PHYSICAL REVIEW B VOLUME 23, NUMBER 11 1 JUNE 1981

Reentrant phase transition of granular superconductors

E. Šimánek
Department of Physics, University of California, Riverside, California 92521

(Received 30 June 1980)

It is shown that the effects of the charging energy on the mean-field transition temperature of a granular superconductor depend in a profound manner on the choice of the interval for the phase ϕ of the order parameter. For $-\infty < \phi < \infty$ a well pronounced reentrant behavior is obtained for the diagonal model, in which the Coulomb interaction is neglected. The reentrance disappears in this model when the interval is taken to be $-\pi < \phi < \pi$. Dipolar excitations of the nondiagonal model, considered recently by Efetof are shown to diminish the extent of reentrance for the $-\infty < \phi < \infty$ model and to produce a weak reentrance in the $-\pi < \phi < \pi$ case. The reentrant behavior is shown to be due to the thermally induced phase coherence via the low-lying excited states characterized by the vanishing of the frequency of the phase rotation.

I. INTRODUCTION

As first pointed out by Abeles,[1] the electrostatic energy necessary to add an electron to the grain of a granular superconductor acts to disrupt the long-range phase coherence. The first quantitative understanding of this effect comes from the ideas of deGennes[2] who proposed a pseudospin $S=1$ model for an ordered array of grains. In the mean-field approximation this model predicts that the superconducting long-range order at $T=0$ is quenched when the charging energy $U > zE_1$ where z is the number of nearest neighbors in the array and E_1 is the Josephson coupling energy. We have independently considered a similar model of an ordered array described by the Hamiltonian[3]

$$\mathcal{H}=\frac{U}{2}\sum_i \hat{n}_i^{\,2}+\sum_{ij} E_{ij}[1-\cos(\phi_i-\phi_j)] \quad , \qquad (1.1)$$

where $\hat{n}_i$ is the operator describing the deviation from the average number of electrons on the ith grain and $E_{ij}=E_1\delta_{i,j\pm 1}$. To calculate the effects of the charging energy on the transition temperature T_c we have used a mean-field approximation which replaces the second term of Eq. (1.1) by $-2zE_1\langle\cos\phi\rangle\sum_i\cos\psi_i$. The average order parameter $\langle\cos\phi\rangle$ of the array is calculated with the use of the expression

$$\langle\cos\phi\rangle=\frac{\sum_m e^{-E_m/T_c}\langle\Psi_m|\cos\phi|\Psi_m\rangle}{\sum_m e^{-E_m/T_c}} \quad , \qquad (1.2)$$

where Ψ_m and E_m are the eigenstates and eigenvalues of the mean-field Hamiltonian, describing the motion of a fictitious particles of mass $1/4U$ in a $\cos\phi$ potential.

Including in Eq. (1.2) all periodic solutions of the corresponding Mathieu equation up to $m=2$ the following self-consistency equation for the temperature T_c is obtained[3]

$$1=\alpha\frac{1+(\frac{1}{2}+2x)e^{-x}-\frac{2}{3}e^{-4x}}{1+2(e^{-x}+e^{-4x})} \quad , \qquad (1.3)$$

where $x=U/2T_c$ and $\alpha=zE_1/U$. The interesting feature of this equation is that it leads to a phase diagram with a pronounced reentrant behavior (see curve a of Fig. 1). The relatively broad range of the α values over which there are double-valued solutions for x and T_c makes this result of considerable experimental interest.

Recently Efetof[4] studied an extension of the above model which includes the Coulomb interaction between the charged neighboring grains. Specifically, he considered a Hamiltonian

$$\mathcal{H}=\frac{1}{2}\sum_{ij} U_{ij}\hat{n}_i\hat{n}_j+\sum_{ij} E_{ij}[1-\cos(\phi_i-\phi_j)] \qquad (1.4)$$

and used the method of the "phase correlator" to derive the self-consistency equation for T_c in the mean-field approximation. In the diagonal limit, $U_{ij}=U\delta_{ij}$, he does not find any reentrant behavior, which makes him suspect a numerical error in the calculations of Ref. 3. For the nondiagonal case he shows that an important role is played by the low-lying excitation, corresponding to the transfer of a Cooper pair between neighboring grains. By taking into account these dipolar excitations for an array of close-packed grains, Efetof[4] reports a numerical evidence for reentrant behavior.

The main purpose of the present paper is to clarify the origin of the reentrant phase transition of the diagonal model predicted in Ref. 3 and to resolve the

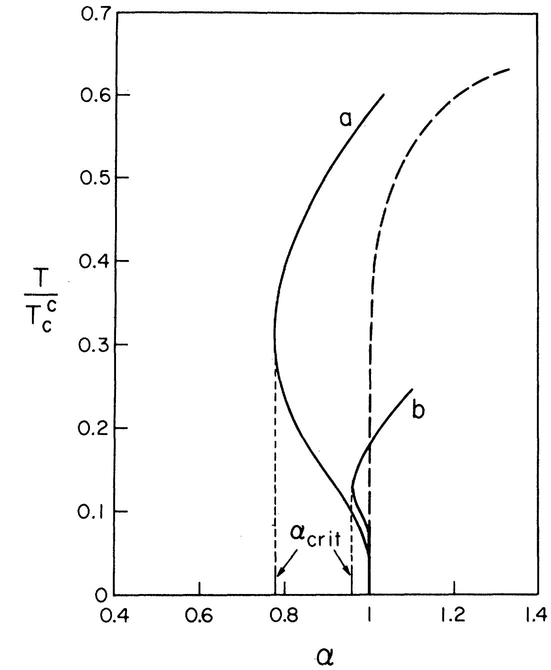

FIG. 1. The phase diagrams for the various models of a granular superconductor. Curve a presents the solution of the self-consistency equation (1.3) corresponding to the diagonal model with the phase ϕ varying from $-\infty$ to ∞. Curve b is the result of Eq. (4.3), corresponding to the nondiagonal model including the lowest-energy dipolar excitation and assuming $-\infty < \phi < \infty$. The broken curve is the solution of Eq. (2.4) for the diagonal model with the phase varying from $-\pi$ to π. The parameter $\alpha = zE_1/U_{11}$ and $T_c^c = zE_1$ is the mean-field transition temperature of a granular system without charging effects [Eq. (1.1) with $U=0$]. The superconducting phase is to the right of the above curves.

discrepancy between the latter and Ref. 4. We also investigate the effect of the dipolar excitations on the reentrance of the phase transition in the nondiagonal model. In Sec. II we discuss the diagonal model using the method of the phase correlation[4] and show that the reentrance of Ref. 3 stems from the inclusion of special excited states resulting when the phase of the order parameter is allowed to vary from $-\infty$ to ∞. Section III is devoted to an analysis of the physical mechanism underlying the phenomenon of reentrance. The role of dipolar excitations in the nondiagonal model is studied in Sec. IV. The self-consistency equation of Efetof's formulation[4] is, for the sake of completeness, derived in the Appendix.

II. PHASE TRANSITION IN THE DIAGONAL MODEL

The diagonal form of the charging energy is the analog of the Coulomb part of the Hubbard Hamiltonian of an atomic array. For a granular system it has been previously postulated by Kawabata[5] to discuss the metal-insulator transition in the normal state. To see to what extent is the diagonal approximation valid we consider the charging energy needed to transfer an electron between two equivalent nearest-neighbor grains of the array

$$E_c^{(1)} = \frac{1}{2}\sum_{ij} U_{ij} n_i n_j = U_{11} - U_{12} \ . \tag{2.1}$$

The energy $E_c^{(1)}$ has been estimated by Abeles *et al.*[6] who considered a pair of grains embedded in a medium of effective dielectric constant $K = \epsilon(1 + d/2s)$, where ϵ is the dielectric constant of the insulator, d is the grain diameter and s is the spacing between the grains. For a large range of the ratio d/s Ref. 6 shows that $E_c^{(1)} \simeq \frac{1}{2} E_c^{(0)}$ where $E_c^{(0)} = U_{11}$ is the energy to transfer an electron from one grain to another one an infinite distance away. This result and Eq. (2.1) imply that, for a large range of compositions, it is reasonable to assume

$$U_{12} \simeq \frac{1}{2} U_{11} \ . \tag{2.2}$$

It is only when $s >> d$ that the diagonal approximation holds, as easily seen from Ref. 6. This limit may be difficult to realize in practice because of the small Josephson coupling expected for such an array. Nevertheless, the diagonal model is theoretically interesting because of its simplicity, allowing a rather accurate determination of its mean-field phase diagram.

A. Case of $(-\pi < \phi < \pi)$

We start from the self-consistency condition for the transition temperature of the nondiagonal model derived, using the method of phase correlator, in the Appendix [Eq. (A14)]. By letting $U_{ij} = U\delta_{ij}$ in this equation we obtain its "diagonal" version

$$1 = \frac{zE_1}{Z_0} \sum_{n_1} \frac{1 - \exp\left[-\frac{2U}{T}(1+n_1)\right]}{2U(1+n_1)} \exp\left[-\frac{Un_1^2}{2T}\right] \ , \tag{2.3}$$

where n_1 is the eigenvalue of the electron number operator $\hat{n}_1 = -2i\partial/\partial\phi_1$. If the phase ϕ_1 is restricted to the interval $-\pi$ to π the mean-field approximation of the Hamiltonian (1.1) describes a plane rotator model, for which the eigenstates must be 2π-periodic functions of ϕ_1. This implies that only even values of n_1 are allowed. This is also the case considered by Efetof.[4] Including in the sum of Eq. (2.3) the terms $n_1 = 0$, ± 2, and ± 4 we obtain the self-consistency condition

$$1=\alpha\frac{1-\frac{2}{3}e^{-4x}}{1+2e^{-4x}} \quad . \tag{2.4}$$

We note that we have retained in this equation only the leading exponential terms. The phase diagram resulting from Eq. (2.4) is shown in Fig. 1 (broken curve). In agreement with the results of Refs. 3 and 4 it does not exhibit a reentrant behavior.

B. Case of $(-\infty<\phi<\infty)$

It is customary to assume that the phase-locking transition of an array of superconducting grains is isomorphous to the phase transition of the $x-y$ model.[7] In the latter the angular variable defining the orientation of the spins is restricted to the interval $-\pi$ to π. For the superconducting order parameter $|\Psi_i|e^{i\phi_i}$ of the ith grain in the array such a restriction does not necessarily apply,[8,9] so that we may extend the range of ϕ_i to $-\infty<\phi_i<\infty$. This has important consequences for the phase transition of the models described by the Hamiltonians (1.1) and (1.4). The mean-field theory of the diagonal model with the condition $-\infty<\phi<\infty$ has been formulated in terms of the Mathieu equation in Ref. 3. It is known that periodic solutions Ψ_n of this equation are not all 2π-periodic functions of ϕ, but there is a set of 2π-antiperiodic (i.e., 4π-periodic) solutions $\Psi_1,\Psi_3,\ldots$. Such solutions are linear combinations of the eigenfunctions $e^{i\phi n_1/2}$ of the Hamiltonian (A2) where $n_1=\pm1,\pm3,\ldots$. This implies that odd eigenvalues of the electron number operator are also allowed when the phase can vary from $-\infty$ to ∞. Including in Eq. (2.3) the configurations $n_1=0$, ±1, ±2, ±3, and ±4, we in fact obtain the self-consistency equation (1.3), which verifies the correctness of our previous result.[3] Numerical analysis of the solutions of Eq. (1.3) shows that the reentrant behavior (curve a of Fig. 1) is brought about by the presence of the $2xe^{-x}$ term in the numerator. This can also be seen analytically by considering an approximate version of Eq. (1.3), valid for large values of x:

$$\frac{1}{\alpha}=\frac{1+(2x+\frac{1}{2})e^{-x}}{1+2e^{-x}}\simeq[1+(2x-\tfrac{3}{2})e^{-x}] \quad . \tag{2.5}$$

As long as $x>\frac{7}{4}$, the right-hand side of Eq. (2.4) is an increasing function of T_c (its derivative with respect to x is negative). This implies a decrease of α with increase of T_c, explaining the reentrant behavior near the α axis of the phase diagram of Fig. 1.

III. PHYSICAL ORIGIN OF REENTRANCE

In deriving Eq. (1.3) from Eq. (2.3) we observe that the $2xe^{-x}$ term, essential for reentrant behavior, originates from the configuration $n_1=-1$. For the latter the characteristic energy $2U(1+n_1)$ vanishes so that the corresponding contribution to $\langle\cos\phi\rangle$ becomes

$$\lim_{n_1\to-1}\frac{1-\exp\left[-\frac{2U}{T}(1+n_1)\right]}{2U(1+n_1)}=\frac{1}{T}=\frac{2x}{U} \quad . \tag{3.1}$$

The physical meaning of this result is that the order parameter $|\Psi_i|e^{i\phi_i}$ in the excited configuration $n_1=-1$ can rotate freely thus exhibiting a Curie-like polarizability with respect to the molecular field. An additional understanding of this effect comes from the inspection of Eq. (A13). The exponents, given by the expression

$$2\left[U_{ij}+\sum_j U_{ij}n_j\right]=\omega(n_i,n_j) \tag{3.2}$$

can be interpreted as the angular frequencies $\omega(n_i,n_j)$ of the phase rotation in the excited state (n_i,n_j) (see Ref. 4). In the ground state $(n_i=0,n_j=0)$ the quantity ω has a nonzero value of $2U_{ij}$. The presence of an extra hole on the grain is therefore capable of canceling this "zero-point" frequency of the phase rotation. This result suggests that the phase correlator theory,[4] leading to Eq. (A14), suffers from a lack of particle-hole symmetry.

In the Appendix we derive a version of the self-consistency condition in which the latter defect is removed. This condition [Eq. (A16)] shows that it is both the extra electron $n_1=1$ and extra hole, $n_1=-1$ configurations which lead to terms proportional to x. We note that our previous formulation[3] of the diagonal model also exhibits the particle-hole symmetry. In the latter theory it is the doublet of the lowest excited states $\Psi_1^{\rm even}$ and $\Psi_1^{\rm odd}$, which splits under the action of the molecular field, yielding the Curie-like polarizability proportional to x. The strongly pronounced reentrant behavior of the phase diagram (Fig. 1, curve a) is due to the low value of the excitation energy of the above states.

IV. ROLE OF DIPOLAR EXCITATIONS

We now consider the experimentally interesting nondiagonal model described by Hamiltonian (1.4). The mean-field theory of this model leads to the expression (A14). There are two types of excited configurations to be considered in the summation over (n_i,n_j) in the latter equation.

(i) Charge-nonconserving configurations

$(n_i \neq 0, n_j = 0)$ for which the terms on the right-hand side of Eq. (A14) agree with those of the diagonal model.

(ii) Charge-conserving configurations $(n_i, -n_i)$, which are the dipolar excitations of Efetof's theory.[4] To see the most important trends we consider only the lowest-energy excitation caused by the charge transfer between the nearest-neighbor grains. To be specific we also use the following relation

$$U_{12} = \tfrac{1}{2} U_{11} \ , \tag{4.1}$$

which replaces the approximate relation (2.2) by an exact equality.

A. $(-\pi < \phi < \pi)$ case

In this case only even values of n_i and n_j are allowed. The lowest-energy configurations and the corresponding phase rotation frequencies defined by Eq. (2.6) are displayed in Table I. We see that the dipolar excitation $(n_i = -2, n_j = 2)$ is characterized by the vanishing of the frequency ω and thus it is expected to produce some reentrant behavior of the phase diagram. Using the configurations of Table I in expression (A14) we arrive at the following self-consistency relation:

$$1 = \alpha \frac{1 + e^{-4x}(2zx + \frac{1}{4}z - \frac{5}{6})}{1 + (2z+2)e^{-4x}} \ . \tag{4.2}$$

The presence of the $2zx$ term in the numerator is due to the above $(n_i = -2, n_j = 2)$ excitation of multiplicity z. Numerical analysis of Eq. (4.2) yields a phase diagram with a very weakly pronounced reentrant behavior. The double-valued transition temperature occurs over a narrow range $0.99 < \alpha < 1$. The main reason for this is the relatively high value of the excitation energy (equal to $2U_{11}$) producing a small Boltzmann factor e^{-4x} in the expression (4.2). For $\alpha > 1$ the phase diagram almost coincides with that of Eq. (2.4) (broken curve of Fig. 1).

B. $(-\infty < \phi < \infty)$ case

The configurations relevant for this case also include the odd values of n_i and n_j. They are displayed in Table II, where we use the relation (4.1) to calculate the energies of the configurations and the corresponding frequencies $\omega(n_i, n_j)$. Including the configurations of Table II in the expression (A14) we obtain

$$1 = \alpha \frac{1 + e^{-x}(\frac{1}{4} + 2x + 4z/3) - ze^{-3x} + e^{-4x}(2zx + z/4 - \frac{5}{6})}{1 + (2z+2)e^{-x} + (2z+2)e^{-4x}} \ . \tag{4.3}$$

Again the configuration $(n_i = -1, n_j = 0)$, familiar from the diagonal model, is responsible for the presence of the $2xe^{-x}$ term which produces the reentrant behavior of this model. The part of the phase diagram for small values of T_c and $z = 6$ is shown as curve b in Fig. 1. The reentrant behavior, obtained in this case, is stronger than the one of the nondiagonal $(-\pi < \phi < \pi)$ model but still considerably smaller than that of the diagonal model (curve a). This is due to the role of the dipolar excitations $(n_i = \pm 1, n_j = \mp 1)$ which are of the same energy as the $(n_i = \pm 1, 0)$ configurations but have a greater multi-

TABLE I. The ground- and excited-state configurations (n_i, n_j) used in the evaluation of the self-consistency condition (A14) for the mean-field theory of the Hamiltonian (1.4). The phase of the order parameter is allowed to vary from $-\pi$ to π. The configuration energies and phase rotation frequencies shown in the third and fourth columns, respectively, are calculated using the relation (4.1). The multiplicity of the configurations is denoted by N.

n_i	n_j	$\frac{1}{2}\sum_{ij} U_{ij} n_i n_j$	$\omega(n_i, n_j)$	N
0	0	0	$2U_{11}$	1
2	0	$2U_{11}$	$6U_{11}$	1
−2	0	$2U_{11}$	$-2U_{11}$	1
2	−2	$2U_{11}$	$4U_{11}$	z
−2	2	$2U_{11}$	0	z

TABLE II. The ground- and excited-state configurations (n_i, n_j) included in the evaluation of expression (A14) for the mean-field theory of Hamiltonian (1.4) and allowing the phase of the order parameter to vary from $-\infty$ to ∞. Equation (4.1) is used to evaluate the entries of the third and fourth columns.

n_i	n_j	$\frac{1}{2}\sum U_{ij} n_i n_j$	$\omega(n_i, n_j)$	N
0	0	0	$2U_{11}$	1
1	0	$\frac{1}{2}U_{11}$	$4U_{11}$	1
-1	0	$\frac{1}{2}U_{11}$	0	1
1	-1	$\frac{1}{2}U_{11}$	U_{11}	z
-1	1	$\frac{1}{2}U_{11}$	U_{11}	z
2	0	$2U_{11}$	$6U_{11}$	1
-2	0	$2U_{11}$	$-2U_{11}$	1
2	-2	$2U_{11}$	$4U_{11}$	z
-2	2	$2U_{11}$	0	z

plicity z. The finite phase rotation frequency of these dipolar excitations masks the phase reinforcing effect of the $(n_i = -1, 0)$ configuration. For smaller values of z, which are perhaps possible in planar arrays $(z = 4)$ this masking effect is diminished so that the reentrant behavior becomes somewhat more pronounced.

From a practical point of view it is useful to consider also the case when the equality (4.1) holds only approximately, implying an incomplete vanishing of the frequency $\omega(n_i = -2, n_j = 2)$. It can be shown that the weak reentrance persists as long as $\omega << U_{11}$.

V. SUMMARY AND COMMENTS

It is shown that the effects of the charging energy on the phase diagram of a granular superconductor depend on the model Hamiltonian and the choice of the interval for the phase of the order parameter. The strongest reentrant behavior is obtained for the diagonal Hamiltonian (1.1) with $-\infty < \phi < \infty$. The mechanism for the increase of the phase coherence with temperature is found to be the thermal occupation of the low-lying excited states in which the phase rotation frequency vanishes. When the phase is confined to $-\pi < \phi < \pi$ the diagonal model is equivalent to the plane rotator model and no reentrance is observed in accord with Refs. 2 and 4. The low-lying dipolar excitations corresponding to electron transfer between nearest-neighbor grains tend to diminish the reentrant behavior in the nondiagonal model with $-\infty < \phi < \infty$. For $-\pi < \phi < \pi$ the excitations caused by transfer of a Cooper pair induce a weak reentrant behavior. At $T = 0$ all the above models predict the same critical value 1 for the parameter α. This parameter is expected to increase with the metal volume fraction of the granular films. Experimentally, the superconducting transition temperature is known to decrease rapidly when this fraction is decreased to the point where the sample becomes semiconducting.[10] This behavior is in qualitative accord with the phase diagrams of Fig. 1. An experimental distinction between the $(-\pi < \phi < \pi)$ and the $(-\infty < \phi < \infty)$ models can be perhaps made through the different dependence of T_c upon α exhibited near the metal-semiconductor transition. This will require an extension of the above theory to include the effects of disorder on the localization transition. Finally, let us discuss the various choices for the interval of ϕ from a physical point of view. First we note that for a macroscopic wave function $|\psi|\exp[i\phi(\vec{r})]$ of a superfluid the phase $\phi(\vec{r})$ need not be single valued. The extension of its range to $-\infty < \phi < \infty$ is needed to establish the notion of the vortices and the phase slippage.[8–11] However, the macroscopic wave function itself must be single valued in the sense that it does not change its value as the phase ϕ changes by 2π. In the present work the macroscopic wave function is proportional to the quantity $\langle\cos\phi\rangle$ evaluated with the use of Eq. (1.2). Since the matrix elements $\langle\psi_m|\cos\phi|\psi_m\rangle$ are single valued (even for $m = 1$) so is the quantity $\langle\cos\phi\rangle$ in keeping with the above general requirement. Only when the phase is restricted to the range $(-\pi, \pi)$, the $m = 1$ solutions must be rejected on a mathematical ground since they do not satisfy the requirement of continuity. For Josephson-junction arrays this restriction does not apply since the interval of the local phase is $(-\infty, \infty)$ as required by the ac Josephson effect and phase slippage. However the 2π-

antiperiodic states are meaningful only for Cooper pair tunneling as implied by the fact that they correspond to an odd number of electrons added or renewed from a neutral grain. In the case of a Josephson tunneling of bosons such as that between droplets of superfluid helium only the 2π-periodic solutions have a physical meaning. It is interesting that single-electron excitations (similar to the $m=1$ states) have been considered previously by Bari[12] in a study of a superconductor-semiconductor transition of a Hubbard model extended by a local BCS interaction.

ACKNOWLEDGMENTS

The author acknowledges the correspondence with P. G. deGennes and W. L. McLean, which stimulated the present investigation and wishes to thank N. Bui and K. A. Müller for interesting discussions.

APPENDIX

In this Appendix we derive the self-consistency equation of the nondiagonal model, using the phase correlator method of Efetof.[4] This result is based on the mean-field approximation to the Hamiltonian (1.4):

$$\mathcal{H}_{\rm MF}=\mathcal{H}_0+\mathcal{H}_1 \ , \tag{A1}$$

where

$$\mathcal{H}_0=\frac{1}{2}\sum_{ij}U_{ij}\hat{n}_i\hat{n}_j \tag{A2}$$

and

$$\mathcal{H}_1=-2zE_1\langle\cos\phi\rangle\sum_i\cos\phi_i \ . \tag{A3}$$

Near the transition temperature the average order parameter is small and can be calculated using the thermodynamic perturbation theory to first order in $\mathcal{H}_1$

$$\langle\cos\phi\rangle=\mathrm{Tr}\left[e^{-\beta\mathcal{H}_0}\left(1-\int_0^\beta\hat{\mathcal{H}}_1(\tau)d\tau\right)\cos\phi\right]\Big/Z_0 \ , \tag{A4}$$

where

$$\mathcal{H}_1(\tau)=e^{\tau\mathcal{H}_0}\mathcal{H}_1e^{-\tau\mathcal{H}_0} \tag{A5}$$

and

$$Z_0=\mathrm{Tr}(e^{-\beta\mathcal{H}_0}),\quad \beta=1/T \ . \tag{A6}$$

Introducing for $\mathcal{H}_1$ the expression (A3) we obtain from Eq. (A4) the self-consistency condition of Efetof

$$1=zE_1\int_0^\beta\pi(\tau)d\tau \ , \tag{A7}$$

where

$$\pi(\tau)=\left(\frac{2}{Z_0}\right)\mathrm{Tr}[e^{-\beta\mathcal{H}_0}\cos\phi(\tau)\cos\phi(0)]$$

$$=\langle e^{-i\phi(\tau)}e^{+i\phi(0)}\rangle \ . \tag{A8}$$

To calculate the phase correlator $\pi(\tau)$ we observe that the phase $\phi_i(\tau)$ satisfies the equation of motion

$$\frac{\partial\phi_i}{\partial\tau}=[\mathcal{H}_0,\phi_i] \ . \tag{A9}$$

Using in this equation the commutation relation between the phase and number operators

$$[\phi_i,\hat{n}_j]=2i\delta_{ij} \tag{A10}$$

we have

$$\phi_i(\tau)=\phi_i(0)-2i\sum_{ij}U_{ij}\hat{n}_j(0)\tau \ . \tag{A11}$$

With use of Eq. (A11) and the identity

$$\langle e^{-i\phi_i(\tau)}e^{\phi_i(0)}\rangle=\langle e^{-i[\phi_i(\tau)-\phi_i(0)]}\rangle e^{1/2[\phi_i(\tau),\phi_i(0)]} \tag{A12}$$

we obtain the formula of Efetof[4]

$$\pi(\tau)=\frac{1}{Z_0}\sum_{n_in_j}\exp\left[-2\tau\left(U_{ii}+\sum_jU_{ij}n_j\right)-\frac{1}{2T}\sum_{ij}U_{ij}n_in_j\right] \ , \tag{A13}$$

where n_i and n_j are all allowed eigenvalues of the operators $\hat{n}_i$ and $\hat{n}_j$. Integrating this result over τ the self-consistency equation (A8) takes the following explicit form:

$$1=\frac{zE_1}{Z_0}\sum_{n_in_j}\frac{1-\exp\left[-(2/T)\left(U_{ii}+\sum_jU_{ij}n_j\right)\right]}{2\left(U_{ii}+\sum_jU_{ij}n_j\right)}\exp\left(-(1/2T)\sum_{ij}U_{ij}n_in_j\right) \ . \tag{A14}$$

As noted in Sec. III this result lacks the particle-hole symmetry. This formal defect can be traced back to Eq. (A8) where a particular choice of signs in the exponents of the correlation function $\pi(\tau)$ was made. The particle-hole symmetry can be restored by taking $\pi(\tau)$ in a symmetric form

$$\pi(\tau)=\frac{1}{2}\left(e^{i\phi(\tau)}e^{-i\phi(0)}+e^{-i\phi(\tau)}e^{i\phi(0)}\right) . \tag{A15}$$

Consequently the expression (A14) is replaced by

$$1=\frac{zE_1}{2Z_0}\sum_{n_i n_j}\left\{\frac{1-\exp\left[-(2/T)\left(U_{ii}+\sum_j U_{ij}n_j\right)\right]}{2\left(U_{ii}+\sum_j U_{ij}n_j\right)}+\frac{1-\exp\left[-(2/T)\left(U_{ii}-\sum_j U_{ij}n_j\right)\right]}{2\left(U_{ii}-\sum_j U_{ij}n_j\right)}\right\}\exp\left(-(1/2T)\sum_{ij}U_{ij}n_i n_j\right) . \tag{A16}$$

For the diagonal model, we see that both the configurations $n_1=1$ and -1 contribute in Eq. (A16) a term proportional to $2x$, showing that the particle-hole symmetry is restored. Similar conclusions hold for the nondiagonal model, where for example the configurations ($n_i=2$, $n_j=-2$) and ($n_i=-2$, $n_1=2$) contribute symmetrically to vanishing of the phase rotation frequencies [see Eq. (4.2)]. Although conceptually more satisfactory, this formulation leads to the same numerical form of the final self-consistency condition as the original Efetof's expression (A14). For the sake of simplicity we are using in this paper the latter equation.

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