Macropscopic Quantum Tunneling (MQT) in Josephson systems \(^1\) has been studied in detail both experimentally \(^2\) and theoretically \(^3\) in the eighties but has gained renewed interest very recently \(^4\) since the exponential dependence of the MQT rate on parameters allows for a high fidelity readout of qubits based on superconducting circuits. In this context a new variety of quantum tunneling problem arises, namely, barrier penetration in presence of coupling to a spin-\(\frac{1}{2}\) system. It is shown that when the diabatic potentials for fixed spin intersect in the barrier region, Landau-Zener transitions lead to an enhancement of the tunneling rate. The effect of these spin flips in imaginary time is in qualitative agreement with experimental observations.

Motivated by recent realizations of qubits with a readout by macroscopic quantum tunneling in a Josephson junction, we study the problem of barrier penetration in presence of coupling to a spin-\(\frac{1}{2}\) system. It is shown that they cause an enhancement of the tunneling rate in the appropriate parameter range in agreement with experimental observations.

In contrast to the well-studied problem of LZ transitions where the diabatic potentials intersect in the barrier region so that Landau-Zener (LZ) transitions may arise, however, there is an interesting parameter range where the diabatic potentials intersect in the barrier region.

Within the subspace spanned by the eigenvectors \(\ket{0}, \ket{1}\) of the operator \(N\), the qubit can be described by Pauli matrices \(\sigma_i\). Further, measuring all energies in units of \(E_J\), we obtain the dimensionless Hamiltonian

\[
H = \epsilon \sigma_z - j \cos \left( \frac{\theta + \phi}{2} \right) \sigma_x + \frac{p_0^2}{2m} - \cos(\theta) - i_b \theta \]

with the dimensionless parameters \(\epsilon = (E_C/E_J)(N_g - \frac{1}{2})\), \(j = E_J/E_J\), and \(i_b = hI_b/2eE_J\). The variables \(p_0 = Q/2e\) and \(\theta\), the with the commutator \([p_0, \theta] = -i\) may be viewed as dimensionless momentum and coordinate of a particle with dimensionless mass \(m = C'E_J/4e^2\). We do not discuss here the manipulations of the qubit done for \(i_b = 0\), but address the readout when the bias current is increased to a value slightly below the dimensionless critical current \(i_c = 1\). The problem at hand then is tunneling of this ficticious particle through a barrier of the potential \(\cos(\theta) - i_b \theta\) in presence of the interaction with the spin.

In view of the large mass \(m\) the coordinate \(\theta\) is almost a classical variable. When the kinetic energy \(p_0^2/2m\) is neglected, the Hamiltonian \(^1\) can easily be diagonalized with the eigenvalues

\[
\lambda_\pm(i_b, \theta) = -\cos(\theta) - i_b \theta \pm \sqrt{\epsilon^2 + j^2 \cos^2[\theta + \phi]/2}
\]

that determine two adiabatic potential surfaces. At zero temperature and for vanishing bias current the system will approach the minimum of the lower surface \(\lambda_- (i_b = 0, \theta)\) which for small \(\epsilon\) and \(j\) lies close to \(\theta = 0\). As usual in MQT experiments, the switching of the bias current...
form 0 to a value close to \( i_e = 1 \) is slow compared to the characteristic time scales of the circuit. When the system follows the bias current adiabatically, the particle lies at finite bias \( i_b \) near the minimum \( \theta_0 (i_b) \) of the adiabatic potential \( \lambda_-(i_b, \theta) \). This state serves as the initial state for the calculation of the tunneling rate.

For this initial state it is natural to use the spin eigenvectors \( |\theta_-, +\rangle, |\theta_-, -\rangle \) associated with the eigenvalues \( \lambda_\pm(i_b, \theta_-) \) as a basis for a matrix representation of the Hamiltonian \( H \). We then find

\[
H = \begin{pmatrix}
\frac{p_\theta^2}{2m} + V_+(\theta) & \Delta(\theta) \\
\Delta(\theta) & \frac{p_\theta^2}{2m} + V_-(\theta)
\end{pmatrix}
\]  

(2)

where

\[
V_\pm(\theta) = -\cos(\theta) - i_b \theta \pm \left( \sqrt{\epsilon^2 + V_0^2} + \kappa_0 [V(\theta) - V_0] \right)
\]

are now two diabatic surfaces corresponding to the two spin orientations \( |\theta_-, +\rangle, |\theta_-, -\rangle \), and

\[
\Delta(\theta) = \epsilon \kappa_0 \left[ 1 - \frac{V(\theta)}{V_0} \right]
\]

is the \( \theta \) dependent coupling between them. For convenience, we introduced

\[
V(\theta) = j \cos[(\theta + \phi)/2],
\]

and \( V_0 = V(\theta_-) \), as well as

\[
\kappa_0 = 2V_0 \frac{\epsilon + \sqrt{\epsilon^2 + V_0^2}}{(\epsilon + \sqrt{\epsilon^2 + V_0^2})^2 + V_0^2}.
\]

Apparently, for \( \theta = \theta_- \) the Hamiltonian \( H \) is diagonal. It further becomes diagonal in the limits \( \epsilon \to 0 \) or \( j \to 0 \).

Depending on the external flux \( \phi \) and \( \epsilon/j \) the two diabatic potentials \( V_\pm \) may intersect. As can be seen from Fig. 1 this is always the case for \( \phi \) near \( \frac{\pi}{2} \) and \( \epsilon \) small compared to \( j \). Near such a crossing point \( \theta_* \), which is determined by

\[
\frac{\epsilon}{j} = \left[ -\cos \left( \frac{\theta_- + \phi}{2} \right) \cos \left( \frac{\theta_- + \phi}{2} \right) \right]^{1/2},
\]

the diabatic potential surfaces are strongly coupled by the off-diagonal element of the Hamiltonian \( H \). To quantify the strength of this coupling we may introduce the parameter

\[
g(\theta) = \frac{\Delta(\theta)}{V_+(\theta) - V_-(\theta)}
\]

which diverges at the crossing point \( \theta_* \). A LZ region where spin-flips may occur can then be defined by the condition \( g(\theta) > 1 \). We assume that this region is restricted to the vicinity of \( \theta_- \). In fact, when the bias current is sufficiently far from the critical current to allow for several states in the metastable minimum, the LZ region turns out to be narrow except near the boundary between the regions \( I \) and \( II \) in Fig. 1. This crossover region will be discussed further below.

To determine the tunneling rate we employ the “bounce technique” \( \text{[8]} \) which relates the rate \( \Gamma \) essentially to an imaginary time trajectory in the inverted potential, the so-called bounce. This method is equivalent to WKB and starts out form the partition function of the metastable system

\[
Z = \text{Tr} \left[ |\theta_-,-\rangle \langle \theta_-,-| e^{-\beta H} \right]
\]

which has to be evaluated in the semiclassical limit for \( \beta \to \infty \). Within the path integral representation this takes the form

\[
Z = \int D[\theta] e^{-S_-[\theta]} \left\{ 1 + \sum_{n=1}^{\infty} \int_0^\beta ds_2n \cdots \int_0^{s_21} ds_1 \Delta[\theta(s_2n)] \cdots \Delta[\theta(s_1)] \times \exp \left[ \sum_{k=1}^{n} \int_{s_{2k-1}}^{s_{2k}} d\tau (V_-[\theta] - V_+[\theta]) \right] \right\}
\]

where the path sum runs over all orbits with period \( \beta \) switching \( 2n \) times between \( V_- \) and \( V_+ \) at times \( s_1 < s_2 < \ldots < s_{2n} \). The Euclidian action on \( V_- \) is

\[
S_- = \int_0^\beta d\tau \left[ \frac{p_\theta^2}{2m} + V_-(\theta) \right]
\]
In the semiclassical limit $Z$ decomposes into $Z_{sc} \approx Z_w + Z_0 + Z_2$. Here $Z_w$ is the partition function of the well which is obtained by summing over paths in the vicinity of the trivial trajectory $\theta(\tau) = \theta_0$ sitting at the well minimum. $Z_0$ is the contribution of paths in the vicinity of the standard non-flip bounce trajectory in $V_-$. In region II we also have to take into account the contribution $Z_2$ from paths that flip when the bounce traverses the LZ region. Trajectories with four and more spin-flips can be neglected away from the boundary between regions I and II. Both the bounce and spin-flip bounce are saddlepoint trajectories with an unstable fluctuation mode which after an analytical continuation \cite{3} yield imaginary and, compared to $Z_w$, exponentially small contributions that determine the rate. Following standard procedures, we obtain for the dimensionless rate, in units of $E_s'/\hbar$,

$$
\Gamma = \lim_{\beta \to \infty} \frac{2}{\beta} \Im(Z_0 + Z_2)/Z_w = \Gamma_0 + \Gamma_2. \quad (5)
$$

To evaluate this explicitly, we first note that within the barrier region the potentials $V_\pm$ can very accurately be approximated by cubic polynomials. It is convenient to introduce for each diabatic potential the frequency at the well bottom

$$
\omega_s^2 = V'_\pm(\theta_s)/m,
$$

and a scaled distance

$$
x_s^\pm = (\theta_s - \theta_s)/\theta_0^\pm - \theta_s^\pm \]

between the well bottom and the “exit point” $\theta_0^\pm$, where $V_\pm(\theta_0^\pm) = V_\pm(\theta_s)$. Further, $V_0^\pm$ is the barrier height with respect to the minimum $V_\pm(\theta_s)$.

Since we are interested in the limit $\beta \to \infty$, it is natural to look for solutions in the time interval $s \in [-\beta/2, \beta/2]$. The simple bounce trajectory in the inverted potential $-V_-\theta)$ then reads (see Fig. 2)

$$
\theta_{\text{bounce}}(s) = \theta_+ + (\theta_0^+ - \theta_-)/\cosh^2(\omega_- s/2).
$$

This trajectory dominates the non-flip contribution $Z_0$ that has been evaluated previously yielding the well-known MQT rate in the absence of damping \cite{3}

$$
\Gamma_0 = 6 \sqrt{6 \omega_- V_0^- / \pi} \exp \left( -\frac{36 V_-}{5 \omega_-} \right) \quad (6)
$$

which determines the rate in region I of Fig. 1.

In region II the semiclassical trajectory may switch to the potential surface $V_+(\theta)$ in the LZ region. The lowest order flip contribution reads

$$
Z_2 = \int D[\theta] e^{-S_{\text{sc}}[\theta]} \int_0^\beta ds_1 \int_0^{s_2} ds_1 \Delta[\theta(s_2)] \Delta[\theta(s_1)] \times \exp \left( \int_{s_1}^{s_2} d\tau (V_-[\theta] - V_+[\theta]) \right).
$$

To determine $Z_2$ we proceed as follows: First, the action for the flip bounce is calculated for arbitrary flipping times $s_1 < s_2$. Due to energy conservation and the periodic boundary condition one finds that the restriction $\theta(s_1) = \theta(s_2)$ applies. For a path running in the interval $[-\beta/2, \beta/2]$ this means that the flips have to occur symmetrically around $s = 0$. Second, as a function of $s_1$ the action has a minimum at an optimal flipping time $s_1^*$ determined by

$$
p_\theta \frac{\partial t_+}{\partial \theta} \left\{ (V_+ - V_-)[\theta] \right\}_{s=s_1^*} = 0 \quad (7)
$$

where $t_+\theta$ is the time the bounce spends on the $V_+$ surface. As one might have guessed, Eq. (7) yields $V_+\theta = V_-\theta$, so that the optimal flips occur at the intersection point $\theta_*$ of the diabatic potentials. Then $\theta_* = \theta(s_1^*)$ and $s_2^* - s_1^* = t_+ (\theta_*) := t_+$. Other solutions of Eq. (7) with $p_\theta(s_1^*) = 0$ mean that flips either occur in the well or at the turning point. In both cases the orbit has no energy to run on $V_+$ and one regains the simple bounce action on $V_-$. Further, solutions with $\partial t_+ / \partial \theta = 0$ corresponds to a maximum of the action.

This way the trajectory at the saddlepoint of the action is obtained as

$$
\theta_{\text{flip}}(s) = h(|s| - t_+ s) \theta_{\text{flip}}(s) + h(t_+ s - |s|) \theta_{\text{flip}}(s).
$$

Here the step functions $h(\cdot)$ select the time segments spend on the two potential surfaces, where

$$
t_+ = \frac{2}{\omega_+ \lambda} F(\phi|m)|m). \quad (8)
$$

The parameter $\lambda = [P'(x_0)]^{1/4}$ is determined by the slope $P'$ of the polynomial

$$
P(x) = x^3 - x^2 - \frac{4}{27} \rho, \text{with } \rho = \frac{V_+(\theta_*) - V_-(\theta_-)}{V_0^+} \quad (9)
$$

at its zero where $P(x_0) = 0$, and $F(\phi|m)$ is the elliptic integral of the first kind with modulus $m = 1/2 + P''(x_0)/8x_0^2$ and angle $\cos(\phi) = [\lambda^2 - (x_0 + x_0^+)]/[\lambda^2 + (x_0 + x_0^+)]$. Further, $\theta_{\text{flip}}(s) = \theta_{\text{bounce}}(s - \text{sign}(s) \alpha)$ describes the segments of the flip bounce on the surface $V_-$ where it coincides with the simple bounce apart from a phase

$$
\alpha = \frac{t_+ \phi}{2} - \frac{2}{\omega_+ \lambda} \arccosh(\sqrt{x_+}).
$$

Finally, the segment running on $V_+$ follows as

$$
\theta_{\text{flip}}^+(s) = \theta_+ + (\theta_0^+ - \theta_+ \left[ x_0 + \lambda^2 \frac{\text{cn}((\lambda s_0^+ + \phi)|m) - 1}{\text{cn}(\lambda s_0^+ + \phi) + 1} \right]
$$

where $\text{cn}(\cdot)$ is a Jacobi function (see Fig. 2).
For the action of this flip bounce one finds
\[ S_* = \frac{18 V_b^-}{5 \omega_-} \left[ \sqrt{(1-x_-^3)} \left( 3 \sqrt{(1-x_+^3)} - 5 \right) + 2 \right] \]
\[ + \frac{18 V_b^+}{5 \omega_+} \left[ 2x_0 - 2\lambda^2 + 9\rho \right] F(\varphi|\tilde{m}) + 2\lambda E(\varphi|\tilde{m}) \]
\[ - \frac{1}{2} \sqrt{-P(x_+^3)} \left( \frac{4}{\lambda^2 + x_0 - x_+^2} + P''(x_+^3) \right). \]

Here, \( E(\cdot) \) is the elliptic integral of the second kind.

Next, the action is expanded around \( S_* \) with respect to variations of the flipping times up to second order. For this purpose it is convenient to introduce sum, to variations of the flipping times up to second order or the bounce in time. Hence, like the conventional non–flip \( \phi \)

\[ \omega_\pm (s) = 1 + s \left( \frac{3V_b^-}{\omega_-} \right) \text{erfc} \left[ \frac{\Omega_1 t_+ + \Delta(\theta_\pm)}{\sqrt{2}} \right] e^{-S_*}. \]

This can be combined with \( \Omega \) to yield the central result of this paper, namely, the decay rate in region \( \text{II} \)

\[ \Gamma = \Gamma_0 \left\{ 1 + \frac{\Delta(\theta_\pm)^2}{\Omega^2} \right\} \text{erfc} \left[ \frac{\Omega_1 t_+ + \Delta(\theta_\pm)}{\sqrt{2}} \right] e^{(S_--S_*)} \]

with \( S_- = \frac{36 V_b^-}{\omega_-} \). The corresponding rate enhancement is shown in Fig. 3. Apparently, there is a pronounced exponential increase of the total rate due to spin flips in the LZ range along the bounce. This is in agreement with experimental findings of the peak current variation with magnetic flux in the quantronium device.

As one approaches the boundary between \( \text{I} \) and \( \text{II} \) the LZ region grows and in a narrow boundary layer the parameter \( g(\theta) \) in (11) is larger than 1 in the entire barrier range. Then, multi–spin flips can occur anywhere along the bounce and also during the switching on of the bias current. However, since the exponential factors of \( \Gamma_0 \) and \( \Gamma_2 \) coincide at the boundary, this breakdown of the nonadiabatic approach utilized here, essentially reduces to a prefactor effect smoothing the transition between the results in region \( \text{I} \) and \( \text{II} \). A more interesting extension of the present work would consider initial states where due to manipulations via the charge gate the system moves on the upper adiabatic potential surface \( \lambda_+(i_b, \theta) \). This will be addressed in future work.

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