Effect of quantum fluctuations on even-odd energy difference in a Cooper-pair box

R. M. Lutchyn

W.I. Fine Theoretical Physics Institute, University of Minnesota, Minneapolis, Minnesota 55455, USA (Received 4 March 2007; published 5 June 2007)

We study the effect of quantum charge fluctuations on the discrete spectrum of charge states of a small superconducting island (Cooper-pair box) connected to a large finite-size superconductor by a tunnel junction. In particular, we calculate the reduction of the even-odd energy difference δE due to virtual tunneling of electrons across the junction. We show that the renormalization effects are important for understanding the quasiparticle "poisoning" effect because *E* determines the activation energy of a trapped quasiparticle in the Cooper-pair box. We find that renormalization of the activation energy depends on the dimensionless normalstate conductance of the junction g_T and becomes strong at $g_T \gg 1$.

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Recently, superconducting quantum circuits have attracted considerable interest (see Refs. [1](#page-3-0) and 2 , and references therein). From the viewpoint of quantum many-body phenomena, these circuits are good systems to study the effect of quantum fluctuations of an environment on the discrete spectrum of charge states $3-7$ $3-7$ (similar to the Lamb shift in a hydrogen atom). While most of the studies of superconducting nanostructures focus on smearing of the charge steps in the Coulomb staircase measurements, $\frac{8}{3}$ here we consider another observable quantity—even-odd-electron energy difference δE in the Cooper-pair box (CPB). This quantity is important for understanding the quasiparticle "poisoning" effect, $9-13$ $9-13$ and it has been recently studied experimentally. $14,15$ $14,15$ It was conjectured that δE may be reduced in the strong tunneling regime $g_T = R_a / R_N > 1$ by quantum fluctuations of the charge.¹⁴ Here R_q and R_N are the resistance quantum, R_q $=h/e²$, and normal-state resistance of the tunnel junction, respectively.

In this Brief Report, we study the renormalization of the discrete spectrum of charge states of the Cooper-pair box by quantum charge fluctuations. We show that virtual tunneling of electrons across the tunnel junction may lead to a substantial reduction of the even-odd energy difference δE . We consider here the case of the tunnel junction with a large number of low transparency channels.¹⁶

The dynamics of the system is described by the Hamiltonian

$$
H = H_C + H_{BCS}^b + H_{BCS}^r + H_T.
$$
 (1)

Here H_{BCS}^b and H_{BCS}^r are BCS Hamiltonians for the CPB and superconducting reservoir; $H_C = E_c(\hat{Q}/e - N_g)^2$ with E_c , N_g , and \hat{Q} being the charging energy, dimensionless gate voltage, and charge of the CPB, respectively. The tunneling Hamiltonian H_T is defined in the conventional way. We assume that the island and reservoir are isolated from the rest of the circuit, i.e., total number of electrons in the system is fixed. At low temperature $T < T^*$, thermal quasiparticles are frozen out. [Here $T^* = \frac{\Delta}{\ln(\Delta/\delta)}$, with Δ and δ being the superconducting gap and mean level spacing in the reservoir, respectively. If the total number of electrons in the system is even, then the only relevant degree of freedom at low energies is the phase difference across the junction φ . In the case of an odd number of electrons, a quasiparticle resides in the system even at zero temperature. The presence of 1*e*-charged carriers changes the periodicity of the CPB energy spectrum $(see Fig. 1)$ $(see Fig. 1)$ $(see Fig. 1)$ since an unpaired electron can reside in the island or in the reservoir. Note that at $N_e = 1$, a working point for the charge qubit, the odd-electron state of the CPB may be more favorable, resulting in trapping of a quasiparticle in the island. $14,15,17$ $14,15,17$ $14,15,17$ In order to understand the energetics of this trapping phenomenon, one has to look at the ground-state energy difference δE between the even-charge state (no quasiparticles in the CPB) and odd-charge state (with a quasiparticle in the CPB):

$$
\delta E = E_{\text{even}}(N_g = 1) - E_{\text{odd}}(N_g = 1),\tag{2}
$$

see also Fig. [1.](#page-1-0) For equal gap energies in the box and the reservoir $(\Delta_r = \Delta_b = \Delta)$, the activation energy δE is determined by the effective charging energy of the CPB. Note that tunneling of an unpaired electron into the island shifts the net charge of the island by 1e. Thus, one can find δE of Eq. ([2](#page-0-0)) as the energy difference at two values of the induced charge, N_g =1 and N_g =0, on the even-electron branch of the spectrum (see Fig. 1):

$$
\delta E = E_{\text{even}}(N_g = 1) - E_{\text{even}}(N_g = 0). \tag{3}
$$

Here we assumed that subgap conductance due to the presence of an unpaired electron is negligible.¹⁸

In order to find the activation energy δE given by Eq. ([3](#page-0-1)), we calculate the partition function $Z(N_g)$ for the system, island and reservoir, with even number of electrons. For the present discussion, it is convenient to calculate the partition function using the path-integral description developed by Ambegaokar *et al.*^{[19](#page-3-12)} In this formalism, the quadratic in \hat{Q} interaction in Eq. (1) (1) (1) is decoupled with the help of Hubbard-Stratonovich transformation by introducing an auxiliary field φ (conjugate to the excess number of Cooper pairs on the island). Then, the fermion degrees of freedom are traced out, and around the BCS saddle point, the partition function becomes

FIG. 1. (Color online) Energy of the Cooper-pair box as a function of dimensionless gate voltage N_g in units of e . The solid line corresponds to even-charge state of the box; dashed line corresponds to the odd-charge state of the box. Here, δE is the groundstate energy difference between the even-charge state (no quasiparticles in the CPB) and odd-charge state (an unpaired electron in the CPB) at N_g =1. (We assume here equal gap energies in the box and reservoir, $\Delta_r = \Delta_b = \Delta.$)

$$
Z(N_g) = \sum_{m=-\infty}^{\infty} e^{i\pi N_g m} \int d\varphi_0 \int_{\varphi(0)=\varphi_0}^{\varphi(\beta)=\varphi_0+2\pi m} D\varphi(\tau) e^{-S}.
$$
 (4)

Here, the summation over winding numbers accounts for the discreteness of the charge²⁰ and the action *S* reads $(h=1)$

$$
S = \int_0^\beta d\tau \left[\frac{C_{\text{geom}}}{2} \left(\frac{\dot{\varphi}(\tau)}{2e} \right)^2 - E_J \cos \varphi(\tau) \right] + \int_0^\beta d\tau \int_0^\beta d\tau' \alpha(\tau - \tau') \left\{ 1 - \cos \left[\frac{\varphi(\tau) - \varphi(\tau')}{2} \right] \right\}, \tag{5}
$$

with β being the inverse temperature, $\beta = 1/T$. Here C_{geom} is the geometric capacitance of the CPB, which determines the bare charging energy $E_c = e^2 / 2C_{\text{geom}}$, and E_J is the Josephson coupling given by the Ambegaokar-Baratoff relation. The last term in Eq. (5) (5) (5) accounts for single-electron tunneling with kernel $\alpha(\tau)$ decaying exponentially at $\tau \gg \Delta^{-1}$.^{[19](#page-3-12)} For sufficiently large capacitance, the evolution of the phase is slow in comparison with Δ^{-1} and we can simplify the last term in Eq. (5) (5) (5) as

$$
\int_0^\beta d\tau \int_0^\beta d\tau' \alpha(\tau - \tau') \left\{ 1 - \cos \left[\frac{\varphi(\tau) - \varphi(\tau')}{2} \right] \right\}
$$

$$
\approx \frac{3\pi^2}{128} \frac{1}{2\pi e^2 R_N \Delta} \int_0^\beta d\tau \left[\frac{d\varphi(\tau)}{d\tau} \right]^2.
$$
 (6)

It follows from here that virtual tunneling of electrons be-

tween the island and reservoir leads to the renormalization of the capacitance¹⁹

$$
C_{\text{geom}} \to \tilde{C} = C_{\text{geom}} + \frac{3\pi}{32} \frac{1}{R_N \Delta}.
$$
 (7)

Within the approximation (6) (6) (6) , the effective action acquires simple form

$$
S_{\text{eff}} = \int_0^\beta d\tau \left\{ \frac{\tilde{C}}{2} \left[\frac{\dot{\varphi}(\tau)}{2e} \right]^2 - E_J \cos \varphi(\tau) \right\}.
$$
 (8)

To calculate $Z(N_g)$, one can use the analogy between the present problem and that of a quantum particle moving in a periodic potential, and write the functional integral as a quantum-mechanical propagator from $\varphi_i = \varphi_0$ to $\varphi_f = \varphi_0$ +2 π *m* during the (imaginary) "time" β

$$
\int_{\varphi(0)=\varphi_0}^{\varphi(\beta)=\varphi_0+2\pi m} D\varphi(\tau) \exp(-S_{\rm eff}) = \langle \varphi_0 | e^{-\beta \hat{H}_{\rm eff}} | \varphi_0 + 2\pi m \rangle.
$$
\n(9)

The time-independent "Schrödinger equation" corresponding to such problem has the form 21

$$
\hat{H}_{\rm eff}\Psi(\varphi) = E\Psi(\varphi), \quad \hat{H}_{\rm eff} = \left(-4\tilde{E}_c \frac{\partial^2}{\partial \varphi^2} - E_J \cos \varphi\right).
$$
\n(10)

Here, \tilde{E}_c denotes renormalized charging energy

$$
\widetilde{E}_c = \frac{E_c}{1 + \frac{3}{32} g \cdot \frac{E_c}{\Delta}}.
$$
\n(11)

One can notice that Eq. (10) (10) (10) corresponds to the well-known Mathieu equation for which eigenfunctions $\Psi_{k,s}(\varphi)$ are known.²² Here, quantum number *s* labels Bloch band (*s* $=0,1,2,...$), and *k* corresponds to the "quasimomentum." By rewriting the propagator (9) (9) (9) in terms of the eigenfunctions of the Schrödinger equation (10) (10) (10) , we obtain

$$
\langle \varphi_0 | e^{-\beta \hat{H}_{\rm eff}} | \varphi_0 + 2 \pi m \rangle = \sum_{k,k'} \langle \varphi_0 | | k \rangle \langle k | e^{-\beta \hat{H}_{\rm eff}} | k' \rangle \langle k' | | \varphi_0 + 2 \pi m \rangle
$$

$$
= \sum_{k,s} \Psi_{k,s}^* (\varphi_0) \Psi_{k,s} (\varphi_0 + 2 \pi m)
$$

$$
\times \exp[-\beta E_s(k)]. \qquad (12)
$$

Here $E_s(k)$ are eigenvalues of Eq. ([10](#page-1-3)).

According to the Bloch theorem, the eigenfunctions should have the form $\Psi_{k,s}(\varphi) = e^{ik\varphi/2}u_{k,s}(\varphi)$, with $u_{k,s}(\varphi)$ being 2π -periodic functions, $u_{k,s}(\varphi) = u_{k,s}(\varphi + 2\pi)$. We can now rewrite Eq. ([4](#page-1-5)) as

FIG. 2. (Color online) Dependence of the even-odd energy difference δE on the dimensionless parameter $E_J/2\tilde{E}_c$.

$$
Z(N_g) = \sum_{m=-\infty}^{\infty} e^{i\pi N_g m} \int d\varphi_0 \sum_{k,s} \Psi_{k,s}^*(\varphi_0) \Psi_{k,s}(\varphi_0 + 2\pi m)
$$

$$
\times \exp[-\beta E_s(k)] = \sum_{s=0,1}^{\infty} \exp[-\beta E_s(N_g)]. \tag{13}
$$

The eigenvalues $E_s(N_g)$ are given by the Mathieu characteristic functions $M_A(r,q)$ and $M_B(r,q)$.^{[23](#page-3-16)} At $N_g=0$ and $N_g=1$, the exact solution for the lowest band reads

$$
E_0(N_g = 0) = \widetilde{E}_c M_A \left(0, -\frac{E_J}{2\widetilde{E}_c} \right),
$$

$$
E_0(N_g = 1) = \widetilde{E}_c M_A \left(1, -\frac{E_J}{2\widetilde{E}_c} \right).
$$
 (14)

The activation energy δE can be calculated from Eq. ([13](#page-2-0)) by evaluating the free energy at *T*=0:

$$
\delta E = \widetilde{E}_c \left[M_A \left(1, -\frac{E_J}{2\widetilde{E}_c} \right) - M_A \left(0, -\frac{E_J}{2\widetilde{E}_c} \right) \right].
$$
 (15)

The plot of δE as a function of $E_J/2\tilde{E}_c$ is shown in Fig. [2.](#page-2-1) Even-odd energy difference δE has the following asymptotes:

 δE

$$
\approx \begin{cases} \tilde{E}_c - \frac{1}{2} E_J, & E_J/2\tilde{E}_c \ll 1, \\ 2^5 \sqrt{\frac{2}{\pi}} \tilde{E}_c \left(\frac{E_J}{2\tilde{E}_c}\right)^{3/4} \exp\left(-4\sqrt{\frac{E_J}{2\tilde{E}_c}}\right), & E_J/2\tilde{E}_c \gg 1. \end{cases}
$$

These asymptotes can also be obtained using perturbation theory and Wentzel-Kramers-Brillouin approximation, respectively.

As one can see from Eq. (15) (15) (15) , δE can be reduced by quantum charge fluctuations. For realistic experimental parameters,¹⁴ $\Delta \approx 2.5$ K, $E_c \approx 2$ K, and $g_T \approx 2$, we find that even-odd energy difference δE is 15% smaller with respect to its bare value, i.e., $\delta E \approx 1.45$ K and $\delta E^{\text{bare}} \approx 1.7$ K. Since the reduction of the activation energy by quantum fluctuations is much larger than the temperature, this effect can be observed experimentally. The renormalization of δE can be studied systematically by decreasing the gap energy Δ , which can be achieved by applying magnetic field *B*. [3](#page-3-2) The dependence of the activation energy δE on $\Delta(B)$ in Eq. ([15](#page-2-2)) enters through the Josephson energy E_I , which is given by the Ambegaokar-Baratoff relation, and renormalized charging energy \tilde{E}_c of Eq. ([11](#page-1-6)).

The renormalization of the discrete spectrum of charge states in the CPB becomes more pronounced in the strong tunneling regime. However, the adiabatic approximation leading to the effective action S_{eff} ([8](#page-1-7)) is valid when the evolution of the phase is slow, i.e., the adiabatic parameter ω_I/Δ is small. (Here, ω_I is the plasma frequency of the Josephson function, $\omega_j \sim \sqrt{E_c E_j}$. Thus, at large conductances g_T , the adiabatic approximation holds only when the geometric capacitance is large, $C_{\text{geom}} \geq e^2 g_T / \Delta$. Under such conditions, the renormalization effects lead to a small correction of the capacitance, see Eq. ([7](#page-1-8)). If $\omega_J/\Delta > 1$, the dynamics of the phase is described by the integral equation (5) (5) (5) , and retardation effects have to be included.

In a similar circuit corresponding to the Cooper-pair box qubit, $1,2$ $1,2$ it is possible to achieve strong tunneling regime, $g_T \gg \Delta C_{\text{geom}}/e^2$, and satisfy the requirements for adiabatic approximation $(\omega_J/\Delta \ll 1)$. In this circuit, a single Josephson junction is replaced by two junctions in a loop configuration.^{1[,2](#page-3-1)} This allows one to control the effective Josephson energy using an external flux Φ_{r} . For the CPB qubit, the Josephson energy E_J in Eq. ([8](#page-1-7)) should be replaced with $E_J(\Phi_x) = 2E_J^0 \cos(\pi \Phi_x / \Phi_0)$; here, Φ_0 is the magnetic flux quantum, $\Phi_0 = h/2e$, and E_J^0 is the Josephson coupling per junction.] In this setup, even at large conductance g_T $\gg \Delta C_{\text{geom}}/e^2$ one can decrease $\omega_J \sim \sqrt{E_c E_J(\Phi_x)}$ by adjusting the external magnetic flux to satisfy $\omega_J/\Delta \ll 1$. Under such conditions, the quantum contribution to the capacitance *C˜* [see Eq. (7) (7) (7)] becomes larger than the geometric one, while the dynamics of the phase is described by the simple action of Eq. (8) (8) (8) . It would be interesting to study experimentally the renormalization of the discrete energy spectrum of the qubit in this regime. We propose to measure, for example, the even-odd energy difference δE . In this case, δE is determined by the conductance of the junctions g_T , superconducting gap Δ , and magnetic flux Φ_x , and is given by Eq. ([15](#page-2-2)) with $E_c \approx 32\Delta/3g_T$ [see Eq. ([11](#page-1-6))] and E_J $= 2E_J^0 \cos(\pi \Phi_x / \Phi_0).$

In conclusion, we studied the renormalization of the discrete spectrum of charge states of the Cooper-pair box by virtual tunneling of electrons across the junction. In particular, we calculated the reduction of even-odd energy difference δE by quantum charge fluctuations. We showed that under certain conditions, the contribution of quantum charge fluctuations to the capacitance of the Cooper-pair box may become larger than the geometric one. We propose to study this effect experimentally using the Cooper-pair box qubit.

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