Coupled-cluster expansions for the self-charging model of a Josephson junction chain

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The critical behavior of the self-charging model of a chain of Josephson junctions is studied by the coupled-cluster expansion method. It is shown that the system displays a Kosterlitz-Thouless transition, and the critical point as well as the critical parameters are determined. The results agree reasonably well with those obtained by other methods. [S0163-1829(97)01117-X]

I. INTRODUCTION

The coupled-cluster expansions with the eigenvalue equations truncated according to the continuum limit have proved to be efficient in investigating the ground state, mass gaps, and scaling behavior of lattice gauge theory[1,2] and the O(3) nonlinear σ model on lattice.[3]

In this paper, we study the critical behavior of the self-charging model of chains of Josephson junctions[4] by the coupled-cluster expansions method. Our purpose is to demonstrate the effectiveness of our method in phase transitions with an essential singularity of correlation length so as to provide a technique to analyze the scaling behavior near the critical point. Calculations were done for the mass gaps up to tenth-order approximation. It is shown that the system displays a Kosterlitz-Thouless (KT) transition. The critical point as well as the critical parameters are determined, and the results agree reasonably well with that obtained by other methods.[5–13]

This paper is organized as follows. Section II contains a description of the Hamiltonian of the self-charging model of Josephson junction chains, and the truncated eigenvalue equations. In Sec. III, expressions are derived from these truncated eigenvalue equations for the ground state wave function and mass gaps. Finally, in Sec. IV, we give a discussion of the results and the conclusions.

II. THE HAMILTONIAN AND THE TRUNCATED EIGENVALUE EQUATIONS

We consider a linear array with lattice spacing a of N superconducting grains embedded in an insulator.[4] The ith grain is described by a superconducting order parameter $\psi_i \equiv |\psi| e^{i\phi}$ and contain n_i Cooper pairs of charge $2e$. The ith and jth grains are coupled by a Josephson junction with critical current I_0. Even if at some low temperature the individual islands of the array are superconducting, it may require still lower temperature for the global phase coherence to establish across the whole array. It is interesting to predict the critical behavior and the phase transition of the array.

In the self-charging model, the behavior of the array is approximated by the following Hamiltonian:[4]

$$H=\alpha_0 \sum_i n_i^2 - 2J_0 \sum_i \cos(\phi_{i+1}-\phi_i), \quad \text{with } [n_i,\phi_i]=-i\delta_{ij}, \tag{1}$$

where n_i is the number operator for excess Cooper pairs on the ith grain and α_0 is, in general, related to the inverse of the capacitance of assembly of grains. The second term is specified by the Josephson coupling energy $J_0=\hbar I_0/e$, here J_0 is assumed to be the same for all nearest-neighbor pairs of grains $\langle ij \rangle$.

The Hamiltonian (1) has been studied by strong-coupling expansions,[5] mean-field theory,[6] the variational method,[7,11] and the equivalent partition function method.[4]

It is well known that the Hamiltonian (1) is the lattice version of the $(1+1)$-dimensional $O(2)$ nonlinear σ model,[7] which is defined by the following action:

$$S=\frac{1}{2g^2}\int \Delta\vec{\phi}\cdot\Delta\vec{\phi}\,dx\,dt \quad \text{with } \vec{\phi}\cdot\vec{\phi}=1, \tag{2}$$

where $\vec{\phi}$ is a two-component field. The action (2) on a discrete space-time lattice can be approximated as

$$S=-\frac{1}{g^2}\sum_i \left\{ \frac{\delta x}{\delta t}\vec{\phi}_i\cdot\vec{\phi}_{i+\hat{t}} + \frac{\delta t}{\delta x}\vec{\phi}_i\cdot\vec{\phi}_{i+\hat{x}} \right\}, \tag{3}$$

where δx and δt are the spacings in the space and time directions, respectively. An inessential constant has been dropped in Eq. (3). If we take $\delta t=\delta x$, then the lattice theory is now equivalent to the statistical mechanical problem of two-component spins interacting via nearest-neighbor coupling on a two-dimensional lattice, i.e., the two-dimensional XY model

$$H=-J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j=-J\sum_{\langle ij\rangle}\cos(\phi_i-\phi_j). \tag{4}$$

The two-dimensional XY model is conjectured to experience a KT phase transition,[8] characterized by a very weak singularity in the free energy and an exponential divergence of the correlation length ξ at a finit β, i.e.,

$$\xi \sim \exp\left(\frac{b}{\tau^{\sigma}}\right), \tag{5}$$

with $0<\tau \equiv 1-\beta/\beta_c \ll 1$, $\sigma=1/2$, and $b \simeq 1.5$.

The critical behavior of the two-dimensional XY model has long been studied numerically by Monte Carlo (MC) simulations,[7] by high-temperature expansions,[9] and by renormalization group methods.[10] All these studies have produced increasing accurate verifications of the KT transition. However, another method, the coupled-cluster expansion truncated according to the continuum limit for calculating the mass gap and the scaling behavior of the Hamiltonian (1) may still be valuable.

Before studying the one-dimensional chain with the Hamiltonian (1), we first discuss its relation with the physically interesting two-dimensional case. There exist comprehensive recent reviews on the two-dimensional Josephson junction arrays with charging effects.[14,15] The two-dimensional arrays display interesting physics, such as the KT phase transition caused by vortices, the charge unbinding phase transition, charge-vortex duality, Aharonov-Casher effects, etc. In the critical region, the Hamiltonian (1) for the one-dimensional chain with a charging effect is equivalent to the ''classical'' two-dimensional arrays without the charging term, i.e., the Hamiltonian (4). We will show, by explicit calculation of the energy gap of the Hamiltonian (1), that the system displays a phase transition at some critical value of J_0/α_0 caused by competition between charge order and phase order. This phase transition corresponds to the KT phase transition of the ''classical'' two-dimensional arrays. We will leave the more interesting two-dimensional Josephson junction arrays with charging effects for future investigation.

We now calculate the mass gap of the Hamiltonian (1) using the coupled-cluster expansion. Defining $U_i=e^{i\phi_i}$ and $E_i=n_i$ for convenience, the Hamiltonian (1) is

$$H=\alpha_0 \sum_i E_i^2 - J_0 \sum_i (U_i U_{i+1}^{+} + U_i^{+} U_{i+1}), \tag{6}$$

$$W \equiv \frac{H}{\alpha_0} = \sum_i E_i^2 - \frac{1}{g^4} \sum_i (U_i U_{i+1}^{+} + U_i^{+} U_{i+1}),$$

$$\text{with } \frac{1}{g^4} = \frac{J_0}{\alpha_0} \equiv Q^2, \tag{7}$$

$$[E_i, U_j] = U_j \delta_{ij}, \quad [E_i, U_j^{+}] = -U_j^{+} \delta_{ij}. \tag{8}$$

The Hamiltonian (6) with the commutators (8) is very similar to that of U(1) lattice gauge Hamiltonian formalism[2] except that the site variable E_i replaces the link variable E_l, and the link term $U_i U_{i+1}^{+}$ replaces the plaquette term U_p. So the calculations of the mass gap of Eq. (6) are similar to that in Ref. 2. We shall restrict our calculations to the case of zero temperature, $T=0$.

Let us start with a ground state of the form

$$|\psi_0\rangle = e^{R}|0\rangle, \tag{9}$$

where $|0\rangle$ is the bare vacuum satisfying

$$E_i|0\rangle = 0. \tag{10}$$

R is a functon of coupled clusters. The state $|\psi_0\rangle$ satifies the Schrödinger equation

$$W|\psi_0\rangle = w_0|\psi_0\rangle. \tag{11}$$

Substituting Eq. (9) into Eq. (11), we find

$$[E_i,[E_i,R]] + [E_i,R][E_i,R] - \frac{2}{g^4} G_1 = w_0, \tag{12}$$

where the repeated index i implies a summation over all lattice space sites i, and

$$G_1 = \frac{1}{2} \sum_i (U_i U_{i+1}^{+} + U_i^{+} U_{i+1}) \equiv (1,\overline{1}). \tag{13}$$

Defining the order of clusters in the same way as in Refs. 1–3, we expand R as a series of clusters which are the various combinations of U_i with the same symmetry as the ground state

$$R = R_1 + R_2 + R_3 + \cdots, \tag{14}$$

and choose

$$R_1 = c_1 G_1, \tag{15}$$

where c_1 is a coefficient to be determined. The first-order cluster G_1 is the simplest cluster with the symmetry as the vacuum. The term $[E_i,[E_i,G_1]]$ will not produce new clusters

$$[E_i,[E_i,G_1]] = 2G_1, \tag{16}$$

while the term $[E_i,G_1][E_i,G_1]$ will produce new clusters

$$[E_i,G_1][E_i,G_1] = -1 + G_{2,1} - G_{2,2} + G_{2,3}, \tag{17}$$

where

$$G_{2,1} = \frac{1}{2} \sum_k (U_k^2 U_{k+1}^{+2} + U_K^{+2} U_{k+1}^2) \equiv (2,\overline{2}),$$

$$G_{2,2} = \frac{1}{2} \sum_k (U_k U_{k+2}^{+} + U_K^{+} U_{k+2}) \equiv (1,0,\overline{1}),$$

$$G_{2,3} = \frac{1}{2} \sum_k (U_k U_{k+1}^{+2} U_{k+2} + U_K^{+} U_{k+1}^2 U_{k+2}^{+}) \equiv (1,\overline{2,1}). \tag{18}$$

We define these three new clusters as the second-order clusters. We denote a cluster as $G_{n,j}$, where n represent the order and j the serial number of the cluster. Thus R_2 can be written as

$$R_2 = c_{2,1} G_{2,1} + c_{2,2} G_{2,2} + c_{2,3} G_{2,3} = \sum_{j=1}^{3} c_{2,j} G_{2,j}, \tag{19}$$

where $c_{2,j}$ $(j=1,2,3)$ are coefficients to be determined. The terms $[E_i,G_1][E_i,G_{2,j}](j=1,2,3)$ will produce more new clusters which are different from those in R_1 and R_2. They are defined as third-order clusters.

In general,

$$[E_i,R_n][E_i,R_m]=(n+m)\text{th clusters}+\text{lower order clusters}. \tag{20}$$

It has been shown in Ref. 1 that we can make a truncation scheme , which preserves the continuum limit by computing $[E_i,R_n][E_i,R_m]$ only for $n+m\leqslant M$ in Eq. (12), so that no clusters with order higher than M are produced. In this truncation scheme, the Mth-order truncated eigenvalue equation of the vacuum state is

$$\sum_{n=1}^{M}[E_i,[E_i,R_n]]+\sum_{n+m=2}^{M}[E_i,R_n][E_i,R_m]-\frac{2}{g^4}G_1=w_0, \tag{21}$$

with

$$R=R_1+R_2+\cdots+R_M. \tag{22}$$

Next, let us consider the mass gaps. An excited state can be represented by

$$|\psi_F\rangle=F(U)|\psi_0\rangle=F(U)e^R|0\rangle, \tag{23}$$

which satisfies the equation

$$W|\psi_F\rangle=w_F|\psi_F\rangle, \tag{24}$$

where $F(U)$ is a function of U_i with appropriate symmetry so as to make $|\psi_F\rangle$ possessing the required quantum numbers. The expansion of F in terms of coupled clusters up to Mth order is

$$F=F_1+F_2+\cdots+F_M. \tag{25}$$

The Mth-order truncated eigenvalue equation for the $|\psi_F\rangle$ in the scheme preserving the continuum limit is

$$\sum_{n=1}^{M}[E_i,[E_i,F_n]]+\sum_{n+m=2}^{M}2[E_i,F_n][E_i,R_m]=w_{F0}\sum_{n=1}^{M}F_n, \tag{26}$$

$$w_{F0}=w_F-w_0. \tag{27}$$

We do the calculation for the antisymmetric and symmetric lowest-lying excited states of the model under a parity transformation, denoted by m_A and m_s, respectively. The lowest order term F_1 in expansion (25) is

$$S_1=s_1G_1 \quad \text{for } m_s$$

and

$$A_1=a_1\cdot\frac{1}{2}\sum_i\,(U_iU_{i+1}^{+}-U_i^{+}U_{i+1}) \quad \text{for } m_A, \tag{28}$$

where s_1 and a_1 are coefficients to be determined. Higher order terms can be produced in the same way as in the case of the vacuum state.

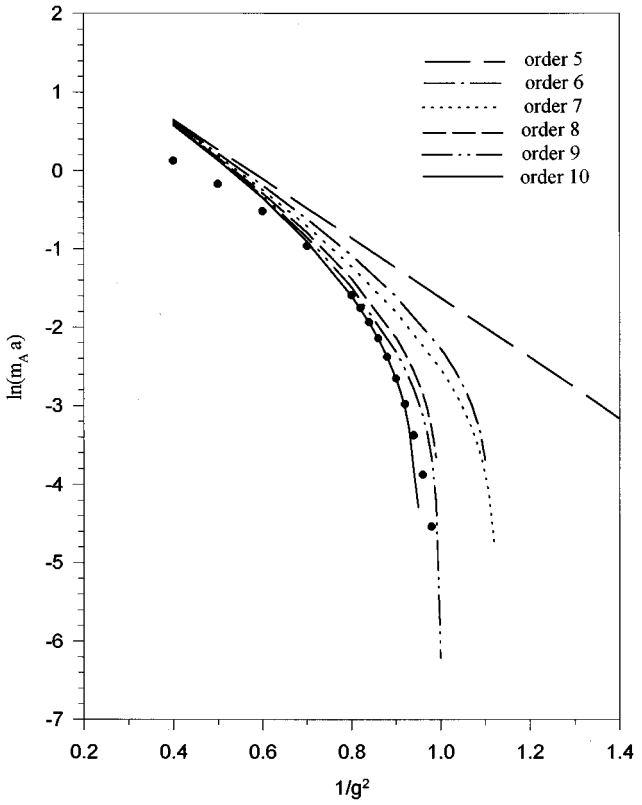

FIG. 1. Calculated values of $\ln(m_Aa)$ vs $1/g^2$. The plot composed of solid circles is the fitting of Eq. (30) to the tenth-order curve.

III. CALCULATION OF THE VACUUM WAVE FUNCTION AND MASS GAPS

To compute the mass gaps, we must first determine the vacuum state. The left-hand side of Eq. (21) can be expressed as a linear combinaton of clusters with order $1\sim M$. All those clusters are independent from one another. Therefore, the coefficient of each cluster in both sides of Eq. (21) should be equal to each other. This led to a system of nonlinear equations for $\{c_{n,j},\ n=1,2,\ldots,M\}$. Solving these equations, we get the coefficients of the Mth order expansion of R, and hence the state $e^R|0\rangle$. After obtaining the vacuum wave function, we determine the mass gaps by solving the eigenvalue equation (26). Generally, there are many solutions when the order M is larger than three, we take the smallest non-negative real number as the value of w_{F0} in Eq. (26). The mass gap is $ma=(g^2/2a)w_{F0}$.

We carry out the calculation for $M=3,4,5,6,7,8,9,10$. The larger M is, the more the number of independent clusters increases as the order rises. For example, the number of indepedent clusters for the vacuum state is 10 for $M=3$, and 30 for $M=4$, but 7355 for $M=9$. The plots of $\ln(m_Aa)$ and $\ln(m_sa)$ against $1/g^2$ with $M\geqslant 5$ are presented in Fig. 1 and Fig. 2, respectively. The results with $M\geqslant 6$ show that the system displays a clear phase transition. Since the curves apparently exhibit the trend of convegence as the order is increasing, we think the results are meaningful and the tenth-order results can be taken as good approximations to the mass gap.

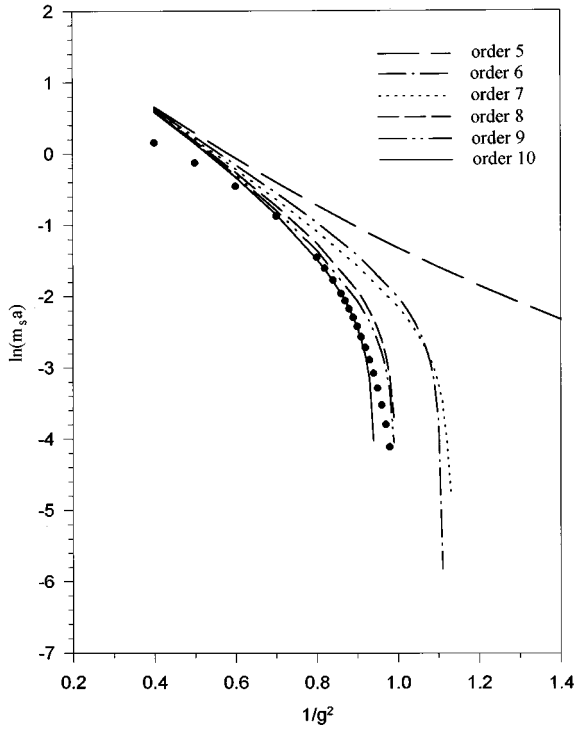

FIG. 2. The mass gap $\ln(m_s a)$ vs $1/g^2$. The plot with solid circles is the fitting of Eq. (30) to the tenth-order curve.

Both tenth-order results of m_A and m_s show a phase transition at

$$\frac{1}{g_c^2} \sim 1. \tag{29}$$

Near the phase transition point, the mass gaps exhibit essential singularities characterized by[4,8]

$$ma \simeq c \exp\left\{ -\frac{b}{(g^2 - g_c^2)^{\sigma}} \right\}. \tag{30}$$

The values of Q_c, σ, b, and c determined by fitting Eq. (30) to the tenth curve in Fig. 1 are

$$Q_c = \frac{1}{g_c^2} = 1.0641, \quad \sigma = 0.4928, \quad b = 1.7551, \quad \ln\ c = 1.5372, \tag{31}$$

and to the tenth curve in Fig. 2 are

$$Q_c = \frac{1}{g_c^2} = 1.064, \quad \sigma = 0.467, \quad b = 1.755, \quad \ln c = 1.578, \tag{32}$$

We have plotted the results of Eq. (30) with its parameters taking the values in Eq. (31) and Eq. (32) in Fig. 1 and Fig. 2, respectively. The fit for m_A is quite well up to correlation length $\xi \simeq 40$.

The results in Eq. (31) differ slightly from those in Eq. (32). It is because the mass of m_s is larger than that of m_A. Generally, the larger the mass gap is, the more complicated and larger coupled clusters are needed to obtain results with the same accuracy. Therefore, the results for the critical point and the critical exponent in Eq. (31) are more reliable.

IV. CONCLUSIONS AND DISCUSSION

By using the coupled-cluster expansion with the eigenvalue equations truncated according to the continuum limit, we have shown that, at $T=0$, the self-charging model of Josephson junction chains has a KT transition at $Q_c \simeq 1.064$, and the critical exponent $\sigma \simeq 0.493$. The chain is superconducting for $Q \geqslant Q_c$, and is insulating for $Q < Q_c$, and the correlation length is exponential devergent near the critical point Q_c. The result is not surprising, because $Q < Q_c$ means the Coulomb coupling between the grains in the chain is strong enough comparing to the Josephson coupling even at zero temperature. The transition to a superconducting state can be suppressed entirely in favor of an insulating state in which there is an energy gap (mass gap) for transfer of charge between grains.

It is interesting to compare our results with those of other works. The variational calculation by Kampf and Schön[11] gives $Q_c = 0.725$ and the mean-field theory[6] gives $Q_c = 0.5$, but does not give the critical behavior of the correlation length. The analytic method gives[8] $Q_c = 1.11$. A recent MC simulation also gives this result.[13]

Bradly and Doniach[4] found that the self-charging model of the Josephson junction chain is equivalent to the isotropic two-dimensional XY model with coupling constant $(J_0/\alpha_0)^{1/2}$ and lattice constant a, if $\alpha_0 \ll \Delta$ and $J_0 \ll \Delta$, where Δ is the superconducting energy gap at $T=0$. They then conclude that the system has a KT transition at $Q_c = 1.11$, which is well known for the two-dimensional XY model. All previous investigations on the critical exponent and critical point refer to the two-dimensional XY model. On the other hand, in our method, there is no such restriction for the value of α_0 and J_0, and the critical behavior of the KT transition is naturally derived in the Hamiltonian formulation.

It is known that the critical coupling constant Q_c depends on regulation schemes while the critical exponent such as σ is independent of the schemes. For example, in Ref. 12, the strong-coupled expansion was used to study the lattice XY model in action formulation. When the lattice is square, triangular, and honeycomb, the value of Q_c is about 1.11, 0.67, and 1.44, respectively. Since the lattice Hamiltonian formulation and the action formulation are two different regulation schemes,[16] our result of Q_c is not unreasonable.

Besides the antisymmetric mass gap m_A which is related to the inverse correlation length of the two-dimensional XY model, we have also calculated the symmetric mass gap m_s. Near the critical point, m_s shows the same behavior as m_A. This provides further evidence for the scaling characteristics of the system near its critical point. The results of this paper also show that the coupled-cluster expansion with appropriate truncaton scheme is effective for studying the critical behavior of physical systems with phase transitions.

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