Charge-excess superconductors and the pseudo-angular-momentum approach to Josephson tunneling

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(Received 5 October 1981; revised manuscript received 28 December 1981)

This work addresses the problem of describing the Josephson junction with a pseudo-angular-momentum formalism. An alternate approach to the existing pseudo-angular-momentum theory is begun with a modification of the fundamental operators upon which the method is based. Along with this, a new state vector, which affords a more complete description of the constant-charge-imbalance mode of the junction, is explicitly constructed. Certain inconsistencies which arise within the existing pseudo-angular-momentum theory are discussed in the context of this new formulation. Finally, a method is suggested for employing the charge-imbalance state in problems where the pair difference between the junction sides is allowed to vary.

I. INTRODUCTION

During the late sixties, a new approach to Josephson tunneling was initiated by addressing the problem from a quantum optical perspective.[1] This was done by trying to extend the Anderson pseudospin method in superconductivity[2] to a point where certain operators associated with the Josephson junction, $S'^{\pm}$ and S'_Z, could be identified as the Bloch vector for the system. Once this analogy to atomic systems was established, it was felt that much of the formalism developed for the quantum theory of the laser[3] could be brought to bear on the Josephson problem. Thus it was hoped that new physics would emerge.

This paper is the first in a series which will develop an alternate approach to extending Anderson's original pseudospin model. This new approach will be based on the following: (i) an explicit construction of a state vector to represent the constant-charge-imbalance mode of the junction, and (ii) a description of junction dynamics using the coupling of two macroscopic pseudoangular momenta. By use of these concepts we hope to:

(a) provide an alternate physical picture to the dynamics of the Josephson junction,

(b) study degrees of freedom not present in Anderson's (n,ϕ) theory of the junction,[4]

(c) provide a microscopic model for describing the dynamics of a three-superconductor two-insulator sandwich [a problem which is not easily formulated in the context of the (n,ϕ) theory],

(d) give a simple and transparent derivation of Feynman's two-level model of the Josephson junction,[5] starting from a microscopic picture, and

(e) apply many of the theoretical techniques of quantum optics and magnetic resonance to junction problems.

This paper deals only with (i). Part (ii) of the formulation and the specific problems that will be addressed with it will follow in a future work. We have chosen to publish part (i) now because the construction of a charge-imbalance state solves a problem that has been pointed out in the existing pseudo-angular-momentum theory.[6]

To this end, Sec. II gives a short exposition of the existing pseudo-angular-momentum theory, which concentrates on only its most basic aspects. Even so a serious difficulty is discovered in that the expectation value of one of the fundamental operators S'_Z (when taken with respect to any of the conventional states used to describe the superconductors of the junction) is shown to be identically zero.

Section III starts by pointing out that $\langle S'_Z \rangle = 0$ is only a symptom of a larger problem. This problem has two parts. First, all basic operators of the theory are, to a certain degree, incorrectly defined. Second, the state used to describe the junction when an ideal battery is placed across it (i.e., there are no voltage fluctuations), is in fact incomplete. Finally, methods are proposed to surmount these difficulties while at the same time retaining the basic integrity of the pseudo-angular-momentum picture. In Sec. IV a suggestion is made on how to apply the charge-imbalance state to a specific non-steady-state problem. Section V gives a short summary of the work.

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II. A BRIEF HISTORY OF THE PSEUDO-ANGULAR-MOMENTUM THEORY

In this section the early development of the theory is outlined. A historical approach is used as a means of stating approximations and assumptions which were made. This then allows a more systematic analysis of the problems that eventually arise.

A. Anderson's pseudospin notation

In 1957 Bardeen, Cooper, and Schrieffer[7] proposed a theory of superconductivity based on the highly specialized state vector

$$|\varphi\rangle=\prod_{\vec{k}}[U(\vec{k})+V(\vec{k})e^{i\varphi}C^\dagger_{\vec{k}\uparrow}C^\dagger_{-\vec{k}\downarrow}]|0\rangle\ , \tag{1}$$

where $C^\dagger_{\vec{k}s}$ is the usual fermion creation operator for an electron with momentum $\vec{k}$ and spin s, and $U^2(\vec{k})+V^2(\vec{k})=1$. This state was constructed to emphasize the central role of pairing[8] in superconductivity.

Shortly after the success of the Bardeen, Cooper, and Schrieffer (BCS) theory, Anderson[2] observed that each momentum subspace factor of $|\varphi\rangle$ could be viewed as a state vector for an imaginary two-level system. That is,

$$|\varphi\rangle=\prod_{\vec{k}}|\chi\rangle_{\vec{k}}$$

with

$$|\chi\rangle_{\vec{k}}=U(\vec{k})|0\rangle_{\vec{k}}+V(\vec{k})e^{i\varphi}C^\dagger_{\vec{k}\uparrow}C^\dagger_{-\vec{k}\downarrow}|0\rangle_{\vec{k}}\ .$$

He then took full advantage of this analogy by realizing that a complete set of operators for the theory could be written in terms of a spin-$\frac{1}{2}$ angular-momentum notation. These pseudospin operators are as follows:

$$\sigma^+_{\vec{k}}=C^\dagger_{\vec{k}\uparrow}C^\dagger_{-\vec{k}\downarrow}\ , \tag{2a}$$

which creates a pair and raises spin,

$$\sigma^-_{\vec{k}}=C_{-\vec{k}\downarrow}C_{\vec{k}\uparrow}\ , \tag{2b}$$

which destroys a pair and lowers spin, and

$$\sigma_{\vec{k}z}=\tfrac{1}{2}(n_{\vec{k}\uparrow}+n_{-\vec{k}\downarrow}-1)\ , \tag{2c}$$

which acts like a number operator for electron pairs or equivalently is the z component of the angular momentum operator ($n_{\vec{k}s}=C^\dagger_{\vec{k}s}C_{\vec{k}s}$). The exact pair-number operator $N_{\vec{k}}$ for the $\vec{k}$th subspace becomes

$$N_{\vec{k}}=\tfrac{1}{2}(n_{\vec{k}\uparrow}+n_{-\vec{k}\downarrow})$$
$$=\sigma_{\vec{k}z}+\tfrac{1}{2}$$

in this notation. (Note: The definitions given here differ slightly from those given by Anderson but are completely equivalent to them.)

By using the fermion anticommutation relations

$$[C_{\vec{k}s},C^\dagger_{\vec{k}'s'}]_+=\delta_{\vec{k}\vec{k}'}\delta_{ss'}\ ,$$
$$[C^\dagger_{\vec{k}s},C^\dagger_{\vec{k}'s'}]_+=0\ ,$$

it is easy to show that the σ's do in fact satisfy angular momentum commutation rules,

$$[\sigma^+_{\vec{k}},\sigma^-_{\vec{k}'}]=2\sigma_{\vec{k}z}\delta_{\vec{k}\vec{k}'}\ ,$$
$$[\sigma_{\vec{k}z},\sigma^\pm_{\vec{k}'}]=\pm\sigma^\pm_{\vec{k}}\delta_{\vec{k}\vec{k}'}\ . \tag{3}$$

With the above pseudospin operators the state vector for the imaginary two-level system can now be written as

$$|\chi\rangle_{\vec{k}}=U(\vec{k})|0\rangle_{\vec{k}}+V(\vec{k})e^{i\varphi}\sigma^+_{\vec{k}}|0\rangle_{\vec{k}}\ ,$$
$$=U(\vec{k})|\downarrow\rangle_{\vec{k}}+V(\vec{k})e^{i\varphi}|\uparrow\rangle_{\vec{k}}\ , \tag{4}$$

where $|\downarrow\rangle_{\vec{k}}$ and $|\uparrow\rangle_{\vec{k}}$ are the spin states of the system. This then allows $|\varphi\rangle$ to be viewed as a state representing an ensemble of such imaginary two-level systems,

$$|\varphi\rangle=\prod_{\vec{k}}[U(\vec{k})+V(\vec{k})e^{i\varphi}\sigma^+_{\vec{k}}]|0\rangle\ . \tag{5}$$

B. The tunneling Hamiltonian

Shortly after Josephson's[9] original discovery of coherent tunneling, several authors[10,11] started work on the junction problem by incorporating a tunneling term into the usual many-body Hamiltonian for superconductivity. Typically this term was written as

$$H_g=\sum_{\vec{k},\vec{q},s}g_{\vec{k}\vec{q}}(C^\dagger_{\vec{k}s}C_{\vec{q}s}+C^\dagger_{\vec{q}s}C_{\vec{k}s})\ . \tag{6}$$

On the surface at least, it appears to be an operator for single-electron tunneling. This apparent lack of emphasis on pair tunneling has made H_g a cumbersome operator to use when dealing with the Josephson problem.

In an attempt to simplify the junction calculations by stressing the fact that the process being described strictly involves paired electrons, Wallace and Stavn[12] introduced a new Hamiltonian,

$$H_T''=\sum_{\vec{k},\vec{q}} T_{\vec{k}\vec{q}}(\sigma_{\vec{k}}^{+}\sigma_{\vec{q}}^{-}+\sigma_{\vec{k}}^{-}\sigma_{\vec{q}}^{+}) , \tag{7}$$

where a $\vec{k}$ subscript refers to the left superconductor and a $\vec{q}$ subscript refers to the right. (It is assumed in using this Hamiltonian that all operators dealing with one superconductor automatically commute with those operators dealing with the other.) This Hamiltonian, which is derived from Eq. (6) by a canonical transformation, explicitly illustrates the paired electron nature of the Josephson problem by using the pseudospin formalism of Anderson.

Before employing their Hamiltonian, Wallace and Stavn made the approximation that

$$T_{\vec{k}\vec{q}}=T ,$$

i.e., $T_{\vec{k}\vec{q}}$ is in fact independent of $\vec{k}$ and $\vec{q}$. This approximation is usually followed by the proviso that the momentum sums be restricted to a small region about the Fermi momentum of each superconductor. [As Wallace and Stavn point out a similar approximation and restriction is made in the underlying BCS theory (see Ref. 13, p. 153).] This restriction will be denoted by a "prime" on the summation symbol $\sum'_{\vec{k},\vec{q}}$ which implies the only allowed momenta are those whose associated energies lie within a region of width $2\hbar\omega_D$ about the Fermi energy. (More will be said about this later.) Thus they obtain the final form,

$$H_T'=T\sum_{\vec{k},\vec{q}}{}' (\sigma_{\vec{k}}^{+}\sigma_{\vec{q}}^{-}+\sigma_{\vec{k}}^{-}\sigma_{\vec{q}}^{+}) . \tag{8}$$

C. Extension of the pseudospin approach

Motivated by the close analogy of the BCS state, Eq. (5), to that for a system of two-level atoms, Scully and collaborators[14-16] attempted to extend the Anderson pseudospin treatment of the junction problem to a point where quantum optical techniques could be employed. The idea being that these techniques, developed primarily for the quantum theory of the laser,[3] would lend themselves to a class of problems not easily handled within the framework of the usual thermodynamic equilibrium many-body theories.

To see how this extension was accomplished, consider first the tunneling Hamiltonian of Eq. (8),

$$H_T'=T\sum_{\vec{k},\vec{q}}{}' (\sigma_{\vec{k}}^{+}\sigma_{\vec{q}}^{-}+\sigma_{\vec{k}}^{-}\sigma_{\vec{q}}^{+}) .$$

This can be written as

$$\begin{aligned} H_T' &= C(J_L'^{+}J_R'^{-}+J_L'^{-}J_R'^{+}) ,\\ &= C(S'^{+}+S'^{-}) , \end{aligned} \tag{9}$$

if the following identifications are made:

$$J_L'^{\pm}=\frac{1}{N^*}\sum_{\vec{k}}{}'\sigma_{\vec{k}}^{\pm} , \tag{10a}$$

$$J_R'^{\pm}=\frac{1}{N^*}\sum_{\vec{q}}{}'\sigma_{\vec{q}}^{\pm} , \tag{10b}$$

$$S'^{+}=J_L'^{+}J_R'^{-} , \tag{11a}$$

$$S'^{-}=J_R'^{+}J_L'^{-} , \tag{11b}$$

(in these relations, C and N^* are constants which do not bear on the problem being discussed in this paper).

Along with these, three other operators can be defined:

$$J_{LZ}'=\sum_{\vec{k}}{}'\sigma_{\vec{k}z} , \tag{12a}$$

$$J_{RZ}'=\sum_{\vec{q}}{}'\sigma_{\vec{q}z} , \tag{12b}$$

$$S_Z'=\tfrac{1}{2}(J_{LZ}'-J_{RZ}') . \tag{12c}$$

As is stated in Ref. (15), $J_{LZ}'(J_{RZ}')$ "describes the number of electron pairs in excess of the value required to maintain charge neutrality." Imposing charge conservation on these equations implies $S_Z'=J_{LZ}'$. Since, as will be seen in the next section, these are the operators of interest to this work, the physical interpretation of the other operators will be omitted except to say that the operators of each set (e.g., $J_L'^{\pm}$ and J_{LZ}') are related to each other by means of commutation relations.[14] Finally, it is through the operators S'^{+}, S'^{-}, and S_Z', which form the Bloch vector, that the above authors attempt to make the connection between the Josephson junction problem and the calculational techniques of quantum optics.

D. An inconsistency in the theory

The existing pseudo-angular-momentum theory, as defined in the literature,[14,15] has a fundamental inconsistency in it. This problem, though, does not become apparent until explicit numerical values are obtained for certain physical quantities. It is an error that appears already in the steady-state mode of the junction, and therefore is unrelated to such topics as frequency pulling[1] and transient phenomena.[16] *(Here, and throughout this paper, "steady state" is taken to mean that the pair difference between the sides of the junction is constant, i.e., neither voltage fluctuations nor charge buildup is being described.)* Consequently, the nature of the problem is fundamental to the groundwork on which the theory rests and, as will be shown in Sec. III, relates to the basic definition of the operators and the states used to calculate their expectation values. In this and the next section, unambiguous systematic calculations that clearly display this difficulty will be given. The following two conditions are imposed which serve only to simplify the calculations and do not in any way effect the physics of the situation:

(i) The superconductors of the junction are assumed to be identical. That is, not only are they made of the same material but their volumes are the same too.

(ii) The Thouless strong-coupling model,[17] described below, is assumed for both superconductors, with all calculations being carried out at $T=0$ K.

1. Strong-coupling model superconductor

Consider a charge neutral superconductor at $T=0$ K. Within the strong-coupling model the state of this system is described by the BCS ground state, Eq. (5), with $U^2(\vec{k})$ and $V^2(\vec{k})$ as shown in Fig. 1. To be specific, the occupation distributions of the BCS theory have been approximated as step functions in the region about k_F. The region, in energy, over which this step occurs is of length 2Δ, where Δ is the energy-gap parameter. The boundaries of this region in momentum space are given by

$$k_U=\left[\left[\frac{2m_e}{\hbar^2}\right](\epsilon_F+\Delta)\right]^{1/2}\simeq k_F+k_\Delta\ ,$$
$$k_L=\left[\left[\frac{2m_e}{\hbar^2}\right](\epsilon_F-\Delta)\right]^{1/2}\simeq k_F-k_\Delta\ , \tag{13}$$

with

$$k_\Delta=\frac{1}{2}\left[\frac{2m_e}{\hbar^2}\right]^{1/2}\left[\frac{\Delta}{\epsilon_F^{1/2}}\right]$$
$$=\frac{1}{2}\left[\frac{\Delta}{\epsilon_F}\right]k_F\ .$$

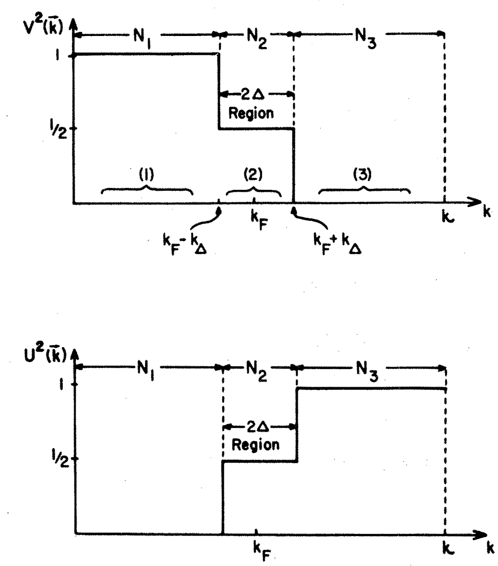

FIG. 1. $U^2(\vec{k})$ and $V^2(\vec{k})$ are shown for a charge-neutral superconductor in the strong-coupling limit. N_1, N_2, and N_3 are the number of pseudospin systems ($\vec{k}$ vectors) in their respective regions of $\vec{k}$ space. k_Δ is the momentum associated with the energy-gap parameter $k_\Delta=\frac{1}{2}(\Delta/\epsilon_F)k_F$, and κ is the chosen cut-off in momentum space.

The number of pseudospin systems in a given region of momentum space will be needed in the calculations that follow. It is easy to see that this number is equal to the number of momentum vectors in the given region. As an example of this, the diagrams show three regions with, respectively, N_1, N_2, and N_3 momentum vectors in each. (κ is at this point an arbitrary cut-off in momentum space. It has no effect in the following calculations but will be needed in Sec. III.)

2. dc Josephson effect

As is shown in Ref. 15, the pseudospin notation can now be effectively employed to obtain the dc Josephson current. In particular, the state of the junction at $T=0$ K and biased at zero voltage is taken to be

$$|\psi\rangle_0=|\varphi\rangle^L\otimes|\varphi\rangle^R\ , \tag{14}$$

with

$$|\varphi\rangle^L=\prod_{\vec{k}}[U(\vec{k})+V(\vec{k})e^{i\varphi_L}\sigma^+_{\vec{k}}]\,|0\rangle\ ,$$

$$|\varphi\rangle^R=\prod_{\vec{q}}[U(\vec{q})+V(\vec{q})e^{i\varphi_R}\sigma^+_{\vec{q}}]|0\rangle\ .$$

By defining the current as $I=-2e\dot{N}_L$, where N_L is the total pair-number operator for the left superconductor

$$N_L=\sum_{\vec{k}}(\sigma_{\vec{k}z}+\tfrac{1}{2})\ ,$$

the current operator becomes

$$\begin{aligned}I&=-2e(i/\hbar)[H'_T,N_L]\\&=C_1\sum_{\vec{k},\vec{q}}{}'(\sigma^+_{\vec{k}}\sigma^-_{\vec{q}}-\sigma^+_{\vec{q}}\sigma^-_{\vec{k}})\ .\end{aligned}\tag{15}$$

It is now straightforward to show that

$$\begin{aligned}\langle I\rangle&={}_0\langle\psi|I|\psi\rangle_0\\&=j'_1\sin(\varphi_R-\varphi_L)\ ,\end{aligned}\tag{16}$$

where

$$\begin{aligned}j'_1&=C_2\sum_{\vec{k},\vec{q}}{}'[U(\vec{k})V(\vec{k})][U(\vec{q})V(\vec{q})]\\C_1,C_2&=\text{const}\ .\end{aligned}\tag{17}$$

This, then, is the desired dc Josephson current.

Before going on to the ac Josephson current it would be worthwhile to calculate $\langle S'_Z\rangle$. Remember $\langle S'_Z\rangle$ supposedly measures the number of pairs in excess of that required to maintain charge neutrality, and thus should be zero in this case. Using S'_Z as defined in Eq. (12c) and the state as given above, this expectation value becomes

$$\begin{aligned}\langle S'_Z\rangle&={}_0\langle\psi|S'_Z|\psi\rangle_0\\&=\tfrac{1}{2}[{}^L\langle\varphi|J'_{LZ}|\varphi\rangle^L-{}^R\langle\varphi|J'_{RZ}|\varphi\rangle^R]\ .\end{aligned}$$

To continue, note that

$$\begin{aligned}{}^L\langle\varphi|\sigma_{\vec{k}z}|\varphi\rangle^L&=-\tfrac{1}{2}[U^2(\vec{k})-V^2(\vec{k})]\ ,\\{}^R\langle\varphi|\sigma_{\vec{q}z}|\varphi\rangle^R&=-\tfrac{1}{2}[U^2(\vec{q})-V^2(\vec{q})]\ ,\end{aligned}\tag{18}$$

and consequently by Eq. (12),

$$\begin{aligned}\langle J'_{LZ}\rangle&=\sum_{\vec{k}}{}'\{-\tfrac{1}{2}[U^2(\vec{k})-V^2(\vec{k})]\}\ ,\\\langle J'_{RZ}\rangle&=\sum_{\vec{q}}{}'\{-\tfrac{1}{2}[U^2(\vec{q})-V^2(\vec{q})]\}\ .\end{aligned}\tag{19}$$

These give

$$\langle J'_{LZ}\rangle=0\ ,$$

$$\langle J'_{RZ}\rangle=0\ ,$$

by using Fig. 1 and remembering that $\sum'$ means that $\vec{k}$ and $\vec{q}$ are restricted to the symmetric $2\hbar\omega_D$ region about the Fermi momenta. Thus

$$\langle S'_Z\rangle=\tfrac{1}{2}[\langle J'_{LZ}\rangle-\langle J'_{RZ}\rangle]=0\ ,$$

as expected.

3. *ac Josephson effect*

Consider the situation where an ideal battery maintains a constant voltage V between the left and right superconductors. Since the junction acts as a capacitor, an additional term must be added to the Hamiltonian to describe this[14]:

$$H'_V=-eV\left[\sum_{\vec{k}}{}'\sigma_{\vec{k}z}-\sum_{\vec{q}}{}'\sigma_{\vec{q}z}\right]\ .\tag{20}$$

Approaching this as strictly a steady-state problem (i.e., how the charge buildup occurred is not of interest), the state of the junction in the interaction picture becomes

$$|\psi\rangle'=\exp(iH'_Vt/\hbar)|\psi\rangle_0\ .\tag{21}$$

Basically this is the direct product of two phase-rotated BCS ground states. Thus $|\psi\rangle'$ looks exactly like $|\psi\rangle_0$ but with the following substitutions:

$$\begin{aligned}\varphi_L&\to\varphi_L(t)=\varphi_L-eVt/\hbar\ ,\\\varphi_R&\to\varphi_R(t)=\varphi_R+eVt/\hbar\ .\end{aligned}\tag{22}$$

Using this state to calculate the expectation value of the current operator gives

$$\langle I\rangle=j'_1\sin[(\varphi_R-\varphi_L)+2eVt/\hbar]\ ,\tag{23}$$

which again is the expected result.

But consider once more the expectation value of S'_Z. Since there is a constant voltage across the junction, there must be a constant charge difference between the two sides (if it is assumed that this voltage is maintained by an ideal battery). Taking the potential energy to be higher on the left implies that there must be a charge excess on that side. Consequently, it is expected that

$$\langle S'_Z\rangle=n\ ,$$

where n is the number of excess pairs on the left side.

The expectation value is given by

$$\langle S'_Z\rangle=\langle\psi|S'_Z|\psi\rangle'\ .\tag{24}$$

Since this is a steady-state problem, the above can be evaluated at any time t, in particular at $t=0$.

Doing so gives

$$\begin{aligned}\langle S_Z' \rangle &\doteq \langle \psi(0) \,|\, S_Z' \,|\, \psi(0) \rangle' \\ &= {}_0\langle \psi \,|\, S_Z' \,|\, \psi \rangle_0 \\ &= 0 \,. \end{aligned} \tag{25}$$

The last equality follows from Sec. II D 2 above.

This apparent inability of S_Z' to measure the excess charge[6] is the fundamental inconsistency mentioned above. It is a serious defect in the theory and must be dealt with.

III. MODIFICATION OF THE THEORY

As Anderson[4] has pointed out, one of the dynamical variables governing the motion of the Josephson junction is $N_L - N_R$, the difference between the total number of pairs on the left and right superconductors. Consequently, any proposed extension of the Anderson (n,ϕ) formalism must reflect this fact. As has been shown above, the existing formulation of the pseudo-angular-momentum theory does not manifestly exhibit this variable. The source of this problem is investigated below and a method for correcting it is suggested.

A. Source of the problem

As was seen in Sec. II, $\langle S_Z' \rangle = 0$. This problem arises from the following two sources, either one of which alone would ensure $\langle S_Z' \rangle = 0$:

(i) The insistence on using only the BCS ground state or a phase-rotated BCS ground state to represent the superconductors of the junction (note: A third state has been used and will be discussed at the end of Sec. III C), and

(ii) unnecessarily restricting the range of the momentum sums in the definition of the operators.

To see how these force $\langle S_Z' \rangle = 0$, consider first (i). The number operator for a given pair is

$$N_{\vec{k}} = \sigma_{\vec{k}z} + \tfrac{1}{2} \,,$$

and therefore the operator for the total number of pairs in a superconductor is

$$N = \sum_{\vec{k}} (\sigma_{\vec{k}z} + \tfrac{1}{2}), \tag{26}$$

where the summation is *unrestricted* in $\vec{k}$ space. To check that this is indeed the total pair-number operator, consider its expectation value with respect to the BCS ground state:

$$\begin{aligned}\langle N \rangle &= \langle \varphi \,|\, N \,|\, \varphi \rangle \\ &= \sum_{\vec{k}} V^2(\vec{k}) \\ &= N_1 + m/2 \,. \end{aligned} \tag{27}$$

The last equality follows by using the values of $V^2(\vec{k})$ from Fig. 1. This is exactly what is expected for the total pair number. (Note that had the product index of the BCS ground state been restricted to a small region about k_F; as is stated in Ref. 13, this expectation value would have yielded an incorrect result for the total number of pairs.)

Now consider the phase-rotated BCS state $|\psi\rangle'$, Eq. (21). This state supposedly represents the junction when a constant charge imbalance exists between the two sides. In particular, consider the case described above Eq. (24), i.e., n pairs have been added to the left side and n have been removed from the right. Hence the expectation values of N_L and N_R with respect to this state should be

$$\begin{aligned}\langle N_L \rangle &= N_1 + m/2 + n \,, \\ \langle N_R \rangle &= N_1 + m/2 - n \,. \end{aligned} \tag{28}$$

But

$$\begin{aligned}\langle N_L \rangle &\doteq \langle \psi \,|\, N_L \,|\, \psi \rangle' \\ &= {}^L\langle \varphi \,|\, N_L \,|\, \varphi \rangle^L \\ &= N_1 + m/2 \end{aligned} \tag{29}$$

and

$$\langle N_R \rangle = N_1 + m/2,$$

where the second equality of Eq. (29) follows by evaluating at $t = 0$.

Thus it is seen that even though $|\psi\rangle'$ leads to the correct frequency relationship for the ac Josephson effect, it fails to measure the change in the total number of pairs on either side. It is in this sense that $|\psi\rangle'$ gives an incomplete description of the junction operating in a constant-charge-imbalance mode. Consequently, another state must be found to describe this situation.

Source (ii) above deals with the operators themselves. It is not clear how the operators J_{LZ}', J_{RZ}', and S_Z' get the physical interpretations given to them in Ref. 15 and quoted in Sec. II C of this paper. But for S_Z' it might be surmised that the following argument was used:

$$\frac{1}{2}(N_L-N_R)=\frac{1}{2}\left[\sum_{\vec{k}}(\sigma_{\vec{k}z}+\tfrac{1}{2})-\sum_{\vec{q}}(\sigma_{\vec{q}z}+\tfrac{1}{2})\right]$$
$$=\frac{1}{2}\left[\sum_{\vec{k}}\sigma_{\vec{k}z}-\sum_{\vec{q}}\sigma_{\vec{q}z}\right]$$
$$=S_Z' \; . \tag{30}$$

Assume, for the moment, that a state exists which does accurately describe the constant-charge-imbalance mode of the junction, i.e., Eq. (28) gives the expectation values of the total pair-number operators with respect to this state. Then $\langle S_Z'\rangle$ would measure the charge excess on the left side since

$$\langle S_Z'\rangle=\tfrac{1}{2}(\langle N_L\rangle-\langle N_R\rangle)$$
$$=n \; . \tag{31}$$

Unfortunately though, the last equality in Eq. (30) does not hold. To see this, note that the summations in N_L and N_R are *unrestricted* while those in the definition of S_Z', Eq. (12c), are *restricted* to momenta whose associated energy falls in the range

$$\epsilon_F-\hbar\omega_D\le\epsilon_{\vec{k}}\le\epsilon_F+\hbar\omega_D$$

(this restriction on $\vec{k}$ is clearly stated in Ref. 15, p. 770). Consequently, even if the problem of what state to use were solved there would still be difficulty with the operator S_Z'.

B. The charge-imbalance state

To provide a concrete model for the state used to characterize a junction in the presence of a constant charge imbalance, first consider a neutral, isolated, nearly-free-electron metal, at $T=0$ K. If n extra electron pairs are deposited on this metal, one can, in principle, solve for the self-consistent one-electron orbitals using, for example, a density-functional formalism.[18] Filling these orbitals with electrons up to the Fermi momentum k_{nF} would then produce the electron charge density inside the metal. The resulting charge density would correspond to having a total charge $-2|e|n$ localized near the surface. This excess charge density need not, however, be associated with single electrons localized near the surface. Rather, it can be thought of as the result of a large number of itinerant bulk electrons whose weakly perturbed self-consistent wave functions result in an excess charge density near the surface. This is the physical interpretation that will be used in the remainder of this work.[19]

Now imagine turning on the electron-phonon interaction in the charged metal. Since all the electron orbitals are delocalized, we may take as one model for the state vector of the superconductor

$$|\varphi\rangle_n=\prod_{\vec{k}}[U_n(\vec{k})+V_n(\vec{k})e^{i\varphi}\sigma^+_{\vec{k}}]\,|0\rangle \; . \tag{32}$$

That is, $|\varphi\rangle_n$ is a BCS-like state, but with $U_n^2(\vec{k})$ and $V_n^2(\vec{k})$ now referred to the shifted Fermi momentum, k_{nF}, as shown in Fig. 2.

Using the states $|\varphi\rangle_n$, the exact pair-number state of Anderson[4] can also be generated

$$|N_0+\frac{m}{2}+n\rangle=\int_0^{2\pi}e^{-i(N_0+m/2+n)\varphi}\,|\varphi\rangle_n d\varphi \tag{33}$$

Thus it is seen that there are really two requirements which the desired state vector must satisfy if it is ultimately to be acceptable as a description of one side of the junction. These are as follows:

(a) The algebraic form of this state vector must be the same as that of the BCS ground state (if a state with a well-defined φ is required).

(b) The expectation value of the total pair-

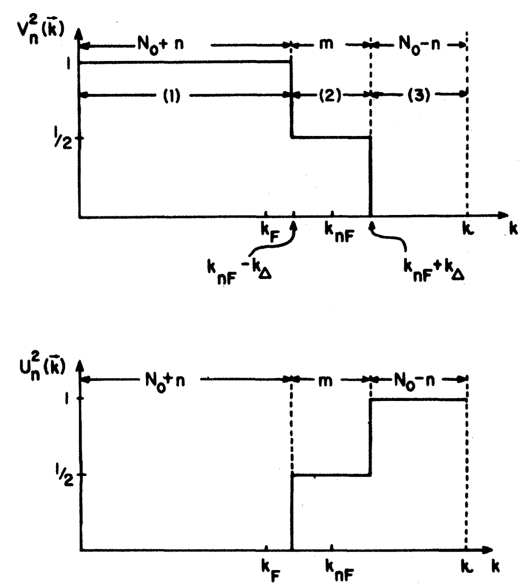

FIG. 2. Occupation distributions, now labeled $U_n^2(\vec{k})$ and $V_n^2(\vec{k})$, are shown for a superconductor which has had n pairs added, at $T=0$ K. The 2Δ region is now centered about k_{nF} but its width is the same as in Fig. 1. (Note: κ has now been chosen such that $N_1=N_3$ of Fig. 1, and these are set equal to N_0.)

number operator with respect to this state must reflect the excess in the number of pairs.

The state $|\varphi\rangle_n$, given in Eq. (32), satisfies both of these requirements, (a) being satisfied by definition. The fact that $|\varphi\rangle_n$ is not a well-defined pair-number state is not a serious problem since it shall only be used in connection with the Josephson junction (i.e., the pair number on either side of the junction is, indeed, not well defined).[20]

To see how $|\varphi\rangle_n$ satisfies criterion (b), return momentarily to Fig. 1 and the BCS ground state. The momentum space in these diagrams has been broken up into three regions, with κ, the upper bound of region (3), being unspecified. In regards to these regions and the cutoff κ, the following ansatz is now made:

(i) For a given charge-neutral superconductor at $T=0$ K, even though κ can be chosen almost arbitrarily, choose it such that $N_1=N_3$ and relabel them as N_0. Then, once κ has been defined, it remains fixed regardless of how the physical state of the superconductor changes.

(ii) The three regions of $\vec{k}$ space are always defined in the same way, that is,

$$\begin{aligned}&(1)\ \ 0\le k<k_F-k_\Delta\ ,\\&(2)\ \ k_F-k_\Delta\le k\le k_F+k_\Delta\ ,\\&(3)\ \ k_F+k_\Delta<k\le\kappa\ ,\end{aligned}\tag{34}$$

where it is understood that k_F may change depending on the state of the system (i.e., if excess charge is added then k_F is replaced by k_{nF}, and Fig. 1 is replaced by Fig. 2). If N_2 is now relabeled as m, then the consequences of the above are that regardless of how the physical state of the system may change the total number of $\vec{k}$ states from 0 to κ is fixed at $2N_0+m$.

This then specifies $|\varphi\rangle_n$, the shifted-BCS state. Even though it may be an oversimplified model for the problem, it does contain the essential physics. As an example, consider taking the expectation value of the total pair-number operator N, with respect to this state,

$$\begin{aligned}\langle N\rangle&={}_n\langle\varphi|N|\varphi\rangle_n\\&=\sum_{\vec{k}}V_n^2(\vec{k})\\&=(N_0+n)+(m/2)+(0)\\&=N_0+m/2+n\ .\end{aligned}\tag{35}$$

Thus both requirements (a) and (b) are satisfied.

If charge is depleted from a superconductor, the state $|\varphi\rangle_{-n}$ is obtained in a similar fashion to $|\varphi\rangle_n$. Here $|\varphi\rangle_{-n}$ is defined as

$$|\varphi\rangle_{-n}=\prod_{\vec{k}}[U_{-n}(\vec{k})+V_{-n}(\vec{k})e^{i\varphi}\sigma_{\vec{k}}^{+}]|0\rangle\ ,\tag{36}$$

with $U_{-n}^2(\vec{k})$ and $V_{-n}^2(\vec{k})$ given in Fig. 3.

Finally, $|\varphi\rangle_n$ and $|\varphi\rangle_{-n}$ can be used to build a state vector for the junction

$$|\psi\rangle_n=|\varphi\rangle_n^L\otimes|\varphi\rangle_{-n}^R\ .\tag{37}$$

The state $|\psi\rangle_n$ is meant to represent the junction when n pairs have been added to the left and n have been removed from the right. It can be considered as the time-independent part of the state vector for the junction when an ideal battery maintains a constant charge imbalance between the sides. *This state should be viewed as characterizing the constant-charge-imbalance mode of the junction in the same spirit that* $|\psi\rangle_0$, *Eq. (14), has been used previously*[20] *to characterize the charge-neutral mode.*

In conclusion, with both conditions (a) and (b) satisfied, $|\varphi\rangle_n$ and the resulting charge-imbalance state $|\psi\rangle_n$ become appealing instruments through which calculations on the Josephson junction can be carried out within the framework of the pseudo-angular-momentum approach. Unfortunately, though, this state alone is not sufficient to remove the problem of $\langle S_Z'\rangle=0$.

C. Redefining the operators

The problem mentioned in Sec. III A, on the improper definition of the pseudo-angular-momentum operators, will now be addressed. As was seen in that section, the momentum sums in S_Z' differed from those in the total pair-number operators N_L and N_R. This in itself is unappealing, but *the real consequence of using restricted momentum sums is that they force the expectation value of* S_Z' *to be zero,* even when taken with respect to the charge-imbalance state $|\psi\rangle_n$. To see this note that if the definition of the operators[15] is taken literally, then each momentum sum of Eq. (12) is centered about the Fermi momentum of the corresponding superconductor. In the case of a charge imbalance described by $|\psi\rangle_n$, J_{LZ}' would be centered on k_{nF} while J_{RZ}' would be centered on k_{-nF}. This plus the fact that each sum is restricted to symmetric $2\hbar\omega_D$ region about its respective Fermi momentum ensures that the pseudo-angular-momentum operators J_{LZ}' and J_{RZ}' always see the same truncated occupation distributions regardless of the state used. With this view of the operators J'_{LZ}, J'_{RZ} and S'_Z, it is easy to show that their expectation values with respect to $|\psi\rangle_n$, or any other BCS-like state, are zero.

In the above, one interpretation of the definitions of the operators, in light of the charge-imbalance state, has been used. Alternate interpretations are possible. Apparently, though, none of these interpretations allow for a consistent set of angular-momentum operators which at the same time yield nonzero expectation values for S'_Z. Consequently the definitions must be modified in such a way as to overcome these difficulties.

The change contemplated is that instead of using the definitions of Eq. (12) the following are used:

$$J_{LZ}=\sum_{\vec{k}}\sigma_{\vec{k}z}\ , \tag{38a}$$

$$J_{RZ}=\sum_{\vec{q}}\sigma_{\vec{q}z}\ , \tag{38b}$$

$$S_Z=\tfrac{1}{2}(J_{LZ}-J_{RZ})\ , \tag{38c}$$

where the summations over $\vec{k}$ and $\vec{q}$ are now *unrestricted,* except that they terminate at κ. This change will be justified below, but first consider how this will affect the expectation values.

For the charge-neutral superconductor, described by the BCS ground state and Fig. 1, the expectation values of these three operators become

$$\begin{aligned}\langle J_{LZ}\rangle &= {}^L\langle\varphi|J_{LZ}|\varphi\rangle^L\\ &=\sum_{\vec{k}}\{-\tfrac{1}{2}[U^2(\vec{k})-V^2(\vec{k})]\}\\ &=0\ ,\end{aligned} \tag{39}$$

$$\langle J_{RZ}\rangle=0\ ,$$

$$\langle S_Z\rangle=0\ ,$$

as they should be according to their definitions in terms of excess charge.

For the charge-imbalance state, though, the results are now different from those obtained in Eq. (25), where just the phase rotated BCS state $|\psi\rangle'$ and the old definition of the operators were used. Using the operators of Eq. (38) and Figs. 2 and 3 gives

$$\begin{aligned}\langle J_{LZ}\rangle &= {}^L_n\langle\varphi|J_{LZ}|\varphi\rangle^L_n\\ &=\sum_{\vec{k}}\{-\tfrac{1}{2}[U_n^2(\vec{k})-V_n^2(\vec{k})]\}\\ &=\{-\tfrac{1}{2}[-(N_0+n)]+(0)\\ &\quad-\tfrac{1}{2}[(N_0-n)]\}=n\end{aligned} \tag{40a}$$

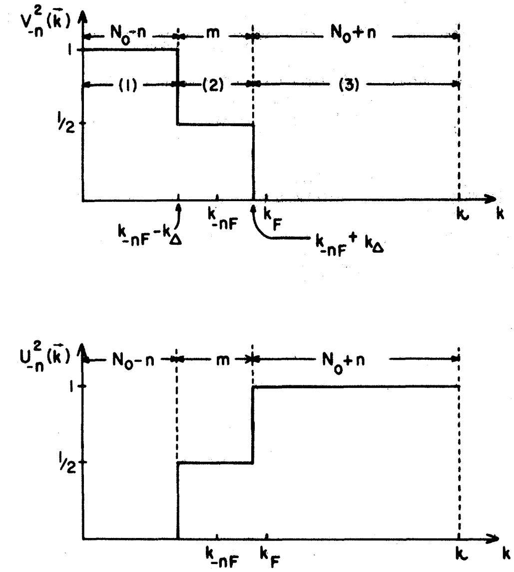

FIG. 3. Occupation distributions, labeled $U^2_{-n}(\vec{k})$ and $V^2_{-n}(\vec{k})$, are shown for a superconductor which has had n pairs removed, at $T=0$ K.

and

$$\begin{aligned}\langle J_{RZ}\rangle &= {}^R_{-n}\langle\varphi|J_{RZ}|\varphi\rangle^R_{-n}\\ &=\sum_{\vec{q}}\{-\tfrac{1}{2}[U^2_{-n}(\vec{q})-V^2_{-n}(\vec{q})]\}\\ &=-n\ .\end{aligned} \tag{40b}$$

With these the expectation value of S_Z becomes

$$\begin{aligned}\langle S_Z\rangle &= {}_n\langle\psi|S_Z|\psi\rangle_n\\ &=\tfrac{1}{2}[\langle J_{LZ}\rangle-\langle J_{RZ}\rangle]\\ &=n\ .\end{aligned} \tag{41}$$

Now these operators yield results consistent with their physical definitions. Also, note that the identification

$$S_Z=\tfrac{1}{2}(N_L-N_R)$$

is valid, unlike Eq. (30).

Return now to the question of changing from restricted to unrestricted sums. Section II C shows that the restrictions on $\vec{k}$ and $\vec{q}$, in $J'^{\pm}_L$ and $J'^{\pm}_R$, arise ultimately from restrictions on the sums in H'_T. These, in turn, were based on having made the approximation $T_{\vec{k}\vec{q}}=T$. The restrictions on J'_{LZ} and J'_{RZ} then resulted from the fact that these operators are related to $J'^{\pm}_L$ and $J'^{\pm}_R$ through commutation relations[14] (i.e., all the operators must have the same range of momenta). Consequently, it might be argued that changing the sums in two of the operators requires changing the sums in all of them. But since the approximation $T_{\vec{k}\vec{q}}=T$ prevents this, none of the sums can be changed.

The last statement in the above argument is invalid. To see this consider Eq. (8), but now let the sums be unrestricted. That is, define H_T as

$$H_T=T\sum_{\vec{k},\vec{q}}(\sigma^+_{\vec{k}}\sigma^-_{\vec{q}}+\sigma^-_{\vec{k}}\sigma^+_{\vec{q}})\ . \tag{42}$$

If this change is going to have a physical effect it will certainly show up in the calculation of the Josephson current, in particular its magnitude. Following the derivation leading to Eq. (17), which uses H'_T, gives

$$j'_1=C_2\sum_{\vec{k},\vec{q}}{}'\,[U(\vec{k})V(\vec{k})][U(\vec{q})V(\vec{q})]\ ,$$

while using H_T it gives

$$j_1=C_2\sum_{\vec{k},\vec{q}}[U(\vec{k})V(\vec{k})][U(\vec{q})V(\vec{q})]\ .$$

But as can be seen by using the values of $U^2(\vec{k})$ and $V^2(\vec{k})$ from Fig. 1, $j'_1=j_1$.

Consequently, the restrictions placed on the sums in H'_T, which ultimately led to those on J'_{LZ}, J'_{RZ}, and S'_Z, are unnnecessary. This has come about because the algebraic form of the BCS ground state has led to a current which is proportional to

$$\sum_{\vec{k}}U(\vec{k})V(\vec{k})\ ,$$

and the numerical values of $U(\vec{k})$ and $V(\vec{k})$ automatically then ensure that only those $\vec{k}$ states near k_F contribute to the tunneling process.

One final note on this subject. Since the algebraic form of $|\varphi\rangle_n$ is the same as that of $|\varphi\rangle$, and since the numerical values of $U_n(\vec{k})$ and $V_n(\vec{k})$ near k_{nF} are the same as $U(\vec{k})$ and $V(\vec{k})$ near k_F, the magnitude of the Josephson current calculated with respect to $|\psi\rangle_n$ will be the same as that given by using $|\psi\rangle_0$.

[Note: At the beginning of Sec. III A it was claimed that a third state vector besides $|\psi\rangle_0$, Eq. (14), and $|\psi\rangle'$, Eq. (21), had been used to describe the junction. This state is $|k\rangle$ of Ref. 1, p. 24. It is described as:

(i) being composed of strongly coupled BCS states, and

(ii) representing a situation where there are k excess pairs on the left side of the junction.

Also "only the electron pairs within a narrow region $(\epsilon_F\pm\hbar\omega_D)$ of the Fermi surface" are considered when using this state.

In regards to $|k\rangle$ it is not exactly clear what these authors mean by a "BCS state with k excess pairs," and since no explicit construction of $|k\rangle$ is given a direct calculation of $\langle k|S_Z|k\rangle$ is not possible. But one thing can be said. The restrictions on the pairs of interest (i.e., only those in the $2\hbar\omega_D$ region) along with the BCS nature of the state impose an unphysical symmetry on the problem which ensures $\langle k|S_Z|k\rangle=0$ for every $|k\rangle$. (This is the same problem which arises when restrictions are placed on the momentum sums of operators.) Thus $|k\rangle$, as defined in Ref. 1, appears to be an unacceptable state on which to base a pseudo-angular-momentum formalism. *In conclusion, our differences with Scully and Lee are not in the concept of a constant-charge-imbalance state or in how such a state is used, rather it is in how this state is defined.]*

IV. AN APPLICATION OF THE CHARGE-IMBALANCE STATE

As an example of how the charge-imbalance state might be employed in non-steady-state situations consider the following problem. A Josephson junction is initially charged such that n_0 pairs have been added to the left side and n_0 have been removed from the right. The junction is then freed from all external circuits and allowed to evolve via tunneling and radiative transitions.

As has been shown above, the charge-imbalance state $|\psi\rangle_n$ [Eq. (37)] describes the junction when the average charge difference between then two sides is held constant. But in this case the charge difference is not constant since the junction will eventually relax back into equilibrium (i.e., both sides will be neutral) through the interaction of the tunneling current with the radiation field.

Consequently, it would be expected that the state of the junction could be approximated as a linear combination of charge-imbalance states:

$$|\Psi\rangle=\sum_{n=0}^{n'}a_n(t)|\psi\rangle_n\ . \tag{43}$$

In the above equation $a_n(t)$ are time-dependent coefficients, n' may differ from n_0 due to the initial direction of the current, and

$${}_n\langle\psi\,|\,S_Z\,|\,\psi\rangle_n = n\ .$$

However, Eq. (43) is not quite the case. Remember that the magnitude of the Josephson current, j_1, is independent of the charge difference between the sides. Therefore, it is conceivable that enough pairs will tunnel through, during part of a cycle, that the polarity of the sides would become reversed. That is, the right side now has excess pairs while the left is deficient in pairs. Taking these additional physical situations into account finally gives

$$|\Psi\rangle = \sum_{n=-n'}^{n'} a_n(t)\,|\,\psi\rangle_n\ . \tag{44}$$

The importance of this is that by solving for the $a_n(t)$ it allows for the construction of an explicit state to use in computing expectation values.

V. CONCLUDING REMARKS

This paper deals with the states and operators needed to develop a pseudo-angular-momentum approach to Josephson tunneling. As has been shown above, there is a problem with the expectation value of one of the fundamental operators of the existing pseudo-angular-momentum theory.[1,15] This difficulty arises from two sources. First, the truncation of momentum sums in operators, and second, the state used to describe the junction when a constant charge imbalance exists. Either of these is capable of eliminating, from the formulation, essential information on the charge difference between the junction sides.

The first source was removed by realizing that the original restrictions on the momentum sums were unnecessary. That is, the algebraic form of $|\,\varphi\rangle$ and the numerical values of $U(\vec{k})$ and $V(\vec{k})$ automatically made any necessary restrictions. This then allowed S_Z', Eq. (12c), to be replaced by S_Z, Eq. (38c). Elimination of the second source required the construction of a state, $|\,\varphi\rangle_n$, that would accurately reflect an increase in the total number of pairs when a single superconductor carries a charge excess. With this shifted-BCS state, the junction having a constant pair imbalance between its sides could be represented by the state vector

$$|\,\psi\rangle_n = |\,\varphi\rangle_n^L \otimes |\,\varphi\rangle_{-n}^R\ .$$

Thus, by using the state $|\,\psi\rangle_n$ and the operator S_Z the inconsistency in the original theory was corrected. *What effect, if any, these changes would have if employed in the remainder of the existing pseudo-angular-momentum theory is not clear at the present time.* Finally, the set of operators and states developed in this work form a base from which the remainder of the program, outlined in the Introduction, can now be carried out.

ACKNOWLEDGMENTS

The authors wish to thank Dr. R. H. Parmenter and Dr. M. O. Scully for many helpful discussions. Also Dr. R. A. Ferrell is gratefully acknowledged for providing a copy of his work in advance of publication.

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Consider an energy axis and a symmetric region about ϵ_F. For a neutral superconductor at $T=0$ K, align k_F (of the BCS occupation distribution) with ϵ_F of this axis. The spin system being considered is now defined in terms of this energy axis and not the momentum axis of the BCS distribution. The distribution serves only to tell the orientation of each spin subsystem. The operators corresponding to this pseudo-angular-momentum system are also now defined in terms of the energy axis.

For the situation where n pairs have been added to the superconductor, the energy of each bulk electron has changed so that $\epsilon'_{\vec{k}}=\epsilon_{\vec{k}}+$ const. Consequently, the entire BCS distribution is shifted with respect to this energy axis, i.e., k_F is now aligned with $\epsilon'_F=\epsilon_F+$ const. This induces an asymmetry between the subsystems with spin-up and those with spin-down which results in $\langle J_Z \rangle = n$.

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