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

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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 $\delta E$ due to virtual tunneling of electrons across the junction. We show that the renormalization effects are important for understanding the quasiparticle “poisoning” effect because $\delta E$ 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 normal-state conductance of the junction $g_r$, and becomes strong at $g_r \gg 1$.

Recently, superconducting quantum circuits have attracted considerable interest (see [1,2] 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 [4,5] (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, here we consider another observable quantity - even-odd-electron energy difference $\delta E$ in the Cooper-pair box (CPB). This quantity is important for understanding the quasiparticle “poisoning” effect [9,10,11,12,13], and it has been recently studied experimentally [13-15]. It was conjectured that $\delta E$ may be reduced in the strong tunneling regime $g_r = R_g/R_N > 1$ by quantum fluctuations of the charge [14]. Here $R_q$ and $R_N$ are the resistance quantum, $R_q = h/e^2$, and normal-state resistance of the tunnel junction, respectively.

In this paper, 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 $\delta E$. 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

$$\label{eq:1} H = H_C + H_{\text{BCS}}^b + H_{\text{BCS}}^r + H_r.$$ 

Here $H_{\text{BCS}}^b$ and $H_{\text{BCS}}^r$ are BCS Hamiltonians for the CPB and superconducting reservoir; $H_C = E_c (Q/e - N_g)^2$ with $E_c$, $N_g$ and $Q$ being the charging energy, dimensionless gate voltage and charge of the CPB, respectively. The tunneling Hamiltonian $H_r$ 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 $\Delta$ and $\delta$ being superconducting gap and mean level spacing in the reservoir, respectively.)

If 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 $\varphi$. In the case of an odd number of electrons a quasiparticle resides in the system even at zero temperature. The presence of 1e-charged carriers changes the periodicity of the CPB energy spectrum (see Fig. 1) since an unpaired electron can reside in the island or in the reservoir. Note that at $N_g = 1$, 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]. In order to understand energetics of this trapping phenomenon, one has to look at the ground state energy difference $\delta E$ between the even-charge state (no quasiparticles in the CPB), and odd-charge state (with a quasiparticle in the CPB):

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

see also Fig. 1. For equal gap energies in the box and the reservoir ($\Delta_r = \Delta_b = \Delta$) the activation energy $\delta E$ 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 $e$. Thus, one can find $\delta E$ of Eq. (2) 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):

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

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

In order to find activation energy $\delta E$ given by Eq. (3), 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, Eckern and Schön [18]. In this formalism the quadratic in $\hat{Q}$ interaction in Eq. (1) is decoupled with the help of Hubbard-Stratonovich transformation by introducing an auxiliary field $\varphi$ (conjugate to the excess number of Cooper pairs on the island). Then, the fermion degrees of Cooper pairs are traced out, and around the BCS saddle-point the partition function be-
comes

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

(4)

Here the summation over winding numbers accounts for the discreteness of the charge, and the action \( S \) reads (\( \hbar = 1 \))

\[ S = \int_0^\beta d\tau \left[ \frac{C_{\text{geom}}}{2} \left( \frac{\varphi(\tau)}{2e} \right)^2 - E_J \cos \varphi(\tau) \right] \]

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

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

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

(6)

It follows from here that virtual tunneling of electrons between the island and reservoir leads to the renormalization of the capacitance

\[ C_{\text{geom}} \to \tilde{C} = C_{\text{geom}} + \frac{3\pi}{32} \frac{1}{R_N \Delta}. \]

(7)

Within the approximation, 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 \( \varphi_f = \varphi_0 + 2\pi m \) during the (imaginary) “time” \( \beta \)

\[ \int_{\varphi(0)=\varphi_0}^{\varphi(\beta)=\varphi_0+2\pi m} D\varphi(\tau) \exp(-S_{\text{eff}}) = \langle \varphi_0 | e^{-\beta \tilde{H}_{\text{eff}}} | \varphi_0 + 2\pi m \rangle. \]

(9)

The time-independent “Shrödinger equation” corresponding to such problem has the form

\[ \tilde{H}_{\text{eff}} \Psi(\varphi) = E \Psi(\varphi), \quad \tilde{H}_{\text{eff}} = \left( -4 \tilde{E}_c \frac{\partial^2}{\partial \varphi^2} - E_J \cos \varphi \right). \]

(10)

Here \( \tilde{E}_c \) denotes renormalized charging energy

\[ \tilde{E}_c = \frac{E_c}{1 + \frac{3}{32} g_r \frac{E_c}{\Delta}}. \]

(11)

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

\[ \langle \varphi_0 | e^{-\beta \tilde{H}_{\text{eff}}} | \varphi_0 + 2\pi m \rangle = \sum_{k,k'} \langle \varphi_0 | k \rangle \langle k | e^{-\beta \tilde{H}_{\text{eff}}} | k' \rangle \langle k' | \varphi_0 + 2\pi m \rangle \]

\[ = \sum_{k,k,s} \Psi_{k,s}(\varphi_0) \Psi_{k,s}(\varphi_0 + 2\pi m) \exp(-\beta E_s(k)). \]

Here \( E_s(k) \) are eigenvalues of Eq. (10).

According to the Bloch theorem, the eigenfunctions should have the form \( \Psi_{k,s}(\varphi) = e^{ik\varphi/\beta} u_{k,s}(\varphi) \) with \( u_{k,s}(\varphi) \) being 2\( \pi \)-periodic functions, \( u_{k,s}(\varphi) = \)
The eigenvalues $E_s(N_g)$ are given by the Mathieu characteristic functions $M_A(r, q)$ and $M_B(r, q)^\ast$. At $N_g = 0$ and $N_g = 1$, the exact solution for the lowest band reads

$$E_0(N_g = 0) = \tilde{E}_c, M_A(0, -\frac{E_J}{2E_c}),$$

$$E_0(N_g = 1) = \tilde{E}_c, M_A(1, -\frac{E_J}{2E_c}).$$

The activation energy $\delta E$ can be calculated from Eq. (13) by evaluating free energy at $T = 0$:

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

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

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

These asymptotes can be also obtained using perturbation theory and WKB approximation, respectively.

As one can see from Eq. (15), $\delta E$ can be reduced by quantum charge fluctuations. For realistic experimental parameters $\Delta \approx 2.5K$, $E_c \approx 2K$ and $g_J \approx 2$, we find that even-odd energy difference $\delta E$ is $15\%$ smaller with respect to its bare value, i.e. $\delta E \approx 1.45K$ and $\delta E^\text{bare} \approx 1.7K$. 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 $\delta E$ can be studied systematically by decreasing the gap energy $\Delta$, which can be achieved by applying magnetic field $B$ [3]. The dependence of the activation energy $\delta E$ on $\Delta(B)$ in Eq. (15) enters through the Josephson energy $E_J$, which is given by Ambegaokar-Baratoff relation, and renormalized charging energy $\tilde{E}_c$ of Eq. (11).

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 $S_{\text{eff}}$ [8] is valid when the dimensionless parameter $E_J/2\tilde{E}_c$. In conclusion, we studied the renormalization of the discrete spectrum of charge states of the Cooper-pair box with virtual tunneling of electrons across the junction. In particular, we calculated the reduction of even-odd energy difference $\delta E$ 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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