Macroscopic quantum dynamics of $\pi$-junctions with ferromagnetic insulators

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We theoretically investigate the macroscopic quantum dynamics of a $\pi$ junction with a superconductor (S) and a multiferroic material or a ferromagnetic insulator (FI). By deriving the effective action from a microscopic Hamiltonian, a $\pi$-junction qubit (a S-FI-S superconducting quantum interference device ring) is proposed. In this qubit, a quantum two-level system is spontaneously generated and the effect of the quasiparticle dissipation is found to be very weak. These features make it possible to realize a quiet qubit with high coherency. We also investigate macroscopic quantum tunneling (MQT) in current-biased S-FI-S $\pi$ junctions and show that the influence of the quasiparticle dissipation on MQT is negligibly small.

When two superconductors are weakly coupled via a thin insulating barrier, a direct current can flow even without bias voltage. The driving force of this supercurrent is the phase difference in the macroscopic wave function. The supercurrent $I$ and the phase difference $\phi$ across the junction have a relation $I = I_C \sin \phi$ with $I_C > 0$ being the critical current. If the weak link consists of a thin ferromagnetic metal (FM) layer, the result can be a Josephson junction with a built-in phase difference of $\pi$. Physically this is a consequence of the phase change of the order parameter induced in the FM by the proximity effect. Superconductor (S)-FM-S Josephson junctions presenting a negative coupling or a negative $I_C$ are usually called $\pi$ junctions and such behavior has been reported experimentally.

As proposed by Bulaevskii et al., a superconducting ring with a $\pi$ junction [a $\pi$ superconducting quantum interference device (SQUID)] exhibits a spontaneous current without an external magnetic field and the corresponding magnetic flux is half a flux quantum $\Phi_0$ in the ground state. Therefore it is expected that a S-FM-S $\pi$ SQUID system becomes a quiet qubit that can be efficiently decoupled from the fluctuation of the external field. From the viewpoint of quantum dissipation, however, the structure of S-FM-S junctions is inherently identical with S-N-S junctions (where N is a normal nonmagnetic metal). Therefore a gapless quasiparticle excitation in the FM layer is inevitable. This feature gives a strong Ohmic dissipation and the coherence time of S-FM-S qubits is bound to be very short. In practice the current-voltage characteristic of a S-FM-S qubit is bound to be very short.

First, we will calculate the effective action for S-FI-S Josephson junctions by using the functional integral method. S-FI-S Josephson junctions consist of two superconductors (L and R) and a thin FI barrier [Fig. 1(a)]. The Hamiltonian of S-FI-S junctions is conveniently given by $H = H_L + H_R + H_T + H_Q$, where $H_L(R)$ is the Hamiltonian describ-
ing the left (right) superconductor electrodes: $\mathcal{H}_L = \sum_x \int dr \psi_L^\dagger(r) \left(-\frac{h^2 \nabla^2}{2m} - \mu\right) \psi_L(r) - \left(g_\ell/2\right) \sum_x \int dr \psi_L^\dagger (r) \psi_L^\dagger (r) \psi_L (r) \psi_L (r)$, where $\psi_L$ is the electron field operator for the spin $\sigma = \uparrow, \downarrow$, $m$ is the electron mass, and $\mu$ is the chemical potential. The coupling between two superconductors is due to the transfer of electrons through the FI barrier and to the Coulomb interaction term $\mathcal{H}_Q = (Q_L - Q_R)^2/2C$, where $C$ is the capacitance of the junction and $Q_{L(R)} = e \sum_x \int dr \psi_{L(R)}^\dagger (r) \psi_{L(R)} (r)$ is the operator for the charge on the superconductor L(R). The former is described by the tunneling term $\mathcal{H}_T = \sum_x \int dxd\tau' [T_\sigma(r, r') \psi_L^\dagger (r) \psi_R (r')] + H.C.$, where $H.C.$ stands for higher correlated terms. The FI barrier can be described by a potential $\mathcal{V}_\rho(r) = \rho_s V \delta(x)$, where $\rho_s = 1$ and $\rho_\parallel = -1$ [see Fig. 1(b)]. In the high-barrier limit ($Z \equiv mV/h^2k_F \gg 1$), the tunneling matrix element is given by $T_\sigma(k, k') = i \rho_s k_x / (k_F Z) \delta_{k_x, k'_x} \delta_{k_y, k'_y}$, where $k_F$ is the Fermi wave number. The spin dependence of $T_\sigma$ is essential for the formation of the $\pi$ coupling.

Examples of FIs include the $f$-electron systems EuX (X=O, S, and Se)\textsuperscript{25,26} ferrites,\textsuperscript{27} earth rare-nitrides (e.g., GdN),\textsuperscript{28,29} insulating barriers with magnetic impurities\textsuperscript{27} (e.g., amorphous FeSi alloys),\textsuperscript{28} Fe-filled semiconductor carbon nanotubes\textsuperscript{30} and single molecular magnets (e.g., Mn$_{12}$ derivatives).\textsuperscript{31} Multiferroic materials\textsuperscript{32,33} and the Jahn-Teller orbital-ordered systems (e.g., Ti oxides\textsuperscript{34} and Mn oxides\textsuperscript{35,36}), and the spinels (e.g., CdCr$_2$S$_4$\textsuperscript{37} and CoCr$_2$O$_4$\textsuperscript{38,39}) can serve as a FI. It has been recently shown theoretically that a FI can be also induced by doping in wide band-gap semiconductors such as ZnO and GaN\textsuperscript{40}. However, it is still an open question whether any of these materials posses the spin dependent potential shown in Fig. 1(b). This problem will be addressed in a future study.

The partition function $Z$ of the junction can be written as an imaginary time path integral over the complex Grassmann fields:\textsuperscript{30} $Z = \int D\bar{\psi} D\psi \exp(-\int_0^{\beta} d\tau \mathcal{L}[\bar{\psi}, \psi]/\hbar)$, where $\beta = 1/k_B T$ and the Lagrangian is given by $\mathcal{L} = \sum_x \int dr \left(\bar{\psi}_x \psi_x \partial_\tau \bar{\psi}_x \psi_x - H[\bar{\psi}, \psi]\right)$. In order to write the partition function as a functional integral over the macroscopic variable (the phase difference $\phi$), we apply the Stratonovich-Hubbard transformation. This introduces a complex order parameter field $\Delta(r, \tau)$. Next the integrals over the Grassmann fields and $|\Delta| \equiv \Delta_0$ are performed by using the Gaussian integral and the saddle point approximation, respectively. Then we obtain the partition function as $Z = \int D\phi \exp(-S_{\text{eff}}[\phi]/\hbar)$, where the effective action $S_{\text{eff}}$ is given by

$$S_{\text{eff}}[\phi] = \int_0^{\beta} d\tau \left[\frac{C}{2} \left(\frac{\hbar}{2e} \partial_\tau \phi(\tau)\right)^2 - E_J \cos \phi(\tau)\right] + S_\alpha[\phi],$$

$$S_\alpha[\phi] = -\sum_{\sigma} \int_0^{\beta} dr \partial_\tau' \alpha_{\sigma} (\tau - \tau') e^{i \phi_{\sigma}(\tau, \tau')} e^{i \phi_{\sigma}(\tau - \tau')}.$$  

Here the Josephson coupling energy $E_J = (\hbar/2e) I_C$ is given in terms of the anomalous Green’s function in the left (right) superconductor $F_{L(R)}(k, \omega_n) = \hbar \Delta_0/[\hbar \omega_n + \xi_{k}^2 + \Delta_0^2]$ ($\xi_k = \hbar^2 k^2/2m - \mu$ and $\hbar \omega_n = (2n + 1)\pi/\beta$ is the fermionic Matsubara frequency):

$$E_J = \frac{2}{\hbar} \int_0^{\beta} d\tau \sum_{k, k'} T_\uparrow(k, k') T_\downarrow(k, k') \times F_{L}(k, \tau) F_{R}(k', -\tau) \approx -\frac{\Delta_0 R_Q}{4\pi R_N} < 0.$$  

In this equation, $R_Q = \hbar/4e^2$ is the resistance quantum, and $R_N$ is the normal state resistance of the junction. As expected, $E_J$ becomes negative. The formation of the $\pi$ junction can be attributed to the spin-discriminating scattering processes in the spin-dependent potential $V_\sigma(r)$. Therefore S-FI-S junctions can serve as $\pi$ junctions similar to S-FM-S junctions. $S_{\alpha}$ is the dissipation action and describes the tunneling of quasiparticles which is the origin of the quasiparticle dissipation. In Eq. 2, the dissipation kernel $\alpha_{\sigma}(\tau)$ is given by

$$\alpha_{\sigma}(\tau) = -\frac{2}{\hbar} \sum_{k, k'} \left| T_\sigma(k, k') \right|^2 G_{L}(k, \tau) G_{R}(k', -\tau),$$

where $G_{L(R)}(k, \omega_n) = \hbar i \omega_n / [\hbar \omega_n - \xi_{k}^2 + \Delta_0^2]$ is the diagonal component of the Nambu Green’s function. In the high-barrier limit ($Z \gg 1$), we obtain

$$\alpha_{\sigma}(\tau) = \frac{\Delta_0^2}{4\pi^2 e^2 R_N} K_1 \left(\frac{\Delta_0}{\hbar \tau}\right)^2,$$

where $K_1$ is the modified Bessel function. For $|\tau| \gg \hbar/\Delta_0$ the dissipation kernel decays exponentially as a function of the imaginary time $\tau$, i.e., $\alpha_{\sigma}(\tau) \sim \exp(-2\Delta_0 |\tau|/\hbar)$. If the phase varies only slowly with the time scale given by $\hbar/\Delta_0$, we can expand $\phi(\tau) \rightarrow \phi(\tau')$ in Eq. 2 about $\tau = \tau'$.

This gives $S_{\alpha}[\phi] \approx (\delta C/2) \int_0^{\beta} d\tau' [\hbar (2e) \partial_\tau \phi(\tau')/\partial \tau']^2$. Hence the dissipation action $S_{\alpha}$ acts as a kinetic term so that the effect of the quasiparticles results in an increase of the capacitance, $C \rightarrow C + \delta C$. This indicates that the quasiparticle dissipation in S-FI-S junctions is qualitatively weaker than that in S-FM-S junctions in which the strong Ohmic dissipation appears\textsuperscript{15,16}. At zero temperature, the capacitance increment $\delta C$ can be easily calculated using Eq. 5 and we can obtain

$$\delta C = \frac{3}{32\pi} \frac{e^2 R_Q}{\Delta_0 R_N}.$$  

As will be shown in later, $\delta C/C < 1$. Therefore the effect of the quasiparticle dissipation on the quantum dynamics of S-FI-S junctions is very small.

By using the above result, we propose a different type of flux qubit\textsuperscript{40}. In Fig. 2(a), we show the schematic of the $\pi$ SQUID qubit. In this proposal, the qubit consists of the superconducting rf SQUID loop (the inductance
two minima at \( \phi \) phase difference \( n \pi \) which describes this qubit is given by counterclockwise persistent currents circulating in the equal energy levels when tunneling between the wells split, and a two-level system (the tunneling between two wells is switched on, the levels (\( \uparrow \) state composed from the two low-lying energy levels qubit. The resultant action describes the quantum dynamics of a fictive particle (the macroscopic phase difference \( \phi \)) with mass \( M = C_{ren}(\hbar/2e)^2 \) moving in the tilted washboard potential \( U(\phi) = -E_J(\cos \phi - \eta \phi) \), where \( \eta \equiv I_{ext}/|I_C| \).

The MQT escape rate from this metastable potential at zero temperature is given by \( \Gamma = \lim_{\beta \to \infty} (2/\beta) \Im \ln Z \).

By using the semiclassical (instanton) method, the MQT rate is approximated as

\[
\Gamma(\eta) = \frac{\omega_p(\eta)}{2\pi} \sqrt{120\pi B(\eta)} \ e^{-B(\eta)},
\]

where \( \omega_p(\eta) = \sqrt{\hbar C/2eM(1 - \eta^2)^{1/4}} \) is the Josephson plasma frequency and \( B(\eta) = -\delta C/\hbar \) is the bounce exponent, that is, the value of the action \( S_{eff} \) evaluated along the bounce trajectory \( \phi_B(\tau) \). The analytic expression for the exponent \( B \) is given by

\[
B(\eta) = \frac{12}{3e} \sqrt{\frac{\hbar}{2e} I_C C_{ren} (1 - \eta^2)^{\frac{3}{4}}}. 
\]

In MQT experiments, the switching current distribution \( P(\eta) \) is measured. \( P(\eta) \) is related to the MQT rate \( \Gamma(\eta) \) as

\[
P(\eta) = \frac{1}{v} \Gamma(\eta) \exp \left(-\frac{1}{v} \int_0^\eta \Gamma(\eta')d\eta' \right),
\]

where \( v \equiv |d\eta/dt| \) is the sweep rate of the external bias current. The average value of the switching current is expressed by \( \langle \eta \rangle \equiv \int_0^\infty d\eta' P(\eta') \eta' \).

At high temperature regime, the thermally activated decay dominates the escape process. Then the escape rate is given by the Kramers formula \( \Gamma = (\omega_p/2\pi) \exp(-U_0/k_BT) \), where \( U_0 \) is the barrier height. Below the crossover temperature \( T^* \), the escape process is dominated by MQT and the escape rate is given by Eq. (11). The crossover temperature \( T^* \) is defined by

\[
T^* = \frac{5\hbar \omega_p(\eta = \langle \eta \rangle)}{36k_B}. 
\]

As was shown by Caldeira and Leggett, in the presence of a dissipation, \( T^* \) is suppressed.

In order to see explicitly the effect of the quasiparticle dissipation on MQT, we numerically estimate \( T^* \). Currently no experimental data are available for S-FI-S junctions. Therefore we estimate \( T^* \) by using the parameters for a high-quality Nb/Al2O3/Nb junction \( (\Delta_0 = 1.30\text{ meV}, C = 1.61 \text{pF}, |I_C| = 320 \text{mA}, R_N = \Delta_0/4\pi |I_C|, v |I_C| = 0.245 \text{A/s}) \). By substituting these data into Eq. (10) we obtain \( \delta C/C = 0.0145 \ll 1 \). Then from Eq. (13) we get the crossover temperature \( T^* = 245 \text{mK} \) for the dissipationless case \((C_{ren} = C)\) and \( T^* = 244 \text{mK} \) for the dissipation case \((C_{ren} = C + \delta C)\). We find that, due to the existence of the quasiparticle dissipation, \( T^* \) is reduced, but this reduction is negligibly small. This strongly indicates the high potentiality for the S-FI-S junctions as a phase-type qubit.
To summarize, we have theoretically proposed a π-junction quiet qubit which consists of a superconducting ring with the FI (the S-FI-S π SQUID qubit). Moreover, we have investigated the effect of the quasiparticle dissipation on the quantum dynamics and MQT using the parameter set for a high-quality Nb junction with Al2O3 barrier, and showed that this effect is considerably smaller compared with S-FM-S junction cases. This feature and the quietness of this system make it possible to realize a quiet qubit with long coherence time.

Finally, we would like to comment on the possibility of a quiet qubit using a S-I-FM-S junction. Recently Weides et al. have fabricated high-quality S-I-FM-S junctions, i.e., Nb/Al2O3/Nb0.5Cu0.4/Nb and Nb/Al/Al2O3/Nb3Al/Nb, respectively. They have clearly observed the 0-π transitions by changing the thickness of the FM layer. In these systems, the quasiparticle tunneling is inhibited due to the existence of the insulating barrier I (Al2O3). Therefore, as in the case of S-FI-S junctions, low quasiparticle dissipation and quietness are also expected in S-I-FM-S junctions. The theory of the qubit and MQT in such systems will be the subject of future studies.

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41 From a practical point of view, one drawback of the flux qubit with a single π junction described in this paper concerns the large inductance $L_{loop}$, the energy of which must be comparable to $|E_f|$ to form the required double-well potential profile. This implies a large size of the qubit loop, which makes the qubit vulnerable to decoherence by magnetic fluctuations of the environment. One way to overcome this difficulty is usage of one π junction and two S-I-S 0 junctions connected in series in a superconducting ring. The inductive energy of the ring is chosen to be much smaller than $|E_f|$ of the junctions.
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