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Superconducting charge qubits from a microscopic many-body perspective

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Abstract

The quantized Josephson junction equation that underpins the behaviour of charge qubits and other tunnel devices is usually derived through canonical quantization of the classical macroscopic Josephson relations. However, this approach may neglect effects due to the fact that the charge qubit consists of a superconducting island of finite size connected to a large superconductor. We show that the well-known quantized Josephson equation can be derived directly and simply from a microscopic many-body Hamiltonian. By choosing the appropriate strong-coupling limit we produce a highly simplified Hamiltonian that nevertheless allows us to go beyond the mean-field limit and predict further finite-size terms in addition to the basic equation.

The Josephson effect [1] is still one of the phenomena that make superconductors such a fascinating area of study. For instance, after some 40 years of intensive basic and applied research there are still new features of the coherent tunnelling of Cooper pairs coming to light in connection with junctions involving small superconducting grains. The new complications arise from the fact that when one side of a Josephson junction is sufficiently small for the charging energy to be relevant, quantum interplay between charging and tunnelling begins to appear [2]. The standard approach to describing these junctions is to take the classical equations of motion of the superconducting phase difference ϕ_D across the junctions and apply canonical quantization rules to ϕ_D as a 'position' variable. Of course, the classical Josephson equations for such a phase difference are first derived from microscopic theory [1], and so this standard approach represents a 're-quantization' of 'classical' equations that were in turn derived from quantum mechanical microscopic theory using a mean-field theory that does not take into account the charging energy of the island. Consequently, in such approaches the description of quantum fluctuations is at best semi-phenomenological. In what follows we examine the limitations of the above procedure on the basis of a simple model which permits an exact treatment of a superconducting island coupled weakly to a bulk superconductor.

To motivate our interest in the problem we note that much current experimental and theoretical attention is focused on nanoscale superconducting grains coupled to large superconductors as such ‘Cooper Pair Boxes’ are becoming realistic candidates for being useful qubits in Quantum Information devices [3–6]. Starting with the work of Nakamura *et al* [7], over the last few years there have been a number of impressive experiments [8–13] demonstrating appropriate charge qubit behaviour and macroscopic tunnelling. As experiments continue to improve, it is now pertinent to re-examine the standard approach to describing quantum fluctuations in superconducting charge qubits and related systems. Clearly, in the course of such investigation one would expect to reproduce the basic quantum phenomenology from a fully microscopic approach within a well controlled approximation, as there is already good experimental support for this. Nevertheless, a generalized theory will also yield new additional terms due to the finite size of the superconducting islands and for future experiments they could have significant consequences. To shed light on these, we examined a simple microscopic model of a Cooper Pair box, showing how the familiar phenomenology emerges, along with new finite-size effects.

1. Quantizing the Josephson relations

In the interest of clarity, we start our discussion by recalling, briefly, the usual phenomenological approach to the problem at hand. The standard way to obtain the Hamiltonian describing a small superconductor connected through Josephson tunnel junctions to a bulk superconductor is by starting with the Josephson equations for ϕ_D and V , the difference in phases of the two superconducting regions and the voltage across the junction,

$$I = I_C \sin \phi_D \quad (1)$$

$$\frac{d\phi_D}{dt} = \frac{2eV}{\hbar}, \quad (2)$$

where I_C is the critical current of the junction. Although derived from a quantum mechanical microscopic treatment, as evidenced by the appearance of \hbar , these equations can be regarded as classical equations of motion. We follow the standard procedure for canonical quantization and first find the Lagrangian that leads to these equations. Namely, we take,

$$\mathcal{L} = \frac{1}{2} \frac{\hbar^2 C}{4e^2} \left(\frac{d\phi_D}{dt} \right)^2 + \frac{\hbar I_C}{2e} \cos \phi_D, \quad (3)$$

where we have introduced the total island capacitance, C . If we choose the phase ϕ_D to be the canonical position variable, we can identify the canonical momentum $\pi = \partial \mathcal{L} / \partial \dot{\phi}_D$,

$$\pi = \frac{\hbar^2 C}{4e^2} \dot{\phi}_D = \frac{\hbar CV}{2e} = \hbar(N - n_g), \quad (4)$$

and it is seen that the phase of the condensate and the excess number of Cooper pairs on the island, $(N - n_g)$, are conjugate variables [3, 4]. The term n_g represents an applied gate voltage (in dimensionless units) and so the canonical momentum $\pi = (N - n_g)$ is effectively the charge on the device, viewed as a capacitor, in units of $2e$. Note that if the total charge on the system is zero, this can be rewritten in terms of the charge difference. To quantize the system, we introduce the commutation relation between conjugate variables $[\phi_D, \pi] = i\hbar$ and note that this can be satisfied by writing $\pi = -i\hbar \partial / \partial \phi_D - n_g$ (keeping the gate voltage explicit). Then the Hamiltonian, $\hat{H} = \pi \dot{\phi}_D - \mathcal{L}$, is given by,

$$\hat{H} = E_C \left(i \frac{\partial}{\partial \phi_D} - n_g \right)^2 - E_J \cos \phi_D, \quad (5)$$

where the charging energy is given by $E_C = 2e^2/C$ and E_J is defined as $E_J = \hbar I_C/2e$. The Schrödinger's equation for the amplitude $\psi(\phi_D)$ is then,

$$\hat{H}\psi(\phi_D) = i\hbar \frac{d}{dt}\psi(\phi_D). \quad (6)$$

Evidently, the probability that the phase difference takes on a certain value is given by $|\psi(\phi_D)|^2$.

This is the desired standard quantum description of the Josephson junction. In the remainder of this paper, we show how the above quantized Josephson junction equation can be rederived directly from the microscopic theory in a way that includes finite-size effects.

2. Finite superconductors as spins

We wish to produce a description of a finite superconductor that is simple enough to solve exactly but retains properties due to its finite size. Specifically, we wish to be able to capture effects that go beyond the mean-field approximation. Our starting point is the well-known BCS Hamiltonian [14]:

$$\hat{H} = \sum_{k, \sigma} \epsilon_k c_{k, \sigma}^\dagger c_{k, \sigma} - \sum_{k, k'} V_{k, k'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}, \quad (7)$$

where $c_{k, \sigma}^\dagger$ and $c_{k, \sigma}$ create and annihilate electrons, respectively, with spin σ in the state k with energy ϵ_k and the matrix element $V_{k, k'}$ describes an attractive two body interaction. As we are discussing a finite superconducting island, the label k, \uparrow does not refer to a free electron wavevector but to a generic single-electron eigenstate, with $-k, \downarrow$ representing the corresponding time-reversed state.

A common approximation to this equation is made by assuming the pairing potential $V_{k, k'}$ is equal for all k, k' in a region around the Fermi energy determined by the cutoff energy $\hbar\omega_c$ and zero outside this region. That is, $V_{k, k'} = V$ for $|\epsilon_k - \epsilon_F| < \hbar\omega_c$ and $V_{k, k'} = 0$ otherwise. This greatly simplifies matters whilst retaining the essential physics. We now adopt a similar philosophy in making a further approximation, and take all the single-electron energy levels ϵ_k within the cutoff region around the Fermi energy to be equal to the Fermi energy ϵ_F .

The interaction term, $V_{k, k'}$ acts only within the cutoff region around the Fermi energy. Outside this region the Hamiltonian is diagonal and trivially solved. Writing the single-electron energy as $\epsilon_k = \epsilon_F + (\epsilon_k - \epsilon_F)$, we note that within the cutoff region $|\epsilon_k - \epsilon_F| < \hbar\omega_c$, and thus if $V \gg \hbar\omega_c$, then $|\epsilon_k - \epsilon_F| \ll V$ and we can discard the variation of ϵ_k . Thus in this strong-coupling approximation, our Hamiltonian becomes,

$$\hat{H} = \epsilon_F \sum_k c_{k, \sigma}^\dagger c_{k, \sigma} - V \sum_{k, k'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}, \quad (8)$$

where the dashes on the sums indicate that they are only taken over states within the cutoff region.

Although this caricature of a realistic Hamiltonian represents an uncontrolled approximation, we will show that it allows us to derive a Josephson junction equation that goes beyond mean field, and that the results it produces agree in the strong-coupling limit with known results in two important cases. Namely, the mean-field solution of this Hamiltonian agrees with the BCS solution, and the exact solution agrees with the Richardson solution [15].

It should be noted that although many superconductors can be described as having strong coupling, the BCS Hamiltonian is not necessarily appropriate for their description. Equation (8) is hence not intended as a description of this particular class of superconductors, but rather as a generic model that, although simplified, allows an exact solution and a description of the physics we are trying to capture.

As a consequence of the above simplifications equation (8) can now be written in terms of the three operators [16],

$$\begin{aligned}\widehat{S}^Z &= \frac{1}{2} \sum_k^l \left(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow} - 1 \right) \\ \widehat{S}^+ &= \sum_k^l c_{k\uparrow}^\dagger c_{-k\downarrow} \\ \widehat{S}^- &= \sum_k^l c_{-k\downarrow} c_{k\uparrow}.\end{aligned}\quad (9)$$

Note that these operators obey the commutation relations, and therefore the algebra, of quantum spin operators of size $l/2$, where l is the number of levels in the cutoff region. Thus the main result of this section is the effective Hamiltonian,

$$\widehat{H}_{\text{sp}} = 2(\epsilon_F - \mu) \left(\widehat{S}^Z + \frac{l}{2} \right) - V \widehat{S}^+ \widehat{S}^-, \quad (10)$$

where we have introduced a chemical potential μ to describe coupling to a reservoir.

3. Exact solution

The eigenstates of equation (10) are the eigenstates of the spin operator \widehat{S}^Z , $|\frac{l}{2}, m_N\rangle$, where the component of the spin along the Z axis is given by $m_N = N - l/2$ and N denotes the number of Cooper pairs on the island. The eigenenergies corresponding to these eigenstates are,

$$E_N = 2(\epsilon_F - \mu)N - VN(l - N + 1). \quad (11)$$

A chemical potential allows us to specify the average number of Cooper pairs on the island in equilibrium. In the case of the exact solution, where N is a good quantum number, this means choosing a state with a particular value of N to be the ground state. We choose μ so that the ground state is the state with a chosen value of N , which we label \bar{N} . The eigenenergies E_N therefore become,

$$E_N = -VN(2\bar{N} - N), \quad (12)$$

and the ground state is $|\frac{l}{2}, m_{\bar{N}}\rangle$, with energy,

$$E_{\text{gs}} = -V\bar{N}^2. \quad (13)$$

We can also easily see that although the pairing parameter $\langle \widehat{S}^+ \rangle = 0$ in all eigenstates, i.e. there is no symmetry breaking, we still have fluctuations as expected for a finite superconductor which are given by $\langle \widehat{S}^+ \widehat{S}^- \rangle = N(l - N + 1)$ for a general eigenstate N and

$$\left\langle \frac{l}{2}, m_{\bar{N}} \left| \widehat{S}^+ \widehat{S}^- \right| \frac{l}{2}, m_{\bar{N}} \right\rangle = \bar{N}(l - \bar{N} + 1) \quad (14)$$

for the ground state. We also see that the operator \widehat{S}^+ which couples eigenstates, corresponds (when appropriately normalized) to the quasiparticle creation operator for the system.

4. Comparison to standard results

To generate confidence in this simple model, we compare its solutions to the solutions of the full Hamiltonian (equation (7)) in two ways. First, we find the mean-field solution and compare it to the BCS results. Second, we compare the exact solution to the Richardson solution in the appropriate limit.

4.1. The mean-field solution

The mean-field approximation arises from the assumption that the operators \widehat{S}^\pm remain close to their expectation values, $\langle \widehat{S}^\pm \rangle$. We write $\widehat{S}^\pm = \langle \widehat{S}^\pm \rangle + (\widehat{S}^\pm - \langle \widehat{S}^\pm \rangle)$, and discard terms to second order or higher in $(\widehat{S}^\pm - \langle \widehat{S}^\pm \rangle)$. Writing $V \langle \widehat{S}^- \rangle = \Delta$, we find the mean-field Hamiltonian for our model,

$$\widehat{H}_{\text{MF}} = 2(\epsilon_F - \mu) \left(\widehat{S}^Z + \frac{l}{2} \right) - \Delta \widehat{S}^+ - \Delta^* \widehat{S}^- + \frac{|\Delta|^2}{V}. \quad (15)$$

Apart from the constant term, this is a linear combination of the spin operators \widehat{S}^Z , \widehat{S}^Y and \widehat{S}^X and is therefore proportional to the projection of a spin operator on an unknown direction specified by the unit vector \hat{n} . Thus denoting $\widehat{S} \cdot \hat{n}$ by \widehat{S}_n^Z , we may write,

$$\widehat{H}_{\text{MF}} = \gamma \widehat{S}_n^Z + \frac{|\Delta|^2}{V} + 2(\epsilon_F - \mu) \frac{l}{2}, \quad (16)$$

and therefore the problem of diagonalizing equation (15) is equivalent to the problem of rotating the axis of quantization for our effective spin operators. Requiring that the commutation relations $[\widehat{S}_n^Z, \widehat{S}_n^\pm] = \widehat{S}_n^\pm$ hold for spin operators in the frame of reference where the axis of quantization is along \hat{n} determines both an expression for \widehat{S}_n^+ and the value of γ ,

$$\begin{aligned} \widehat{S}_n^+ &= \frac{2\Delta}{\gamma} \left(\widehat{S}^Z - \frac{\Delta}{2\xi_F - \gamma} \widehat{S}^+ - \frac{\Delta^*}{2\xi_F + \gamma} \widehat{S}^- \right) \\ \gamma &= 2\sqrt{(\xi_F)^2 + |\Delta|^2}, \end{aligned} \quad (17)$$

where $\xi_F = \epsilon_F - \mu$ and we note that $\gamma = 2E_F$, the energy of a Cooper pair evaluated at the Fermi energy. The ground state of our Hamiltonian can now be trivially found, as it corresponds to the $m = -l/2$ eigenstate of the operator \widehat{S}_n^Z . Recalling that a maximal m state of a spin operator pointing in one direction is a spin coherent state [17] in any other we find,

$$\begin{aligned} |\alpha\rangle &= \frac{1}{\sqrt{(1 + |\alpha|^2)^l}} \sum_{N=0}^l \frac{(\alpha^* \widehat{S}^+)^N |l/2, m_0\rangle}{N!} \\ &= \frac{1}{\sqrt{(1 + |\alpha|^2)^l}} \prod_k (1 + \alpha^* c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) \left| \frac{l}{2}, m_0 \right\rangle. \end{aligned} \quad (18)$$

As one might expect, the second line is a way of writing the BCS ground state wavefunction in the limit where all the levels have equal probability of occupation, i.e. $u_k/v_k = \alpha^*$ for all k . Making use of equation (16) and the fact that $\widehat{S}_n^- |\alpha\rangle = 0$ for the ground state, we find that $\alpha = (\xi_F - E_F)/\Delta$. To complete the calculation, we need to self-consistently determine the values Δ and μ , which is relatively simple in the spin model and gives,

$$|\Delta|^2 = V^2 \bar{N} (l - \bar{N}) \quad (19)$$

$$\epsilon_F - \mu = V (l/2 - \bar{N}) \quad (20)$$

$$H_{\text{SMF}} |\alpha\rangle = -V \bar{N}^2 |\alpha\rangle \quad (21)$$

where \bar{N} is the average occupation of the island. We find equations (18)–(21) are exactly equal to the expressions found if we were to solve the full BCS equation and then take the weak-coupling limit (this is shown in the appendix of [18]). Comparing the mean-field solution to the exact solution, we see that, surprisingly, the exact (equation (13)) and mean field (equation (21)) ground state energies are identical. However, we have a non-zero pairing parameter $\langle S^- \rangle = \Delta/V$ and the expectation value of the mean-field coupling term,

$$\langle \alpha | -\Delta \widehat{S}^+ - \Delta^* \widehat{S}^- + \frac{|\Delta|^2}{V} | \alpha \rangle = -V \bar{N} (l - \bar{N}), \quad (22)$$

neglects the quantum fluctuations present in the exact solution,

$$\left\langle \frac{l}{2}, m_{\bar{N}} \left| -V\widehat{S}^+\widehat{S}^- \right| \frac{l}{2}, m_{\bar{N}} \right\rangle = -V\bar{N}(l - \bar{N} + 1) \quad (23)$$

in much the same way a classical spin neglects the fluctuations present in a quantum spin, i.e. the eigenvalues of \widehat{S}^2 are $S(S + 1)$ and not the classical values S^2 .

4.2. The Richardson solution

Unbeknownst to the condensed matter community for many years, there exists an exact solution to the BCS Hamiltonian (equation (7)) for finite superconductors, first discovered in 1963 by Richardson [15, 19, 20] in the context of nuclear physics. It has been shown that this solution reproduces the BCS result in the bulk limit, but it is difficult to work with for any island occupied by more than a few Cooper pairs. The Richardson solution requires the introduction of operators that diagonalize the full (i.e. not mean field) BCS Hamiltonian,

$$\widehat{H} = \sum_{\nu=1}^N E_{J\nu} \widehat{B}_{J\nu}^+ \widehat{B}_{J\nu}^- \quad (24)$$

$$\widehat{B}_{J\nu}^+ = \sum_k \frac{c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger}{2\epsilon_k - E_{J\nu}}, \quad (25)$$

where the sum in equation (24) runs over ν up to the total number of Cooper pairs on the island. The parameters $E_{J\nu}$ are found by solving the equations,

$$1 + \frac{2V}{E_{J\nu} - E_{J\nu}} = V \sum_k \frac{1}{2\epsilon_k - E_{J\nu}}, \quad (26)$$

for all ν .

Whilst the usual BCS theory has an essential singularity at $V = 0$, the theory is well behaved near $1/V \sim 0$. Thus, following Altshuler *et al* [21] we expand equation (26) in powers of $\hbar\omega_c/V$. Using $\epsilon_k \sim \epsilon_F$ leads to,

$$\frac{1}{V} + \sum_{\nu=1}^N \frac{2}{E_{J\nu} - E_{J\nu}} = \frac{l}{(E_{J\nu} - 2\epsilon_F)} + \sum_{k=1}^l \frac{2(\epsilon_k - \epsilon_F)}{(E_{J\nu} - 2\epsilon_F)^2}. \quad (27)$$

Now discard the second term on the right as negligible, multiply by $E_{J\nu} - 2\epsilon_F$, and sum over the N parameters $E_{J\nu}$ to obtain,

$$\sum_{\eta=1}^N \frac{E_{J\eta} - 2\epsilon_F}{V} + N(N - 1) + 0 = Nl, \quad (28)$$

where the double sums over η, ν have either vanished, or gone to $N(N - 1)$ due to symmetry. Finally, we recall that the energy of the Richardson solution is given by a sum over $E_{J\eta}$, and rewrite equation (28) to get the energy of an island containing N Cooper pairs:

$$E_N = 2\epsilon_F N - V N(l - N + 1). \quad (29)$$

As heralded in the introduction this result matches the exact energy of the spin Hamiltonian as given in equation (11) for $\mu = 0$.

Thus we have shown that although we have made a significant approximation to the Hamiltonian, the results thereby derived are consistent with results obtained by solving the full system in either the mean-field approximation or exactly, and *then* taking the appropriate limit.

5. Phase representation of the spin operators \widehat{S}^+ and \widehat{S}^-

The preceding sections have established our model of a finite superconducting system as a large spin, as given in equation (10). We shall now go on to show how this model can be used to derive a phase-representation description of the Josephson effect in a system comprising a small island coupled to a larger piece of bulk superconductor.

We wish to convert to a representation in terms of the continuous phase variable ϕ , i.e. convert from ket notation to wavefunction $\psi(\phi)$ and differential operator (such as $\frac{d}{d\phi}$) notation. Thus, a ket $|\psi_a\rangle$ will become a wavefunction $\langle\phi|\psi_a\rangle$, and the differential operator must be consistent with this. Defining the state $|\phi\rangle = (2\pi)^{-1/2} \sum e^{i\phi N} |\frac{l}{2}, m_N\rangle$, we find that the wavefunction corresponding to $|\frac{l}{2}, m_N\rangle$ is $(2\pi)^{-1/2} e^{-i\phi N}$. We can then examine how the operators act on this wavefunction.

$$\begin{aligned} \widehat{S}^Z \left\langle \phi \left| \frac{l}{2}, m_N \right. \right\rangle &= \langle \phi | \left(N - \frac{l}{2} \right) \left| \frac{l}{2}, m_N \right\rangle \\ &= \left(N - \frac{l}{2} \right) \left\langle \phi \left| \frac{l}{2}, m_N \right. \right\rangle \\ &= \left(N - \frac{l}{2} \right) \frac{e^{-i\phi N}}{\sqrt{2\pi}} \end{aligned} \quad (30)$$

$$\widehat{S}^Z \psi(\phi) = \left(i \frac{\partial}{\partial \phi} - \frac{l}{2} \right) \psi(\phi).$$

Similarly, we find for the raising operator,

$$\begin{aligned} \widehat{S}^+ \left\langle \phi \left| \frac{l}{2}, m_N \right. \right\rangle &= \langle \phi | \sqrt{(N+1)(l-N)} \left| \frac{l}{2}, m_N \right\rangle \\ \widehat{S}^+ \psi(\phi) &= e^{-i\phi} \sqrt{\left(i \frac{\partial}{\partial \phi} + 1 \right) \left(l - i \frac{\partial}{\partial \phi} \right)} \psi(\phi), \end{aligned} \quad (31)$$

with the lowering operator given by,

$$\begin{aligned} \widehat{S}^- \left\langle \phi \left| \frac{l}{2}, m_N \right. \right\rangle &= \langle \phi | \sqrt{N(l-N+1)} \left| \frac{l}{2}, m_N \right\rangle \\ \widehat{S}^- \psi(\phi) &= e^{i\phi} \sqrt{i \frac{\partial}{\partial \phi} \left(l - i \frac{\partial}{\partial \phi} + 1 \right)} \psi(\phi). \end{aligned} \quad (32)$$

Collecting the differential forms for the operators and rewriting S^+ and S^- into a more convenient form leaves us with,

$$\begin{aligned} \widehat{S}^Z &= \left(i \frac{\partial}{\partial \phi} - \frac{l}{2} \right) \\ \widehat{S}^\pm &= \sqrt{\left(\frac{l}{2} \pm \left(i \frac{\partial}{\partial \phi} - \frac{l}{2} \right) \right)} e^{\mp i\phi} \sqrt{\left(\frac{l}{2} \mp \left(i \frac{\partial}{\partial \phi} - \frac{l}{2} \right) \right)}. \end{aligned} \quad (33)$$

The form of the raising and lowering operators can also be derived by requiring that the commutation relations for quantum spins are enforced. We see that it is the $(i \frac{\partial}{\partial \phi} - \frac{l}{2})$ terms in the S^+ , S^- operators that take into account the finite-size effects and ensure that $[S^+, S^-] \neq 0$.

Writing the operators in this form allows us to take the large size ($l \rightarrow \infty$) limit. In taking this limit we assume that $S^Z \ll \frac{l}{2}$. In the superconducting language, this corresponds to only states close to half filling being occupied. Specifically, we assume,

$$\left| \left\langle \frac{l}{2}, m_N \left| \psi \right. \right\rangle \right| \sim 0 \quad \text{for} \quad \left| N - \frac{l}{2} \right| \gtrsim \left(\frac{l}{2} \right)^{1/2}, \quad (34)$$

a condition which is fulfilled for coherent states with \bar{N} set close to $\frac{l}{2}$. When this is true, we can expand the square root in $(i\frac{\partial}{\partial\phi} - \frac{l}{2})/l$. We see that the leading order terms give $S^\pm = \frac{l}{2}e^{\mp i\phi}$, and we regain the semiclassical large-size limit for which $[S^+, S^-] = 0$ as discussed by Lee and Scully [16].

6. Quantized Josephson junction equation

We can now use the forms of the operators given in equations (33) to write down the quantized Josephson equation. We begin with a Hamiltonian that describes a finite superconducting island coupled to a superconducting reservoir,

$$\hat{H} = \hat{H}_I + \hat{H}_R + \hat{H}_C + \hat{H}_T, \quad (35)$$

where \hat{H}_I and \hat{H}_R are the BCS Hamiltonians on the island and reservoir respectively, and we introduce Hamiltonians representing the charging energy of the island,

$$\hat{H}_C = \frac{4e^2}{2C}(\hat{N}_I - n_g)^2 \quad (36)$$

and the tunnelling between island and reservoir,

$$\hat{H}_T = -T \sum_{k,q} c_k^\dagger c_{-k}^\dagger c_{-q} c_q + c_q^\dagger c_{-q}^\dagger c_{-k} c_k, \quad (37)$$

where T is the standard tunnelling matrix element for Cooper pairs [22], which we assume for simplicity to be real and independent of k, q . If we make our strong-coupling approximation and assume that all the electronic energy levels can be considered equal, we can write these Hamiltonians in terms of spin operators, as follows:

$$\begin{aligned} \hat{H}_I &= 2(\epsilon_{FI} - \mu_I)\hat{S}_I^Z - V_I\hat{S}_I^+\hat{S}_I^- \\ \hat{H}_R &= 2(\epsilon_{FR} - \mu_R)\hat{S}_R^Z - V_R\hat{S}_R^+\hat{S}_R^- \\ \hat{H}_C &= \frac{4e^2}{2C}(\hat{S}_I^Z + l_I/2 - n_g)^2 \\ \hat{H}_T &= -T(\hat{S}_I^+\hat{S}_R^- + \hat{S}_I^-\hat{S}_R^+). \end{aligned} \quad (38)$$

Inserting these expressions into equation (35), we obtain

$$\hat{H} = E'_C(\hat{S}_I^Z - n'_g)^2 - T(\hat{S}_I^+\hat{S}_R^- + \hat{S}_I^-\hat{S}_R^+), \quad (39)$$

where we have incorporated the terms from \hat{H}_I linear and quadratic in \hat{S}_I^Z into the renormalized charging energy and gate voltage represented by E'_C and n'_g respectively. In the limit that both the reservoir and the island can be considered infinite, we regain the standard form for the quantized Josephson junction Hamiltonian,

$$\hat{H} = E'_C \left(i\frac{\partial}{\partial\phi_I} - n'_g \right)^2 - T \frac{l_R l_I}{2} \cos(\phi_I - \phi_R), \quad (40)$$

suggesting that equation (6) can be considered as a large-size limit where the finite size of the island can be neglected. However, we are now able to obtain, using equation (33), the next terms in the series expansion,

$$\begin{aligned} \hat{H} = E'_C \left(i\frac{\partial}{\partial\phi_I} - n'_g \right)^2 - T \frac{l_R}{2} \left\{ (l_I + 1) \cos(\phi_I - \phi_R) - \frac{2}{l_I} \left(i\frac{\partial}{\partial\phi_I} - \frac{l_I}{2} \right)^2 \cos(\phi_I - \phi_R) \right. \\ \left. - \frac{2}{l_I i} \left(i\frac{\partial}{\partial\phi_I} - \frac{l_I}{2} \right) \sin(\phi_I - \phi_R) + \dots \right\}. \end{aligned} \quad (41)$$

We find that the new terms involve products of both the phase and the charge operators. Thus the Josephson tunnelling term effectively depends on the island charge. Making an analogy with a particle in a potential, with a position corresponding to the phase, we see that the extra terms in equation (41) can be thought of as a velocity-dependent potential. This effect also breaks the periodicity of the island energy with n'_g , i.e. the energy now depends on the absolute value of n'_g , rather than merely its value modulo 1. In this derivation we have assumed that the single-electron energies are all equal, and thus the occupations u_k/v_k are all equal. However, these occupations maintain a similar order of magnitude when different, and so we would expect the extra terms in equation (41) to be of a similar size when the strong-coupling approximation is relaxed.

We can make an estimate of the size of these effects for an island of a given size by calculating l_1 , the number of electrons within the cutoff region, by comparing the level spacing to the Debye energy. For an island with a volume equal to that described in [7], we find that $l_1 \approx 6 \times 10^5$, and thus the additional terms in equation (41) (proportional to $1/l_1$) are unlikely to be significant. If we consider instead a nanograin of the type described in [19, 20, 23], we find that $l_1 \approx 400$, and thus the extra terms may be relevant.

7. Conclusions

We have shown how the quantum Josephson junction equation, usually derived by re-quantizing the mean-field equations of motion, can be directly derived from a microscopic description of a superconducting island. We used a simplified Hamiltonian in which the energy of the individual microscopic electron levels is considered equal that allowed an exact solution to be found. We have shown how a mean-field approximation leads to a solution that corresponds to a spin coherent state, which is the BCS state in the appropriate limit. As well as illustrating how the familiar phenomenology emerges through the mean-field approximation, we showed we can describe effects beyond the mean field, such as quantum fluctuations. We went on to rederive the Josephson junction equation and describe size dependent corrections to the familiar terms.

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