Superconducting arrays in a magnetic field: Quantum effects

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We consider a Josephson-coupled superconducting array with finite quantum fluctuations, arising from a nonzero capacitive charging energy, placed in a transverse magnetic field. To estimate the superconducting transition temperature as a function of magnetic field, we introduce a Hartree-type mean-field approximation. With no applied magnetic field, this approximation is very similar to that of Simanek, but unlike the latter, it does not lead to a reentrant normal phase transition. Reentrance is absent because we include no 4π-periodic eigenstates of Mathieu's equation in calculating quantum-statistical expectation values. We argue that these 4π-periodic functions are properly omitted because the original Hamiltonian does not include pair-breaking terms. With charging energies included, we find the transition temperature to be highly nonmonotonic in magnetic field, just as in the zero-capacitance limit. For every field B, there exists an upper critical charging energy $U_c(B)$ above which the array is normal even at $T=0$; this charging energy is highly nonmonotonic in field. A brief comparison is made between our results and other recent calculations involving superconducting arrays in the presence of charging energies.

I. INTRODUCTION

Superconducting arrays, consisting of Josephson- or proximity-coupled superconducting grains embedded in a normal metal or insulating host, form fascinating model systems. Such arrays can readily be prepared in ordered, two-dimensional form by photolithographic techniques.[1-8] They can also be produced in disordered, two- or three-dimensional form, as "granular superconductors."[9-12] The behavior of such systems has been the subject of much study, both experimental and theoretical. It is now known that superconducting arrays have a complex variety of normal-to-superconducting phase transitions. These transitions are affected by many parameters, including charging energies, applied magnetic fields, disorder, and dissipative processes within the weak links.

The purpose of the present paper is to reexamine a simple approximation for treating the effects of charging energies in superconducting arrays, and to apply this approximation to superconducting arrays in a magnetic field. The importance of charging energies is explicit in the resistively-shunted-junction model for a single junction. Their relevance to phase transitions in superconducting arrays was first emphasized by Anderson[13] and by Abeles.[14] The basic idea is that, in addition to the Josephson coupling which tends to align the phases of the ordering parameters on neighboring grains, there is also a capacitive energy which tends to oppose departures of the grains from charge neutrality. Since charge and phase are canonically conjugate, large capacitive energies tend to produce quantum fluctuations in phase and thus to suppress phase ordering.

Various approximations have been developed to treat the quantum Hamiltonian which describes such an array. Simanek,[15] and independently Maekawa *et al.*,[16] proposed a mean-field theory (analogous to a self-consistent Einstein approximation for the "phase phonons" of this system). They found that the phase transition was suppressed to 0 K for sufficiently large capacitive energy U. For certain values of the ratio of U to the Josephson coupling energy J, they also predicted a reentrant (normal-to-superconducting-to-normal) phase transition as a function of temperature. Efetov,[17] Doniach,[18] Wood and Stroud,[19] and Imry and Strongin,[20] all using different methods of analysis, also found an upper critical U/J, but did not recover the reentrant transition. Recent quantum Monte Carlo calculations by Jose and collaborators[21] appear to show *two* separate superconducting transitions at certain values of the ratio U/J but they, too, still show a critical ratio U/J above which no superconducting transition takes place.

In this paper, we reexamine the original mean-field theory of Simanek and extend it to treat superconducting arrays in a magnetic field. We find that when the Hartree wave functions that arise in this mean-field theory are properly restricted to exclude those which break Cooper pairs (since pair-breaking is not included in the original charging Hamiltonian), the reentrant phase transition found by Simanek disappears. We also find, within the mean-field theory, that the critical ratio $(U/J)_c$ is a strong, highly nonmonotonic function of magnetic field. The function describing the magnetic field dependence of $(U/J)_c$ is closely related to the mean-field transition temperature as a function of field at zero capacitance, as calculated by Shih and Stroud.[22] Since $(U/J)_c$ depends on the magnetic field B, one has the possibility of entering and exiting the superconducting state by varying the magnetic field at fixed temperatures.

The mean-field theory is, of course, quite oversimplified, especially for the two-dimensional systems considered here. In the absence of capacitive energies, for example, the mean-field theory certainly overestimates the

transition temperature of the model Hamiltonian it describes.[23–28] Nonetheless, it shows excellent agreement with the trends of experimental measurements, and predicts several experimental peaks[5] in transition temperature as a function of a magnetic field. The mean-field theory thus seems a useful starting point, in the absence of other, more quantitatively precise calculations, for finite capacitance also. Another advantage is that the mean-field approach can easily be extended to the experimentally interesting cases of disordered, two- or three-dimensional granular superconductors.

II. FORMALISM

We consider a superconducting array of N grains, the ith grain centered at $\mathbf{x}_i$, which is described by a complex superconducting order parameter (or gap parameter) $\Delta_i = |\Delta_i| \exp(i\phi_i)$. The Hamiltonian of a Josephson array, far below the bulk transition temperature T_{c0} of the individual grains, may be approximated by assuming that the magnitude of the order parameters, $|\Delta_i|$, is a fixed number, (the same for each grain, if the grains are identical), and that only the phase ϕ_i is a dynamical variable.

The Hamiltonian thus takes the form

$$H = \sum_i (U_i/2) n_i^2 - \sum_{\langle i,j \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \ . \tag{1}$$

In this expression, $U_i = e^2/C_i$, where e is the charge of an electron, C_i is the capacitance of the ith grain; n_i is the excess charge on the ith grain (measured in units of e); J_{ij} is the Josephson coupling energy for the junction between grains i and j; and the phase factor

$$A_{ij} = (2e/hc) \int_{\mathbf{x}_i}^{\mathbf{x}_j} \mathbf{A} \cdot d\mathbf{l} \tag{2}$$

is proportional to the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. The first term in (1) thus represents the electrostatic energy required to charge up the grains to net charges indicated by the n_i's, in the "diagonal approximation"—that is, the grains are assumed to be capacitively coupled to ground, but the capacitive energy associated with the coupling between grains is assumed to be negligible. This limit can be reached if the distance between the grains is sufficiently large that the "off-diagonal" capacitance is negligible. The "diagonal approximation" is more widely studied and easily handled than the off-diagonal case. The second term in (1), which involves a sum over all distinct pairs of grains $\langle i,j \rangle$ is the Josephson coupling energy in the presence of a magnetic field $\mathbf{B}$, in which the phase difference $\phi_i - \phi_j$ is replaced by the gauge-invariant phase difference $\phi_i - \phi_j - A_{ij}$. Hamiltonian (1) is quantum mechanical in the sense that n_i and ϕ_i are canonically conjugate variables, as discussed further below.

The thermodynamic properties of the array described by (1) are determined by a partition function in the canonical ensemble, i.e.,

$$Z = \mathrm{Tr} \exp(-H/k_B T) \ , \tag{3}$$

where the trace is a sum over a complete set of quantum states and T is the temperature. Likewise, quantum statistical averages of operators of the form $O(\phi_1, \phi_2, \ldots, \phi_N)$ (denoted $\overline{O}$) are defined by

$$\overline{O} = Z^{-1} \mathrm{Tr} O \exp(-H/k_B T) \ . \tag{4}$$

We can most conveniently formulate the mean-field theory for (1) by rewriting H (assuming N identical grains) as

$$H = (U/2) \sum_i n_i^2 - \tfrac{1}{2} \sum_{\langle i,j \rangle} J_{ij} [\psi_i \psi_j^* \exp(-iA_{ij}) + \text{c.c.}] \ , \tag{5}$$

where $\psi_i = \exp(i\phi_i)$ and "c.c." denotes "complex conjugate." Now ψ_i can be written as a sum of a thermal average (denoted by triangular brackets, $\langle\ \rangle$) and a fluctuation:

$$\psi_i = \langle \psi_i \rangle + \delta\psi_i \ . \tag{6}$$

Correspondingly H can be decomposed into three terms:

$$H = H_{\mathrm{eff}} + H_1 + H_2 \ , \tag{7}$$

where

$$H_{\mathrm{eff}} \equiv \sum_i H_{\mathrm{eff}}^{(i)} = (U/2) \sum_i n_i^2 - \tfrac{1}{2} \sum_i (\psi_i h_i^* + \text{c.c.}) \ , \tag{8}$$

$$H_1 = \tfrac{1}{4} \sum_i (\langle \psi_i \rangle h_i^* + \text{c.c.}) \ , \tag{9}$$

$$H_2 = -\tfrac{1}{2} \sum_{\langle i,j \rangle} J_{ij} [\delta\psi_i \delta\psi_j^* \exp(-iA_{ij}) + \text{c.c.}] \ , \tag{10}$$

and the effective field h_i is defined by

$$h_i = \sum_j J_{ij} \langle \psi_j \rangle \exp(iA_{ij}) \ . \tag{11}$$

The mean-field approximation consists in replacing H_2 by $\overline{H}_2$. Since $\overline{H}_2$ is now a c-number, H is a sum of one-body operators. Its eigenfunctions are therefore products of one-body eigenfunctions and the canonical averages of any operator are easily computed. For example, $\langle \psi_i \rangle$ is an average of a one-body operator, and therefore, in the mean-field approximation, involves only one-body eigenfunctions:

$$\langle \psi_i \rangle = \overline{\psi}_i \equiv \sum_m \exp(-E_m^{(i)}/k_B T) \langle m_i | \exp(i\phi_i) | m_i \rangle / \sum_m \exp(-E_m^{(i)}/k_B T) \ , \tag{12}$$

where $E_m^{(i)}$ and $|\ m_i\rangle$ satisfy the Schrödinger equation

$$H_{\mathrm{eff}}^{(i)} |\ m_i\rangle = E_m^{(i)} |\ m_i\rangle \ . \tag{13}$$

Note that both H_1 and $\overline{H}_2$, being c numbers, are irrelevant to the averaging procedure, i.e., they appear in both the numerator and denominator of (12) and cancel out.

Equations (12) and (13) are self-consistent equations for

the order parameters $\langle \psi_i \rangle$. These equations represent N complex equations (or $2N$ real equations) which must be solved for the complex order parameters of a Josephson junction array containing N coupled grains. In principle, the equations may be solved for disordered as well as ordered arrays, the disorder arising either from variable grain size (corresponding to random values of U_i) or variable coupling (random J_{ij}'s).

The eigenfunctions and eigenvalues of $H_{\rm eff}^{(i)}$ can be found by using the canonically conjugate relation between the number operator and the phase:

$$n_i = -2id/d\phi_i \ , \tag{14}$$

where the factor of two is present because n_i refers to the number of electrons, whereas it is the Cooper pair-number operator which is canonically conjugate to the phase. With this relation, $H_{\rm eff}^{(i)}$ takes the form

$$H_{\rm eff}^{(i)} = -2U_i d^2/d\phi_i^2 - \sum_{j\,(\neq i)} J_{ij}\{\cos\phi_i \langle \cos(\phi_j + A_{ij})\rangle + \sin\phi_i \langle \sin(\phi_j + A_{ij})\rangle\} \ . \tag{15}$$

The effective Schrödinger equation (13) can now be transformed into Mathieu's equation,

$$d^2y/dx^2 + [2q\cos(2x) + e]y = 0 \tag{16}$$

with the identifications

$$y = \psi_m^{(i)} \equiv \langle \phi_i \mid m_i \rangle, \ e = 2E_m^{(i)}/U_i,$$

$$x = \phi_i/2 - \tfrac{1}{2}\tan^{-1}(b_i/a_i) \ ,$$

and

$$q = (a_i^2 + b_i^2)^{1/2} \ ,$$

where

$$a_i = (1/U_i) \sum_{j(\neq i)} J_{ij} \langle \cos(\phi_i + A_{ij})\rangle \ ,$$

$$b_i = (1/U_i) \sum_{j(\neq i)} J_{ij} \langle \sin(\phi_i + A_{ij})\rangle \ . \tag{17}$$

The solutions of Eq. (16) are standard.[29] Two classes of solutions exist, depending on whether $y(x)$ has period π or 2π. Since ϕ_i is the phase of a Cooper-pair wave function, we demand that $\psi_m^{(i)}$ be 2π-periodic in ϕ_i and hence that y be π-periodic in x.

We pause to comment that Simanek[15] has studied solutions to Eq. (16) in zero field using 4π-periodic wave functions $\psi_m^{(i)}$ as well as others. He justifies the inclusion of these solutions in the quantum-statistical averages on the grounds that the existence of vortices and the phenomenon of phase slippage imply that ϕ_i is not restricted to the range between 0 and 2π but must be allowed to take on all values. We note, however, that the Cooper-pair number operator $n_i/2$, when applied to 4π-periodic wave functions, yields half-integer eigenvalues, i.e., fractional numbers of Cooper pairs. Since our original Hamiltonian (1) is only intended to describe the tunneling of Cooper pairs between grains, and does not take into account the effects of pair-breaking, only eigenfunctions which are 2π periodic in ϕ_i are physically relevant. As for the supposed omission of vortices from this formalism when only 2π-periodic wave functions are included, the vortices are described, not by the gauge-dependent phase ϕ_i but by the gauge-independent sum $\sum(\phi_i - \phi_j - A_{ij})$ around some closed loop. This sum can take on all values even when the phases ϕ_i are restricted.

The inclusion of 4π-periodic solutions would be justified only if we were to incorporate the effects of pair-breaking and normal electron tunneling in the Hamiltonian (1). The extra terms would greatly complicate the task of finding the partition function. By limiting our considerations to the subspace containing integer numbers of Cooper pairs, and hence 2π-periodic solutions, we find no reentrant transitions, as described below.

III. RESULTS

Using the mean-field equations and the solutions of the Mathieu's equation defined above, we can now calculate the transition temperature $T_c(B,U)$, defined as the highest temperature such that $\langle \psi_i \rangle$ takes on a nonzero value. The calculation is done by linearizing the coupled equations (12)—(17) in q, the amplitude of the effective potential in Mathieu's equation; this potential is small near T_c. The self-consistent equations then become (for the case where all the U_i's are identical)

$$\langle \cos\phi_i \rangle = a_i G(k_B T_c/U)/[2k_B T_c/U] \ ,$$

$$\langle \sin\phi_i \rangle = b_i G(k_B T_c/U)/[2k_B T_c/U] \ , \tag{18}$$

where $T_c \equiv T_c(B,U)$, and

$$G(x) = S_1/S_2 \ ,$$

$$S_1 = x\{1 - 2\sum_{m=1}^{\infty} [\exp(-2m^2/x)/(4m^2-1)]\} \ ,$$

$$S_2 = 1 + 2\sum_{m=1}^{\infty} \exp(-2m^2/x) \ . \tag{19}$$

Note that $G(x)$ has the limiting behavior $G(x)\to 1$ as $x\to\infty$; $G(x)\to x$ as $x\to 0$. In general, to obtain T_c as a function of U and B from these equations, (18) must be solved numerically for the array under consideration. The function $G(k_B T_c/U)/k_B T_c$ will then be obtained from the solution of the determinantal equation associated with (19). The relation

$$T_c(B,U)/T_c(B,0) = G(k_B T_c(B,U)/U) \tag{20}$$

holds for any array at any field B, even one with disorder in the coupling strengths (but not for one with disorder in the charging energies). At a critical value $U_c(B) = k_B T_c(B,0)$, $T_c(B,U_c) = 0$. For stronger values of U_c, no superconducting transition occurs. Since $T_c(B,0)$ is a function of magnetic field, it is possible to go from the normal to the superconducting state, at fixed value of the charging energy U, by varying the field. The function $G(x)$ determining this variation is plotted in Fig. 1. The zero-field version of (20) was first found by Imry and Strongin,[20] who also include only 2π-periodic functions.

In order to make these results more concrete, we now specialize to a square lattice with nearest-neighbor couplings J only. In this case, the transition temperature at any U is a periodic function of $f = Ba^2/\phi_0$, where a is the lattice spacing and $\phi_0 = hc/2e$ is the superconducting flux

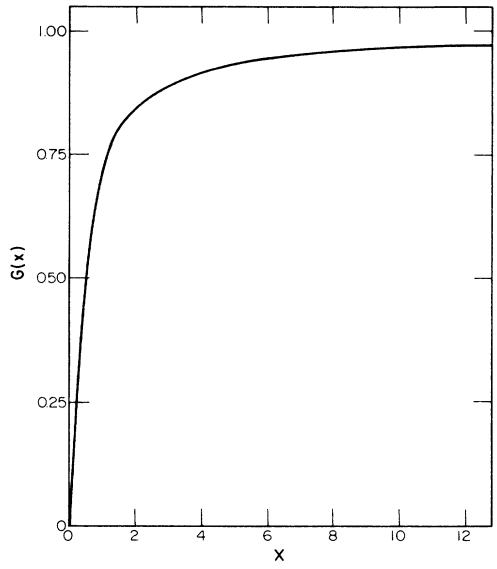

FIG. 1. Variation of the function $G(x)$ with x. $G(x)$ is defined in Eq. (19).

quantum. Shih and Stroud[22] have used mean-field theory to calculate $T_c(f,0)$ for several rational fractions $f=p/q$ by imposing periodic boundary conditions on a unit cell of length nq, where $n>1$ is any integer. Since order-parameter configurations and transition temperatures are numerically found to be independent of n, they take $n=1$. The results for $k_BT_c(f,0)/J$ are reproduced in Fig. 2.

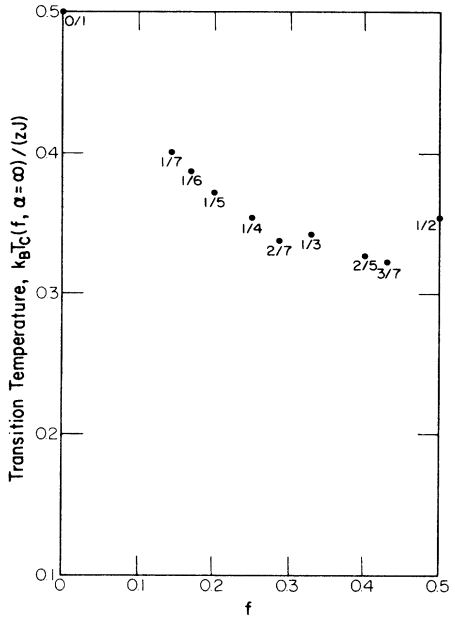

FIG. 2. Transition temperature $k_BT_c(f,\alpha=\infty)/(zJ)$ for various values of the flux per plaquette $f=\Phi/(hc/2e)$, as calculated by the mean-field theory of Ref. 22 for a square lattice. The values of k_BT_c are symmetric about $f=\frac{1}{2}$. $\alpha=zJ/U$, where J is the Josephson coupling energy and U the charging energy, and $z=4$ is the number of nearest neighbors.

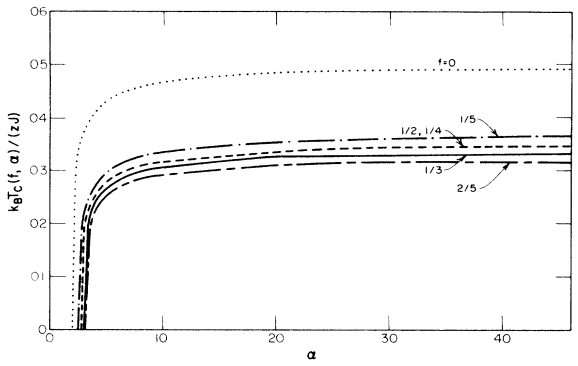

FIG. 3. Normalized transition temperature $k_BT_c(f,\alpha)/(zJ)$ for various values of f as a function of $\alpha=zJ/U$. Other symbols as in Fig. 2.

In order to extend these results to finite U, we introduce the dimensionless parameter $\alpha=4J/U$ to measure the charging energy. From Eq. (20) we find for any f that when $\alpha<\alpha_c=4J/k_BT_c(f,\alpha=\infty)$, the superconducting state is destroyed. This mean-field estimate gives, for example, $\alpha_c=2$ when $f=0$. A plot of $k_BT_c(f,\alpha)/J$ versus α for several values of f is given in Fig. 3.

Following the method of Shih and Stroud, the full nonlinear set of equations for $\langle\exp(i\phi_i)\rangle$ can be solved numerically for $T<T_c$ by imposing periodic boundary conditions on a $q\times q$ unit cell. By minimizing the function $\sum_i(\langle\psi_i\rangle-\bar{\psi}_i)^2$, we can watch the configuration of the order parameters develop as α is decreased. Our starting configurations, for $\alpha=\infty$ were obtained from the results of Teitel and Jayaprakash and of Shih and Stroud. Using the gauge $\mathbf{A}=Bx\hat{\mathbf{y}}$, we obtain the ground-state configurations shown in Fig. 4 for $f=\frac{1}{2}$, $\frac{1}{3}$, and $\frac{1}{4}$ at two values of

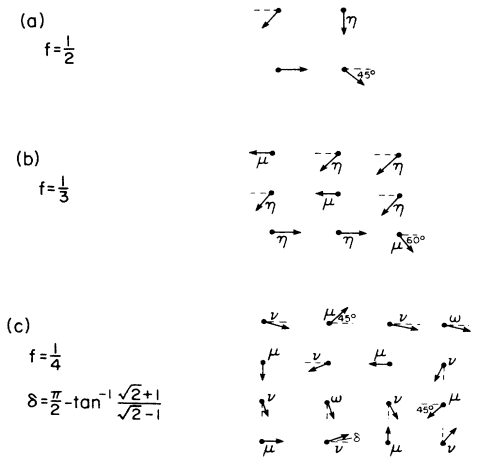

FIG. 4. Order-parameter configurations $\langle e_i^{i\phi}\rangle$ at $T=0$, for $f=\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{4}$, square lattice. (a) $f=\frac{1}{2}$. (b) $f=\frac{1}{3}$; unlabeled angles are 60°. (c) $f=\frac{1}{4}$; unlabeled angles are δ. The magnitudes of the order parameter $|\langle e^{i\phi_i}\rangle|$, given by η, μ, η, and ω in the figure, depend on α as shown in Table I; when $\alpha=\infty$ they are all unity.

α. In the limit of zero charging energy or infinite grain capacitance ($\alpha=\infty$), the "spins" all have unit magnitude at $T=0$, but the angles are the same as those found at finite α with the same value of f. The superconducting state is progressively suppressed as α is reduced, as shown, until it is destroyed at $\alpha=\alpha_c$. For intermediate values of α, the order parameters $\langle\psi_i\rangle$ in each $q\times q$ unit cell split into $q-1$ different populations (at least up to $q=4$), each group having an order parameter of different magnitude. In general, one can show from the general mean-field equations that the directions of the "spins" are independent of α although the magnitudes of the order parameter do depend on α. Various properties of the ground state are listed in Table I.

The absence of reentrant behavior is clearly demonstrated in Fig. 5, which shows the variation of the order parameter $\langle\cos\phi_i\rangle$ with temperature for various values of α, as calculated in the mean-field approximation. Note that this mean-field approximation is too simplified to yield the expected jump at $T=T_c$, $\alpha=\infty$ corresponding to the Kosterlitz-Thouless transition.

IV. VARIATIONAL FORMULATION

In order to check the consistency of this approach, we have rederived our mean-field approximation as a variational bound on the free energy. This can be done by returning to the original Hamiltonian (5) and constructing an appropriate zeroth-order Hamiltonian. The best variational choice is $H_{\rm eff}$ as defined in (8), but with the mean fields h_i now regarded as variational parameters rather than specified quantities. For any choice of the h_i's, we can decompose H as $H=H_{\rm eff}+V$. The appropriate variational principle is then based on the Gibbs-Bogolyubov inequality.[30] This inequality states that

TABLE I. Properties of order-parameter configurations at $T=0$, square lattice. The columns represent $\alpha=U/(zJ)$, where z is the number of nearest neighbors; order parameters; and ground-state energy per grain E_g/J.

		$f=\frac{1}{2}$		
α	η	E_g/J		
∞	1.000	−1.414		
100	0.9386	−1.088		
3	0.2526	−0.0027		
		$f=\frac{1}{3}$		
α	η	μ	E_g/J	
∞	1.0	1.0	−1.333	
100	0.940	0.927	−1.018	
3.5	0.435	0.340	−0.020	
		$f=\frac{1}{4}$		
α	μ	ν	ω	E_g/J
∞	1.0	1.0	1.0	−1.366
100	0.932	0.938	0.949	−1.047
3.5	0.377	0.430	0.538	−0.027

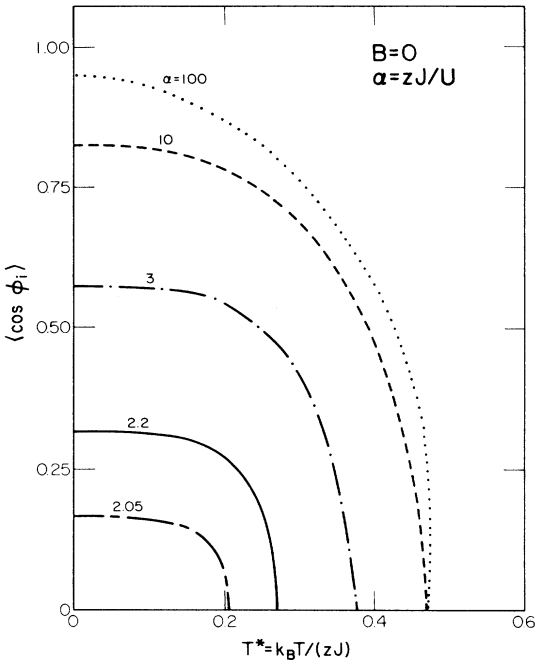

FIG. 5. Variation of the order parameter $\langle\cos\phi_i\rangle$ with temperature $T^*=k_BT/(zJ)$ for various values of $\alpha=zJ/U$, as calculated in the mean-field approximation for a square lattice with no applied field.

$$F\le F_0+\overline{V}\,, \tag{21}$$

where F_0 is the Helmholtz free energy corresponding to $H_{\rm eff}$ and $\overline{V}$ is the quantum-statistical expectation value of the perturbation, $H-H_{\rm eff}$, with respect to the canonical ensemble defined by $H_{\rm eff}$. Since $H_{\rm eff}$ is a sum of single-particle operators, its eigenstates are calculable from solutions to Mathieu's equation, as above. The expectation value $\overline{V}$ is likewise calculable and the right-hand side of (21) can be minimized. The resulting self-consistent equations are the same as those obtained in Sec. II. The advantage of this formulation, however, is that it shows that the self-consistent solutions are indeed at least local minima of the free energy.

V. SUMMARY

We have described a mean-field theory for a Josephson junction array in a magnetic field, including the effects of finite capacitance. We find that, above a critical, field-dependent value of the capacitive energy U, the superconductive state is destroyed. The field dependence of U_c allows the possibility of superconductor-normal transitions at fixed temperature as a function of field.

We have also obtained the ground-state configurations for a square lattice at various values of the applied field and at finite capacitance. We find that, while the directions of the effective spins (defined by the ratio of averages $\langle\sin\phi_i\rangle/\langle\cos\phi_i\rangle$) are independent of capacitance, the magnitudes of the order parameters are reduced. This reduction reflects the fact that, at finite capacitance, the

phases of the superconducting order parameters do not point in fixed directions at $T=0$, but rather, because of quantum-mechanical fluctuations, oscillate about preferred directions. These oscillations grow in amplitude until, at the critical capacitance (which varies with field), the oscillations become unstable and superconductivity is destroyed.

It is of interest, finally, to compare our results with other recent work on the behavior of superconducting arrays in the presence of finite charging energies. The quantum Monte Carlo calculations of Jose and collaborators,[21] who predict a superconductor-to-superconductor phase transition at certain values of the ration U/J, are obviously much more accurate, in principle, than our mean-field approach, which gives no such transition. Nevertheless, their method is extremely difficult to use at finite magnetic field, and the present approach, which gives reasonable results, may serve as a guide for future quantum Monte Carlo calculations.

The nonmonotonic behavior of our results in a magnetic field is quite intriguing. Various Monte Carlo and analytic studies suggest that the superconducting transition (with no charging energy) is not only nonmonotonic with field, but is, in fact, suppressed to very low temperatures except at a few magnetic fields corresponding to low-order rational fractions of a flux quantum per lattice cell (flux p/q of a flux quantum, with p and q small integers). Experimentally, there is little evidence of such suppression. We speculate that an additional effect must be included to explain this lack of suppression, namely, quantum dissipation.[31] Such dissipation was recently invoked by Chakravarty *et al.*[32] to explain certain universal features of phase transitions of disordered granular superconductors in the absence of a magnetic field. One can readily add a magnetic field to the formalism of Chakravarty *et al.*, and the resulting action can be variationally estimated using a mean-field approach such as that given here. We hope to include such dissipation in a subsequent paper.

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