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Information-theoretical approach to Josephson tunneling

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A simplified Hamiltonian model of pair tunneling between two weakly coupled superconductors is used to obtain the ac Josephson current. A closed operator algebra is defined through commutation with the Hamiltonian. With the use of information theory, we find a subalgebra (quasi-angular-momentum operators) that allows us to obtain naturally the dependence of the Josephson current on the phase, as well as a geometric interpretation of the phase. The quasi-spin algebra permits us to find a consistent solution for the imbalance of charge without resorting to further constraints.

I. INTRODUCTION

The use of the pseudospin model proposed by Anderson,[1] based on pseudo-angular-momentum operators, to solve the problem of tunneling of pairs of electrons in weakly coupled superconductors, gave rise to extensive discussion[2–6] due to some inconsistencies it presented. The main difficulty is related to the imbalance of charge, which was found to be zero even for voltage-biased junctions.[3,4] It was pointed out by Ferrell that the Josephson-Anderson number phase formalism provides a complete description of pair tunneling when the algebra is properly defined. He argues that the identification of the pair number operator with the commutator of the pair current with the pair tunneling Hamiltonian is wrong since, due to a symmetry of the underlying microscopical theory, this commutator is zero. Here, we show that, taking a simple model Hamiltonian, but using the complete Hamiltonian in the definition of the new operators through commutators, the aforementioned problems can be solved. The model, introduced by Eckmann and Guenin,[7] in spite of its simplifications, allows us to reproduce the main features of the theory. To solve it we define a closed-operator algebra through commutation with the Hamiltonian and use information theory (IT)[8–11] to calculate the expectation value of those operators. Finding the dynamical invariants of the algebra, we define a subspace where the dependence of the Josephson current with the phase arises naturally, as well as a geometrical interpretation of the latter. We show how to find properly the imbalance of charge and point out the difficulties that led to the misinterpretation of the operator, which in turn produced the inconsistencies mentioned previously. Finally the Josephson equation for the phase is also recovered from the theory without further ansätze.

The paper is organized as follows. A brief resume of basic ideas about information theory is given in Sec. II, our model for Josephson tunneling is developed in Sec. III, and finally, some conclusions are drawn in Sec. IV.

II. BRIEF REVIEW OF THE FORMALISM

The inverse problem of reconstructing the density matrix for a system when the expectation value of dynamical operators is known can be approached through information theory. This formalism provides a well-defined prescription by incorporating the principle of maximum entropy,[8–11] which is summarized here briefly. Given the expectation values O_j of operators $\hat{O}_j$ the statistical operator $\hat{\rho}(t)$ is defined by:

$$\hat{\rho}(t)=\exp\left[-\lambda_0-\sum_{j=1}^{M}\lambda_j(t)\hat{O}_j\right] . \tag{2.1}$$

The λ_i's, $M+1$ of them, are Lagrange multipliers which will be determined to fulfill the set of constraints

$$\langle \hat{O}_j \rangle = O_j = \mathrm{Tr}(\hat{\rho}\hat{O}_j), \quad j=1,2,\ldots,M \tag{2.2}$$

and the normalization condition

$$\mathrm{Tr}(\hat{\rho}\hat{I})=\mathrm{Tr}(\hat{\rho}\hat{O}_0)=\mathrm{Tr}\hat{\rho}=1 , \tag{2.3}$$

where $\hat{I}$ is the unity operator. Under the conditions stated through Eqs. (2.1)–(2.3), if the time evolution of the statistical operator is given by

$$i\hbar\frac{d\hat{\rho}}{dt}=[\hat{H},\hat{\rho}]\ , \tag{2.4}$$

the entropy, defined by

$$S(\hat{\rho})=-k_B\mathrm{Tr}(\hat{\rho}\ln\hat{\rho}) \tag{2.5}$$

is maximum, and a constant of the motion.[8,11,12] In Eqs. (2.4) and (2.5), $\hbar$ is Planck's constant, $\hat{H}$ is the Hamiltonian, and k_B, Boltzmann's constant. The relevant question now is which are those operators whose expectation values we need to know in order to construct a density operator that fulfills Eq. (2.4)? The answer is that those "relevant" operators $\hat{O}_j$ belong to a set that closes under commutation with the Hamiltonian,[11] such that

$$[\hat{H},\hat{O}_j]=i\hbar\sum_{i=0}^{M}\hat{O}_i g_{ji}\ , \tag{2.6}$$

in this way defining a Lie algebra of $(M+1)$ elements, whose structure constants are given by the matrix $\underline{G}$,[9,11] which can be time dependent if $\hat{H}$ is. We are restricting ourselves to the case when we know the expectation values of *all* the elements of the algebra. The Liouville equation (2.4) can be substituted by a set of coupled equations for the Lagrange multipliers λ_i as follows:

$$\frac{d\lambda_i}{dt}=\sum_{j=0}^{M}g_{ij}\lambda_j,\quad i=1,\ldots,M\ . \tag{2.7}$$

Solving this set of equations and using the Ehrenfest theorem:

$$\frac{d\langle\hat{O}_i\rangle}{dt}=\sum_{j=0}^{M}\langle\hat{O}_j\rangle g_{ji}\ , \tag{2.8}$$

the entropy becomes

$$S[\hat{\rho}(t)]=\sum_{j=0}^{M}\lambda_j(t)\langle\hat{O}_j\rangle\ . \tag{2.9}$$

Since the entropy is a constant of the motion, Eq. (2.9) provides the constraint in the time evolution of the $\hat{O}_j$'s. The equations for the commutators Eq. (2.6) are defined through commutation with the Hamiltonian. As shown by Cerdeira *et al.*[13] in a different context, the relevant set is generated taking the operation (adH) $\hat{O}_n$ $(\equiv[\hat{H},\hat{O}_n]_-)$, $M+1$ times until we close the subalgebra. $\hat{O}_n$ is the operator whose dynamical evolution we want to study. Therefore the set contains all the $\hat{O}_j$'s that are relevant to the knowledge of $\hat{O}_n$.

It has been shown that the mean value of the operators and the Lagrange multipliers are related by[8,14]

$$-\frac{\partial\lambda_0}{\partial\lambda_i}=\langle\hat{O}_i\rangle\ . \tag{2.10}$$

Following Duering *et al.*[14] we can write for the time evolution of the $\langle\hat{O}_j\rangle$'s,

$$\langle\hat{O}_j\rangle_t=\sum_i\langle\hat{O}_i\rangle_{t_0}F_{ij}(t,t_0) \tag{2.11}$$

or in vector notation,

$$\langle\hat{O}\rangle_t=\langle\hat{O}\rangle_{t_0}\underline{F}(t,t_0)\ . \tag{2.12}$$

$\underline{F}(t,t_0)$ is a square matrix defined by[8]

$$-\frac{\partial F}{\partial t}=\underline{F}\cdot\underline{G}\ . \tag{2.13}$$

In the Heisenberg representation we can write

$$\hat{O}_t=\hat{O}_{t_0}\underline{F}(t,t_0)\ . \tag{2.14}$$

For the Lagrange multipliers we have

$$\lambda^t=\underline{F}^{-1}(t,t_0)\lambda^{t_0}\ . \tag{2.15}$$

The subscript or superscript t,t_0 in Eqs. (2.11)–(2.15) indicates whether we are working with a covariant or a contravariant vector, respectively. The information about the dynamical behavior of the system is completely contained in the matrix $\underline{F}(t,t_0)$ [or $\underline{G}(t,t_0)$]. This information is obtained through the investigation of the transformation properties (and invariants) of spaces defined by the matrix $\underline{F}$. The covariant or contravariant nature of the vectors is also defined with respect to these transformations.

In order to define vectorial Reimann spaces with $\langle\hat{O}_t\rangle$ (or $\hat{O}_t$) and λ^1 as elements, we need first to specify the form of the scalar products, which are invariants, as

$$\langle\hat{O}\rangle_t\langle\hat{O}\rangle^t=\langle\hat{O}\rangle_0\langle\hat{O}\rangle^0 \tag{2.16}$$

or

$$\hat{O}_t\hat{O}^t=\hat{O}_0\hat{O}^0 \tag{2.17}$$

and

$$\lambda_t\lambda^t=\lambda_0\lambda^0\ , \tag{2.18}$$

where the index zero refers to the time $t=t_0$ before the transformation is applied. Given a covariant vector $\hat{O}_t$ we need to find the metric tensor of the space $\underline{e}$ (such that $\underline{e}\,\underline{e}^{-1}=\underline{1}$) for which

$$\langle\hat{O}\rangle^t=\underline{e}\langle\hat{O}\rangle_t\ . \tag{2.19}$$

In this way we shall be able to construct the invariants of the motion of the system.[8,14,15] Using the invariance of the scalar product we obtain

$$\underline{F}\,\underline{e}\,\underline{\tilde{F}}=\underline{e}\ , \tag{2.20}$$

where $\underline{\tilde{F}}$ indicates transposed matrix. Furthermore

$$\underline{\tilde{F}}^{-1}\underline{e}'\underline{F}^{-1}=\underline{e}'\ , \tag{2.21}$$

where

$$\lambda_t=\lambda^t\underline{e}'\ . \tag{2.22}$$

If we use Eqs. (2.7) and (2.8), we can replace Eqs. (2.20) and (2.21) by

$$\underline{G}\,\underline{e}=-\underline{e}\,\underline{\tilde{G}} \tag{2.23}$$

and

$$\underline{G}\,\underline{e}'=-\underline{e}'\underline{\tilde{G}} \tag{2.24}$$

which are easier to handle. Then, through the use of the metric matrices (which are not uniquely defined) we can express the invariants [Eqs. (2.16)–(2.18)] as

$$\hat{O}_t \hat{O}^{\,t} = \hat{O}_t \underline{e} \hat{O}_t \tag{2.25}$$

and

$$\lambda_t \lambda^t = \lambda^t \underline{e}' \lambda^t \ . \tag{2.26}$$

In the next section we shall apply this formalism to a tunneling Hamiltonian in order to calculate the Josephson current. We shall compare our results to some of the existing pseudo-angular-momentum theories.[2–4]

III. JOSEPHSON TUNNELING

In the early sixties Anderson put forward a pseudospin model to discuss tunneling between two superconductors.[1] Recently, several authors pointed out some inconsistencies of the model.[2–4,16] The most serious difficulty arises when the expectation value of the operator representing charge imbalance is found to be zero, even when a constant voltage between both superconductors is maintained, as found by Ferrell.[3] Di Rienzo and Young[4] refer to the source of the problem as being the insistence in using only the BCS ground state to represent the superconductors and the unnecessary restriction of the range of momentum sums in the definition of the operators. To solve the problem they lifted these restrictions and proposed a new state vector to represent the charge imbalance. They still assume that this new state vector is a direct product of the state vector of the left and right superconductor. Here, we present a calculation where the dynamical evolution of the system is properly taken into account. The charge-imbalance operator will be obtained from the invariants of the transformation which governs the dynamics and show that those inconsistencies disappear.

In this section we use a simplified model Hamiltonian for tunneling across the junctions introduced earlier by Eckmann and Guenin.[7] It is a one-momentum Hamiltonian which can be solved defining a closed-operator algebra as presented in Sec. II. This method does not introduce any constraint on the time evolution of the wave function. We show that the main aspects of the problem come out in a natural way already in this simple model. model.

A. The model

Consider two coupled superconductors, described by the Hamiltonian

$$\hat{H} = \hat{H}_l^0 + \hat{H}_r^0 + \hat{H}_t \ . \tag{3.1}$$

Here $\hat{H}_l^0$ and $\hat{H}_r^0$ describe the superconductors to the left and right to the junction and have the form:

$$\hat{H}^0 = \varepsilon \hat{N} + \theta \hat{S}^{+} \hat{S} \ . \tag{3.2}$$

ε is the energy of a quasiparticle measured from the Fermi surface, θ is the BCS coupling constant,

$$\hat{N} = \hat{a}_\uparrow^\dagger \hat{a}_\uparrow + \hat{a}_\downarrow^\dagger \hat{a}_\downarrow \tag{3.3}$$

is the density operator, and

$$\hat{S}^\dagger \hat{S} = \hat{a}_\uparrow^\dagger \hat{a}_\downarrow^\dagger \hat{a}_\downarrow \hat{a}_\uparrow \tag{3.4}$$

is the pair number operator and $\hat{a}_\sigma^\dagger$ ($\hat{a}_\sigma$) is the creation (annihilation) operator of quasiparticles of spin σ.

The last term of Eq. (3.1) $\hat{H}_t$, given by

$$\hat{H}_t = \rho(\hat{S}_l^\dagger \hat{S}_r + \hat{S}_r^\dagger \hat{S}_l) \ , \tag{3.5}$$

is the pair tunneling Hamiltonian, which represents a two-step tunneling of single electrons across the barrier.[17] Notice that this Hamiltonian is generally accepted as describing the dc as well as the ac tunneling. A comparison with Ferrell[3] and Di Rienzo and Young[4] shows that when the zeroth-order Hamiltonian $\hat{H}_l^0 + \hat{H}_r^0$ is explicitly written, we are including an ideal battery maintaining a constant voltage V between the left and right superconductors, if we define

$$\varepsilon_l = \varepsilon_l^0 - eV/2, \quad \varepsilon_r = \varepsilon_r^0 + eV/2 \ . \tag{3.6}$$

Di Rienzo and Young[4] considered only the case when $\varepsilon_l = \varepsilon_r$, while Ferrell,[3] even considering different superconductors, does not take into account the zeroth-order Hamiltonian in the definition of the operator algebra, in this way missing the proper definition of the pseudo-angular-momentum subalgebra. We show in Sec. III C that this Hamiltonian reproduces the ac Josephson tunneling when the appropriate limits are taken. Instead, the dc tunneling cannot be obtained using this particular Hamiltonian as we shall see below.

Here we study the dynamics of some key physical quantities whose expectation values are known. These relevant quantities for this problem are the number of particles on each side of the junction, the number of pairs, and the tunneling term. The corresponding operators are

$$\hat{O}_1 = \hat{N}_l \ , \tag{3.7a}$$

$$\hat{O}_2 = \hat{N}_r \ , \tag{3.7b}$$

$$\hat{O}_3 = \hat{S}_l^\dagger \hat{S}_l \ , \tag{3.7c}$$

$$\hat{O}_4 = \hat{S}_r^\dagger \hat{S}_r \ , \tag{3.7d}$$

$$\hat{O}_5 = \hat{S}_l^\dagger \hat{S}_r + \hat{S}_r^\dagger \hat{S}_l \ . \tag{3.7e}$$

Following the formalism presented in Sec. II, we can define a closed algebra, formed by linear combinations of operators. These operators are found through initial commutation of one of the operators, let us say $\hat{O}_1$, with the Hamiltonian.[7,13] The equation of motion for the complete set is

$$[\hat{H}, \hat{O}_1] = 2i\rho \hat{O}_6 \ , \tag{3.8a}$$

$$[\hat{H}, \hat{O}_2] = -2i\rho \hat{O}_6 \ , \tag{3.8b}$$

$$[\hat{H}, \hat{O}_3] = i\rho \hat{O}_6 \ , \tag{3.8c}$$

$$[\hat{H}, \hat{O}_4] = -i\rho \hat{O}_6 \ , \tag{3.8d}$$

$$[\hat{H}, \hat{O}_5] = i\alpha \hat{O}_6 \ , \tag{3.8e}$$

$$[\hat{H}, \hat{O}_6] = -i\alpha \hat{O}_5 - 2i\rho \hat{O}_7 \ , \tag{3.8f}$$

$$[\hat{H}, \hat{O}_7] = 2i\rho \hat{O}_6 \ , \tag{3.8g}$$

where

$$\hat{O}_6 = i(\hat{S}_l^\dagger \hat{S}_r - \hat{S}_r^\dagger \hat{S}_l) , \tag{3.9}$$

$$\hat{O}_7 = \hat{S}_l^\dagger \hat{S}_l (\hat{1} - \hat{N}_r) - \hat{S}_r^\dagger \hat{S}_r (\hat{1} - \hat{N}_l) , \tag{3.10}$$

and

$$\alpha = -[2(\varepsilon_l - \varepsilon_r) + \theta_l - \theta_r] . \tag{3.11}$$

Here, it appears clearly that α can be interpreted as the voltage across the junction when $V \neq 0$, even if the superconductors are the same. The operators $\hat{O}_6$ and $\hat{O}_7$ had been generated to close the algebra necessary to the knowledge of the time evolution of the expectation values of the observables $\hat{O}_1 - \hat{O}_5$. Therefore we define the set of $M+1$ relevant operators as $\{\hat{O}_0 = \hat{1}, \hat{O}_1, \hat{O}_2, \hat{O}_3, \hat{O}_4, \hat{O}_5, \hat{O}_6, \hat{O}_7\}$. The matrix $\underline{G}$ is defined by

$$\begin{aligned} &g_{16} = g_{17} = -g_{26} = -g_{67} = 2i\rho , \\ &g_{36} = -g_{46} = i\rho , \\ &g_{56} = -g_{65} = i\alpha , \end{aligned} \tag{3.12}$$

all other elements being zero. Using Eqs. (2.8) and (3.12) we obtain for the expectation values

$$\langle \hat{O}_1 \rangle = \langle \hat{O}_1 \rangle_0 - f(\alpha,\rho) - w(\alpha,\rho,t) , \tag{3.13a}$$

$$\langle \hat{O}_2 \rangle = \langle \hat{O}_2 \rangle_0 + f(\alpha,\rho) + w(\alpha,\rho,t) , \tag{3.13b}$$

$$\langle \hat{O}_3 \rangle = \langle \hat{O}_3 \rangle_0 - \tfrac{1}{2} f(\alpha,\rho) - \tfrac{1}{2} w(\alpha,\rho,t) , \tag{3.13c}$$

$$\langle \hat{O}_4 \rangle = \langle \hat{O}_4 \rangle_0 + \tfrac{1}{2} f(\alpha,\rho) + \tfrac{1}{2} w(\alpha,\rho,t) , \tag{3.13d}$$

$$\langle \hat{O}_5 \rangle = \langle \hat{O}_5 \rangle_0 - \frac{\alpha}{2\rho} f(\alpha,\rho) - \frac{\alpha}{2\rho} w(\alpha,\rho,t) , \tag{3.13e}$$

$$\langle \hat{O}_6 \rangle = \langle \hat{O}_6 \rangle_0 \cos(\omega t) + \frac{\hbar\omega}{2\rho} f(\alpha,\rho) \sin(\omega t) , \tag{3.13f}$$

$$\langle \hat{O}_7 \rangle = \langle \hat{O}_7 \rangle_0 - f(\alpha,\rho) - w(\alpha,\rho,t) \tag{3.13g}$$

with

$$f(\alpha,\rho) = \frac{2\rho}{(\hbar\omega)^2} (\alpha \langle \hat{O}_5 \rangle_0 + 2\rho \langle \hat{O}_7 \rangle_0) , \tag{3.14a}$$

$$w(\alpha,\rho,t) = \frac{2\rho}{\hbar\omega} \langle \hat{O}_6 \rangle_0 \sin(\omega t) - f(\alpha,\rho) \cos(\omega t) , \tag{3.14b}$$

and

$$\hbar^2 \omega^2 = \alpha^2 + 4\rho^2 . \tag{3.14c}$$

We now calculate the partition function, which enters in the density matrix.

B. The partition function

Since this subsection is very technical we summarize here the results, and refer to Appendix A for details. We consider the Hilbert space spanned by the 16 eigenvectors

$$|l_1 l_2 r_1 r_2\rangle = |l_1\rangle \otimes |l_2\rangle \otimes |r_1\rangle \otimes |r_2\rangle , \tag{3.15}$$

where l_1 and r_1 take the values 0 or 1. In this basis all operators are diagonal with the exception of $\hat{O}_5$ and $\hat{O}_6$. The matrix elements for the operators as well as those of $\ln\hat{\rho}$ are given in Appendix A. Diagonalizing $\ln\hat{\rho}$, we evaluate $e^{\lambda 0}$, resulting in the formula:

$$\begin{aligned} e^{\lambda 0} = {} & 1 + e^{-2(\lambda_1+\lambda_2)-(\lambda_3+\lambda_4)} + 2e^{-\lambda_1-2\lambda_2-\lambda_4} \\ & + 2e^{-2\lambda_1-\lambda_2-\lambda_3} + 4e^{-\lambda_1-\lambda_2} + 2e^{-\lambda_2} \\ & + 2e^{-\lambda_1} + 2e^{-\lambda_1-\lambda_2} e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]} \cosh a . \end{aligned} \tag{3.16a}$$

Here

$$a = \{[\lambda_1 - \lambda_2 + (\lambda_3 - \lambda_4)/2 + \lambda_7]^2 + \lambda_5^2 + \lambda_6^2\}^{1/2} \tag{3.16b}$$

and the λ_i's are the Lagrange multipliers. From Eqs. (3.16) and (2.10) we can calculate the expectation value of the operators we want to study as a function of the Lagrange multipliers (see Appendix B). The time dependence of the latter is evaluated in Appendix C. Having these elements we go on to calculate the second-order invariants of the system as described in Sec. II, Eqs. (2.25) and (2.26). We shall show that some of them are associated with the conservation of electrons, pairs, and energy. We shall obtain two extra invariants, whose meaning we shall explain in the next section. This will allow us to obtain a geometrical interpretation for the Josephson tunneling.

C. Dynamical invariants of the Josephson junction: The pseudoangular momentum approach

As shown in Sec. II, in order to obtain the dynamical invariants it is necessary to know the metric tensors e and e' of the dual space of operators and Lagranger multipliers [see Eqs. (2.23) and (2.24)]. Solving Eqs. (2.23)–(2.26), those invariants are given by

$$\hat{O}_1 - \frac{2\rho}{\alpha} \hat{O}_5 , \tag{3.17a}$$

$$\hat{O}_2 + \frac{2\rho}{\alpha} \hat{O}_5 , \tag{3.17b}$$

$$\hat{O}_3 - \frac{\rho}{\alpha} \hat{O}_5 , \tag{3.17c}$$

$$\hat{O}_4 + \frac{\rho}{\alpha} \hat{O}_5 , \tag{3.17d}$$

$$\hat{O}_7 - \frac{2\rho}{\alpha} \hat{O}_5 , \tag{3.17e}$$

$$\hat{O}_5^2 + \hat{O}_6^2 + \hat{O}_7^2 \tag{3.17f}$$

and

$$\lambda_7 - \frac{2\rho}{\alpha} \lambda_5 \tag{3.18a}$$

and

$$a^2 = [\lambda_1 - \lambda_2 + (\lambda_3 - \lambda_4)/2 + \lambda_7]^2 + \lambda_5^2 + \lambda_6^2 . \tag{3.18b}$$

It can be seen from equations of the operators and their definition [see Eqs. (3.17)] that the first five invariants are associated to the conservation of the number of electrons, number of pairs, and energy. From the invariants given by Eqs. (3.17f) and (3.18b) and using the expectation values calculated in Appendix B, it is possible to define two interrelated three-dimensional spaces, one of operators, one of Lagrange multipliers. The space of operators, composed of $\hat{O}_5$, $\hat{O}_6$, and $\hat{O}_7$ have the following commutation relations:

$$[\hat{O}_5,\hat{O}_6]=-2i\hat{O}_7 \ , \tag{3.19a}$$

$$[\hat{O}_6,\hat{O}_7]=-2i\hat{O}_5 \ , \tag{3.19b}$$

$$[\hat{O}_7,\hat{O}_5]=-2i\hat{O}_6 \ , \tag{3.19c}$$

with the constraint

$$[\hat{O}_5^2+\hat{O}_6^2+\hat{O}_7^2,\hat{O}_i]=0, \quad i=1,2,3 \ . \tag{3.20}$$

This operator space is isomorphic with that of the angular momentum, where the Casimir operator is given by Eq. (3.17f). In this way we can make, without any external imposition (i.e., not necessarily forcing its definition), the following association between a closed-compact semisimple Lie algebra, defined by Eqs. (3.19), and the SO(3) group [see Eqs. (B5)–(B7)]:

$$\hat{O}_5 \leftrightarrow \hat{J}_x \ , \tag{3.21a}$$

$$\hat{O}_6 \leftrightarrow \hat{J}_y \ , \tag{3.21b}$$

$$\hat{O}_7 \leftrightarrow \hat{J}_z \ , \tag{3.21c}$$

thus showing that the pseudo-momentum approach arises naturally from the invariants of the space, and correctly finding those operators. We shall see below that one of these operators $\hat{O}_6$ is associated to the pair current across the junction and that $\hat{J}_z$ cannot be identified with the charge-imbalance operator. The dual space of the Lagrange multipliers can be defined from the invariance of a as

$$\lambda_5=\mathbf{x}\lambda_5 \ , \tag{3.22a}$$

$$\lambda_6=\mathbf{y}\lambda_6 \ , \tag{3.22b}$$

$$\lambda_7=\mathbf{z}[\lambda_1-\lambda_2+(\lambda_3-\lambda_4)/2+\lambda_7] \ , \tag{3.22c}$$

where $(\mathbf{x},\mathbf{y},\mathbf{z})$ are the Cartesian orthogonal unit vectors. It is equivalent to work with any of the spaces as shown in Ref. 14. In both cases, the magnitude of the radial vector is an invariant of the motion, as shown in Eqs. (3.17f) and (3.18b). From Eqs. (3.21) and the calculation of the initial expectation values, we can define the new operators $\hat{\theta}$ and $\hat{\phi}$ through

$$\hat{O}_5=R_0\sin\hat{\theta}\cos\hat{\phi} \ , \tag{3.23}$$

$$\hat{O}_6=R_0\sin\hat{\theta}\sin\hat{\phi} \ , \tag{3.24}$$

$$\hat{O}_7=R_0\cos\hat{\theta} \ , \tag{3.25}$$

where R_0 relates the magnitude of the radial vectors of the dual spaces (R_0 and a) and is given by [see Eqs. (3.18b) and (B5)–(B7)],

$$R_0=-2\exp[-\lambda_0-(\lambda_1+\lambda_2)-(\lambda_3-\lambda_4)/2]\sinh a \ . \tag{3.26}$$

Using the fact that λ_0, λ_1, λ_2, λ_3, and λ_4 are constants in time, as shown in Appendix C, and Eq. (3.18b) we see that R_0 is also an invariant, thus reinforcing the result of Eq. (3.20), i.e., that the Casimir operator is an invariant. The pair current operator[3,4,7]

$$I=\frac{d\langle \hat{S}_l^\dagger \hat{S}_l\rangle}{dt} \tag{3.27a}$$

can be obtained from Eqs. (3.14) and found to be

$$I=\frac{d\langle \hat{O}_3\rangle}{dt}=-\frac{\rho}{\hbar}\langle \hat{O}_6\rangle \ . \tag{3.27b}$$

Substituting Eq. (3.24) and (3.27a) we find that

$$I=-\frac{\rho}{\hbar}R_0\langle \sin\hat{\theta}\sin\hat{\phi}\rangle \ . \tag{3.27c}$$

Thus obtaining the Josephson relation[18] between the pair current and the phase, $\hat{\phi}$ is associated to the Josephson's phase.

Summarizing, we have calculated, with the use of information theory[11,12,14] a basis of operators forming a closed Lie algebra, whose associated groups have an SO(3) symmetry. One of the components $\langle \hat{O}_6\rangle$ is associated to the pair current across the junction. The corresponding phase, or Josephson phase, is a consequence of an invariant relationship between the Lagrange multiplires, this in turn being a result of maximizing the entropy. Therefore we find a dynamical definition of the Josephson current which does not depend on particular approximations of the problem, and the form of I (the pair current) is always proportional to $\sin\phi$, independent of the voltage bias. To make contact with Ferrell's argument, we notice that Eq. (3.8f) (which now we know to represent the commutator of the pair current operator with the Hamiltonian) is *not* the number of pairs, defined by $\langle \hat{O}_3\rangle+\langle \hat{O}_4\rangle$. Even so it is a strictly to zero-for-zero bias function, in this way agreeing with Ferrell.

In the next section we show how the equation of motion for the phase is obtained from the theory.

D. dc and ac tunneling

1. *Time dependence of the phase of the Josephson current: ac tunneling*

Having calculated the current as a function of the phase, we need to evaluate the behavior of its derivative, one of the main points discussed by Ferrell.[3] From Eq. (3.8f) we obtain

$$\frac{d\langle \hat{O}_6\rangle}{dt}=\frac{\alpha}{n}\langle \hat{O}_5\rangle+\frac{2\rho}{\hbar}\langle \hat{O}_7\rangle \tag{3.28}$$

which can be written as

$$\frac{d\langle \hat{O}_6\rangle}{dt}=\left\langle R_0\left[\frac{\alpha}{n}\sin\theta\cos\phi+\frac{2\rho}{\hbar}\cos\theta\right]\right\rangle \ . \tag{3.29}$$

The angles ϕ, the Josephson's phase, and θ are defined by

$$\phi=\arctan\frac{\langle \hat{O}_6\rangle}{\langle \hat{O}_5\rangle} \tag{3.30}$$

or

$$\phi=\arctan\frac{\lambda_6(t)}{\lambda_5(t)} \tag{3.31}$$

and

$$\cos\theta=[\lambda_1-\lambda_2+(\lambda_3-\lambda_4)/2+\lambda_7]/a \ , \tag{3.32}$$

where a is defined in Eq. (3.18b). Equations (3.30)–(3.32) had been found from (3.21)–(3.25). To study the time dependence of the phase of the Josephson current, we see that

$$\frac{d\phi}{dt}=\frac{1}{\langle\hat{O}_5\rangle^2+\langle\hat{O}_6\rangle^2}\left[\langle\hat{O}_5\rangle\frac{d\langle\hat{O}_6\rangle}{dt}-\langle\hat{O}_6\rangle\frac{d\langle\hat{O}_5\rangle}{dt}\right] \tag{3.33}$$

which can be written as

$$\frac{d\phi}{dt}=\frac{\alpha}{\hbar}+\frac{2\rho}{\hbar}\frac{\cos\theta}{\sin\theta}\cos\phi \ . \tag{3.34}$$

If we consider a weakly coupled biased junction, i.e., $\alpha \gg \rho$, we obtain, after averaging over time

$$\frac{d\phi}{dt}=\frac{\alpha}{\hbar} \ , \tag{3.35}$$

which agrees with Josephson's equation.

2. *Nonbiased junction limit*

As it was said above, several references suggest that the Hamiltonian given by Eq. (3.1) reproduces the Josephson dc current. However, the information-theoretical approach gives a different result. Let us take into consideration the following. If α is zero, which means no applied voltage across the junction, there is no time evolution provided there is no interaction at all between the junctions (i.e., $\rho=0$) [see Eqs. (3.8)]. If instead we suppose that only α is zero, which means that we make the ansätz that the dc current is induced by some portion of the interaction, we obtain [$\rho\neq 0$, but $\alpha=0$ using Eqs. (3.13)],

$$I=-\frac{\rho}{\hbar}\left[\langle\hat{O}_6\rangle_0\cos(\omega t)+\frac{2\rho}{\hbar\omega}\langle\hat{O}_7\rangle_0\sin(\omega t)\right] \tag{3.36}$$

and as it can be seen the current is time dependent. Thus we can conclude that this Hamiltonian cannot reproduce the dc Josephson tunneling.

3. *Proper definition of the charge imbalance*

As we mentioned earlier the point that gave rise to controversies in the existing literature is the incorrect result for the imbalance charge. This is given by the mean value of the operator

$$\hat{S}_z=\tfrac{1}{2}(\hat{S}_l^\dagger\hat{S}_l-\hat{S}_r^\dagger\hat{S}_r)=\tfrac{1}{2}(\hat{O}_3-\hat{O}_4) \ . \tag{3.37}$$

To analyze the physical meaning of the results obtained in the previous section, it is necessary to emphasize that the subset of relevant operators related to SO(3) are $\hat{O}_5$, $\hat{O}_6$, and $\hat{O}_7$. A quick comparison of Eq. (3.37) with Eq. (3.10) shows that $\hat{O}_7$ does not describe the imbalance of charge. Using our results from Appendix B, we obtain for $\langle\hat{S}_z\rangle$

$$\langle\hat{S}_z\rangle=e^{-\lambda 0}(e^{-2\lambda_1-\lambda_2-\lambda_3}-e^{-\lambda_1-2\lambda_2-\lambda_4} -e^{-\lambda_1-\lambda_2-(\lambda_3+\lambda_4)/2}\sinh a\cos\theta) \ . \tag{3.38}$$

Also using the results from Appendix B we may notice that the mean value of $\hat{O}_7$ is

$$\langle\hat{O}_7\rangle=-2e^{-\lambda 0}e^{-\lambda_1-\lambda_2-(\lambda_3+\lambda_4)/2}\sinh a\cos\theta \ . \tag{3.39}$$

When both superconductors are the same, the first two terms of Eq. (3.38) cancel and $\langle\hat{S}_z\rangle=\langle\hat{O}_7\rangle$. It is then clear that this may lead to the confusion of thinking that the imbalance of charge is the third operator of the algebra. Notice also that

$$\begin{aligned}\hat{O}_7&=\hat{O}_3-\hat{O}_4-\hat{O}_3\hat{O}_1+\hat{O}_4\hat{O}_2\\&=\hat{O}_3-\hat{O}_4-\tfrac{1}{2}[\hat{O}_3,\hat{O}_1]_++\tfrac{1}{2}[\hat{O}_4,\hat{O}_2]_+ \ ,\end{aligned} \tag{3.40}$$

where the last two terms represent the statistical correlations between those operators. For this reason, it is not possible to factorize these products when mean values are taken. Although they have the same result when both superconductors are equal, since the knowledge of $\hat{O}_7$ has not been used by previous authors, it led to inconsistencies in the theories and had to appeal to a different ansätze to solve the problem. Notice from Eq. (3.38) that when the two superconductors are the same, the imbalance of charge vanishes with α, therefore giving no excess of charge on one side of the junction unless the system has been voltage biased.

IV. SUMMARY AND CONCLUSIONS

The application of the pseudo-angular-momentum model[1] to the problem of pair tunneling between superconductors gave rise to some inconsistencies in the description of charge excess,[2–6] as well as in the derivation of the equation of motion of the Josephson's phase and in the time derivative of the Josephson's current. Ferrell noticed some of these inconsistencies and pointed out the importance of a proper definition of the operators necessary to solve the problem. He showed that the operators $\hat{O}_5$, $\hat{O}_6$ and the imbalance of charge $\hat{O}_3-\hat{O}_4\equiv\hat{S}_z$ [Eqs. (3.37)–(3.38)] play important roles in the dynamics of a Josephson junction and that they should be taken into account to avoid the appearance of spurious effects.[3] Here we show that the operators which are important to study the dynamical evolution of the system are $\hat{O}_5$, $\hat{O}_6$, and $\hat{O}_7$ [see Eq. (3.10)] and not $\hat{O}_5$, $\hat{O}_6$ and the imbalance of charge as it was previously proposed. To solve the problem we use a simplified model Hamiltonian of pair tunneling between weakly coupled superconductors and solve it with the help of information theory. As a consequence of the closure relation, given by Eq. (2.6), we obtain a closed algebra consisting of seven operators and define an angular-momentum subalgebra $(\hat{O}_5,\hat{O}_6,\hat{O}_7)$, which arises naturally from the dynamical invariants of the theory. We show that, in the case of voltage bias and equal superconductors both operators ($\hat{O}_7$ and the charge imbalance) have the same expectation values. Ferrell, in spite of pointing out the importance of the three operators, did not use the complete Hamiltonian, in this way failing to see the importance of $\hat{O}_7$ in the consistency of the solution. When this is used we obtain a description for the ac tunneling, and the imbalance of charge is properly accounted for. The relation of the current with the phase, as well as a geometrical interpretation of the latter, follows from finding the dynamical invariants of the theory. The Josephson's equation appears for the weak-coupling limit as time-averaged relationships. Finally, we conclude that this Hamiltonian is inadequate to describe the dc tunneling, as was demonstrated in Sec. III D 2.

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APPENDIX A: CALCULATION OF THE MATRIX ELEMENTS

To calculate the partition function it is necessary to calculate the matrix elements of all the operators $\hat{O}$ in a base. To do that we consider the Hilbert space spanned by the 16 eigenvectors

$$|l_\uparrow l_\downarrow r_\uparrow r_\downarrow\rangle = |l_\uparrow\rangle \otimes |l_\downarrow\rangle \otimes |r_\uparrow\rangle \otimes |r_\downarrow\rangle \; , \tag{A1}$$

where l_i and R_i take the value 0 or 1. The basis is defined by $|m\rangle$, where m takes the values 1–16 such that the state $|1\rangle \equiv |1,1,1,1\rangle$, $|2\rangle \equiv |1,1,1,0\rangle$, $|3\rangle \equiv |1,1,0,1\rangle, \ldots, |16\rangle \equiv |0,0,0,0\rangle$. In this basis we define

$$\langle i|\hat{O}^n|j\rangle = O^n_{i;j} \tag{A2}$$

and find

$$O^1_{i;i} = \begin{cases} 2, & i=1;2;3;4 & \text{(A3)} \\ 1, & i=5;6;7;8;9;10;11;12 \; , & \text{(A4)} \end{cases}$$

$$O^2_{i;i} = \begin{cases} 2, & i=1;5;9;13 & \text{(A5)} \\ 1, & i=2;3;6;7;10;11;14;15 \; , & \text{(A6)} \end{cases}$$

$$O^3_{i;i} = 1, \quad i=1;2;3;4 \; , \tag{A7}$$

$$O^4_{i;i} = 1, \quad i=1;5;9;13 \; , \tag{A8}$$

$$O^7_{4;4} = -O^7_{13;13} = 1 \; , \tag{A9}$$

$$O^5_{4;13} = O^5_{13;4} = 1 \; , \tag{A10}$$

$$O^6_{4;13} = -O^6_{13;4} = i \; . \tag{A11}$$

all other matrix elements being zero. For the density matrix operator we find

$$\langle 1|\ln\hat{\rho}|1\rangle = -\lambda_0 - 2(\lambda_1+\lambda_2) - (\lambda_3+\lambda_4) \; , \tag{A12}$$

$$\langle 2|\ln\hat{\rho}|2\rangle = \langle 3|\ln\hat{\rho}|3\rangle = -\lambda_0 - 2\lambda_1 - \lambda_2 - \lambda_3 \; , \tag{A13}$$

$$\langle 4|\ln\hat{\rho}|4\rangle = -\lambda_0 - 2\lambda_1 - \lambda_3 - \lambda_7 \; , \tag{A14}$$

$$\langle 5|\ln\hat{\rho}|5\rangle = \langle 9|\ln\hat{\rho}|9\rangle = -\lambda_0 - \lambda_1 - 2\lambda_2 - \lambda_4 \; , \tag{A15}$$

$$\langle 6|\ln\hat{\rho}|6\rangle = \langle 7|\ln\hat{\rho}|7\rangle = \langle 10|\ln\hat{\rho}|10\rangle = \langle 11|\ln\hat{\rho}|11\rangle = -\lambda_0 - \lambda_1 - \lambda_2 \; , \tag{A16}$$

$$\langle 8|\ln\hat{\rho}|8\rangle = \langle 12|\ln\hat{\rho}|12\rangle = -\lambda_0 - \lambda_1 \; , \tag{A17}$$

$$\langle 13|\ln\hat{\rho}|13\rangle = -\lambda_0 - 2\lambda_2 - \lambda_4 + \lambda_7 \; , \tag{A18}$$

$$\langle 14|\ln\hat{\rho}|14\rangle = \langle 15|\ln\hat{\rho}|15\rangle = -\lambda_0 - \lambda_2 \; , \tag{A19}$$

$$\langle 16|\ln\hat{\rho}|16\rangle = -\lambda_0 \; , \tag{A20}$$

$$\langle 4|\ln\hat{\rho}|13\rangle = \langle 13|\ln\hat{\rho}|4\rangle^* = -(\lambda_5 + i\lambda_6) \; . \tag{A21}$$

APPENDIX B: EXPECTATION VALUE OF THE RELEVANT OPERATORS

The expectation values of the operators $\hat{O}_i$ can be found using Eqs. (3.16) and (2.10). We obtain

$$\begin{aligned}\langle\hat{O}_1\rangle = \langle\hat{N}_l\rangle &= -\frac{\partial\lambda_0}{\partial\lambda_1} \\ &= 2e^{-\lambda 0}[\, e^{-2(\lambda_1+\lambda_2)-(\lambda_3+\lambda_4)} + e^{-\lambda_1-2\lambda_2-\lambda_4} + 2e^{-2\lambda_1-\lambda_2-\lambda_3} \\ &\quad + 2e^{-\lambda_1-\lambda_2} + e^{-\lambda_1} + e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\cosh(a) - e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\cos(\theta)] \; ,\end{aligned} \tag{B1}$$

$$\begin{aligned}\langle\hat{O}_2\rangle = \langle\hat{N}_r\rangle &= -\frac{\partial\lambda_0}{\partial\lambda_2} \\ &= 2e^{-\lambda 0}[\, e^{-2(\lambda_1+\lambda_2)-(\lambda_3+\lambda_4)} + 2e^{-\lambda_1-2\lambda_2-\lambda_4} + e^{-2\lambda_1-\lambda_2-\lambda_3} \\ &\quad + 2e^{-\lambda_1-\lambda_2} + e^{-\lambda_2} + e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\cosh(a) - e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\cos(\theta)] \; ,\end{aligned} \tag{B2}$$

$$\langle \hat{O}_3 \rangle = \langle \hat{S}_l^\dagger \hat{S}_l \rangle = -\frac{\partial\lambda_0}{\partial\lambda_3}$$
$$= e^{-\lambda_0}[e^{-2(\lambda_1+\lambda_2)-(\lambda_3+\lambda_4)} + 2e^{-2\lambda_1-\lambda_2-\lambda_3}$$
$$+ e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4/2]}\cosh(a) - e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\cos(\theta)] , \quad \text{(B3)}$$

$$\langle \hat{O}_4 \rangle = \langle \hat{S}_r^\dagger \hat{S}_r \rangle = -\frac{\partial\lambda_0}{\partial\lambda_4}$$
$$= e^{-\lambda_0}[e^{-2(\lambda_1+\lambda_2)-(\lambda_3+\lambda_4)} + 2e^{-\lambda_1-2\lambda_2-\lambda_4}$$
$$+ e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4/2]}\cosh(a) - e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\cos(\theta)] , \quad \text{(B4)}$$

$$\langle \hat{O}_5 \rangle = \langle \hat{S}_l^\dagger \hat{S}_r + \hat{S}_r^\dagger \hat{S}_l \rangle = -\frac{\partial\lambda_0}{\partial\lambda_5} = -2e^{-\lambda_0}e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\sin(\theta)\cos(\phi) , \quad \text{(B5)}$$

$$\langle \hat{O}_6 \rangle = \langle i(\hat{S}_l^\dagger \hat{S}_r - \hat{S}_r^\dagger \hat{S}_l) \rangle = -\frac{\partial\lambda_0}{\partial\lambda_6} = -2e^{-\lambda_0}e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\sin(\theta)\sin(\phi) , \quad \text{(B6)}$$

$$\langle \hat{O}_7 \rangle = \langle \hat{S}_l^\dagger \hat{S}_l(1-\hat{N}_r) - \hat{S}_r^\dagger \hat{S}_r(1-\hat{N}_l) \rangle = -\frac{\partial\lambda_0}{\partial\lambda_7} = -2e^{-\lambda_0}e^{-\lambda_1-\lambda_2-[(\lambda_3+\lambda_4)/2]}\sinh(a)\cos(\theta) , \quad \text{(B7)}$$

where

$$\cos\theta = [\lambda_1 - \lambda_2 + (\lambda_3 - \lambda_4)/2 + \lambda_7]/a \quad \text{(B8)}$$

and

$$\tan\phi = \frac{\lambda_6(t)}{\lambda_5(t)} . \quad \text{(B9)}$$

APPENDIX C: THE LAGRANGE MULTIPLIERS

As seen in Sec. II, the evolution of the Lagrange multipliers can be determined through the knowledge of the matrix $\underline{G}$, since they follow the equation

$$\frac{d\lambda_i}{dt} = \sum_{l=0}^{M} g_{il}\lambda_l . \quad \text{(C1)}$$

Therefore, we obtain

$$\frac{d\lambda_0}{dt} = \frac{d\lambda_1}{dt} = \frac{d\lambda_2}{dt} = \frac{d\lambda_3}{dt} = \frac{d\lambda_4}{dt} = 0 , \quad \text{(C2)}$$

$$\frac{d\lambda_5}{dt} = -\frac{\alpha}{\hbar}\lambda_6 , \quad \text{(C3)}$$

$$\frac{d\lambda_6}{dt} = \frac{2\rho}{\hbar}(\lambda_1 - \lambda_2) + \frac{\rho}{\hbar}(\lambda_3 - \lambda_4) + \frac{\alpha}{\hbar}\lambda_5 + \frac{2\rho}{\hbar}\lambda_7 , \quad \text{(C4)}$$

$$\frac{d\lambda_7}{dt} = -\frac{2\rho}{\hbar}\lambda_6 , \quad \text{(C5)}$$

the solution of these equations being

$$\lambda_i(t) = \lambda_i^0, \quad i = 1,2,3,4 , \quad \text{(C6)}$$

$$\lambda_5(t) = \lambda_5^0 - \frac{\alpha}{\hbar\omega}\{d(\lambda)[1-\cos(\omega t)] + \lambda_6^0\sin(\omega t)\} , \quad \text{(C7)}$$

$$\lambda_6(t) = \lambda_6^0\cos(\omega t) + d(\lambda)\sin(\omega t) , \quad \text{(C8)}$$

$$\lambda_7(t) = \lambda_7^0 - \frac{2\rho}{\hbar\omega}\{d(\lambda)[1-\cos(\omega t)] + \lambda_6^0\sin(\omega t)\} , \quad \text{(C9)}$$

where

$$d(\lambda) = \frac{1}{\hbar\omega}\{2\rho[\lambda_1^0 - \lambda_2^0 + (\lambda_3^0 - \lambda_4^0)/2 + \lambda_7^0] + \alpha\lambda_5^0\} \quad \text{(C10)}$$

and

$$\hbar^2\omega^2 = \alpha^2 + 4\rho^2 . \quad \text{(C11)}$$

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