Quantum Tunneling between Paramagnetic and Superconducting States of a Nanometer-Scale Superconducting Grain Placed in a Magnetic Field

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We consider the process of quantum tunneling between the superconducting and paramagnetic states of a nanometer-scale superconducting grain placed in a magnetic field. The grain is supposed to be weakly coupled to a normal metallic contact that plays the role of the spin reservoir. Using the instanton method, we find the probability of the quantum tunneling process and express it in terms of the applied magnetic field, order parameter of the superconducting grain, and conductance of the tunneling junction between the grain and metallic contact.

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Recent advances in manufacturing small electronic devices posed several questions in the theory of nanometer-size superconductors related to their prospective applications [1]. One of the key issues is the effect of quantum fluctuations on the dynamic behavior of ultrasmall superconductors of the dimensions much less than the coherence length ξ. Of special interest from both fundamental and practical points of view are dynamical processes of switching between the superconducting and paramagnetic states in the presence of a magnetic field. Small grains can experience spontaneous transitions due to quantum fluctuations. In this Letter, we investigate quantum tunneling between the superconducting and paramagnetic states of an ultrasmall superconductor.

Tunneling switching effects occur in the paramagnetic limit where, at magnetic fields exceeding $H_{\rm spin} = \Delta_0/\sqrt{2}\mu_B$, the Zeeman effect plays a major role in suppression of superconductivity (Δ_0 is the order parameter and $\mu_B = |e|\hbar/2mc$) [2–4]. This limit is characterized by the condition $H_{\rm spin} \ll H_{\rm orb}$, where $H_{\rm orb}$ is the critical magnetic field due to the orbital effect. In dirty small superconductors $H_{\rm orb} \sim \Phi_0/(r\sqrt{D/\Delta_0})$ [5], where $\Phi_0 = hc/2e$, D is the diffusion coefficient, and r is the characteristic size of the grain. For a spherical grain, thus, the paramagnetic limit means $\sqrt{\Delta_0/d}\sqrt{l/r} \ll 1$, where d is the mean energy level spacing. In a ballistic case ($l \simeq r$), the paramagnetic limit is achieved only if $\Delta_0 < d$, i.e., in a strongly fluctuating regime [6]. However, in a platelet geometry with the magnetic field parallel to a film $H_{\rm spin}/H_{\rm orb} \sim \sqrt{\Delta_0/d}\sqrt{lb/S}$ (b is the thickness and S is the area of the sample), and the paramagnetic limit can be achieved even in the ballistic case together with the condition $\Delta_0 \gg d$ provided the ratio $b/\sqrt{S}$ is sufficiently small.

Thus, the paramagnetic limit can be achieved along with the condition $\Delta \gg d$ in the case of (i) dirty grain and (ii) ballistic grain of a platelet geometry. We focus on this limit and investigate the quantum tunneling of the grain between superconducting and paramagnetic states. Since these two states have different values of the total spin, such tunneling can occur only if the total spin of the grain does not conserve. We consider a model where the main mechanism for spin nonconservation is provided by coupling of the superconducting grain to a metallic plate that plays the role of a spin bath.

Our final result for the probability of the quantum tunneling between the superconducting and paramagnetic states is

$$P \sim \exp[N \ln(\beta\, \delta E G/\Delta_0)], \qquad (1)$$

where the numerical coefficient $\beta \approx 1.1$, the factor N is the number of polarized electrons in the paramagnetic state of the grain, G is the conductance of the tunneling junction between the grain and the metallic lead measured in units e^2/h, and $N\delta E$ is the total energy difference between the grain's superconducting and paramagnetic states (see Fig. 1). We assume that the grain and plate are weakly coupled such that $G \ll 1$. The factor N is related to $H_{\rm spin}$ and Δ_0 as $N = 2\mu_B H_{\rm spin}/d = \sqrt{2}\Delta_0/d$. The energy difference per one state $\delta E > 0$ is expressed through the applied magnetic field as $\delta E = \mu_B(H - H_{\rm spin})$. The result (1) holds as long as $\delta E/\Delta_0 \ll 1$; the general case $\Delta_0 \sim \delta E$ is more complicated and we leave it for future study.

Written in a form $P \sim (\delta E G t_{\rm eff})^N$, where the effective tunneling time $t_{\rm eff} = \beta/\Delta_0$, our result can be viewed as

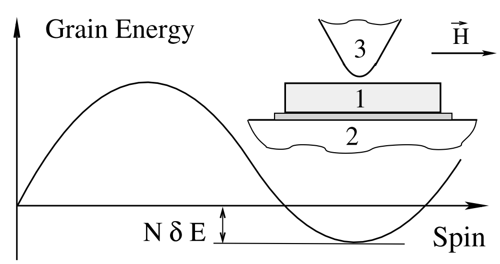

FIG. 1. Energy of an isolated superconducting grain as a function of its total spin. The inset shows a possible experimental setup: An STM tip (3) and superconducting grain separated by an insulating layer from metallic plate (2).

the probability of N simultaneous single electron tunneling processes characterized by elementary probabilities $\delta EGt_{\rm eff}$. The relation between $t_{\rm eff}$ and Δ_0 is found by the instanton method that naturally describes the physics of the quantum "underbarrier" tunneling process taking place in the grain (see Fig. 1).

A possible experimental setup is shown in Fig. 1. The conductance G that controls the tunneling probability is determined by the largest value among the two normal-state conductances of contacts either between the grain and the tip (G_{13}), or between the grain and the plate (G_{21}). The switch from the superconducting state to the paramagnetic one results in a disappearance of the gap Δ, and it can be detected by measuring the total conductance between the tip and plate similar to the spectroscopic measurements by [1].

The model.—The Hamiltonian describing a system of a superconducting grain coupled via weak tunneling to a metallic plate is

$$\hat{H} = \hat{H}_g + \hat{H}_M + \sum_{k,k'} \mathcal{T}_{kk'}[\hat{\psi}^\dagger_{k\sigma}\hat{d}_{k'\sigma} + \hat{d}^\dagger_{k'\sigma}\hat{\psi}_{k\sigma})], \quad (2)$$

where $\hat{H}_g$ is the BCS Hamiltonian of the grain,

$$H_g = \sum_k \hat{\psi}^\dagger_{k\alpha}[\xi_k - h\sigma^z_{\alpha\alpha}]\hat{\psi}_{k\alpha} - \lambda \sum_{k1,k2} \hat{\psi}^\dagger_{k1\uparrow}\hat{\psi}^\dagger_{k1\downarrow}\hat{\psi}_{k2\downarrow}\hat{\psi}_{k2\uparrow},$$

where ξ_k are the exact eigenvalues (measured with respect to the Fermi energy) of the noninteracting Hamiltonian, σ^z is the Pauli matrix, and λ is the interaction constant. The magnetic field h, pointing along the z axis, is measured in the energy units $h = \mu_B H$. Electrons in the metal are described by the free fermion model $\hat{H}_M = \sum_{k'\alpha} \hat{d}^\dagger_{k'\alpha}\,\zeta_{k'}\,\hat{d}_{k'\alpha}$. Since the Zeeman splitting of electrons of the metal is much less than the Fermi energy, the contribution from the field penetrating the metal can be omitted.

Quantum tunneling.—The probability of the quantum tunneling process is determined by $P = \sum_f |A|^2$ with the amplitude

$$A = \langle f|T_t e^{-i\int_{t_i}^{t_f} \hat{H}(t)\,dt}|i\rangle, \quad (3)$$

and the sum taken over all final states of the system. Since coupling between the grain and metal is weak, the last term in the Hamiltonian (2) can be treated as a perturbation. The paramagnetic state has a nonzero total spin S formed by the polarized electrons with $|\xi_k| < \tilde{\xi}$ such that $S = \tilde{\xi}/d$. During tunneling, the spin of the grain increases from zero to S; thus there must be $2S$ electron tunneling processes between the grain and metal, and the first nonzero contribution in the expansion of Eq. (3) in the tunneling element should appear only in the $N = 2S$ order. The paired states which are destroyed by electron tunneling are those with $|\xi| < \tilde{\xi}$. Expanding the exponent in Eq. (3) with respect to electron tunneling, we obtain

$$A = \langle f|T_t \prod_{|\xi_k|<\tilde{\xi}} \int dt_k\, e^{-i\int_{t_i}^{t_f}[\hat{H}_M(t)+\hat{H}_g(t)]dt} \sum_{k'} \mathcal{T}_{kk'} \times [\hat{\psi}^\dagger_{k\,\sigma}(t_k)\hat{d}_{k'\sigma}(t_k) + \hat{d}^\dagger_{k'\sigma}(t_k)\hat{\psi}_{k\,\sigma}(t_k)]|i\rangle. \quad (4)$$

In the absence of coupling between the grain and metal, the initial and final states of the system are the products of the corresponding initial and final states of the grain and metal, respectively, $|i\rangle = |i_G\rangle|i_M\rangle$, $|f\rangle = |f_G\rangle|f_M\rangle$, and the quantum mechanical average of the operators $\hat{d}$ in (4) can be done straightforwardly. Since the total spin of the metallic plate decreases during the tunneling process, the only relevant matrix elements are those corresponding to creation of electrons with spin-down, $\langle f_M|d^\dagger_{k\downarrow}(t)|i_M\rangle = e^{i\zeta_k t}$, $\zeta_k > 0$, and holes with spin-up, $\langle f_M|d_{k\uparrow}(t)|i_M\rangle = e^{i|\zeta_k| t}$, $\zeta_k < 0$. The initial state of the metal is the Fermi sea while its final state is characterized by the set of N electron-hole excitation with energies $\{\zeta^1_{k'}, \zeta^2_{k'}, \ldots, \zeta^N_{k'}\}$, such that $\zeta_{k'} > 0$ correspond to spin-down electrons, while $\zeta_{k'} < 0$ correspond to spin-up holes. Assuming that tunneling matrix elements are index independent, $\mathcal{T}_{kk'} = \mathcal{T}$, we arrive at

$$A = \mathcal{T}^N \langle f_G|T_t \prod_{|\xi_k|<\tilde{\xi}} \int dt_k e^{-i\int_{t_i}^{t_f} \hat{H}_g(t)dt} \sum_{\text{Per } p} e^{i|\zeta^p_{k'}|t_k} \times [\hat{\psi}^\dagger_k(t_k)\theta(-\zeta^p_{k'}) + \hat{\psi}_k(t_k)\theta(\zeta^p_{k'})]|i_G\rangle, \quad (5)$$

where the sum goes over all excitation permutations. Since we consider only the case $\delta E \ll \Delta_0$, we can simplify the problem assuming that the energy of a typical excitation in the metal is much less than Δ_0. We then neglect the energies $\zeta^p_{k'}$ in the exponents of Eq. (5), and the sum over permutation simply reduces to the factor $N!$. The probability P of the tunneling process is obtained by integrating $|A|^2$ over the final states of the metal:

$$P \sim \frac{\nu_M^N}{N!} \int d\zeta^1 \cdots d\zeta^N A^* A \delta\left(N\delta E - \sum_p |\zeta^p|\right), \quad (6)$$

where ν_M is the density of states of the metal.

The amplitude A now is given by the matrix element (5) representing the transition between the superconducting and paramagnetic states of the grain in the presence of electron hoppings. This is an example of quantum underbarrier tunneling processes, typically described by the instanton method. Turning to the Euclidean time $t \to -i\tau$ and taking initial and final times as $\tau_i = -\infty$, $\tau_f = 0$, we present the amplitude A as

$$A = N!\mathcal{T}^N \langle f_G|S(0, -\infty)|i_G\rangle,$$

with the evolution operator

$$S(\tau_2, \tau_1) = \prod_{|\xi_k|<\tilde{\xi}} \int_{\tau_1}^{\tau_2} d\tau_k [\hat{\psi}^\dagger_{k\uparrow}(\tau_k)\theta(-\zeta^p_{k'}) + \hat{\psi}_{k\downarrow}(\tau_k)\theta(\zeta^p_{k'})].$$

In principle, the instanton method should be applied to the amplitude A directly, but it is more convenient to consider the product A^*A presenting A^* as $A^* = N!\mathcal{T}^N\langle i_G|S^\dagger(\infty,0)|f_G\rangle$ and writing A^*A as

$$A^*A = \langle i_G|S^\dagger(\infty,0)|f_G\rangle\langle f_G|S(0,-\infty)|i_G\rangle \\ = \langle i_G|S^\dagger(\infty,0)S(0,-\infty)|i_G\rangle,$$

where it was used that by construction the Euclidean evolution operator S brings the grain from the initial state to the final one; $|f_G\rangle$ state: $S|i_G\rangle = |f_G\rangle$. Now the instanton process has the following structure (see Fig. 2): The evolution begins at $\tau = -\infty$ from the superconducting state, then at $\tau \approx -T$ the system turns into the paramagnetic state and stays there until it turns back to the superconducting state at $\tau \approx T$. The artificial part of the process ($\tau > 0$) is the mirror reflection of the "physical" process with $\tau < 0$. The advantage of this representation is that now the new initial ($\tau = -\infty$) and final ($\tau = \infty$) states are identical, and therefore we can use the convenient functional representation for A^*A:

$$A^*A = [N!\mathcal{T}^N]^2 \int D\Delta D\psi^\dagger D\psi e^{\int \mathcal{L}dt} \prod_{|\xi_k|<\tilde{\xi}} \times \int d\tau_{1k}d\tau_{2k}[\psi_{k\uparrow}(\tau_{1k})\psi^\dagger_{k\uparrow}(\tau_{2k})\theta(-\zeta^p_{k'}) + \psi^\dagger_{k\downarrow}(\tau_{1k})\psi_{k\downarrow}(\tau_{2k})\theta(\zeta^p_{k'})], \quad (7)$$

with the Lagrangian,

$$\mathcal{L} = -\frac{1}{\lambda}\Delta^*\Delta - \sum_k \psi^\dagger_k[\partial_\tau + \xi_k - h\sigma_z]\psi_k - \Delta\psi^\dagger_{k\uparrow}\psi^\dagger_{k\downarrow} - \Delta^*\psi_{k\downarrow}\psi_{k\uparrow}. \quad (8)$$

Using integral representation of delta function in (6) and integrating over ζ^p and over the fermionic fields, we find $\ln P$ as a functional of $\Delta(\tau)$:

$$\ln P = N\ln(N\delta E t^2\nu_M) + \sum_k \mathrm{Tr}\ln[\partial_\tau + \mathcal{H}_k] - \frac{1}{\lambda}\int d\tau\Delta^*(\tau)\Delta(\tau) + \sum_k \ln Z_k, \quad (9)$$

where $N\delta E = \sum_p|\zeta^p|$ is the energy difference between superconducting and paramagnetic states of the grain $Z_k = \mathrm{Tr}\int d\tau_1 d\tau_2 \hat{G}_k(\tau_1,\tau_2)$ and

$$\mathcal{H}_k(\tau) = \begin{bmatrix} \xi_k - h & \Delta(\tau) \\ \Delta^*(\tau) & -\xi_k - h \end{bmatrix}. \quad (10)$$

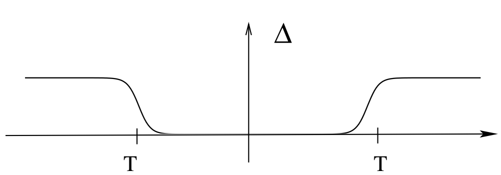

FIG. 2. Dependence of the order parameter Δ on time τ. The region $\tau > 0$ is the mirror reflection of the "physical" region $\tau < 0$. The superconducting state corresponds to the regions $|\tau| > T$ while the paramagnetic one to $|\tau| < T$.

The matrix Green function,

$$\hat{G}_k(\tau_1,\tau_2) = \begin{bmatrix} G_k(\tau_1,\tau_2) & F_k(\tau_1,\tau_2) \\ F^\dagger_k(\tau_1,\tau_2) & \bar{G}_k(\tau_1,\tau_2) \end{bmatrix}, \quad (11)$$

is defined by the equation

$$[\partial_{\tau_1} + \mathcal{H}_k(\tau_1)]\hat{G}_k(\tau_1,\tau_2) = \delta(\tau_1 - \tau_2). \quad (12)$$

Instanton equations.—To find instanton equations, we take the functional derivative of Eq. (9) with respect to Δ^* obtaining

$$\Delta(\tau) = \lambda\sum_k f_{1k}(\tau) + f_{2k}(\tau), \quad (13)$$

where the Green function $f_1(\tau) = F(\tau,\tau)$ emerges from the variation derivative of $\mathrm{Tr}\ln[\partial_\tau + \mathcal{H}_k]$ in (9), and f_2 emerges from the functional derivative of $\hat{G}$:

$$f_{2k}(\tau) = Z_k^{-1}\frac{\delta}{\delta\Delta^*(\tau)}\int d\tau_1 d\tau_2 \,\mathrm{Tr}\,\hat{G}_k(\tau_1,\tau_2). \quad (14)$$

Combining Eq. (12) with the same equation written in the transposed form, one finds the equation defining f_1 in terms of equal time Green functions only:

$$\partial_\tau\hat{g}_{1k}(\tau) + [\mathcal{H}_{0k}(\tau), \hat{g}_{1k}(\tau)] = 0, \quad (15)$$

where

$$\hat{g}_{1k}(\tau) = \begin{bmatrix} g_{1k}(\tau) & f_{1k}(\tau) \\ f^\dagger_{1k}(\tau) & \bar{g}_{1k}(\tau) \end{bmatrix} = \hat{G}_k(\tau,\tau), \quad (16)$$

and $\mathcal{H}_0$ is given by Eq. (10) with $h = 0$. Writing Eq. (15) in components, we get

$$\partial_\tau\tilde{g}_{1k} + \Delta f^\dagger_{1k} - \Delta^* f_{1k} = 0, \\ \partial_\tau f_{1k} + 2\xi_k f_{1k} - 2\Delta\tilde{g}_{1k} = 0, \\ -\partial_\tau f^\dagger_{1k} + 2\xi_k f^\dagger_{1k} - 2\Delta^*\tilde{g}_{1k} = 0, \quad (17)$$

$$\partial_\tau s_{z1k} = 0, \quad (18)$$

where the variables $\tilde{g}_1 = [g_{1k} - \bar{g}_{1k}]/2$, $s_{z1k} = -[g_{1k} + \bar{g}_{1k}]/2$ were introduced instead of components g_1 and $\bar{g}_1$. Equations (17) are similar to the well-known Eilenberger equations [7] and have the same invariant $\tilde{g}^2_{1k} + f^\dagger_{1k}f_{1k} = \mathrm{const}$. Now we turn to the function $f_2(\tau)$: Using the definition of the Green function (12), one can take the variational derivative in Eq. (14) and get

$$f_{2k}(\tau) = -Z_k^{-1}[f^{II}_k(\tau)g^I_k(\tau) + \bar{g}^{II}_k(\tau)f^I_k(\tau)], \quad (19)$$

where g^I_k, f^I_k are the components of the matrix Green function,

$$\hat{g}^I_k(\tau) \equiv \begin{bmatrix} g^I_k(\tau) & f^I_k(\tau) \\ f^{\dagger I}_k(\tau) & \bar{g}^I_k(\tau) \end{bmatrix} = \int d\tau_2\hat{G}_k(\tau,\tau_2), \quad (20)$$

and $f^{II}_k, \bar{g}^{II}_k$ are the components of the matrix Green function $\hat{g}^{II}_k(\tau) = \int d\tau_1\hat{G}_k(\tau_1,\tau)$. Equations determining functions $\hat{g}^I$ and $\hat{g}^{II}$ are easily found by integrating Eq. (12) over τ_2 and transposing Eq. (12) over τ_1:

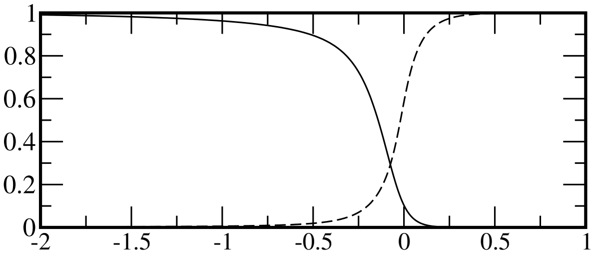

FIG. 3. The normalized order parameter $\Delta(\tau)/\Delta_0$ (dashed line) and the normalized total spin $2S(\tau)/N$ of the grain as functions of $\tau' = \tau - T$ at the boundary $\tau \sim T$ between the superconducting (left) and paramagnetic (right) states.

$$\partial_\tau \hat{g}_k^I(\tau) + \mathcal{H}_k(\tau)\hat{g}_k^I(\tau) = 1,$$
$$-\partial_\tau \hat{g}_k^{II}(\tau) + \hat{g}_k^{II}(\tau)\mathcal{H}_k(\tau) = 1. \quad (21)$$

Initial and final conditions.—The proper instanton configuration is determined by the initial and final conditions for the Green function $\hat{g}_k^{\alpha,\beta}(\tau)$,

$$\hat{g}_k^{\alpha,\beta}(\tau) = \frac{\langle i_G | S^\dagger(\infty, 0) S(0,\tau) \tilde{\psi}_k^\alpha \tilde{\psi}_k^{\beta\dagger} S(\tau, -\infty) | i_G \rangle}{\langle i_G | S^\dagger(\infty, 0) S(0, -\infty) | i_G \rangle},$$

where α, β are indices of the Nambu spinor $\tilde{\psi}$ and a negative τ is chosen for concreteness. To find $\hat{g}_k(\tau)$ in a functional representation, we add the source term $\int d\tau \mu_k^{\alpha\beta}(\tau)\tilde{\psi}_\alpha(\tau)\tilde{\psi}_\beta^\dagger(\tau)$ to the Lagrangian (8) and take the variation derivative of (9) with respect to $\mu_k^{\alpha\beta}(\tau)$:

$$\hat{g}_k(\tau) = \hat{g}_{1k}(\tau) + \hat{g}_{2k}(\tau),$$

where $\hat{g}_{1k}$ is defined by Eq. (16), and the matrix function $\hat{g}_{2k}$ that emerges from variation of Z_k in (9) is related to g^I and g^{II} via

$$\hat{g}_{2k} = -\hat{g}_k^I \hat{g}_k^{II} / Z_k. \quad (22)$$

In the superconducting phase ($|\tau| \gg |T|$), the function $\hat{g}_k$ should coincide with the equilibrium superconducting Green functions,

$$\tilde{g}_k = \xi_k / 2E_k, \qquad f_k = \Delta / 2E_k, \qquad f_k^\dagger = f_k^*, \qquad s_z = 0, \quad (23)$$

where $E_k = \sqrt{\xi_k^2 + \Delta^2}$, $\tilde{g}_k = [g_k - \bar{g}_k]/2$, $s_{zk} = -[g_k + \bar{g}_k]/2$. The function $\tilde{g}$ is directly related to electron density on the level k by $n_k = 1 - 2\tilde{g}_k$, and the function s_{zk} is the z component of the spin on the level k. Analogously, in the paramagnetic phase the Green function $\hat{g}$ is

$$\tilde{g}_k = f_k = f_k^\dagger = 0, \qquad s_{zk} = 1/2 \quad \text{for } |\xi_k| < \tilde{\xi} \quad (24)$$

$$\tilde{g}_k = \text{sign}\,\xi_k/2, \qquad s_{zk} = f_k = f_k^\dagger = 0 \quad \text{for } |\xi_k| > \tilde{\xi}. \quad (25)$$

In the absence of tunneling, the physical Green function $\hat{g}$ coincides with $\hat{g}_1$ which obeys Eqs. (17) and (18), conserving the quasiparticle spin. Therefore the function $\hat{g}_1$ in the paramagnetic state obeys the boundary condition (25) for any ξ, while in the superconducting state it obeys the boundary conditions (23), so that $\hat{g}_2 \to 0$ in the superconducting phase.

Numerical solution.—The solution of Eqs. (17) satisfying the necessary boundary conditions for a given configuration $\Delta(\tau)$ can be easily found numerically. To find the function $\hat{g}_2$, one first needs to solve Eqs. (21) numerically and then find $\hat{g}_2$ according to Eq. (22). Knowing the functions $\hat{g}_1$ and $\hat{g}_2$ for a given configuration $\Delta(\tau)$, one can find the self-consistent configuration of $\Delta(\tau)$ satisfying Eq. (13) which is shown on Fig. 3 along with the dependence of the total spin $S(\tau)$ at the right instanton boundary (solution at the left boundary is the mirror reflection of that on the right one). The final answer (1) follows from Eq. (9), where the most complicated term $\mathrm{Tr}\ln[\partial_\tau + \mathcal{H}_k]$ can be expressed in terms of components of $\hat{g}_1(\tau)$ using the method described in Ref. [8].

Conclusions.—In conclusion, we have developed an instanton approach describing quantum tunneling dynamics of a small superconducting grain placed in a contact with a normal metallic plate that plays the role of a spin bath. Our result (1) obtained formally in the limit of $T \to 0$ holds also at finite temperatures as long as $T \ll \delta E$. At higher temperatures, $\delta E \ll T \ll \Delta_0$, the characteristic energy δE in the exponent of Eq. (1) has to be substituted by temperature T. However, finding the numerical coefficient β in this case requires a more advanced study.

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