilon}}{a} & \frac{-a + b}{\sqrt{\epsilon}} & \frac{\sqrt{\epsilon}}{a} 
\end{pmatrix}
\]

wherein, \( a = \frac{1}{\epsilon}(\sqrt{1 - 2\epsilon} - 1) \) and \( b = \frac{1}{\epsilon}(\sqrt{1 - 2\epsilon} + 1) \), for \( \epsilon \to 0 \) the system and reservoir are decoupled while for \( \epsilon \to 0.5 \) the system and reservoir are strongly coupled. The above S-Matrix satisfies the conservation of current and accounts for the possibility of strong to weakly coupled reservoirs through the coupler “\( \epsilon \)”. One of the important conclusions of the work was that the magnitude of persistent current flowing in the loop decreases with increasing coupling strength \( \epsilon \) but without any change in their nature, i.e., diatomic or paramagnetic. This effect is solely due to exchange of carriers between reservoir and ring (dephasing), and also this is true if the lead connecting reservoir to ring has a charging energy much less than the level spacing. Experimentally persistent currents in both open and closed systems have been observed and these observations have given rise to a spurt in theoretical activities.

![FIG. 1: One dimensional mesoscopic ring coupled to a bubble with a lead connected to a reservoir at chemical potential \( \mu \). The localized flux \( \phi \) penetrates the ring.](image)

**IV. MODEL**

Let us consider the double ring system as shown in FIG. 1. The static localized flux piercing the loop is necessary to break the time reversal symmetry and induce a persistent current in the system. The geometry we consider is a one-dimensional ring with an attached bubble and a lead connected to a reservoir at chemical potential \( \mu \). The reservoir acts as an inelastic scatterer and as a source of energy dissipation. All the scattering processes in the leads including the loop are assumed to be elastic. Hence there is complete spatial separation between the elastic and inelastic processes. The loops J1J2aJ3J1 and J1J2bJ3J1 enclose the localized flux \( \Phi \). However, the bubble J2aJ3bJ2 does not enclose the flux \( \Phi \). The same S-Matrix coupler couples the double ring to the reservoir, i.e., \( S_f = S_J \), for the other two junctions we take symmetric couplers.

\[
S_{J2} = S_{J3} = \begin{pmatrix} 
-1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 
\end{pmatrix}
\]

The waves in the four arms of the system depicted in FIG. 1 are related as follows: The waves incident into the branches of the double ring system are related by the S-Matrices for J1J2 arm by:

\[
\begin{pmatrix} 
y_1 \\
v_1 
\end{pmatrix} = \begin{pmatrix} 
e^{ikl_1}e^{i\alpha_1} & 0 \\
0 & e^{-ikl_1}e^{-i\alpha_1} 
\end{pmatrix} \begin{pmatrix} 
x_1 \\
u_1 
\end{pmatrix}
\]

for J2bJ3 arm by:

\[
\begin{pmatrix} 
y_2 \\
v_2 
\end{pmatrix} = \begin{pmatrix} 
e^{ikl_2}e^{i\alpha_2} & 0 \\
0 & e^{-ikl_2}e^{-i\alpha_2} 
\end{pmatrix} \begin{pmatrix} 
x_2 \\
u_2 
\end{pmatrix}
\]

for J2aJ3 arm by:

\[
\begin{pmatrix} 
y_3 \\
v_3 
\end{pmatrix} = \begin{pmatrix} 
e^{ikl_3}e^{i\alpha_3} & 0 \\
0 & e^{-ikl_3}e^{-i\alpha_3} 
\end{pmatrix} \begin{pmatrix} 
x_3 \\
u_3 
\end{pmatrix}
\]

for J3J1 arm by:

\[
\begin{pmatrix} 
y_4 \\
v_4 
\end{pmatrix} = \begin{pmatrix} 
e^{ikl_4}e^{i\alpha_4} & 0 \\
0 & e^{-ikl_4}e^{-i\alpha_4} 
\end{pmatrix} \begin{pmatrix} 
x_4 \\
u_4 
\end{pmatrix}
\]

Here \( kl_1, kl_2, kl_3 \) and \( kl_4 \) are the phase increments of the wave function in the absence of flux. \( \alpha_1, \alpha_2, \alpha_3 \) and \( \alpha_4 \) are the phase shifts due to flux in the arms of the considered double ring system. Clearly, \( \alpha_1 + \alpha_2 + \alpha_4 = 2\pi\phi \), where \( \Phi \) is the flux piercing the loop and \( \phi_0 \) is the flux quantum \( \frac{\tau}{2e} \). Also \( \alpha_1 + \alpha_3 + \alpha_4 = 2\pi\phi \), thus \( \alpha_2 = 0 \).

The current densities in dimensionless form in the various arms of the system are given as follows:

\[
\begin{align*}
I_1 &= |x_1|^2 - |y_1|^2, \\
I_2 &= |x_2|^2 - |y_2|^2, \\
I_3 &= |x_3|^2 - |y_3|^2, \\
I_4 &= -|x_4|^2 + |y_4|^2
\end{align*}
\]

wherein complex amplitude for propagating waves \( x_1, x_2, x_3, x_4, y_1, y_2, y_3, y_4 \) are as depicted in Fig. 1. The induced current densities in the various arms of the loop are assigned labels \( I_1, I_2, I_3 \) and \( I_4 \), while
V. THEORY

We know that magnetic moment is the derivative of free energy with respect to magnetic field, \( \mu = -\frac{1}{2} F(H) \), wherein \( F \) is the free energy and \( H \) is the magnetic field enclosed by the system. From text books we know that a current carrying loop behaves as a magnet, in other words Amperes law which states- magnetic moment is current multiplied by the area enclosed. The orbital magnetic moment density for a system coupled to reservoir can be calculated in two ways, first from the formulation of Akkermans, et al\textsuperscript{27,28} one can calculate it as follows-

\[
d\mu = \frac{1}{2\pi i} \frac{\partial \ln |\det S|}{\partial \phi} dE
\]  

(1)

Here, \( d\mu \) is the differential contribution to the magnetic moment at energy \( E \), and \( S \) is the on-shell scattering matrix. In the system considered in Fig. 1, the on-shell scattering matrix is just the complex reflection amplitude \( r \). Also from Amperes law one can calculate the orbital magnetic moment density via the local currents in a loop, depends strongly on the topology of the system, whereas the magnetic moment densities calculated from the eigen spectrum as also in the formulation of Akkermans, et al, do not. This is special to only one-dimensional geometry where the eigen-spectrum is independent of variation in topology of the system. In fact there are infinitely many topological structures possible\textsuperscript{27,28}. If we consider our system as depicted in Fig. 1, to be planar and lying in the x-y plane then the magnetic moment density \( \mu_1 \) can be viewed as being generated by current density \( I_1 \) enclosing an area \( A_r \) and by current density \( I_2 \) enclosing area \( A_b \), i.e., \( \mu_1 = \frac{1}{\pi} (I_1 A_r + I_2 A_b) \), wherein \( A_r \) and \( A_b \) are the areas enclosed by the ring \( (J1J2aJ3) \) and the bubble \( (J2aJ3bJ2) \) respectively. Another orientation of the system in which the arm \( J2bJ3 \) is in the x-z plane gives \( \mu_2 = \frac{1}{\pi} (I_1 A_r + I_2 A_r)/2 = I_r A_r/2 \) wherein \( I_r = I_1 + I_2 \) is said to be the most appropriate generalization of the equilibrium persistent current and which is consistent\textsuperscript{29} with Eq. 1, see \textsuperscript{29} for further details. Several other orientations are possible, for example, if the bubble lies in x-y plane and the ring lies in x-z plane, then \( \mu_x = \frac{1}{\pi} (I_3 A_r - I_2 A_r)/2 \) and \( \mu_y = \frac{1}{\pi} I_1 A_r \). Even when our system lies in the x-y plane for fixed \( l_1, l_2, l_3 \) by deforming their shapes we can have different values of magnetic moment density along the z direction. It is also worth mentioning that the total magnetic moment (at temperature \( T = 0 \)) of a representative system is obtained by integrating the magnetic moment densities up-to the Fermi wave-vector \( k_f \).

VI. RESULTS

From the Amperes law we calculate the orbital magnetic moment density for some length parameters. After calculating we plot the orbital magnetic moment densities obtained for the case of \( \mu_2 = \frac{1}{\pi} (I_1 A_r + I_2 A_r)/2 = I_r A_r/2 \). In Fig. 2(a) we depict the plot of the energy-eigen values (normalised by \( \pi^2 \)) of the closed system, and in Fig. 2(b) we plot the dimensionless orbital magnetic moment density \( \mu_2 \) obtained via the local persistent current densities as a function of the dimensionless Fermi wave-vector \( kl \) for different coupling parameters. Now lets test the equivalence of these definitions as \( \epsilon \to 0 \), i.e., the reservoir and system are almost decoupled. We see complete agreement. It can be noted from Fig. 2(a) that the ground state carries diamagnetic current while 1st, 2nd and 3rd excited states carry paramagnetic current for small values of flux (which is obvious from their slopes), the 4th excited state carries diamagnetic currents while the fifth paramagnetic current. Similarly from the top most panel of Fig. 2(b), the \( \epsilon \to 0 \) limit, it can be seen that the ground state carries diamagnetic current (magnitute is negative) while 1st, 2nd and 3rd excited states carry paramagnetic currents (magnitude is positive), the 4th carries diamagnetic current while the fifth paramagnetic current. Indeed the two definitions are completely equivalent as far as the \( \epsilon \to 0 \) limit (henceforth referred to as the weak coupling case) is considered. Now as we increase \( \epsilon \), we notice a dramatic change from the weak coupling case (see middle panel in FIG. 2(b)). There are paramagnetic-diamagnetic jumps at those Fermi energies wherein one would have expected pure diamagnetic or paramagnetic current. This behavior is more seen as one increases the coupling till the maximum (\( \epsilon = 0.5 \)) is reached, see lowest panel of Fig. 2(b). Looking closely at the middle panel of Fig. 2(b), one can notice that the peaks broaden, noticeably the ground, 1st, 3rd and 5th, while the nature of the currents carried at 2nd and 4th levels changes qualitatively. Also, as one approaches the \( \epsilon = 0.5 \) limit the 1st, 3rd and 5th levels disappear completely, these are some of the other qualitative features which distinguish the cases depicted in Fig. 2(a) and (b). This reaffirms that predictions from equilibrium
thermodynamics are in general not valid for a quantum system strongly coupled to a bath. In the conventional equilibrium treatment the properties of the bath appear only through a single parameter namely, the temperature $T$ and nowhere the coupling parameter appears in the magnitude of equilibrium physical quantities. Our results reaffirm that equilibrium properties are determined by the coupling parameter in the quantum domain. The finite coupling can lead to qualitative changes (and not just the broadening of levels or persistent current peaks) from that of the predictions of equilibrium statistical mechanics as shown above.

We have verified separately that the orbital magnetic moment density calculated by the formulation of Akkermans, et al, (Eq. 1) is similar to that in Fig. 2(b), for the geometry considered here. In addition we also have calculated the orbital magnetic moment density for different topological configurations, e.g., $\mu_1, \mu_z, \mu_y$ (see the Theory section for further details) and obtained results not in consonance with that calculated from the eigen-spectrum (equilibrium statistical mechanics), thus bolstering the fact that the orbital magnetic moment density calculated from the local current densities is inherently linked to the topology of the system. As already pointed out, the orbital magnetic moment density calculated through the local current densities is qualitatively different (nature) from that calculated from the closed system energy eigen-spectrum which is independent of topological variations.

We have seen these novel features not only for one set of length parameters but for many different set of length parameters. In Fig. 3(a), we plot the energy eigenvalues (normalised by $\pi^2$) as a function of flux, and in Fig. 3(b) the dimensionless orbital magnetic moment densities as a function of the dimensionless Fermi wavevector $kl$ for different length parameters. Herein also it can be seen from Fig. 3(a) that the ground and the first excited states carry diamagnetic currents while 2nd and 3rd carry paramagnetic currents for small values of flux (which is obvious from their slopes), the 4th and
5th again carry diamagnetic currents. Similarly from the top most panel of Fig. 3(b), the $\epsilon \to 0$ limit, it can be seen that the ground and first excited state carry diamagnetic current (magnitude is negative) while 2nd and 3rd carry paramagnetic currents (magnitude is positive), the 4th and 5th carry diamagnetic currents. The two definitions are again completely equivalent as far as the $\epsilon \to 0$ limit is considered. Again as we increase $\epsilon$, we notice the same change from the weak coupling case (see middle panel in FIG. 3(b)). There are paramagnetic-diamagnetic jumps at those Fermi energies wherein one would have expected pure diamagnetic or paramagnetic current. This behavior is more seen as one increases the coupling till the maximum ($\epsilon = 0.5$) is reached, see lowest panel of Fig. 3(b). Thus, in contrast, to the case of a single quantum ring coupled to a reservoir as was considered by B"{u}ttiker, wherein coupling only led to a broadening of energy levels\textsuperscript{12}, in the case of a quantum double ring system considered here, in addition to level broadening one also sees a change in nature of currents as one increases the strength of coupling to the reservoir.

One should also mention here that there is a drawback in modeling the inelastic effects by this model, if one changes the position of attachment of lead and the double ring system. Qualitatively, different results for the orbital magnetic moment density would be obtained as by definition it involves the length parameters of our system. These length parameters will of-course change with position of junction (J1). Only in the very weakly coupled regime can the specific position of lead to reservoir attachment be ignored. Of-course this drawback does not exist for the system investigated by B"{u}ttiker in Ref.\textsuperscript{12} wherein the orbital magnetic moment density would be same irrespective of the position where lead is attached. However, this simple model for coupling between system and reservoir is enough in order to bring out the importance of finite coupling between system and bath, \textit{vis a vis} equilibrium thermodynamics.
VII. CONCLUSIONS

In this work we have shown using a very simple model of system-reservoir coupling that the equilibrium properties are determined by the strength of coupling parameter. This is consistent with the recent findings,10,11 that in the quantum domain, equilibrium properties of the sub-system are related to dissipative coefficients arising due to subsystem-bath coupling, unlike the predictions of conventional statistical mechanics. These fully dynamical studies in the quantum domain invoke coherence and entanglement between system and bath). However these finite coupling induced qualitative changes can be observed only in hybrid rings which exhibit current magnification effect, a purely quantum phenomena, in equilibrium.21 We have verified separately that multiple ring structures which do not exhibit current magnification effect do not show these qualitative changes apart from features expected from broadening of energy levels.20 These results can be verified experimentally by attaching a voltage probe coupled to a nanoscopic semi-conducting system as depicted in Fig. 1. Here the voltage probe serves the purpose of a reservoir. One can change the parameters of the junction between system and lead by applying appropriate gate voltage (to simulate the effects of coupling parameter) beneath the junction and measure the orbital magnetic response as function of the gate voltage.

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* Electronic address: colin@iopb.res.in
† Electronic address: jayan@iopb.res.in

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