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Suppression of level hybridization due to Coulomb interactions

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Abstract. We investigate an ensemble of systems formed by a ring enclosing a magnetic flux. The ring is coupled to a side stub via a tunnelling junction and via Coulomb interaction. We generalize the notion of level hybridization due to the hopping, which is naturally defined only for one-particle problems, to the many-particle case, and we discuss the competition between the level hybridization and the Coulomb interaction. It is shown that strong enough Coulomb interactions can isolate the ring from the stub, thereby increasing the persistent current. Our model describes a strictly canonical system (the number of carriers is the same for all ensemble members). Nevertheless for small Coulomb interactions and a long side stub the model exhibits a persistent current typically associated with a grand canonical ensemble of rings and only if the Coulomb interactions are sufficiently strong does the model exhibit a persistent current which one expects from a canonical ensemble.

1. Introduction

Hybridization of levels or elementary excitations is encountered in many problems of physics [1–6] and chemistry [7–9] in which two weakly coupled subsystems interact with one another. In this work we are interested in the hybridization of electronic levels and in particular in the case in which a passage through the hybridization point is associated with the displacement of charge in real space. If hybridization invokes the transfer of charge between two weakly coupled systems, the Coulomb interaction can be expected to play a dominant role: the charge transfer is permitted only if it is associated with a charge distribution which exhibits a smaller interaction energy than the original configuration. If this is not the case the Coulomb interaction can be expected to suppress the hybridization.

To investigate this question we consider a simple model system shown in figure 1. A ring pierced by an Aharonov–Bohm flux [10] is weakly coupled to a side branch [11]. Of interest are the processes of charge transfer between the ring and the stub and their effect on the persistent current. The simple model shown in figure 1 permits us to investigate the interplay between highly mobile electron states and states in which the electron is localized. In this model, a state in which the electron is predominantly in the ring is very sensitive to the flux and provides a strong contribution to the persistent current, whereas a state in which the electron is predominantly localized in the stub is nearly insensitive to a variation of the flux. In the absence of Coulomb interaction the hybridization of these two types of state leads to a small persistent current. If now the Coulomb interactions are switched on, transfer of charge into and out of the localized states is generally not energetically favourable. As a consequence the model exhibits an increased persistent current in the

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presence of Coulomb interaction. For a sufficiently strong Coulomb interaction the presence of the side branch is irrelevant; the persistent current is that of a loop without a side branch. Thus the larger persistent current can be viewed as a consequence of the suppression of hybridization of highly mobile states with localized states. It is well appreciated that many-ring experiments [12] as well as experiments on single metallic diffusive rings [13] yield a value for the persistent current which is much larger than predicted by theories which neglect interactions. In contrast, the measurements on single ballistic semiconductor rings [14] seem in accord even with the predictions of non-interacting theories. Possibly, discussions of the persistent current in the absence of interactions find a very small value for the current, since hybridization of levels is not inhibited. In the absence of interactions, arbitrary charge distribution patterns are permitted. If, as is shown in this work, Coulomb interactions can effectively inhibit level hybridization of flux-sensitive states with flux-insensitive localized states, this might offer a mechanism which permits the much larger currents observed in experiments and found in discussions which take Coulomb interactions into account [15]. The discussion presented here is limited to the simple example shown in figure 1 and does not address the case of metallic diffusive systems. We point out, however, that the work of Pascaud and Montambaux [16], which considers metallic diffusive conductors with a geometry similar to the one of interest here, gives results which are in accord with the findings reported below.

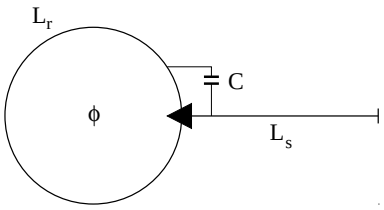

Figure 1. A ring pierced by a flux ϕ and coupled to a (finite-length) side stub. The triangle represents the three-way tunnelling junction and the Coulomb interaction is taken into account via the capacity C.

The model system, proposed in [11], has been analysed in a number of works. Reference [11] treated interactions on the Hartree level in a random-phase approximation. A discussion which takes the effect of charge quantization in the charge transfer explicitly into account and treats interactions within a quantum coherent charging model was subsequently provided by Stafford [17, 18] in collaboration with one of the authors. A computational investigation in which interactions are treated in a Hubbard-like model is provided by Anda *et al* [19]. Without interactions, the geometry of figure 1 represents an elementary system which has also found some interest [20]. There are a number of closely related geometries. First instead of a ring and a side branch one can investigate two coupled rings as has been done by Canali *et al* [21]. Alternatively, two quantum dots in parallel [22] or in series [6, 23–26], usually attached to leads to investigate transport, have been considered. A system very similar to ours, with the side stub replaced by a quantum dot, is investigated in [17, 18]. These authors also treat the case in which the quantum dot is incorporated into one of the arms of the ring and where the dot and ring are each separately coupled to a gate. Throughout, we focus on the closed system of figure 1 in which the level spectrum is discrete. If the stub attached to the ring is not closed but connected to a reservoir [27], we have an open grand canonical system in which the spectrum of the wire connecting the reservoir and the ring is continuous. Effects of Coulomb charging in such models have

been discussed by Beenakker *et al* [28] and by Moskalets [29]. Charge transfer between a Luttinger liquid ring and a reservoir is discussed by Sandström and Krive [30] and Krive *et al* [31].

The purpose of the present work is to extend the discussion of [17, 18] which focused on quantum coherent resonant charge transfer between subsystems to the case of off-resonant charge transfer. The main difficulty in further advancing the notions put forward above is that level hybridization is a single-particle concept. Thus we can only compare the different properties of the interacting system with those of the non-interacting system and show that the signatures of level hybridization encountered in the non-interacting system disappear with increasing interaction strength. To demonstrate this it is necessary to investigate charge transfer not only under resonant conditions but over a wide parameter range of the model. Furthermore, it is necessary to consider an ensemble of systems rather than a single system. It is well known that the size of the persistent currents depends sensitively on the ensemble considered [32, 33]. The present model, although it is strictly a canonical one, since the overall charge is conserved, nevertheless, as far as the persistent current is concerned, shows aspects usually associated with a grand canonical ensemble in the limit of weak interactions and for a sufficiently long stub.

2. The model

We consider the following model. A ring is coupled to a side stub via particle hopping and via electrostatic energy. In the absence of coupling between the ring and the stub both subsystems are perfect, disorder-free conductors. The energy levels of the ring are denoted by $\epsilon_n^{(r)}(\phi)$. They are periodic in the flux ϕ with period $\phi_0 = hc/e$. The eigenstates of the stub are extended along its entire length and their energies are denoted by $\epsilon_n^{(s)}$. For simplicity, the electrons are considered as spinless. We introduce the operators $\hat{a}_i^\dagger$ which create an electron in state i of the ring and the operators $\hat{b}_j^\dagger$ which create an electron in the stub. The Hamiltonian is the sum of the kinetic energy $\hat{K}$ of the electrons in the ring and the stub, the hopping energy $\hat{\Gamma}$ and the Coulomb energy $\hat{H}_C$. With the energies and operators introduced above, we have a kinetic energy

$$\hat{K} = \sum_i \epsilon_i^{(r)}(\phi)\hat{a}_i^\dagger \hat{a}_i + \sum_j \epsilon_j^{(s)}\hat{b}_j^\dagger \hat{b}_j \tag{1}$$

and a coupling energy

$$\hat{\Gamma} = \sum_{i,j}(t_{ij}\hat{a}_i^\dagger \hat{b}_j + \text{HC}). \tag{2}$$

The one-particle spectra $\epsilon_i^{(r)}$ and $\epsilon_j^{(s)}$ of the ring and the stub are given by the spectra of the free particle. If the particle numbers N_r in the ring and N_s in the stub are large, the spectra may be linearized. Denoting the velocity of the topmost occupied state in the stub by $v_F^{(s)}$, we find for a stub of length L_s a level spacing

$$\Delta = \frac{\pi\hbar v_F^{(s)}}{L_s}. \tag{3}$$

We characterize the spectrum of the ring of circumference L_r by the width w of the levels which they obtain as a function of flux. For a ballistic ring in which the topmost state has a velocity $v_F^{(r)}$, the level width is given by

$$w \equiv |\epsilon_{N_r}^{(r)}(\phi_0/2) - \epsilon_{N_r}^{(r)}(0)| = \frac{\pi\hbar v_F^{(r)}}{L_r}. \tag{4}$$

Below we frequently use Δ and w to characterize the spectrum of the system.

The Coulomb energy is taken into account with the help of a geometrical capacitance C and is obtained as follows. The N_r electrons on the ring and N_s electrons on the stub are held in place by an ionic background charge eN_r^+ on the ring and eN_s^+ on the stub. We consider a system that is overall charge neutral and, therefore,

$$N = N_r + N_s = N_s^+ + N_r^+.$$

The Coulomb energy of these charges is

$$E_C = (1/2)[(N_r - N_r^+)eU_r + (N_s - N_s^+)eU_s].$$

Relating the charge imbalance $Q = e(N_r - N_r^+)$ to the potential difference $U_r - U_s$ via the geometrical capacitance C, $Q = C(U_r - U_s)$, and using the charge-neutrality condition gives

$$\hat{H}_C = \frac{e^2}{2C}(\hat{N}_r - N_r^+)^2 \qquad \hat{N}_r = \sum_i \hat{a}_i^\dagger \hat{a}_i. \tag{5}$$

Note that this energy is equal to

$$\hat{H}_C = \frac{e^2}{2C}(\hat{N}_s - N_s^+)^2.$$

Below we discuss various simple limits of this Hamiltonian.

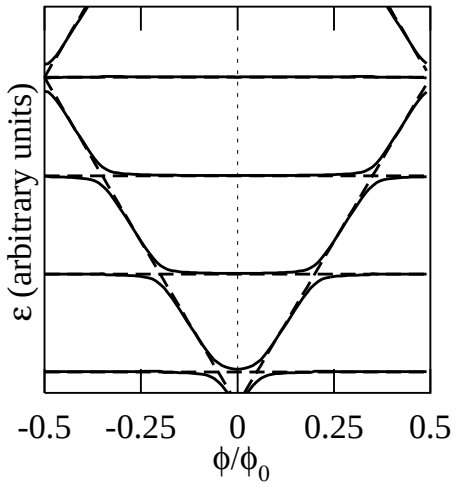

Figure 2. Part of the single-particle energy spectrum of a ring connected to a stub (full lines). The dashed lines represent the spectra of the uncoupled ring (levels 21 and 22) and stub (levels 30 to 33), respectively. The spectrum of the Hamiltonian including tunnelling was calculated by matrix diagonalization with a level width w in the ring, a level spacing $\Delta = 2w/3$ in the stub and a coupling energy $|t| = 0.1w$.

For vanishing Coulomb interaction ($e^2/2C = 0$) the problem reduces to a one-particle problem which we discuss now. In the absence of hopping between the ring and the stub ($\hat{\Gamma} = 0$), the spectrum consists of the flux-sensitive spectrum of a perfect ring and a completely flux-insensitive spectrum of the stub. This spectrum is indicated by broken lines in figure 2. From their flux dependence the ring states behave like extended states, whereas the stub states behave like completely localized states. If we now turn on the coupling

between the stub and the ring, the states of these two subsystems hybridize. Instead of an intersection of two nearby levels, a gap of the order of $|t|$ opens up. The solid lines in figure 2 represent the spectrum of the ring and the stub for a finite coupling strength $|t|$ obtained by matrix diagonalization. As a consequence, the wave function describing a carrier initially in an (extended) ring state changes its character at the hybridization point and turns into a wave function which describes a carrier localized on the stub. As we pass the hybridization point a carrier is thus transferred from the ring into the stub. Separated in energy by a gap of the order of the coupling energy $|t|$, there is a second wave function which describes the transfer of a carrier initially localized on the stub into the ring as we pass the hybridization point. For weak coupling and if both states are occupied, the net charge transferred vanishes. Thus for weak coupling the effect of hybridization is only relevant for the topmost occupied level.

It is the purpose of this work to investigate the suppression of the hybridization when the Coulomb energy is present. Clearly, if the transfer of the topmost electron from the ring to the stub leads to a marked deviation of charge distribution away from a locally electroneutral solution, the charge transfer will effectively be inhibited in the presence of strong Coulomb interaction. The complication which is encountered in the characterization of this phenomenon arises from the fact that level hybridization, as it is typically discussed and shown in figure 2, applies to a non-interacting system. In an interacting system we can in general not follow single-particle levels. Thus we can discuss the suppression of hybridization only indirectly by showing that the features in the ground-state energy which are typical for hybridization in the large-capacitance limit vanish with increasing Coulomb interaction. Alternatively, we can investigate properties of the ground-state wave function, in particular the fluctuations of the charge on the ring as a function of the Coulomb interaction.

Therefore we discuss now the behaviour of our system in the case where the charging energy is non-vanishing. In a first step, the tunnelling energy is neglected. This is the limit of the standard incoherent Coulomb blockade description [34, 35]. It permits us to discuss the charging states of the model. Later on we will include the quantum mechanical transmission to find small corrections to this quasi-classical picture. At zero temperature the free energy is given by

$$F(N_r, \phi) = \sum_{n=1}^{N_r} \epsilon_n^{(r)}(\phi) + \sum_{m=1}^{N_s} \epsilon_m^{(s)} + \frac{e^2}{2C}(N_r - N_r^+)^2. \tag{6}$$

The operator $\hat{N}_r$ has been replaced by its eigenvalue N_r, and $N_s = N - N_r$. For a given flux ϕ, the state with N_r particles on the ring is realized if its free energy is smaller than all of the other free energies obtained with different particle numbers N_r'. It is clear that for very large Coulomb energies the state with $N_r = N_r^+$ for which the electronic charge exactly compensates the ionic background charge will be the state with minimal free energy. The Coulomb energy of this state vanishes, whereas for the neighbouring states $N_r^+ \pm 1$ we have to pay an additional energy $e^2/2C$. Thus for large Coulomb energies we have $F(N_r^+, \phi) \ll F(N_r^+ \pm 1, \phi)$. If we now lower the Coulomb energy, either $F(N_r^+ + 1, \phi)$ or $F(N_r^+ - 1, \phi)$ might become smaller than $F(N_r^+, \phi)$. Thus a charge transfer into or out of the ring occurs at the points of energetic degeneracies for which

$$F(N_r^+, \phi) = F(N_r^+ \pm 1, \phi). \tag{7}$$

Using (6) yields

$$\epsilon_{N_r^+ + 1}^{(r)}(\phi) - \epsilon_{N_s^+}^{(s)} + \frac{e^2}{2C} = 0 \qquad \text{for '+'} \tag{8}$$

$$\epsilon^{(s)}_{N_s^+ +1} - \epsilon^{(r)}_{N_r^+}(\phi) + \frac{e^2}{2C} = 0 \qquad \text{for '}-\text{'} \tag{9}$$

with $N_r^+ + N_s^+ = N$. Since the energies of the ring depend on the flux, these equations might have a solution only for a particular flux $\pm\phi^*$. At this flux the topmost filled stub state has an energy $\epsilon^{(s)}_{N_s^+}$ which is equal to the first empty state of the ring $\epsilon^{(r)}_{N_r^+ +1}(\phi^*)$ augmented by the Coulomb energy $e^2/2C$. Alternatively the topmost occupied ring state $\epsilon^{(r)}_{N_r^+}(\phi^*)$ has an energy which is equal to the topmost empty stub state augmented by the charging energy. In the limit of infinite capacitance the flux ϕ^* corresponds to a hybridization point in figure 2. In the quasi-classical model which neglects phase coherence between ring and stub states the hybridization region has zero extent: the charge on the ring jumps as the flux is moved through ϕ^*. Quantum mechanically, if phase coherence is taken into account, hybridization extends over a range of flux which is determined both by the strength of the tunnelling matrix element $|t|$ and the magnitude of the Coulomb energy $e^2/2C$. In the next section we will describe these transitions in a quantum coherent model in more detail.

By biasing this system via gates [17, 18], one can essentially create an arbitrary charge imbalance, i.e. $N_r \neq N_r^+$. In this case the Hamiltonian (1)–(5) contains additional terms which describe the coupling of the system to the gate voltage. In such a case the system can exhibit resonances like in (7) at any strength $e^2/2C$ of the interaction, depending only on the value of the gate voltage. For a dot connected via a wire to a reservoir, capacitance fluctuations have been discussed by Gopar, Mello and Büttiker [36] and by Aleiner and Glazman [37]. For large charging energy this Hamiltonian can be cast into a Kondo-like form [38]. The Kondo-like features of this problem have been treated by Matveev [39]. As the system that we are discussing does not contain gates, the resonance condition (7) cannot be fulfilled for large charging energies $e^2/2C$. Therefore it does not exhibit a Kondo effect.

3. Quantum corrections

In this section we the treat quantum corrections to the classical picture developed above. Different treatments apply depending on whether or not the charge transfer is resonant or off-resonant.

3.1. Resonant charge transfer

Hybridization occurs when one of the equations (8), (9) is fulfilled for some $\pm\phi^*$. Without loss of generality we may assume that it is equation (9) that is fulfilled. As shown in recent works [17, 18], in the weak-tunnelling limit it suffices to consider hybridization between a state in the ring and a state in the stub. Then the Hamiltonian reduces to a 2×2 matrix

$$\hat{H}_h = \begin{pmatrix} \epsilon^{(r)}_{N_r^+}(\phi) & t \\ t^* & \epsilon^{(s)}_{N_s^+ +1} + e^2/2C \end{pmatrix} + \left(\sum_{n=1}^{N_r^+ -1} \epsilon^{(r)}_n(\phi) + \sum_{m=1}^{N_s^+} \epsilon^{(s)}_m \right) \mathbf{1} \tag{10}$$

that is easily diagonalized. The eigenvalues of $\hat{H}_h$ show a gap around the hybridization point $\phi = \pm\phi^*$. It is a typical hybridization effect, and gaps of the same kind also open up in the one-particle spectrum of the Hamiltonian $\hat{K} + \hat{\Gamma}$ (equations (1), (2)); see figure 2. The eigenstates of $\hat{H}_h$ are not eigenstates of the (reduced) particle number operators $\hat{N}_r$ (and $\hat{N}_s$): $\hat{N}_r = \hat{N}_h + (N_r^+ - 1)\mathbf{1}$ with

$$\hat{N}_h = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{11}$$

Around $\phi = \pm\phi^*$ the topmost electron is extended over both subsystems. As a consequence, we find in the ground state an expectation value of the charge $e\langle\hat{N}_r\rangle$ which is not an integral multiple of the elementary charge. Furthermore there are strong particle number fluctuations ΔN_r^2 away from the average $\langle\hat{N}_r\rangle$. The particle number fluctuations [18] are determined by

$$\Delta N_r^2 = \left\langle (\hat{N}_r - \langle\hat{N}_r\rangle)^2 \right\rangle = \frac{|t|^2}{(\epsilon^{(s)}_{N_s^+ +1} - \epsilon^{(r)}_{N_r^+}(\phi) + e^2/2C)^2 + 4|t|^2}. \tag{12}$$

Note that at the hybridization point

$$\epsilon^{(s)}_{N_s^+ +1} - \epsilon^{(r)}_{N_r^+}(\phi^*) + e^2/2C = 0$$

we have the maximal fluctuation $(\Delta N_r^2)^{1/2} = 1/2$. The persistent current in the ring is given by $I(\phi) = -c\,\partial F/\partial\phi$, where $F = \langle\hat{H}\rangle$. In the two-level approximation, this reads

$$I(\phi) = -c\frac{\partial\epsilon^{(r)}_{N_r^+}}{\partial\phi}\langle\hat{N}_h\rangle + I_{N_r^+ -1}(\phi). \tag{13}$$

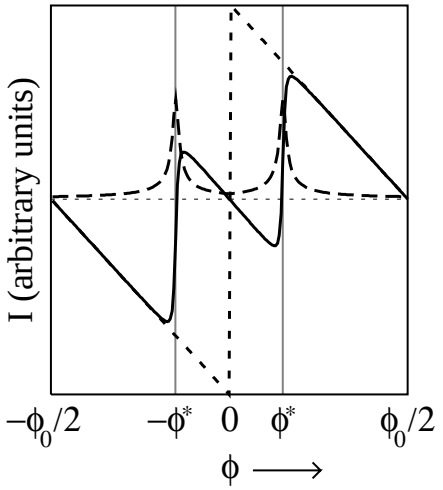

Figure 3. The persistent current (solid line) and its fluctuations $(\Delta I^2)^{1/2}$ (long-dashed line) in the two-level approximation with N_r^+ even and $|t| \approx 0.32w$. For comparison, the persistent current for N_r^+ electrons in the ring and in the absence of hybridization is shown (short-dashed line). The persistent current vanishes near the hybridization points $\pm\phi^*$ ($=\pm\phi_0/6$ in the example) whereas the fluctuations have maxima near the same points, which are of the same order of magnitude as the persistent current in the absence of hybridization.

The total persistent current consists of a contribution of the topmost ring level with an average occupation $\langle\hat{N}_h\rangle$ and of the full persistent current $I_{N_r^+ -1}(\phi)$ of all $N_r^+ - 1$ ring states below the topmost level. This form of the persistent current is a consequence of the weak coupling between the ring and the stub. In this case all ring levels below the topmost level are fully occupied and give rise to a persistent current

$$-c\sum_{n=1}^{N_r^+ -1}\partial\epsilon_n^{(r)}/\partial\phi = I_{N_r^+ -1}(\phi).$$

$I(\phi)$ vanishes near the hybridization points $\phi = \pm\phi^*$, as discussed in [11]. It is interesting to observe what happens to the quantum mechanical current fluctuations when the persistent current itself goes to zero. They are given by [18]

$$\langle \Delta I^2 \rangle = c^2 \left(\frac{\partial \epsilon^{(r)}_{N_r^+}}{\partial \phi} \right)^2 \langle \Delta N_r^2 \rangle. \tag{14}$$

They are maximal near $\phi = \pm\phi^*$ where $I(\phi)$ vanishes, and there $\langle \Delta I^2 \rangle^{1/2}$ is of the same magnitude as $I(\phi)$ is away from $\phi = \pm\phi^*$. The behaviour of $I(\phi)$ and ΔI^2 is summarized in figure 3.

An interesting quantity that is sensitive to hybridization is the flux-induced capacitance [11, 17, 18] $C_\phi = e\,\partial\langle \hat{N}_r \rangle / \partial\phi$. This quantity determines the charge increment (in the ring) in response to a small variation in the flux, much like an electrochemical capacitance coefficient determines the increment in charge in response to a variation of a gate voltage. The flux-induced capacitance is a particularly interesting quantity to consider here since it exhibits a large resonant-like spike at a hybridization point $\phi = \pm\phi^*$. In the two-level approximation considered here, the resonance is determined [17, 18] by

$$C_\phi = -\frac{4|t|^2\, \partial \epsilon^{(r)}_{N_r^+} / \partial\phi}{[(\epsilon^{(s)}_{N_s^+ + 1} - \epsilon^{(r)}_{N_r^+}(\phi) + e^2/2C)^2 + 4|t|^2]^{3/2}}. \tag{15}$$

At resonance, $C_\phi = (\partial \epsilon^{(r)}_{N_r^+} / \partial\phi)/2|t|$. We will not investigate this quantity here any further but note that cC_ϕ has the dimension of conductance and in topological discussions of the Hall effect it is sometimes taken to be the Hall conductance [40].

If we are not close to a hybridization point, however, the two-level approximation is insufficient for discussing the quantities of interest here.

3.2. Off-resonant charge transfer

To discuss the transfer of charge away from the resonant points we decompose the Hamiltonian (1)–(5) as $\hat{H} = \hat{H}_0 + \hat{\Gamma}$ and treat $\hat{\Gamma}$ as a perturbation. Note that $\hat{H}_0 = \hat{K} + \hat{H}_C$ contains the Coulomb energy term. We assume in the following that there are no energetic degeneracies (cf. equation (7)). A complete system of eigenvectors orthonormal to H_0 is constructed as follows. Let $|\psi_0\rangle$ denote the vacuum (no particles) and I_m, J_n index sets with m, n elements, respectively. The basis reads

$$|I_m J_n\rangle = \prod_{i \in I_m} \hat{a}_i^\dagger \prod_{j \in J_n} \hat{b}_j^\dagger |\psi_0\rangle \qquad m + n = N. \tag{16}$$

We need only a small subset of them, one of which is the ground state of the uncoupled system

$$|0\rangle = \prod_{i=1}^{N_r^+} \hat{a}_i^\dagger \prod_{j=1}^{N_s^+} \hat{b}_j^\dagger |\psi_0\rangle \tag{17}$$

with energy

$$E_0 = \sum_{i=1}^{N_r^+} \epsilon_i^{(r)}(\phi) + \sum_{j=1}^{N_s^+} \epsilon_j^{(s)}. \tag{18}$$

We will calculate the corrections to the ground-state energy and the particle number fluctuations to second-order perturbation theory in $\hat{\Gamma}$ [41] (lowest non-vanishing order). We discuss briefly the states that contribute to the ground state of the coupled system. To

first order in $\hat{\Gamma}$, one electron can hop from the stub to the ring or vice versa. We denote the states created from $|0\rangle$ by one electron hopping by $|\alpha\rangle$. They are of the form (16), but they are most easily expressed in terms of the ground state of the uncoupled system

$$|\alpha\rangle = \begin{cases} \hat{a}_i^\dagger \hat{b}_j |0\rangle & \text{with } i > N_r^+,\ j \leqslant N_s^+ \\ \hat{b}_j^\dagger \hat{a}_i |0\rangle & \text{with } i \leqslant N_r^+,\ j > N_s^+. \end{cases} \tag{19}$$

The corresponding eigenvalues are denoted by E_α, i.e. $\hat{H}_0|\alpha\rangle = E_\alpha|\alpha\rangle$. To second order in $\hat{\Gamma}$ one has to consider processes that involve two electrons, namely

(i) one electron hopping from the ring to the stub and back, thereby creating an excitation in the ring,

(ii) one electron hopping from the stub to the ring and back, thereby creating an excitation in the stub,

(iii) one electron hopping from the ring to the stub, the other one hopping from the stub to the ring, creating excitations in the ring and in the stub,

(iv) two electrons hopping from the stub to the ring and

(v) two electrons hopping from the ring to the stub.

We use the summary notation $|\beta\rangle$ for the states emerging from the ground state via these processes. Formally (and in the same order as above)

$$|\beta\rangle = \begin{cases} \hat{a}_k^\dagger \hat{a}_l |0\rangle & \text{with } k > N_r^+, l \leqslant N_r^+ \\ \hat{b}_k^\dagger \hat{b}_l |0\rangle & \text{with } k > N_s^+, l \leqslant N_s^+ \\ \hat{a}_k^\dagger \hat{a}_l \hat{b}_m^\dagger \hat{b}_n |0\rangle & \text{with } k > N_r^+, l \leqslant N_r^+, m > N_s^+, n \leqslant N_s^+ \\ \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{b}_m \hat{b}_n |0\rangle & \text{with } k > l > N_r^+, m < n \leqslant N_s^+ \\ \hat{b}_m^\dagger \hat{b}_n^\dagger \hat{a}_k \hat{a}_l |0\rangle & \text{with } k < l \leqslant N_r^+, m > n > N_s^+ \end{cases} \tag{20}$$

and for the eigenvalue we write $\hat{H}_0|\beta\rangle \equiv E_\beta|\beta\rangle$.

To second order in $\hat{\Gamma}$, the ground-state energy reads

$$E = E_0 + \sum_\alpha \frac{|\langle\alpha|\hat{\Gamma}|0\rangle|^2}{E_0 - E_\alpha} \tag{21}$$

and the ground state $|\Omega\rangle$ of the coupled system

$$|\Omega\rangle = \left(1 - \frac{1}{2}\sum_\alpha \frac{|\langle\alpha|\hat{\Gamma}|0\rangle|^2}{(E_0 - E_\alpha)^2}\right)|0\rangle + \sum_\alpha \frac{\langle\alpha|\hat{\Gamma}|0\rangle}{E_0 - E_\alpha}|\alpha\rangle + \sum_{\alpha,\beta} \frac{\langle\beta|\hat{\Gamma}|\alpha\rangle\langle\alpha|\hat{\Gamma}|0\rangle}{(E_0 - E_\alpha)(E_0 - E_\beta)}|\beta\rangle. \tag{22}$$

Summation over $|\alpha\rangle$ and $|\beta\rangle$ in (21), (22) does not include the ground state $|0\rangle$ of the uncoupled system. Now we can also calculate the particle number fluctuations

$$\Delta N_r^2 = \langle\Omega|\hat{N}_r^2|\Omega\rangle - \langle\Omega|\hat{N}_r|\Omega\rangle^2 = \sum_\alpha \frac{|\langle\alpha|\hat{\Gamma}|0\rangle|^2}{(E_0 - E_\alpha)^2}. \tag{23}$$

The states $|\beta\rangle$ do not appear in second-order perturbation theory in (21), (23). This is true for any observable that is diagonal in the basis (16). However, it is necessary to go to

second order in the perturbation theory to obtain a properly normalized ground state. For the eigenvalues E_α one finds

$$E_\alpha - E_0 = \begin{cases} \dfrac{e^2}{2C} + \epsilon_i^{(r)}(\phi) - \epsilon_j^{(s)} & i > N_r^+,\ j \leqslant N_s^+ \\ \dfrac{e^2}{2C} + \epsilon_j^{(s)} - \epsilon_i^{(r)}(\phi) & i \leqslant N_r^+,\ j > N_s^+. \end{cases} \tag{24}$$

The sums in (21), (23) can be written more explicitly in terms of the eigen-energies (24). We obtain double sums:

$$E_0 - E = \sum_{i>N_r^+, j\leqslant N_s^+} \frac{|t_{ij}|^2}{e^2/2C + \epsilon_i^{(r)}(\phi) - \epsilon_j^{(s)}} + \sum_{i\leqslant N_r^+, j>N_s^+} \frac{|t_{ij}|^2}{e^2/2C + \epsilon_j^{(s)} - \epsilon_i^{(r)}(\phi)} \tag{25}$$

$$\Delta N_r^2 = \sum_{i>N_r^+, j\leqslant N_s^+} \frac{|t_{ij}|^2}{(e^2/2C + \epsilon_i^{(r)}(\phi) - \epsilon_j^{(s)})^2} + \sum_{i\leqslant N_r^+, j>N_s^+} \frac{|t_{ij}|^2}{(e^2/2C + \epsilon_j^{(s)} - \epsilon_i^{(r)}(\phi))^2} \tag{26}$$

that can be interpreted as the effect of an electron *coherently* hopping from the stub into a virtual state in the ring and back (the first sum in the equations (25), (26) or vice versa (second sum). We postpone the explicit evaluation of the above sums until after the discussion of the ensemble.

4. The ensemble

There is little purpose in attempting to characterize an individual sample. If the charging energy $e^2/2C$ is small, the critical flux ϕ^* is very sensitive to changes in the particle densities N_r/L_r and N_s/L_s. For $e^2/2C = 0$ the critical flux covers the entire interval $[0, \phi_0/2]$ when the particle densities in the ring and in the stub are varied independently by $\pm 1/L_r$ and $\pm 1/L_s$, respectively. Many quantities of interest depend crucially on the number of particles in the ring. Let us mention only the persistent current [11]. Any such quantity will depend on ϕ^* which itself is strongly sample dependent. To extract more general results we want to consider an ensemble of rings connected to stubs and to calculate ensemble averages. The construction of an ensemble is thus the next task.

We consider an ensemble of systems having different ring circumferences and stub lengths, but with constant total particle number N, a 'strongly canonical' ensemble according to the classification of Kamenev and Gefen [33]. The spectra in the ring and the stub depend on the circumference of the ring L_r and the length of the stub L_s (see equations (3), (4)). Therefore the topmost occupied energy levels of the ring and the stub shift when L_r and L_s are varied. We describe this shift by the difference $\Delta\epsilon$ between the energy of the topmost occupied ring state at zero flux and the topmost occupied stub level. For consistency with the derivation of the Coulomb energy leading to equation (5), the background charge densities N_r/L_r in the ring and N_s/L_s in the stub are required to be the same for all ensemble members. The double constraint of constant particle number and constant densities puts strong limits on the possible variations of L_r and L_s. These constraints require that the topmost energy levels may vary at most by w in energy for the ring and by Δ for the stub. It follows that $\Delta\epsilon$ can vary at most by $\pm(w + \Delta)$ around 0. Thus $\Delta\epsilon$ lies in an interval of length $2(w + \Delta)$. We consider an ensemble with a uniform distribution of $\Delta\epsilon$ in this interval. From figure 2, one may see that at $e^2/2C \to 0$ and if $\Delta\epsilon$ varies between 0 and $\max\{w, \Delta\}$, $|\phi^*|$ does indeed assume any value between 0 and $\phi_0/2$.

In the limit of vanishing interaction strength and in the limit of a very long stub we show below that our system behaves effectively like a ring coupled to a reservoir. Hence

we will refer to this limit as the 'grand canonical' limit. On the other hand if the stub is very short our system behaves, regardless of the interaction strength, in a canonical manner. Hence we call the limit of a short stub also the canonical limit.

In order to differentiate between quantum mechanical expectation values and ensemble averages, we denote the latter by an overline (e.g. $\overline{x}$) and the former by angular brackets $\langle x \rangle$.

5. Persistent current

It is instructive to compare the Fourier coefficients $\overline{I_n}$ of the average persistent current

$$\overline{I(\phi)} = \sum_{n=1}^{\infty} \overline{I_n} \sin 2\pi n \frac{\phi}{\phi_0} \tag{27}$$

with the Fourier coefficients $I_n^{(0)}$ of the persistent current $I^{(0)}(\phi)$ of an isolated ring containing N_r^+ non-interacting fermions. The $I_n^{(0)}$ are of the form

$$I_n^{(0)} = \frac{2ew}{h}\frac{1}{n\pi} \begin{cases} (-1)^n & \text{for } N_r^+ \text{ odd} \\ 1 & \text{for } N_r^+ \text{ even.} \end{cases} \tag{28}$$

Note that the sign of the $I_n^{(0)}$ depends on the parity of the particle number N_r^+ for odd n, whereas for even n it does not. Therefore, there is also an important difference between the averaged Fourier coefficients $\overline{I_n}$ for odd and even n, respectively. We investigate the Fourier coefficients $\overline{I_n}$ normalized with respect to the $I_n^{(0)}$:

$$\overline{i_n} = \frac{\overline{I_n}}{I_n^{(0)}} \tag{29}$$

and in particular $\overline{i_1}$ and $\overline{i_2}$. The behaviour of these two in the limits $e^2/C \to 0$ and $e^2/C \to \infty$ is representative for all $\overline{i_n}$ with odd and even n, respectively.

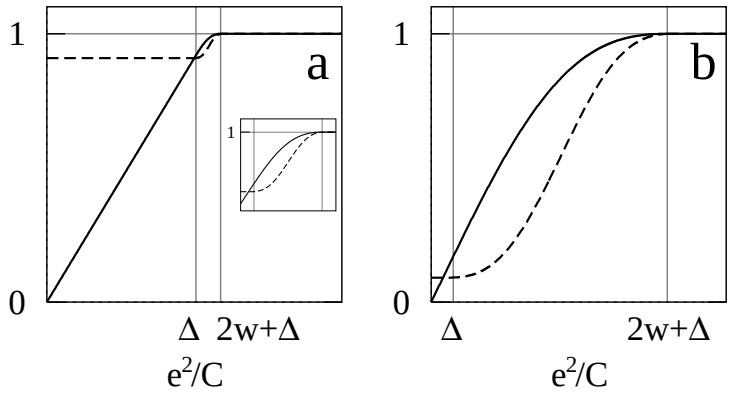

Figure 4. Normalized Fourier coefficients of the persistent current. The full lines stand for $\overline{i_1}$, the dashed ones for $\overline{i_2}$. (a) shows the results for a stub that is much shorter than the ring circumference ($L_r = 10L_s$ or equivalently $\Delta = 10w$). The inset shows the behaviour of $\overline{i_{1,2}}$ in the crossover region $\Delta < e^2/C < 2w + \Delta$. (b) shows the results for a stub that is much longer than the ring circumference: $w = 10\Delta$. In both cases $\overline{i_1} = \overline{i_2} = 1$ for $e^2/C \geqslant 2w + \Delta$. For $e^2/C \leqslant \Delta$ one finds that $\overline{i_1}$ goes linearly to zero whereas $\overline{i_2}$ = constant in both (a) and (b). Note that in the case (b) of the long stub, the second Fourier coefficient is very small ($\overline{i_2} \ll 1$) for $e^2/C \to 0$.

We obtain the $\overline{I_n}$ (and thus the $\overline{i_n}$) by calculating first the average persistent current $\overline{I(\phi)}$ as described in section 4 and then extracting them by Fourier transformation. The first normalized Fourier coefficient $\overline{i_1}$ vanishes linearly for $e^2/C \to 0$ (in fact, for $e^2/C < \Delta$) and goes to 1 for $e^2/C \geqslant 2w + \Delta$. For $\overline{i_2}$ the situation is a little more complicated. It goes to 1 as $e^2/C \geqslant 2w + \Delta$. For small Coulomb energies, however,

$$\overline{i_2} = \frac{\Delta}{w + \Delta} \qquad \text{for } \frac{e^2}{C} < \Delta \tag{30}$$

i.e. for $w \gg \Delta$ one has $\overline{I_2} \ll I_2^{(0)}$, whereas for $w \ll \Delta$ we find $\overline{I_2} \approx I_2^{(0)}$. The results are sketched in figure 4.

We interpret these findings as follows. For e^2/C large enough, the average persistent current becomes insensitive to the side stub. This is true for short as well as for long stubs. In the sense of the 'grand canonical' and 'canonical' limits, introduced in section 4, this indicates that the difference between canonical and grand canonical ensembles is less important for interacting than for non-interacting systems (cf. also [15]). For $e^2/C \to 0$ on the other hand, there is a difference between short and long stubs. If the stub is long, one has $w \gg \Delta$ and $\overline{I_2} \ll I_2^{(0)}$. As $\overline{I_1}$ vanishes in any case in this limit, the average persistent current vanishes, too. This is the behaviour predicted in [42] for a ring in the grand canonical ensemble, i.e. an open ring. If $w \ll \Delta$, that is, for a short stub, $\overline{i_2}$ does not vanish as e^2/C approaches zero but tends to a finite limit which in turn means that the persistent current becomes $(\phi_0/2)$-periodic. This is what one finds for a canonical (closed) ensemble of clean rings containing non-interacting fermions [32, 42]. There is a crossover from $(\phi_0/2)$-periodicity to ϕ_0-periodicity in the energy interval $0 < e^2/C < \Delta$.

Let us point out that in the limit $e^2/C \to 0$ the average persistent current near $\phi = 0$ is positive (it may be very small, though, for small Δ, as discussed above), since $\overline{I_1}$ vanishes, and $\overline{I_2}$ is always positive. Thus, in the absence of Coulomb interactions, the ensemble shows a paramagnetic response, a feature not observed in the experiment [12]. In contrast, in our system, in the case of strong Coulomb interactions, the response of the ensemble can be either diamagnetic or paramagnetic.

We have not taken into account the effect of quantum fluctuations on the persistent current yet. This is done by taking the derivative of (25) with respect to ϕ. The correction is of order $|t|^2$ with respect to $\overline{I(\phi)}$. Even for $e^2/C \geqslant 2w + \Delta$ it causes only small deviations from the quasi-classical result $\overline{i_n} = 1$. The conclusions concerning the persistent current drawn from the quasi-classical picture remain valid. A stronger effect is seen in the particle number fluctuations which we will discuss now.

6. Particle number fluctuations

In the picture of the incoherent Coulomb blockade (no hopping, $\hat{\Gamma} = 0$), the particle number N_r in the ring can be determined using the conditions for incoherent charge transfer (8), (9). Figure 5 shows the domains with definite N_r in the flux–energy plane. The particle number fluctuations can be read off this picture:

$$\overline{(\Delta N_r^2)}_{inc} \equiv \overline{N_r^2} - \overline{N_r}^2 = \max\left\{0, 1 - \left(\frac{e^2}{C} + \Delta + 2w\frac{|\phi|}{\phi_0/2}\right)\Big/ 2(w + \Delta)\right\} \tag{31}$$

the index 'inc' referring to the incoherent Coulomb blockade model. This formula holds for N_r^+ odd; for N_r^+ even, the absolute value of the flux $|\phi|$ is replaced by $\phi_0/2 - |\phi|$.

We shall discuss two cases, depending on the charging energy e^2/C (and on ϕ).

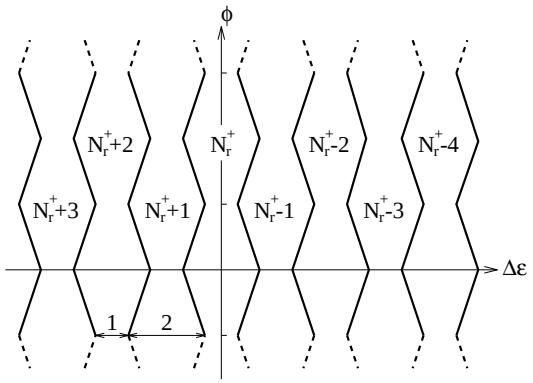

Figure 5. Domains of integer charge states in the ring for N_r^+ odd, in the flux–energy plane. The boundaries of the charge states are indicated by solid lines. The marks on the ϕ-axis are at $n\phi_0/2$, $n = \pm 1, \pm 2, \ldots$. The scale on the abscissa is indicated by the lines 1 and 2, where the length of 1 is $\Delta + e^2/C$, and the length of 2 is $2w + \Delta + e^2/C$.

(i) If e^2/C is sufficiently small we have $\overline{(\Delta N_r^2)_{inc}} > 0$. There is real hopping and equations (8), (9) are fulfilled for some ensemble member. We point out that in this range of e^2/C, quantum contributions to the particle number fluctuations given by equation (31) are irrelevant. If we consider for a moment an individual member of the ensemble, quantum fluctuations are very important (of order 1 in $|t|$) near a resonance; see equation (12). However, the width in energy of the resonance is only of order $|t|$. Thus the quantum contribution of such a resonance to the ensemble average is only of order $|t|/(2w+\Delta) \ll 1$.

(ii) There is only virtual hopping, equations (8) and (9) are never fulfilled, and $\overline{(\Delta N_r^2)_{inc}} = 0$. We can apply the second-order perturbation theory results from section 3.2, giving (26). The sums can be explicitly evaluated, e.g. in a symmetric narrow-band model with band width 2Λ. We assume $\epsilon^{(r)}_{N_r^+}(\phi), \epsilon^{(s)}_{N_s^+} \gg \Lambda \gg w, \Delta$ so that we can linearize the spectra:

$$\epsilon^{(r)}_{N_r^+ + k}(\phi) = \begin{cases} \epsilon^{(r)}_{N_r^+}(\phi) + kw & \text{if } k \text{ is even} \\ \epsilon^{(r)}_{N_r^+ + 1}(\phi) + (k-1)w & \text{if } k \text{ is odd} \end{cases} \tag{32}$$

$$\epsilon^{(s)}_{N_s^+ + l} = \epsilon^{(s)}_{N_s^+} + l\Delta. \tag{33}$$

To evaluate the expression (26) we shall replace the sums by integrals and set $|t_{ij}|^2 = \text{constant} = |t|^2$. With these specifications we obtain

$$\Delta N_r^2 \approx \begin{cases} \dfrac{2|t|^2}{w\Delta} \log\left(\dfrac{\Lambda}{e^2/2C}\right) + \mathrm{O}\left(\dfrac{1}{\Lambda}\right) & \Lambda \gg e^2/2C \gg w, \Delta \\ \dfrac{2|t|^2}{w\Delta}\left(\dfrac{\Lambda}{e^2/2C}\right)^2 + \mathrm{O}\left(\left(\dfrac{e^2}{2C}\right)^{-3}\right) & e^2/2C \gg \Lambda. \end{cases} \tag{34}$$

Thus the result depends crucially on the relation of the band width Λ to the charging energy. It remains to take the ensemble average, but equations (34) do not depend on the ensemble member; thus $\overline{\Delta N_r^2} = \Delta N_r^2$.

The behaviour of the ensemble-averaged particle number fluctuations as a function of e^2/C is summarized in figure 6. The incoherent fluctuations, associated with different particle numbers N_r in the ring in different ensemble members, and thus associated with

resonant charge transfer, vanish linearly for increasing charging energy as discussed in (i) above. In the picture of the incoherent Coulomb blockade, a large enough charging energy therefore suppresses the hybridization completely. A purely quantum mechanical signature of hybridization, however, survives far into the off-resonant region, as demonstrated by equations (34).

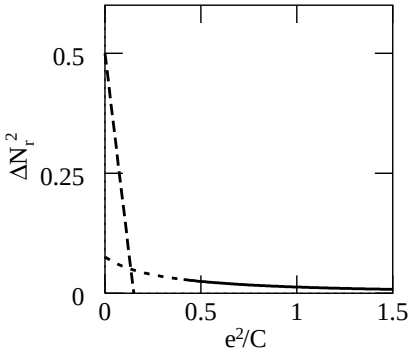

Figure 6. Particle number fluctuations as a function of e^2/C. The result in the incoherent Coulomb blockade model $\overline{(\Delta N_r^2)_{inc}}$ (dashed line) and the off-resonant result $\overline{\Delta N_r^2}$ for $e^2/C > 2w + \Delta$ (solid line), continued beyond its range of validity (short-dashed line) are shown for $\phi = \pm\phi_0/4$, $|t| = 0.02$, $w = 0.1$, $\Delta = 0.2$. All of the energies are given in units of the band width Λ.

7. Potential fluctuations

The electrostatic potential on the ring is connected to the particle number on the ring via

$$U_r = \frac{Q_r}{C} = \frac{e(N_r^+ - N_r)}{C}. \tag{35}$$

Replacing c-numbers by operators, we find that it exhibits therefore fluctuations related to the particle number fluctuations:

$$\Delta U_r^2 \equiv \langle \hat{U}_r{}^2 \rangle - \langle \hat{U}_r \rangle^2 = \frac{4}{e^2}\left(\frac{e^2}{2C}\right)^2 \Delta N_r^2. \tag{36}$$

For intermediate charging energies $w, \Delta \ll e^2/2C \ll \Lambda$, we find potential fluctuations that are *growing* with the charging energy:

$$\Delta U_r^2 = \frac{8|t|^2}{e^2 w \Delta}\left(\frac{e^2}{2C}\right)^2 \log\left(\frac{2\Lambda}{e^2/2C}\right) \tag{37}$$

whereas for higher charging energies $e^2/2C \gg \Lambda$ they tend towards a constant:

$$\Delta U_r^2 = \frac{8|t|^2\Lambda^2}{e^2 w \Delta}. \tag{38}$$

Within the range of validity of the perturbation theory [41], $|t| \ll w, \Delta$, the fluctuations in the single-particle spectrum induced by potential fluctuations $e(\Delta U_r^2)^{1/2}$ are in both cases much smaller than the charging energy $e^2/2C$, but not necessarily smaller than the level width w and the level spacing in the stub Δ.

8. Conclusions

We present an investigation of the competing effects of the Coulomb interaction and the hybridization of the spectra of two coupled subsystems. The model considered consists of a ring penetrated by a magnetic flux and coupled to a side branch. We discuss single systems as well as a canonical ensemble. We identify quantities that are sensitive to hybridization, namely the persistent current (equations (13), (14) and figure 3) and the particle number fluctuations in a subsystem (12) in order to identify hybridization effects not only in a single- but also in a many-particle problem. We show that the Coulomb interaction suppresses hybridization, abruptly in the standard incoherent Coulomb blockade model (equation (31) and figure 4) and smoothly when quantum effects are taken into account (equation (34)). Interestingly, even though our system is strongly canonical, for small charging energies it shows both the behaviour of a grand canonical ensemble of rings for a large side branch and the behaviour of a canonical ensemble of rings for a short side branch. Our results suggest a number of experiments in which either the persistent current (magnetization) or the charge fluctuations are measured. Such experiments can be implemented in mesoscopic structures or in large benzene-like molecules with side branches.

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