Quantum Dynamics of Tunneling between Superconductors

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A functional-integral formulation is used to treat the quantum dynamics of a microscopic model of a Josephson junction, including the dissipative effects of quasiparticle tunneling. The calculation is carried to a point where it makes contact with, and therefore substantiates, recent work by Caldeira and Leggett in which the system is treated by analogy with the quantum Brownian motion of a massive particle coupled to a phenomenological heat bath.

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There is considerable current interest in the theory of the quantum dynamics of tunneling between superconductors. The subject is topical because it applies to the switching of superconducting quantum interference devices at low temperatures, and also because it concerns a situation in which the quantum mechanics of a macroscopic variable—the phase of the order parameter—cannot be decoupled from microscopic degrees of freedom, so that dissipation is an essential part of the dynamics.

In the pioneering work on this subject,[1] the phenomenological dissipation-free equation for the phase variable of a Josephson tunnel junction is treated as a classical equation derivable from a Lagrangian, L_0; terms describing microscopic degrees of freedom and their coupling to the phase are added to this Lagrangian; and quantum mechanics is applied to the enlarged system. Since the phase associated with a Josephson junction is not a classical variable, this procedure raises conceptual questions[2]; in particular, the mass and potential energy in L_0 contain explicit factors of $\hbar$. Furthermore, the phenomenological coupling to the environment leads to model-dependent frequency renormalizations which require good judgment for their correction interpretation. In Ref. 1, these renormalizations are absorbed into the nondissipative zeroth-order problem. However, in more recent work[3] such effects are interpreted, we believe incorrectly (see below), as having physical consequences.[4,5]

In this note, we construct a theory of the quantum mechanics of the phase variable from a microscopic model of superconducting tunneling. We are able to clarify the problems alluded to in the last paragraph. We obtain a result which is somewhat more general than that of Caldeira and Leggett; it reduces to their form when certain simplifying assumptions are made. Our calculation produces the correct barrier against phase fluctuations and contains no additional renormalizations, thus justifying the treatment in Ref. 1. In addition, we cast some light on the approximations inherent in ignoring quantum fluctuations. Thus we make a beginning towards answering the question[6] of the theoretical limit to the accuracy of the measurement of $2e/\hbar$ by the Josephson effect.

We start from a microscopic model described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_T + \mathcal{H}_Q \tag{1}$$

Here $\mathcal{H}_L$ and $\mathcal{H}_R$ describe the superconductors on the left and right of the junction. $\mathcal{H}_T$ is the tunneling Hamiltonian, and $\mathcal{H}_Q$ is the Coulomb energy associated with charge transfer across the junction. Explicitly, we take

$$\mathcal{H}_L = \int d^3x\, \psi_{L\sigma}^\dagger \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu\right]\psi_{L\sigma} - \frac{g_L}{2}\int d^3x\, \psi_{L\sigma}^\dagger(\vec{x})\psi_{L-\sigma}^\dagger(\vec{x})\psi_{L-\sigma}(\vec{x})\psi_{L\sigma}(\vec{x}). \tag{2}$$

Here ψ_σ is the electron field operator for spin σ, and repeated spin indices are summed over; $\mathcal{H}_R$

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$= \mathcal{H}_L(\psi_L \to \psi_R,\ g_L \to g_R);$

$$\mathcal{H}_{\mathcal{T}} = \int_{\vec{x}\subset L,\ \vec{x}'\subset R} d^3x\, d^3x' \,[\mathcal{T}(\vec{x},\vec{x}')\psi_{L\sigma}{}^\dagger(\vec{x})\psi_{R\sigma}(\vec{x}') + \text{H.c.}], \tag{3}$$

$$\mathcal{H}_Q = \frac{1}{2C}\left(\frac{Q_L - Q_R}{2}\right)^2, \tag{4}$$

with $Q_{L(R)}$ the operator for the charge in the left (right) superconductors, i.e.,

$$Q_L = e\int d^3x\, \psi_{L\sigma}{}^\dagger(\vec{x})\psi_{L\sigma}(\vec{x}).$$

To study the low-lying quantum states of this system we calculate the partition function $Z = \text{Tr}[\exp(-\tau\mathcal{H}/\hbar)]$, with τ a real number with the dimension of time. Divide τ into a large number, N, of intervals. In each interval, express the charging energy (4) and the parts of $\mathcal{H}_L$ and $\mathcal{H}_R$ quartic in field operators as Gaussian integrals.[7] In this way, the partition function becomes a multiple functional integral:

$$Z = \int \mathfrak{D}^2\Delta_L \mathfrak{D}^2\Delta_R \mathfrak{D}V\, \text{Tr}\{T\exp[-\int_0^\tau dt\, \mathcal{H}_{\text{eff}}(t)/\hbar]\}. \tag{5}$$

Here Δ_L and Δ_R are complex functions of $\vec{x}$ and t, V is a real function of t,[8] and all three are periodic in t with period τ. The trace is still over the electron variables. T orders operators in time from zero to τ. $\mathcal{H}_{\text{eff}}$ is obtained from the terms in (1) by the following replacements:

$$\mathcal{H}_L \to (\mathcal{H}_L)_{\text{eff}} \equiv K + \int d^3x[\Delta_L{}^*(\vec{x},t)\psi_{L\downarrow}(\vec{x})\psi_{L\uparrow}(\vec{x}) + \text{H.c.}] + \frac{1}{g_L}\int d^3x\, |\Delta_L(\vec{x},t)|^2 \tag{6}$$

[K is the first term in (2)]; $\mathcal{H}_R \to (\mathcal{H}_R)_{\text{eff}}$ in a similar way;

$$\mathcal{H}_Q \to (\mathcal{H}_Q)_{\text{eff}} \equiv \tfrac{1}{2}iV(t)[Q_L - Q_R] + \tfrac{1}{2}CV^2(t); \tag{7}$$

and $\mathcal{H}_{\mathcal{T}}$ is unchanged. The definition of the measure in the functional integrals in (5) is contained in the operations, described above, leading to their construction.[7] Since $\mathcal{H}_{\text{eff}}$ is bilinear in electron operators, the trace can be done exactly. One obtains

$$Z = \int \mathfrak{D}^2\Delta_L \mathfrak{D}^2\Delta_R \mathfrak{D}V \exp\{-\mathfrak{A}[\Delta,\Delta^*,V]\} \tag{8}$$

where[9]

$$-\mathfrak{A} = \text{Tr}\ln \underline{\hat{\mathcal{G}}}^{-1} - \int \frac{dx}{\hbar}\left(\frac{|\Delta_L|^2}{g_L} + \frac{|\Delta_L|^2}{g_R}\right) - \int_0^\tau dt\, \frac{1}{2\hbar}CV^2. \tag{9}$$

Here $dx \equiv d^3x\, dt$, and we have introduced a four-component electron space by adding the Nambu spaces[10] of the left and right superconductors. In particular,

$$\underline{\hat{\mathcal{G}}}^{-1} = \begin{pmatrix} \hat{\mathcal{G}}_L{}^{-1} & -\hat{\mathcal{T}}\,\delta(t-t') \\ -\hat{\mathcal{T}}^\dagger\,\delta(t-t') & \hat{\mathcal{G}}_R{}^{-1} \end{pmatrix}, \tag{10}$$

$$\hat{\mathcal{G}}_{L(R)}{}^{-1} = \left[-\hbar\frac{\partial}{\partial t} + \left(\frac{\hbar^2}{2m}\nabla^2 + \mu (\mp)\frac{ie}{2}V(t)\right)\hat{\tau}_3 - \hat{\Delta}_{L(R)}\right]\delta(x-x'), \tag{11}$$

$$\hat{\Delta}_{L(R)} = \begin{pmatrix} 0 & \Delta_{L(R)} \\ \Delta_{L(R)}{}^* & 0 \end{pmatrix}, \quad \hat{\mathcal{T}} = \begin{pmatrix} \mathcal{T} & 0 \\ 0 & -\mathcal{T}^* \end{pmatrix}. \tag{12}$$

Note that we indicate matrices in the Nambu space of one superconductor by carets, and matrices describing both superconductors by underlines.

We expand the first term of (9) in powers of the tunneling matrix elements, namely the off-diagonal parts of (10). Keeping the lowest nonvanishing term, we obtain

$$-\mathfrak{A} = -\mathfrak{A}_L - \mathfrak{A}_R - \tfrac{1}{2}\text{Tr}\,\underline{\hat{\mathcal{G}}}\,\underline{\hat{\mathcal{T}}}\,\underline{\hat{\mathcal{G}}}\,\underline{\hat{\mathcal{T}}} - \int_0^\tau \frac{dt}{\hbar}\frac{1}{2}CV^2. \tag{13}$$

The third term, which we examine in detail below, contains the effects of pair and quasiparticle tunneling. The first two terms are the time integrals of the bulk free energies of the two uncoupled superconductors. If $V(t)$ is set equal to zero and $\Delta_{L,R}$ taken to be real, it is easy to identify the BCS free energies. Quite generally, we can make gauge transformations to make Δ_L and Δ_R real, whereupon (11) becomes (for the left superconductor)

$$\hat{\mathcal{G}}_L^{-1} = \left\{ -\hbar\frac{\partial}{\partial t} + i\hbar\vec{v}_{SL}\cdot\nabla + \left[\frac{\hbar^2\nabla^2}{2m} + \mu - \frac{m}{2}v_{SL}^2 + \frac{i}{2}\left(\hbar\frac{\partial\varphi_L}{\partial t} - eV\right)\right]\tau_3 - \hat{\Delta}_L\right\}\delta(x-x'). \tag{14}$$

Here $\vec{v}_{SL} \equiv -\hbar(\nabla\varphi_L + e\vec{A}/\hbar c)/2m$, if we allow for a vector potential. In (14) $\hat{\Delta}_L$ is now real, and $-\varphi_L$ is the phase of Δ_L in (12). Expanding (14), and the similar expression with $L \to R$, in powers of the electromagnetic potentials in this preferred gauge we get (for slowly varying potentials)

$$\mathcal{A}_L = \mathcal{A}_L^0 + \int_0^\tau \frac{dt}{\hbar}\int d^3x\left[\frac{N_L(0)}{4}\left(\hbar\frac{\partial\varphi_L}{\partial t} - eV\right)^2 + \tfrac{1}{2}\rho_S{}^L V_{SL}{}^2\right]. \tag{15}$$

Above, $N_L(0)$ is the density of free electron states at the Fermi surface; and $\rho_S\vec{v}_S$, the supercurrent induced by $\vec{v}_S$. Thus we see that bulk energies fix the magnitudes of Δ_L and Δ_R in (8) at their equilibrium values, and also pin $\hbar\dot{\varphi}_{L(R)}$ to $(\pm)\, eV$.[11] When these values are fixed, the multiple functional integral in (8) is reduced to a single one, over $\varphi \equiv \varphi_L - \varphi_R$, and the effective action is given by the last two terms in (13), the last term in (15), and a similar term with $L \to R$. Working out the third term in (13), we find it to be given by (with $|\mathcal{T}|^2$ being the appropriate average[12] of tunneling matrix elements)

$$\mathcal{A}_\mathcal{T} = |\mathcal{T}|^2\int\frac{d^3p_L}{(2\pi\hbar)^3}\int\frac{d^3p_R}{(2\pi\hbar)^3}\int_0^\tau\frac{dt}{\hbar}\int_0^\tau\frac{dt'}{\hbar}\left(\exp\left\{\frac{-i}{2}[\varphi(t)-\varphi(t')]\right\}G_L(t-t',\vec{p}_L)G_R(t'-t,\vec{p}_R)\right.$$
$$\left. - \exp\left\{-\frac{i}{2}[\varphi(t)+\varphi(t')]\right\}F_L(t-t',\vec{p}_L)F_R(t'-t,\vec{p}_R) + (R \leftrightarrow L)\right). \tag{16}$$

Here we have introduced Gorkov's G and F functions.[13]

Equation (16) is the basic result of this paper. It is nothing more or less than the standard tunneling theory: The analytic continuation to real times of the least-action path agrees completely with known results.[12]

Let us pause briefly to summarize what we have done. For the model defined by (1), we considered the partition function, Z. First, we introduced additional fields to eliminate the interaction terms in the Hamiltonian; second, we integrated out the individual electron variables; third, we were able to reduce the multiple functional integral to a single one over the phase difference by noting that large bulk energies determine the magnitude of the order parameter and the phase voltage relation.[14] The result is an effective action for the tunnel junction.

Equation (16) contains the nonlinear quasiparticle resistance and the frequency-dependent critical current characteristic of the tunneling model. To make connection with simpler models in wide use, we evaluate the first term of (16) in the normal state, and the second for zero voltage. With these simplifying assumptions, (16) reduces to

$$\mathcal{A}_\mathcal{T} \to \int_0^\tau dt\left(-\frac{I_0}{2e}\cos\varphi(t) + 2\int_0^\tau dt'\,\alpha(t-t')\sin^2\{\tfrac{1}{4}[\varphi(t)-\varphi(t')]\}\right). \tag{17}$$

Here I_0 is the critical current, and we have dropped a φ-independent constant (via $1-\cos 2x = 2\sin^2 x$). Further,

$$\alpha(t) = \frac{2|\mathcal{T}^2|}{\hbar^2}\int\frac{d^3p_L}{(2\pi\hbar)^3}\int\frac{d^3p_R}{(2\pi\hbar)^3}G_N(t,\vec{p}_L)G_N(-t,\vec{p}_R). \tag{18}$$

Within the approximation (18), $\alpha(t)$ is easily calculated. For t not too small, one may approximate the densities of states by constants, to obtain

$$\alpha(t) = \frac{\hbar}{2\pi e^2 R_N}\frac{1}{t^2}, \quad |t| \gg \frac{\hbar}{\mu}, \tag{19}$$

with $R_N{}^{-1} = 4\pi e^2|\mathcal{T}|^2 N_L(0)N_R(0)/\hbar$ being the normal-state resistance which can be interpreted as the shunt resistance present in many experiments. For simplicity, (19) has been calculated in the zero-temperature limit.

We can also treat a situation in which the external current is fixed. We imagine a one-dimensional geometry (along the x direction), the L and R superconductors occupying the regions $[-l, -\epsilon]$ and

$[+\epsilon, +l]$ $(\epsilon \ll l)$. From the kinetic energy contribution in (15)—and the similar one for R—we then obtain a term given by

$$-\int_0^\tau dt \frac{I}{2e}[\varphi - \varphi_{\text{ext}}], \tag{20}$$

where we have identified the total current, $I = \text{area} \times e/m \times (\rho_S v_S)_{L,R}$, the phase difference $\varphi = \varphi_L(-\epsilon) - \varphi_R(+\epsilon)$, and $\varphi_{\text{ext}} = \varphi(-l) - \varphi(+l)$. The last term in (20) describes the work done from outside to keep the current I constant. It can be dropped in the following, as well as the bulk kinetic energy. The case of a closed loop (SQUID) can be similarly treated, but is slightly more complicated because the magnetic field energy has to be included. We shall discuss these and other details elsewhere.

In conclusion, we have demonstrated that the partition function can be written in the form

$$Z \sim \int D\varphi \exp\{-\mathfrak{A}_{\text{eff}}[\varphi]\} \tag{21}$$

and that the effective action (in a simplified model) is given by

$$\mathfrak{A}_{\text{eff}}[\varphi] = \int_0^\tau \frac{dt}{\hbar}\left[\frac{\hbar^2 C}{8e^2}\left(\frac{\partial\varphi}{\partial t}\right)^2 + \mathfrak{U}(\varphi)\right] + 2\int_0^\tau dt \int_0^\tau dt'\,\alpha(t-t')\sin^2\{\tfrac{1}{4}[\varphi(t) - \varphi(t')]\}; \tag{22}$$

the "potential energy" $\mathfrak{U}(\varphi)$ contains the contributions discussed above. Our derivation gives a microscopic justification for the method used by Caldeira and Leggett[1] to calculate the zero-temperature decay rate of a Josephson junction in the presence of damping. (Their cutoff frequency is seen to be the Fermi energy.) Although our damping term agrees with theirs only in the approximation where the sine is replaced by its argument, the similarities in structure will be apparent. For example, the argument leading to the conclusion that "damping decreases the decay rate" can be easily repeated. Since we have consistently included the oscillatory and damping effects of tunneling, we have illuminated the recent controversy about frequency renormalizations.[3-5] We support the procedure adopted in Ref. 1 of calculating the decay rate as a function of damping constant for fixed renormalized frequency.

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[8]We have introduced V in such a way that for the least-action path (with respect to V) $V = -i\langle Q_L - Q_R\rangle/2C$. This choice reflects the fact that we are working with "imaginary" times.

[9]For the precise meaning of $\text{Tr}\ln\hat{\underline{\mathfrak{g}}}^{-1}$, see, e.g., J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960); G. Baym, Phys. Rev. 127, 1391 (1962).

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[14]Fluctuations about these minima will give small corrections, which we ignore here but which are relevant to the question raised in Ref. 6.