Charging corrections to the Josephson Hamiltonian

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Starting from a microscopic model which includes a charging term, we derive an effective, single-degree-of-freedom Hamiltonian, describing a Josephson junction. We obtain corrections to the standard Josephson Hamiltonian, which hybridize coordinate and momentum operators. The resulting equation of motion is analyzed in the classical limit, and the corresponding $I-V$ characteristics are obtained. We predict that, in a certain range of the parameters, the branching point in the $I-V$ curve and the effective resistance of the junction exhibit reentrant behavior as a function of both the self-capacitance and the normal resistance of the junction.

Recent interest in the behavior of small Josephson junctions came as a result of new developments in several areas. It has been predicted that charging effects in ultrasmall Josephson junctions will give rise to novel effects, some of which have been observed. In addition, experiments on two-dimensional granular systems showed reentrance-like behavior at low temperatures, which has been attributed to the physics of dissipative Josephson junctions.

Theoretical studies of these interesting effects employed the standard Josephson Hamiltonian

\[ H_0 = 4E_c \hat{\theta}^2 - E_J \cos \theta, \quad (1) \]

with $\hat{\theta}$ being the relative phase characterizing the many-body wave functions on the left-hand and right-hand side superconducting electrodes, and $\hat{\theta}$ (measuring the difference in the number of Cooper pairs between the left-hand side and the right-hand side) its canonical conjugate. Here the characteristic scale of the charging energy $E_c = e^2/2C$, with $C$ being the self-capacitance of the junction; the Josephson energy $E_J = 2\Delta|\pi N(0) |^2$, where $\Delta$ is the superconducting gap, $|\pi N(0) |$ is a typical matrix element of the tunneling Hamiltonian, and $N(0)$ is the single-electron density of states near the Fermi level. External bias and coupling to a dissipative environment are usually added as extra terms. Assuming that the energy due to charge differences across the junction is vanishingly small, states of the junction which correspond to different values of $\langle \hat{\theta} \rangle$ are degenerate in the absence of tunneling. $H_0$ is derived by introducing a single-electron tunneling term, employing a second-order degenerate perturbation theory and, finally, adding the charging Hamiltonian as an extra term.

Within present technologies, junctions with self-capacitance $C < 10^{-11}$ F are now being fabricated. Obviously the charging energies associated with such systems are not negligible, and the justification for employing degenerate perturbation theory is dubious. In this work we reexamine the procedure, allowed to above, of deriving $H_0$. We assume that the charging term is small (thus amenable to perturbation theory), yet not vanishingly small, implying that nondegenerate perturbation theory should be employed. In our derivation the charging term is included in the microscopic Hamiltonian [Eq. (3)] right from the start, rather than being added post factum to the macroscopic Josephson Hamiltonian. We find that the Josephson Hamiltonian is given by

\[ H_J = 4\bar{E}_c \bar{\theta}^2 - \bar{E}_J \cos \theta + 2J [i(\sin \theta \bar{\theta} + (\cos \theta) \bar{\theta}^2] \quad (2a) \]

to second order in $\epsilon_c \equiv E_c / \Delta$, with $\bar{E}_c \equiv e^2 / 2\bar{C}$, where

\[ \bar{C} = \frac{C}{(1 - 3E_c \epsilon_c / 2\Delta)}, \]

\[ \bar{E}_J \equiv E_J \left[ 1 + \frac{2}{\pi^2} \epsilon_c + \frac{5}{16} - \frac{8}{\pi^4} \right] \epsilon_c^2, \quad (2b) \]

\[ J \equiv - \bar{E}_c \epsilon_c^2 \left[ \frac{1}{2} - \frac{16}{\pi^4} \right]. \]

The new terms in (2a) are nonstandard hybrids of coordinate and momentum operators.

Equation (2a) has the form of a generalized tight binding Hamiltonian (in $n$ space) with both the on-site energies and the nearest-neighbor hopping matrix elements being site dependent [cf. Eq. (7)]. One may also cast Eq. (2a) in the form

\[ H_J = \bar{\theta}^2 \left[ 4M(\theta) \right]^{-1} + \left[ 4M(\theta) \right]^{-1} \bar{\theta}^2 + V(\theta), \]

where

\[ \left[ 4M(\theta) \right]^{-1} \equiv 2\bar{E}_c + J \cos \theta \]

and

\[ V(\theta) \equiv (\bar{E}_J - J) \cos \theta, \]

thus introducing a coordinate-dependent mass operator. In the latter form we ordered the operators according to the prescription suggested by, e.g., Abers and Lee. Their prescription is based on a convention, which was chosen as an attempt to avoid the problem of ambiguity which arises when nonstandard Hamiltonians are employed in a path-integral formulation. To see the source
of such an ambiguity, note that

\[ \hat{\mathcal{H}}^2 [4 \mathcal{M}(\theta)]^{-1} + [4 \mathcal{M}(\theta)]^{-1} \hat{\mathcal{H}}^2 \neq \hat{\mathcal{H}} [2 \mathcal{M}(\theta)]^{-1} \hat{\mathcal{H}} \]

when \( \mathcal{H} \) and \( \theta \) are operators, whereas for the corresponding classical variables the two expressions are equal.\(^{12}\) In Ref. 11 it was also shown that a careful derivation of the exponent in the path-integral presentation of the time-evolution operator, starting from a Hamiltonian with a coordinate-dependent mass, leads to the appearance of an effective action which differs from

\[ S = \int dt \left[ \frac{1}{2} \mathcal{M}(\theta) \dot{\theta}^2 - V(\theta) \right] . \]

In any case, for our problem the ambiguity and its resolution discussed above are associated with a term in the potential, which is of second order in \( \epsilon_c \) (cf. Eq. (2)). Such a term is of minor physical importance.

We next derive the equation of motion for the above-mentioned Hamiltonian and investigate it in the classical limit, where additional dissipation and external current bias terms are added. In this limit we neglect quantum-mechanical fluctuations of high orders in \( E_c / E_j \ll 1 \), but yet account for the correction terms in the Hamiltonian, whose origin is quantum mechanical. This approach is consistent, since we note that there are two independent small parameters in the problem. One is \( E_c / E_j \), and the other is \( \epsilon_c \equiv E_c / \Delta_c \) which is assumed to be small too. For our analysis to be consistent we have to restrict ourselves to \( \epsilon_c >> E_c / E_j \). This condition implies that \( E_j >> \Delta_c \), hence the normal state resistance of the junction, \( R_n \), must be small compared to \( \hbar / e^2 \).

The results of our analysis are detailed below. One interesting result is that in the light damping limit, \( I_{\min} \) (the branching point in the I-V curve; cf. Fig. 1) exhibits nonmonotonous behavior as a function of both \( \epsilon_c \) and the nominal normal resistance of the junction. This “quasireentrance” behavior is depicted in Fig. 2 and 3. We hope that the new form of the Josephson Hamiltonian, and the rather surprising results based on the classical analysis of the equation of motion that follows, will stimulate further theoretical and experimental investigations of charging effects in the quantum limit. In the following we sketch the main steps of our analysis.

Following the standard derivation of the Josephson Hamiltonian,\(^{5-9}\) we first consider the junction in the absence of tunneling. A many-body state of the system is denoted by \( | n \rangle \) and corresponds to \( N/2 + n \) Cooper pairs in the electrode on the right-hand side and \( N/2 - n \) on the left-hand side. The Hamiltonian of the system is written as \( \mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_e \), where \( \mathcal{H}_L (\mathcal{H}_R) \) is the Hamiltonian of the left (right) uncoupled electrode. \( \mathcal{H}_e \) is the charging term,

\[ \langle \nu | \mathcal{H}_e | \nu' \rangle = E_c \nu^2 \delta_{\nu \nu'} , \]

where \( | \nu \rangle \) is created by starting with \( | n = 0 \rangle \) and transferring \( \nu \) electrons from the left-hand to the right-hand side. \( \mathcal{H}_o \) is diagonal in the particle representation. For \( \mathcal{H}_e = 0 \), the states \( \langle n \rangle \) are degenerate (see, e.g., Ref. 7). Therefore, \( \mathcal{H}_L + \mathcal{H}_R \) will not contribute (apart from a constant term) to the effective Hamiltonian.

We next introduce a tunneling Hamiltonian,

\[ \mathcal{H}_T = \sum_{k,l;\sigma,\tau} \hat{T}_{k,l;\sigma,\tau} , \]

where

\[ \hat{T}_{k,l;\sigma,\tau} = T a_{k,l;\sigma,\tau}^\dagger a_{l,k} + \text{H.c.} \]

Here \( a_{k,l;\sigma,\tau}^\dagger (a_{L,R}) \) creates (annihilates) one electron of momentum \( k \) (l) and spin \( \sigma \) (\( \tau \)) on side right (left). \( \mathcal{H}_T \) connects the state \( | n \rangle \) with \( | n_+ \rangle (| n_- \rangle) \) by transferring a single electron from the left-hand side to the right-hand side (the right-hand to the left-hand side). The corrections to the unperturbed state \( | n \rangle \) due to \( \mathcal{H}_T \) may be calculated, employing nondegenerate perturbation theory. To second order in \( T \) they are
where

\[ E_{n,\pm} = E_e (2n \pm 1)^2 + E_k + E_I \]

\[ E_k (\geq \Delta) \] being the quasiparticle energy.

Our goal here is to construct an effective Hamiltonian, \( H_J \), in the subspace defined by \(|n\rangle\). In order to obtain \( H_J \) from the original Hamiltonian, components of the wave function that contain states \(|n_+\rangle, |n_-\rangle\) should be eliminated. Indeed we note that the \(|n_+\rangle, |n_-\rangle\) components of \(|\delta n^{(2)}\rangle\) are negligible with respect to the second-order terms in Eqs. (5) (i.e., the coefficients of \(|n + 1\rangle\) and \(|n - 1\rangle\)), provided that \(E_e n \ll |T|\). We must also require that the perturbation expansion converges, which implies \(|T| \ll \Delta\). We now pretend that we have found \(H'_J\) of the form \(H_0 + V',\) operating in the subspace \(|n\rangle\). To obtain the matrix elements of \(V'\) we compare first-order corrections to \(|n\rangle\) due to \(V'\) to second-order corrections due to the original Hamiltonian [Eq. (5)], neglecting the \(|n_+\rangle, |n_-\rangle\) components. The latter can be explicitly calculated if we replace \(|n\rangle\) by a product of grand canonical \(\psi_{BCS}^\rho \otimes \psi_{BCS}^L\). The above-mentioned comparison yields, for the nonvanishing off-diagonal matrix elements of \(V'\),

\[ \langle n \pm 1|V'|n\rangle = -4|T|^2 \sum_{k,i} \frac{u_k v_k u_i v_i}{E_k + E_i + 4E_e (1/2 \pm n)} \]

with

\[ E_k = (\epsilon_k^2 + \Delta^2)^{1/2} \]

and

\[ u_k = [\frac{1}{2}(1 + (\epsilon_k/E_k))]^{1/2}, \quad v_k = [\frac{1}{2}(1 - (\epsilon_k/E_k))]^{1/2} \]

being the standard \(\psi_{BCS}\) parameters.\(^6\) The sums in Eq. (6) are replaced by integrals, assuming a constant density of states near the Fermi level, \(N(0)\). We obtain

\[ \langle n \pm 1|V'|n\rangle = -4\Delta[\pi T |N(0)|^2 \times |1 - (2/n^2)|\epsilon_e(1 \pm 4n)] \]

\[ + [\frac{1}{2}\epsilon_e(1 \pm 4n)]^2 \].

The diagonal matrix elements of \(V'\) are calculated by comparing first-order corrections to the energy due to \(V'\), with second-order corrections to the energy due to \(H_T\). The procedure closely follows the derivation of the off-diagonal matrix elements. We find that apart from a constant term, \(\langle n|V'|n\rangle\) contributes a term \(-3E_e [\pi T |N(0)|^2 \epsilon_e \hat n^2 /2\), which can be absorbed in \(E_e\), yielding \(\hat E_e\) [Eq. (2)].

The tridiagonal matrix \(V'\) obtained by truncating the quasiparticle states is not Hermitian. In order to remedy this we apply the similarity transformation

\[ H_J = H_0 + V = S^{-1}(H'_J)S, \]

where

\[ \langle n|S|m\rangle = \delta_{mn}s_n, \quad s_{n+1} = \frac{\langle n|V'|n+1\rangle}{\langle n+1|V'|n\rangle} \]

This transformation does not alter the (real) spectrum of \(H_J\). As a result of this procedure we obtain (up to an additive constant)

\[ \langle m|H_J|n\rangle = \begin{cases} 4\hat E_e n^2, & m = n \\ -\frac{1}{2}E_k J_{n} + J_{m^2}, & m = n \pm 1 \\ 0, & \text{otherwise} \end{cases} \]

which is consistent with the form of Eq. (2).

The equations of motion for the operators \(\hat \sigma\) and \(\hat n\) are

\[ \hat n\hat \sigma = i[H_J, \hat \sigma] = 8\hat E_e \hat n + 2iJ \sin \hat \theta + 4J(\cos \hat \theta) \hat n, \]

\[ \hat n\hat \sigma = i[H_J, \hat \sigma] = 8\hat E_e \hat n + 2iJ \sin \hat \theta + 4J(\cos \hat \theta) \hat n, \quad (8a) \]
\[ \hat{\mathcal{H}} = i [H_J, \hat{\theta}] \]
\[ = -\mathcal{E}_J \sin \theta - 2iJ (\cos \theta) \hat{\theta} + 2J (\sin \theta) \hat{\theta}^2. \]  

We now derive an equation for the expectation value of \( \hat{\theta} \), assuming small fluctuations in \( \hat{\theta} \) (the "classical" limit). To facilitate comparison with an experimental setup we now introduce a biasing d.c. current source, and an external shunt resistor \( R \). Unlike what follows from the standard Josephson Hamiltonian, here \( \hat{\theta} \) is not proportional to \( \hat{\theta} \). The voltage on the junction, defined as the change in energy due to incremental charge transfer, is \( V = \hbar \dot{\theta} / 2e \). The dissipated current is, therefore, \( \hbar \dot{\theta} / 2eR \). To include both the bias and the dissipation, a term \( \hbar I / 2e - \hbar \dot{\theta} / (2eR) \) should be added to the right-hand side of Eq. (8b). After some algebra we obtain (to second order in \( \epsilon_c \))

\[ \hat{\theta} + \frac{\epsilon}{f(\theta)} (\sin \theta)^2 + (\gamma \dot{\theta} + \omega_j^2 \sin \theta) f(\theta) = \omega_j^2 f(\theta) ; \]
\[ \gamma \equiv \frac{8\mathcal{E}_J}{(2e)^2 R}, \quad \omega_j^2 \equiv \frac{8\mathcal{E}_J \mathcal{E}_J}{\hbar^2}, \quad \omega_j^2 \equiv \frac{8\mathcal{E}_J}{(2e) \hbar^2}, \quad \epsilon \equiv \frac{J}{\mathcal{E}_J}, \]  

\[ f(\theta) \equiv 1 + 2e \cos \theta . \]

For any value of \( I \) a solution for \( \hat{\theta} \) (and hence \( V \)) is obtained by integrating Eq. (9). \( I-V \) curves for intermediate damping (\( \gamma / \omega_j = 1 \)) are shown in Fig. 1 for several values of \( \epsilon \). Note the difference from the Stewart-McCumber case (\( \epsilon = 0 \)).

In the heavy damping (\( \gamma \gg \omega_j \)) limit, \( I_{\text{min}} = \mathcal{I}_J \), and since \( \mathcal{I}_J = (2e) \mathcal{E}_J / \hbar \), \( I_{\text{min}} \) is given by Eq. (2b).

The light damping (\( \gamma \ll \omega_j \)) limit can also be studied analytically. We use the variable \( \phi = \theta - \epsilon \sin \theta \) to transform Eq. (9) into

\[ \dot{\phi} + (\gamma \dot{\phi} + \omega_j^2 \sin \phi) f(\phi) = \omega_j^2 (1 + \epsilon \cos \phi) \]

(to first order in \( \epsilon_c \)). For \( \epsilon < 1 \), \( \dot{\phi} = 0 \) if and only if \( \dot{\theta} = 0 \), and consequently one may use (10) to evaluate \( I_{\text{min}} \). Following Stewart (Ref. 13), \( I_{\text{min}} \) (or \( \omega_j^2 \)) corresponds to the bias for which the gain in kinetic energy during one period exactly balances the dissipated energy,

\[ \gamma \int_{-\pi}^{\pi} \dot{\phi}(\phi) f(\phi) d\phi = \omega_j^2 \int_{-\pi}^{\pi} (1 + \epsilon \cos \phi) d\phi. \]

(11)

For small \( \gamma, \omega \) we can substitute for \( \dot{\phi}(\phi) \) the separatrix trajectory (separating running modes from stationary modes in phase space) of the \( \gamma = \omega = 0 \) case. To first order in \( \gamma \),

\[ \dot{\phi}_{\text{ss}}(\phi) = \pm 2^{1/2} \omega \frac{1 + \cos \phi - \frac{\epsilon}{2} \left(1 - \cos(2\phi)\right)}{1 - \cos(2\phi)} \]

Inserting this into (11), we find

\[ I_{\text{min}}(\gamma / \omega_J \rightarrow 0) = \frac{(2e) \hbar \omega_{\text{min}}}{8\mathcal{E}_J} \]
\[ = \frac{8}{\pi(2e)R} \left[ \frac{2DE_j}{\rho_n} \right]^{1/2} \]
\[ \times \left[ 1 + \frac{1}{\pi^2} \left[ \frac{1}{2} + \frac{1}{3} \left[ 1 - \frac{32}{\pi^4} \right] \right] \right] \]
\[ \times \frac{1}{\rho_n} \left[ \frac{E_c}{\Delta} \right], \]

(12)

where

\[ \rho_n \equiv R_n (2e)^2 / \pi \hbar \]

\( R_n \) being the normal resistance of the junction. \( I_{\text{min}} \) is thus a nonmonotonous function of \( C \) and \( \rho_n \), having a maximum at \( E_c / \rho_n \Delta = \frac{1}{4} \). \( I_{\text{min}} \) is plotted as a function of \( \epsilon_c \) (Fig. 2) and \( \rho_n \) (Fig. 3). For a certain range of \( I \) we may observe a nonmonotonous behavior of the effective resistance \( V / I \) as a function of, e.g., \( \epsilon_c \). This is demonstrated in Fig. 4.

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10. Similar (but not identical) capacitance renormalization was previously obtained by U. Eckern, G. Schönh, and V. Ambegaokar, Phys. Rev. B 30, 6419 (1984). We note that their renormalization factor differs from ours by the sign and magnitude of $J$. See also Ref. 5.


12. Only employment of the former form of kinetic energy will yield an identical Hamiltonian exponentiated in the path-integral formulation.

