Long-range order and phase transition in a cooperative Jahn-Teller system

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We have studied the long range order and phase transition in a simple cooperative Jahn-Teller system and show that, as a result of the competition between the intrasite pseudospin tunneling and the phonon-induced intersite pseudospin correlation, a phase transition to the pseudospin long range ordering phase may occur at some critical temperature. An approach, based on a **k**-dependent displacement transformation and then treating the transformed Hamiltonian in perturbation theory, has been proposed to deal with the nonadiabaticity and the retardation effect of the pseudospin-phonon interaction. The approach leads to correct results in both the adiabatic and antiadiabatic limits, as well as a smooth crossover between the limits. It has been pointed out that when phonon frequency is small compared with the intrasite tunneling or the pseudospin-phonon coupling the retardation effect of the pseudospin-phonon interaction is quite important.

I. INTRODUCTION

To understand the mechanism of cooperative phenomena, such as the phase transition and long range ordering, in systems with competing interactions at a microscopic level has been a subject of great interest for many years. Among these systems we mention ferroelectricity (antiferroelectricity),[1–5] conventional superconductors,[6] and structural transformations where the electron-lattice interaction (vibronic interaction) plays an important role.[7–9] The electron-lattice interaction in the case of non-Kramers degeneracy (pseudo-degeneracy) of the electron subsystem is often called the cooperative Jahn-Teller effect[8] and physical properties of the system depend heavily on the nonadiabaticity and the retardation effect of vibronic interaction.

In this work we consider a simple model Hamiltonian of pseudospins interacting with lattice

$$H=-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^{x}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}\left(b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+\frac{1}{2}\right)+\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}g_{\mathbf{k}}\sigma_{\mathbf{j}}^{z}(b_{-\mathbf{k}}^{\dagger}+b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}, \tag{1}$$

which may be the simplest one for the vibronic interaction and the cooperative Jahn-Teller effect. In Eq. (1) N is the number of pseudospins. $\sigma_{\mathbf{j}}^{x}$ and $\sigma_{\mathbf{j}}^{z}$ are the Pauli matrices on site $\mathbf{j}$ with bare tunneling matrix element Δ. $b_{\mathbf{k}}^{\dagger}$ and $b_{\mathbf{k}}$ are the creation and annihilation operators of phonon mode with frequency $\omega_{\mathbf{k}}$. $g_{\mathbf{k}}^{2}=(\alpha/2)\omega_0^2/\omega_{\mathbf{k}}$ and α is the pseudospin-phonon coupling constant. We note that in this Hamiltonian the pseudospin-phonon interaction is an on-site one and the cooperation between different sites is caused by the dispersive phonons. The competing interactions are the intrasite pseudospin tunneling and the phonon-induced intersite pseudospin correlation.

We assume a three-dimensional simple cubic lattice with the phonon frequency[10]

$$\omega_{\mathbf{k}}(\pm)=\omega_0\sqrt{1-\rho(1\pm\gamma_{\mathbf{k}})/2},\quad -\pi\leqslant k_x,k_y,k_z\leqslant\pi, \tag{2}$$

where $\gamma_{\mathbf{k}}=(\cos k_x+\cos k_y+\cos k_z)/3$. ω_0 is the upper limit of phonon frequency, $\omega_0\sim\sqrt{1/M}$ where M is the reduced mass, and ρ measures the size of phonon dispersion. $\omega_{\mathbf{k}}(+)$ lattice mode may induce a ferroelectric ordering $[\omega_{\mathbf{k}}(+)=\omega_0\sqrt{1-\rho}$ at $\mathbf{k}=\mathbf{Q}=(0,0,0)]$ but $\omega_{\mathbf{k}}(-)$ an antiferroelectric ordering $[\omega_{\mathbf{k}}(-)=\omega_0\sqrt{1-\rho}$ at $\mathbf{k}=\mathbf{Q}=(\pi,\pi,\pi)]$.

This model Hamiltonian, and its modified and extended forms, have been used for various cooperative Jahn-Teller systems, such as the proton-lattice interaction in hydrogen-bonded ferroelectrics (antiferroelectrics),[1–5] the structural transformations in ferroelastic (antiferroelastic) crystals,[7–9] etc. Generally, speaking, there are two kinds of theoretical methods to treat the vibronic interactions in cooperative Jahn-Teller systems.[8] One is the displacement transformation method:[8,9] $\tilde{H}=\exp(S')H\exp(-S')$, where

$$S'=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}\frac{g_{\mathbf{k}}}{\omega_{\mathbf{k}}}\sigma_{\mathbf{j}}^{z}(b_{-\mathbf{k}}^{\dagger}-b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}. \tag{3}$$

After the transformation there appears a phonon induced long range correlation and a phonon dressed tunneling. Another is the mean field decoupling to the intersite term in Hamiltonian (1).[8] After the decoupling $H\approx\Sigma_{\mathbf{j}}H_{\mathbf{j}}$, where $H_{\mathbf{j}}$ is a single site Hamiltonian in the mean field. Then, various methods for the single site problem can be used.

In a previous work[10] we proposed a new approach with a **k**-dependent displacement transformation to the cooperative Jahn-Teller effect. In this work the same approach is to be used for studying the long range order in finite temperature and the phase transition. Before our discussions on the model Hamiltonian, we would like to show solutions of Eq. (1) in the adiabatic ($M\rightarrow\infty$) and antiadiabatic ($M\rightarrow 0$) limit. When $M\rightarrow\infty$ the kinetic energy of the lattice can be omitted and the lattice can be treated classically

$$(b_{-\mathbf{Q}}^{\dagger}+b_{\mathbf{Q}})=-\sqrt{N}\frac{2g_{\mathbf{Q}}}{\omega_{\mathbf{Q}}}\sigma_0,\quad (b_{-\mathbf{k}}^{\dagger}+b_{\mathbf{k}})=0\quad\text{for}\quad\mathbf{k}\neq\mathbf{Q}, \tag{4}$$

where $\mathbf{k}=\mathbf{Q}$ makes $g_{\mathbf{k}}^2/\omega_{\mathbf{k}}$ maximum. Then Hamiltonian (1) becomes

$$H(M\to\infty)=\frac{g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x-\sum_{\mathbf{j}}\frac{2g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0\sigma_{\mathbf{j}}^z. \tag{5}$$

It can be solved easily.

The antiadiabatic limit $M\to0$ can be treated by rewriting the Hamiltonian (1) in a functional integral formulation and integrating over the phonon degrees of freedom.[11] Let $M\to0(\omega_0\to\infty)$,

$$H(M\to0)=\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x-\frac{1}{N}\sum_{\mathbf{k}}\sum_{\mathbf{i},\mathbf{j}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}. \tag{6}$$

This is an Ising model with long range interaction in a transverse field. It cannot be solved exactly even in one dimension.[12] Throughout this paper we set $\hbar=1$ and $k_B=1$.

II. THEORETICAL ANALYSIS

First we let the $\mathbf{Q}$-mode phonon be displaced to take into account the long range phonon ordering

$$R=\sqrt{N}\frac{g_{\mathbf{Q}}}{\omega_{\mathbf{Q}}}\sigma_0(b_{-\mathbf{Q}}^\dagger-b_{\mathbf{Q}}), \tag{7}$$

$$\begin{aligned}H&=\exp(R)H\exp(-R)\\&=-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\frac{2g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0\sigma_{\mathbf{j}}^z\\&\quad+\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}g_{\mathbf{k}}[\sigma_{\mathbf{j}}^z-e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0](b_{-\mathbf{k}}^\dagger+b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}\\&\quad+\frac{g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}\sigma_0^2N,\end{aligned} \tag{8}$$

where $\mathbf{k}=\mathbf{Q}$ is the wave vector of long range ordering [$\mathbf{Q}=(0,0,0)$ for ferroelectric or $\mathbf{Q}=(\pi,\pi,\pi)$ for antiferroelectric ordering] which makes $g_{\mathbf{k}}^2/\omega_{\mathbf{k}}$ maximum.

Our treatment is based on the $\mathbf{k}$-dependent displacement transformation,[10]

$$\tilde{H}=\exp(S)H\exp(-S), \tag{9}$$

$$S=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}\frac{g_{\mathbf{k}}}{\omega_{\mathbf{k}}}\delta_{\mathbf{k}}[\sigma_{\mathbf{j}}^z-e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0](b_{-\mathbf{k}}^\dagger-b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}. \tag{10}$$

$\delta_{\mathbf{k}}$ is $\mathbf{k}$ dependent and its form will be determined later. We note that $S+R=S'$ [Eq. (3)] if $\delta_{\mathbf{k}}\equiv1$. The transformation can be done to the end and the result is

$$\tilde{H}=H_0+H_{I1}+H_{I2}, \tag{11}$$

$$H_0=-NV_0+\frac{1}{2}J_{\mathbf{Q}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\eta_0\Delta\sigma_{\mathbf{j}}^x-\sum_{\mathbf{j}}J_{\mathbf{Q}}e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0\sigma_{\mathbf{j}}^z, \tag{12}$$

$$H_{I1}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}g_{\mathbf{k}}(1-\delta_{\mathbf{k}})[\sigma_{\mathbf{j}}^z-e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0](b_{-\mathbf{k}}^\dagger+b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}-\sum_{\mathbf{j}}\eta_0\Delta i\sigma_{\mathbf{j}}^yX_{\mathbf{j}}, \tag{13}$$

$$\begin{aligned}H_{I2}=&-\frac{1}{N}\sum_{\mathbf{k}}\sum_{\mathbf{i},\mathbf{j}}\left(\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}\delta_{\mathbf{k}}(2-\delta_{\mathbf{k}})-V_0\right)[\sigma_{\mathbf{i}}^z-e^{i\mathbf{Q}\cdot\mathbf{i}}\sigma_0]\\&\times[\sigma_{\mathbf{j}}^z-e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0]e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x\{\cosh(X_{\mathbf{j}})-\eta_0\}\\&-\sum_{\mathbf{j}}\Delta i\sigma_{\mathbf{j}}^y\{\sinh(X_{\mathbf{j}})-\eta_0X_{\mathbf{j}}\},\end{aligned} \tag{14}$$

where $J_{\mathbf{Q}}=2(g_{\mathbf{Q}}^2/\omega_{\mathbf{Q}}-V_0)$,

$$X_{\mathbf{j}}=\frac{2}{\sqrt{N}}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}}{\omega_{\mathbf{k}}}\delta_{\mathbf{k}}(b_{-\mathbf{k}}^\dagger-b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}. \tag{15}$$

The last term in H_0 and the first term in H_{I2} describe a long-range Ising-type interaction between pseudospins, in which

$$V_0=\frac{1}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}\delta_{\mathbf{k}}(2-\delta_{\mathbf{k}}) \tag{16}$$

is subtracted because it represents a constant self-coupling since $\sigma_{\mathbf{j}}^z\sigma_{\mathbf{j}}^z=1$ and does not contribute to interaction between pseudospins at different sites.[4] In addition,

$$\eta_0=\exp\left(-\frac{2}{N}\sum_{\mathbf{k}}g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2/\omega_{\mathbf{k}}^2\right) \tag{17}$$

represents the phonon dressing of the bare tunneling matrix element Δ.[4,9]

We treat H_0 as the unperturbed Hamiltonian and both H_{I1} and H_{I2} the perturbation. The perturbation should be small. As is mentioned in Introduction, one of the conventional methods is to let $\delta_{\mathbf{k}}\equiv1$ for all $\mathbf{k}$ in the transformation. Thus the first term in H_{I1} is zero. However, the first order term of $g_{\mathbf{k}}$ still exists in $X_{\mathbf{j}}$. We propose the functional form of $\delta_{\mathbf{k}}$ as[10]

$$\delta_{\mathbf{k}}=\omega_{\mathbf{k}}/(\omega_{\mathbf{k}}+2J_{\mathbf{Q}}), \tag{18}$$

and the reason for this choice will be shown later. Here we show that the main physics is already contained in the unperturbed part H_0 of $\tilde{H}$ in both adiabatic and antiadiabatic limits.

When $M\rightarrow\infty(\omega_0\rightarrow 0)$, $g_{\mathbf{k}}^2/\omega_{\mathbf{k}}$ is a finite quantity but $\delta_{\mathbf{k}}$ goes to zero. Thus $V_0=0,\eta_0=1,H_{I1}=H_{I2}=0$, and

$$H_0=\frac{g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x-\sum_{\mathbf{j}}2\frac{g_{\mathbf{Q}}^2}{\omega_{\mathbf{Q}}}e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0\sigma_{\mathbf{j}}^z. \tag{19}$$

This is the same as $H(M\rightarrow\infty)$ in Eq. (5). It is evident that the order-disorder transition point is at $2g_{\mathbf{Q}}^2/\omega_{\mathbf{Q}}=\Delta$.

When $M\rightarrow 0(\omega_0\rightarrow\infty)$, $g_{\mathbf{k}}^2/\omega_{\mathbf{k}}^2=0$ and $\delta_{\mathbf{k}}\rightarrow 1$. Thus $H_{I1}=0$, $V_0=(1/N)\Sigma_{\mathbf{k}}g_{\mathbf{k}}^2/\omega_{\mathbf{k}}$, $\eta_0=1$, and

$$H_0=-NV_0+\frac{1}{2}J_{\mathbf{Q}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}\Delta\sigma_{\mathbf{j}}^x-\sum_{\mathbf{j}}J_{\mathbf{Q}}e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0\sigma_{\mathbf{j}}^z, \tag{20}$$

$$H_{I2}=-\frac{1}{N}\sum_{\mathbf{k}}\sum_{\mathbf{i,j}}\left(\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}-V_0\right)[\sigma_{\mathbf{i}}^z-e^{i\mathbf{Q}\cdot\mathbf{i}}\sigma_0]\times[\sigma_{\mathbf{j}}^z-e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0]e^{i\mathbf{k}\cdot(\mathbf{i-j})}.$$

H_0+H_{I2} is the same as $H(M\rightarrow 0)$ in Eq. (6). In the mean field approximation (the correlation H_{I2} dropped) H_0 can be solved with the order-disorder transition point at $2(g_{\mathbf{Q}}^2/\omega_{\mathbf{Q}}-V_0)=\Delta$.

As the phonon induced interaction between pseudospins is a long range one, the mean field approximation is good enough for a quantitative analysis of the properties of the system.[8,9] In the mean field approximation the unperturbed part H_0 of $\tilde{H}$ works well in both $M\rightarrow\infty$ and $M\rightarrow 0$ limits. We believe that H_0 should be a good unperturbed Hamiltonian in the intermediate region $\infty>M>0$ and H_{I1} and H_{I2} can be treated as perturbation (we shall return to this point in the last section). We note that the transformation with $\delta_{\mathbf{k}}\equiv 1$ [S' in Eq. (3)] cannot lead to the correct result in the $M\rightarrow\infty$ limit.

H_0 can be easily diagonalized since it is the molecular field approximation for pseudospins plus the free phonons. In this work we are mainly concerned with the case of $J_{\mathbf{Q}}>\eta_0\Delta$, because in this case there exists the long range ferroelectricity (antiferroelectricity). We assume $\exp(i\mathbf{Q}\cdot\mathbf{j})=\pm 1$, that is, the ferroelectric ordering $[\mathbf{Q}=(0,0,0)]$ or antiferroelectric ordering $[\mathbf{Q}=(\pi,\pi,\pi)]$. Then H_0 can be diagonalized by a unitary matrix $U=\Pi_{\mathbf{j}}U_{\mathbf{j}}$, where

$$U_{\mathbf{j}}=\begin{pmatrix}u_{\mathbf{j}} & v_{\mathbf{j}}\\ v_{\mathbf{j}} & -u_{\mathbf{j}}\end{pmatrix}, \tag{21}$$

$$u_{\mathbf{j}}=-\frac{1}{\sqrt{2}}\left[1+\frac{J_{\mathbf{Q}}\sigma_0e^{i\mathbf{Q}\cdot\mathbf{j}}}{W}\right]^{1/2}, \tag{22}$$

$$v_{\mathbf{j}}=-\frac{1}{\sqrt{2}}\left[1-\frac{J_{\mathbf{Q}}\sigma_0e^{i\mathbf{Q}\cdot\mathbf{j}}}{W}\right]^{1/2}, \tag{23}$$

$$W=[J_{\mathbf{Q}}^2\sigma_0^2+\eta_0^2\Delta^2]^{1/2}. \tag{24}$$

The diagonalized H_0 is

$$H_0'=U^\dagger H_0U=-NV_0+\frac{1}{2}J_{\mathbf{Q}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}W\sigma_{\mathbf{j}}^z. \tag{25}$$

H_{I1} is transformed as follows:

$$H_{I1}'=U^\dagger H_{I1}U$$

$$=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}g_{\mathbf{k}}(1-\delta_{\mathbf{k}})\left[\frac{J_{\mathbf{Q}}}{W}\sigma_{\mathbf{j}}^z-1\right]e^{i\mathbf{Q}\cdot\mathbf{j}}\sigma_0(b_{-\mathbf{k}}^\dagger+b_{\mathbf{k}})e^{-i\mathbf{k}\cdot\mathbf{j}}+\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\mathbf{j}}\frac{g_{\mathbf{k}}\delta_{\mathbf{k}}}{\omega_{\mathbf{k}}}\eta_0\Delta e^{-i\mathbf{k}\cdot\mathbf{j}}\left\{\left[\frac{J_{\mathbf{Q}}}{W}-1\right](\sigma_{\mathbf{j}}^+b_{\mathbf{k}}+\sigma_{\mathbf{j}}^-b_{-\mathbf{k}}^\dagger)+\left[\frac{J_{\mathbf{Q}}}{W}+1\right](\sigma_{\mathbf{j}}^+b_{-\mathbf{k}}^\dagger+\sigma_{\mathbf{j}}^-b_{\mathbf{k}})\right\}, \tag{26}$$

where the form of $\delta_{\mathbf{k}}$ [Eq. (18)] has been substituted. We can also get $H_{I2}'=U^\dagger H_{I2}U$. The thermodynamical averaging of $\sigma_{\mathbf{j}}^z$ over the unperturbed H_0' is $(\beta=1/k_BT)$

$$\langle\sigma_{\mathbf{j}}^z\rangle_0=\tanh(\beta W), \tag{27}$$

where $\langle\cdots\rangle_0$ means the thermodynamical averaging

$$\langle\cdots\rangle_0=\mathrm{Tr}[\exp(-\beta H_0')\cdots]/\mathrm{Tr}[\exp(-\beta H_0')].$$

The condition to determine σ_0 is

$$\frac{J_{\mathbf{Q}}}{W}\tanh(\beta W)=1, \tag{28}$$

which makes the thermodynamical average of the factor $(J_{\mathbf{Q}}/W)\sigma_{\mathbf{j}}^z-1$ in the first term of H_{I1}' be zero. The reason for introducing the functional form of $\delta_{\mathbf{k}}$ [Eq. (18)] is that, when $T=0(J_{\mathbf{Q}}/W=1)$, the term $\sigma_{\mathbf{j}}^+b_{\mathbf{k}}+\sigma_{\mathbf{j}}^-b_{-\mathbf{k}}^\dagger$ in H_{I1}' disappears. In addition, $(\sigma_{\mathbf{j}}^+b_{-\mathbf{k}}^\dagger+\sigma_{\mathbf{j}}^-b_{\mathbf{k}})|g_0\rangle=0$ ($|g_0\rangle$ is the ground state of H_0').

In perturbation theory, the free energy F can be calculated as follows:[13]

$$-\beta(F-F_0)=-\int_0^\beta d\tau\langle H_{I1}'(\tau)\rangle_0+\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\langle[H_{I1}'(\tau_1)H_{I1}'(\tau_2)]\rangle_0-\int_0^\beta d\tau\langle H_{I2}'(\tau)\rangle_0+O(g_{\mathbf{k}}^3), \tag{29}$$

where F_0 is the free energy of H_0',

$$F_0=-NV_0+\frac{1}{2}J_{\mathbf{Q}}\sigma_0^2N-\frac{N}{\beta}\ln[2\cosh\beta W]+\frac{1}{\beta}\sum_{\mathbf{k}}\ln[1-\exp(-\beta\omega_{\mathbf{k}})]. \tag{30}$$

$H_{I1}'(\tau)=\exp(H_0'\tau)H_{I1}'\exp(-H_0'\tau)$ is in the interaction picture.

The first order term of H'_{I1} is zero. The second term, which is the second order contribution of H'_{I1}, and the third term can be calculated as

$$F=F_0-\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}(1-\delta_{\mathbf{k}})^2[\coth^2(\beta W)-1]\sigma_0^2$$
$$-\sum_{\mathbf{k}}\frac{2g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta^2\left\{\frac{[\coth(\beta W)-1]^2}{\omega_{\mathbf{k}}+2W}\right.$$
$$\times[1+\coth(\beta\omega_{\mathbf{k}}/2)\tanh(\beta W)]+\frac{[\coth(\beta W)+1]^2}{\omega_{\mathbf{k}}-2W}$$
$$\left.\times[1-\coth(\beta\omega_{\mathbf{k}}/2)\tanh(\beta W)]\right\}$$
$$-N[\eta(T)-\eta_0]\eta_0\frac{\Delta^2}{W}\tanh(\beta W), \qquad (31)$$

$$\eta(T)=\exp\left(-\frac{2}{N}\sum_{\mathbf{k}}g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2\coth(\beta\omega_{\mathbf{k}}/2)/\omega_{\mathbf{k}}^2\right). \qquad (32)$$

In calculation the terms of order $O(g_{\mathbf{k}}^3)$ and higher are neglected. Obviously, when $T=0$ we have $F=F_0$. This is the reason for determining η_0, $\delta_{\mathbf{k}}$ and σ_0 in Eqs. (17), (18), and (28).

The order parameter

$$\langle\sigma_{\mathbf{j}}^z\rangle=\mathrm{Tr}[\exp(-\beta H)\sigma_{\mathbf{j}}^z]/\mathrm{Tr}[\exp(-\beta H)], \qquad (33)$$

where H is the original Hamiltonian, can be calculated as

$$\langle\sigma_{\mathbf{j}}^z\rangle=\frac{J_{\mathbf{Q}}\sigma_0e^{i\mathbf{Q}\cdot\mathbf{j}}}{W}\langle\sigma_{\mathbf{j}}^z\rangle'+\frac{\eta_0\Delta}{W}e^{i\mathbf{Q}\cdot\mathbf{j}}\langle e^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x\rangle'. \qquad (34)$$

Here $\langle\cdots\rangle'$ means the thermodynamical average ($H'=H'_0+H'_{I1}+H'_{I2}$)

$$\langle\cdots\rangle'=\mathrm{Tr}[\exp(-\beta H')\cdots]/\mathrm{Tr}[\exp(-\beta H')]. \qquad (35)$$

$\langle\sigma_{\mathbf{j}}^z\rangle'$ and $\langle e^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x\rangle'$ can be calculated by means of the differentiation

$$\langle\sigma_{\mathbf{j}}^z\rangle'=-\frac{\partial}{\partial h_z}F(h_z,h_x)\bigg|_{h_z=0,h_x=0},$$

$$\langle e^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x\rangle'=-\frac{\partial}{\partial h_x}F(h_z,h_x)\bigg|_{h_z=0,h_x=0}.$$

For calculating $F(h_z,h_x)$ we let

$$H'_0=-NV_0+\frac{1}{2}J_{\mathbf{Q}}\sigma_0^2N+\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}-\sum_{\mathbf{j}}(W+h_z)\sigma_{\mathbf{j}}^z$$
$$-\sum_{\mathbf{j}}h_xe^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x. \qquad (36)$$

The result is

$$\langle\sigma_{\mathbf{j}}^z\rangle=\sigma_0\left\{1-\frac{2}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}(1-\delta_{\mathbf{k}})^2\frac{\beta\sigma_0^2}{\sinh^2(\beta W)}+\frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}(1-\delta_{\mathbf{k}})^2\frac{\eta_0^2\Delta^2}{W^3\sinh(2\beta W)}\right.$$
$$+\frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta^2\frac{[\coth(\beta W)+1]^2}{\omega_{\mathbf{k}}-2W}\left[\frac{\coth(\beta W)-\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}-2W}-\frac{\beta\coth(\beta\omega_{\mathbf{k}}/2)}{\sinh(2\beta W)}\right]$$
$$-\frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta^2\frac{[\coth(\beta W)-1]^2}{\omega_{\mathbf{k}}+2W}\left[\frac{\coth(\beta W)+\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}+2W}-\frac{\beta\coth(\beta\omega_{\mathbf{k}}/2)}{\sinh(2\beta W)}\right]$$
$$-\frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\frac{\eta_0^2\Delta^2}{W^2}J_{\mathbf{Q}}\left[\frac{\coth(\beta W)+1}{\omega_{\mathbf{k}}-2W}(\coth(\beta W)-\coth(\beta\omega_{\mathbf{k}}/2))+\frac{\coth(\beta W)-1}{\omega_{\mathbf{k}}+2W}[\coth(\beta W)+\coth(\beta\omega_{\mathbf{k}}/2)]\right]$$
$$\left.+(\eta(T)-\eta_0)\eta_0\left(\frac{\Delta}{W}\right)^2\left[\frac{2\beta W}{\sinh(2\beta W)}-1\right]\right\}e^{i\mathbf{Q}\cdot\mathbf{j}}. \qquad (37)$$

When $T=0$,

$$\langle\sigma_{\mathbf{j}}^z\rangle=\sigma_0e^{i\mathbf{Q}\cdot\mathbf{j}}=[1-\eta_0^2\Delta^2/J_{\mathbf{Q}}^2]^{1/2}e^{i\mathbf{Q}\cdot\mathbf{j}}. \qquad (38)$$

This means that, for both the free energy F and order parameter $\langle\sigma_{\mathbf{j}}^z\rangle$, the second order contribution $[O(g_{\mathbf{k}}^2)]$ is zero when $T=0$.

The phase transition temperature T_c is determined by Eq. (28) with $\sigma_0=0$. The result is

$$T_c=2\eta_0\Delta/\ln\left[\frac{J_{\mathbf{Q}}+\eta_0\Delta}{J_{\mathbf{Q}}-\eta_0\Delta}\right]. \qquad (39)$$

$T_c=0$ when $J_{\mathbf{Q}}=2(g_{\mathbf{Q}}^2/\omega_{\mathbf{Q}}-V_0)\leqslant\eta_0\Delta$. From it we can get the critical coupling α_c as a function of Δ, ρ, and ω_0 (or the critical tunneling Δ as a function of α, ρ, and ω_0).

Another quantity of physical interest is the thermodynamical average of tunneling matrix $\langle\sigma_{\mathbf{j}}^x\rangle$

$$\begin{aligned}
\langle\sigma_{\mathbf{j}}^x\rangle &= \mathrm{Tr}[\exp(-\beta\tilde{H})\{\sigma_{\mathbf{j}}^x\cosh(X_{\mathbf{j}})+i\sigma_{\mathbf{j}}^y\sinh(X_{\mathbf{j}})\}]/\mathrm{Tr}[\exp(-\beta\tilde{H})]\\
&= \frac{\eta_0^2\Delta}{W}\langle\sigma_{\mathbf{j}}^z\rangle' - \frac{\eta_0 J_{\mathbf{Q}}\sigma_0}{W}\langle e^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x\rangle' + \frac{\eta_0\Delta}{W}\langle\sigma_{\mathbf{j}}^z[\cosh(X_{\mathbf{j}})-\eta_0]\rangle'\\
&\quad - \frac{J_{\mathbf{Q}}\sigma_0}{W}\langle e^{-i\mathbf{Q}\cdot\mathbf{j}}\sigma_{\mathbf{j}}^x[\cosh(X_{\mathbf{j}})-\eta_0]\rangle' - \langle i\sigma_{\mathbf{j}}^y\sinh(X_{\mathbf{j}})\rangle'\\
&= \frac{\eta_0^2\Delta}{W}\tanh(\beta W)\Bigg\{1-\frac{2}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}(1-\delta_{\mathbf{k}})^2\frac{\beta\sigma_0^2}{\sinh^2(\beta W)}\\
&\quad + \frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta^2\frac{[\coth(\beta W)+1]^2}{\omega_{\mathbf{k}}-2W}\left[\frac{\coth(\beta W)-\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}-2W}\right.\\
&\quad \left. - \frac{\beta\coth(\beta\omega_{\mathbf{k}}/2)}{\sinh(2\beta W)}\right] - \frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta^2\frac{[\coth(\beta W)-1]^2}{\omega_{\mathbf{k}}+2W}\left[\frac{\coth(\beta W)+\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}+2W} - \frac{\beta\coth(\beta\omega_{\mathbf{k}}/2)}{\sinh(2\beta W)}\right]\Bigg\}\\
&\quad - \frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}(1-\delta_{\mathbf{k}})^2\frac{\eta_0^2\Delta J_{\mathbf{Q}}\sigma_0^2}{W^3\sinh(2\beta W)} - \frac{4}{N}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}^2\delta_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2}\eta_0^2\Delta\frac{J_{\mathbf{Q}}^2\sigma_0^2}{W^2}\left[\frac{\coth(\beta W)+1}{\omega_{\mathbf{k}}-2W}[\coth(\beta W)-\coth(\beta\omega_{\mathbf{k}}/2)]\right.\\
&\quad \left. + \frac{\coth(\beta W)-1}{\omega_{\mathbf{k}}+2W}[\coth(\beta W)+\coth(\beta\omega_{\mathbf{k}}/2)]\right] + \frac{\eta_0\Delta\,\eta(T)}{\sinh(2\beta W)}\frac{8}{N}\sum_{\mathbf{k}}\left(\frac{g_{\mathbf{k}}\delta_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^2[\exp(\beta\omega_{\mathbf{k}})-1]^{-1}\\
&\quad \times\left\{\frac{\exp[\beta\omega_{\mathbf{k}}]-\exp(2\beta W)}{\omega_{\mathbf{k}}-2W} - \frac{\exp[\beta\omega_{\mathbf{k}}]-\exp(-2\beta W)}{\omega_{\mathbf{k}}+2W}\right\}\\
&\quad + (\eta(T)-\eta_0)\frac{\eta_0\Delta}{W}\left\{\left(\frac{\eta_0\Delta}{W}\right)^2\frac{\beta W}{\cosh^2(\beta W)} + \frac{J_{\mathbf{Q}}\sigma_0^2}{W} + \tanh(\beta W)\right\}.
\end{aligned} \tag{40}$$

Here all the second order contributions have been taken into account. When $T=0$,

$$\langle\sigma_{\mathbf{j}}^x\rangle = \frac{\eta_0^2\Delta}{W} = \frac{\eta_0^2\Delta}{J_{\mathbf{Q}}}. \tag{41}$$

We note that, as is the same case as for F and $\langle\sigma_{\mathbf{j}}^z\rangle$, for $\langle\sigma_{\mathbf{j}}^x\rangle$ the second order contribution $[O(g_{\mathbf{k}}^2)]$ vanishes when $T=0$.

III. NUMERICAL CALCULATIONS AND DISCUSSIONS

All the $\mathbf{k}$ dependence in the calculation is through the frequency $\omega_{\mathbf{k}}$, so we can introduce the density of states (DOS) $N(\omega)$,

$$\begin{aligned}
N(\omega) &= \sum_{\mathbf{k}}\delta(\omega-\omega_{\mathbf{k}}) = \int_{-1}^{1}d\gamma N_\gamma(\gamma)\\
&\quad\times\delta[\omega-\omega_0\sqrt{1-\rho(1\pm\gamma)/2}],
\end{aligned} \tag{42}$$

where $N_\gamma(\gamma)=\Sigma_{\mathbf{k}}\delta(\gamma-\gamma_{\mathbf{k}})$ is the DOS for $\gamma_{\mathbf{k}}$. For simplicity, we assume that $N_\gamma(\gamma)=2\sqrt{1-\gamma^2}/\pi$ is an elliptic DOS. Hence, we have

$$N(\omega) = \frac{8\omega}{\pi\rho\omega_0^2}\left\{1-\left[1-\frac{2}{\rho}\left(1-\left(\frac{\omega}{\omega_0}\right)^2\right)\right]^2\right\}^{1/2} \tag{43}$$

for the region $\omega_0\sqrt{1-\rho}<\omega<\omega_0$. Outside the region $N(\omega)=0$.

Before the numerical results are presented, we would say something about the difference between the physics of $\delta_{\mathbf{k}}\equiv 1$ and that of our choice of Eq. (18). $\delta_{\mathbf{k}}\equiv 1$ means that the phonons can follow completely the intrasite pseudospin tunneling but this should not be the case when ω_0/Δ or ω_0/α is small. $0\leqslant\delta_{\mathbf{k}}\leqslant 1$ of Eq. (18) means that the phonons follow the tunneling motion only partly and there is a retardation effect. In this sense, the theories of $\delta_{\mathbf{k}}\equiv 1$ overestimate the effect of quantum lattice fluctuations, especially for the case when ω_0/Δ or ω_0/α is small.

Figure 1 shows the critical ratio α_c/Δ as a function of ω_0/Δ when $\rho=0.5$. The solid line is our result and the dashed line from the theory of $\delta_{\mathbf{k}}\equiv 1$. The left and right short dotted lines indicate the adiabatic $[\alpha_c/\Delta=0.5$ for $M\to\infty$, Eq. (5) or (19)$]$ and the antiadiabatic $[\alpha_c/\Delta=1.5938$ for $M\to 0$, Eqs. (6) or (20)$]$ limits, respectively. Figure 2 shows the critical ratio Δ_c/α as a function of ω_0/α when $\rho=0.5$. The left and right short dotted lines indicate the adiabatic $[\Delta_c/\alpha=2$ for $M\to\infty$, Eqs. (5) or (19)$]$ and the antiadiabatic

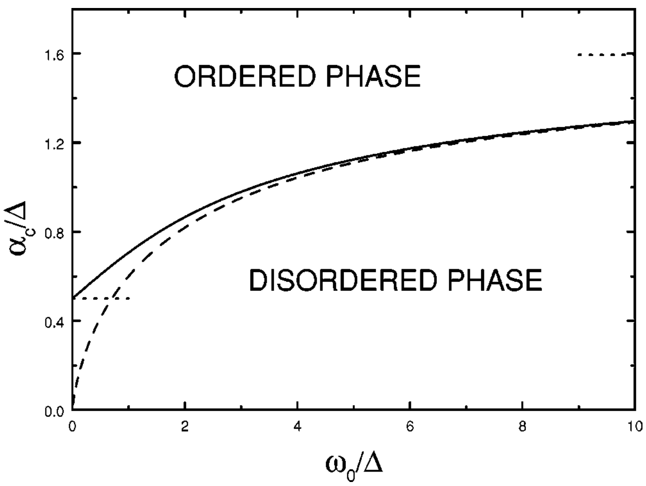

FIG. 1. The critical ratio α_c/Δ as a function of ω_0/Δ when $\rho=0.5$. Solid line: our result; dashed line: the theory of $\delta_{\mathbf{k}}\equiv 1$; left short dotted line: $\alpha_c/\Delta=0.5$ for $M\to\infty$; right short dotted line: $\alpha_c/\Delta=1.5938$ for $M\to 0$.

[$\Delta_c/\alpha=0.6274$ for $M\to 0$, Eqs. (6) or (20)] limits, respectively. One can see from the figures that (i) our theory of $0\le\delta_{\mathbf{k}}\le 1$ leads to the correct critical values in the both limits, as well as a smooth crossover between the limits. (ii) The theory of $\delta_{\mathbf{k}}\equiv 1$ cannot lead to the correct critical value in the adiabatic limit, that is, it is necessary to consider the retardation effect when, roughly speaking, $\omega_0/\Delta<2$ or $\omega_0/\alpha<2$.

Figure 3 shows the ground state average of the pseudospin $\langle\sigma^z\rangle=e^{-i\mathbf{Q}\cdot\mathbf{j}}\langle\sigma^z_{\mathbf{j}}\rangle$ and $\langle\sigma^x\rangle=\langle\sigma^x_{\mathbf{j}}\rangle$ as functions of the ratio ω_0/Δ. One can see that the theory of $\delta_{\mathbf{k}}\equiv 1$ overestimates the long range order $\langle\sigma^z\rangle$ but underestimates the tunneling $\langle\sigma^x\rangle$.

The ground state properties of the model system have already been discussed in an earlier paper.[10] Here we show the phase diagrams and other finite temperature properties.

Figure 4(a) is the T_c/Δ versus ω_0/Δ phase diagram. When $\omega_0/\Delta=0$, $T_c/\Delta=1.243$ from our theory but $T_c/\Delta=0.471$ from the theory of $\delta_{\mathbf{k}}\equiv 1$. The latter predicts a smaller T_c for $\omega_0=0$ because in this limit it predicts the phonon dressing factor $\eta_0=0$. However, our theory predicts $\eta_0=1$ in this limit. T_c/Δ decreases with increasing ratio ω_0/Δ when α/Δ is kept to be a constant, but the decreasing rate for the theory of $\delta_{\mathbf{k}}\equiv 1$ is much lower that that of our

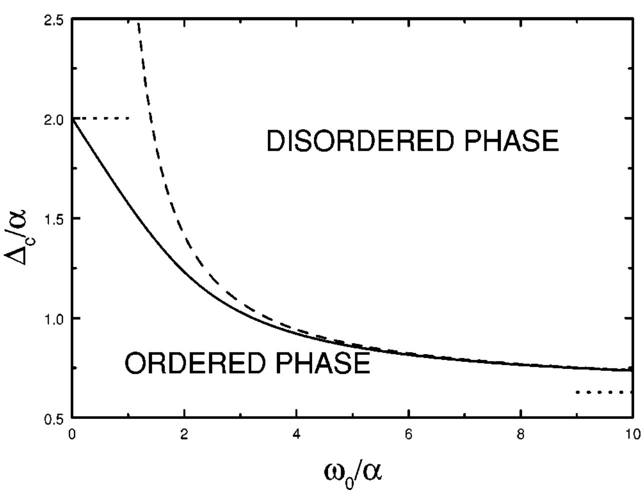

FIG. 2. The critical ratio Δ_c/α as a function of ω_0/α when $\rho=0.5$. Solid line: our result; dashed line: the theory of $\delta_{\mathbf{k}}\equiv 1$; left short dotted line: $\Delta_c/\alpha=2$ for $M\to\infty$; right short dotted line: $\Delta_c/\alpha=0.6274$ for $M\to 0$.

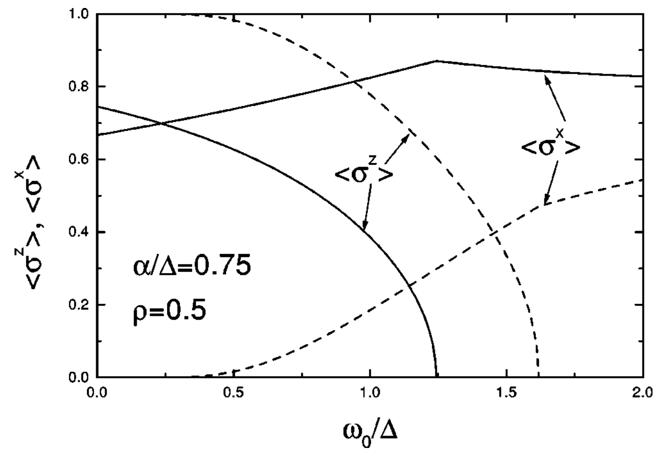

FIG. 3. $\langle\sigma^z\rangle=e^{-i\mathbf{Q}\cdot\mathbf{j}}\langle\sigma^z_{\mathbf{j}}\rangle$ and $\langle\sigma^x\rangle=\langle\sigma^x_{\mathbf{j}}\rangle$ as functions of ω_0/Δ when $T=0$. Solid line: our result; dashed line: the theory of $\delta_{\mathbf{k}}\equiv 1$.

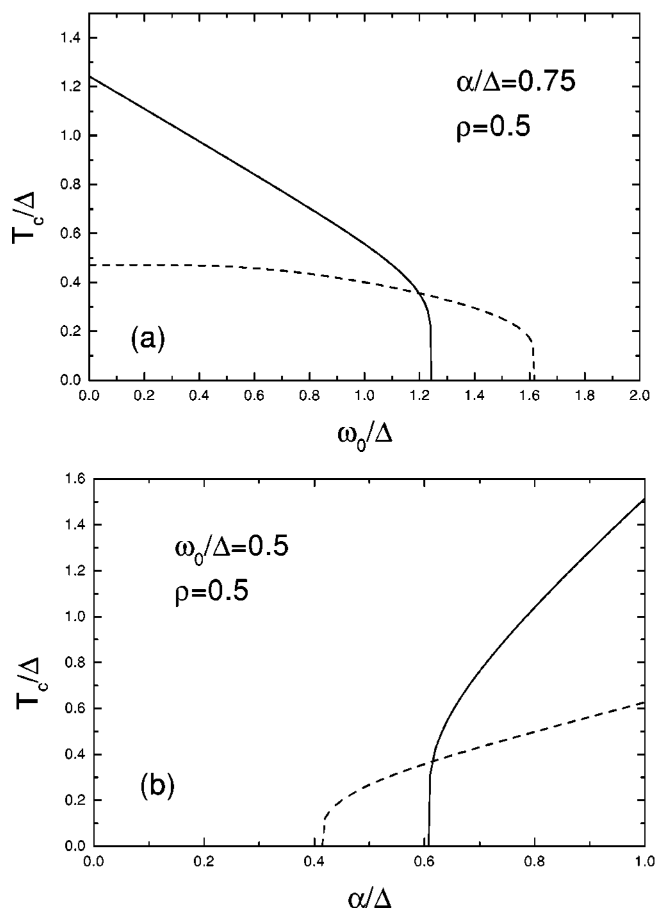

FIG. 4. (a) T_c/Δ versus ω_0/Δ and (b) T_c/Δ versus α/Δ phase diagrams. Solid line: our result; dashed line: the theory of $\delta_{\mathbf{k}}\equiv 1$.

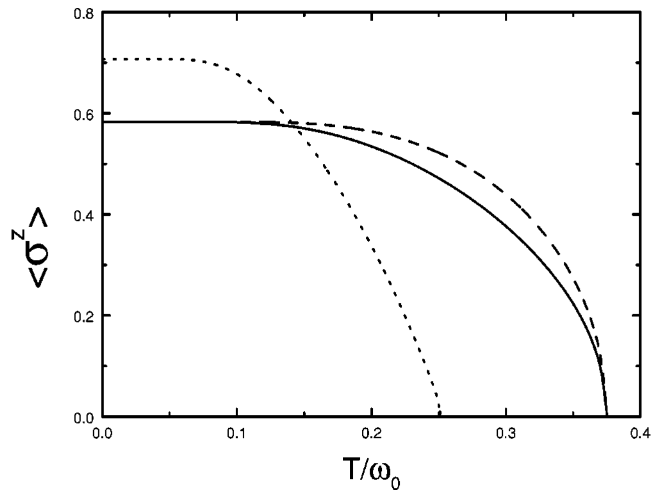

FIG. 5. $\langle\sigma_{\mathbf{j}}^{z}\rangle$ versus temperature (T/ω_0) relations. Solid line: result of second order perturbation; dashed line: result of the zeroth order; dotted line: the theory with $\delta_{\mathbf{k}}\equiv 1$.

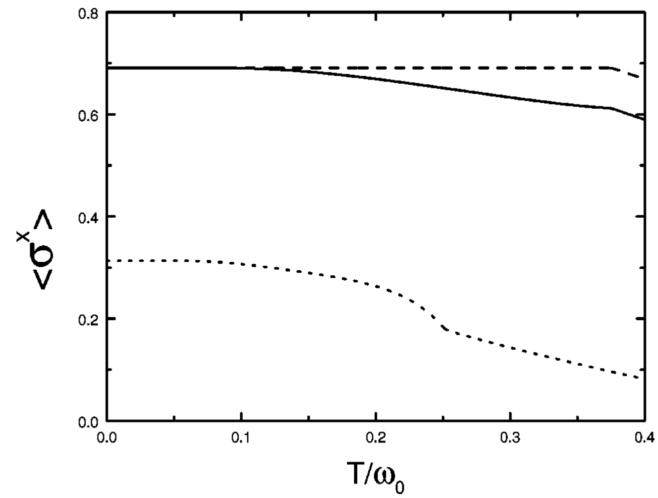

FIG. 6. $\langle\sigma_{\mathbf{j}}^{x}\rangle$ versus temperature (T/ω_0) relations. Solid line: the result of second order perturbation; dashed line: result of the zeroth order; dotted line: the theory with $\delta_{\mathbf{k}}\equiv 1$.

theory. Furthermore, the critical ratio $(\omega_0/\Delta)_c$ where the long range order disappears $(T_c=0)$ is 1.243 for our theory but 1.618 for the theory of $\delta_{\mathbf{k}}\equiv 1$.

The T_c/Δ versus α/Δ phase diagram in Fig. 4(b) is easily to understand. $T_c=0$ when $\alpha/\Delta\leqslant 0.414$ (for the theory of $\delta_{\mathbf{k}}\equiv 1$) or $\alpha/\Delta\leqslant 0.607$ (for our theory). Then T_c/Δ increases with increasing α/Δ when ω_0/Δ is kept to be a constant. The increasing rate for the former is much lower that the latter.

The order parameter $\langle\sigma_{\mathbf{j}}^{z}\rangle$ versus temperature (T/ω_0) relations are shown in Fig. 5. The solid line is the result of second order perturbation and the dashed one that of the zeroth order: $\langle\sigma_{\mathbf{j}}^{z}\rangle=\sigma_0\exp[i\mathbf{Q}\cdot\mathbf{j}]$. One can see that the effect of the second order perturbation is to reduce the long range order. For comparison, the result of the $\delta_{\mathbf{k}}\equiv 1$ theory is also shown by the dotted line. In the disordered phase $T>T_c$ $\langle\sigma_{\mathbf{j}}^{z}\rangle=0$.

$\langle\sigma_{\mathbf{j}}^{x}\rangle$ versus temperature (T/ω_0) relations are shown in Fig. 6. The solid line is the result of second order perturbation and the dashed one that of the zeroth order: $\langle\sigma_{\mathbf{j}}^{x}\rangle=\eta_0^2\Delta\tanh(\beta W)/W$ which is a constant $\langle\sigma_{\mathbf{j}}^{x}\rangle=\eta_0^2\Delta/J_{\mathbf{Q}}$ for $T<T_c$. For comparison, the dotted line is the result of the theory with $\delta_{\mathbf{k}}\equiv 1$. As $\langle\sigma_{\mathbf{j}}^{x}\rangle=1$ for $\alpha=0$, we can use $\langle\sigma_{\mathbf{j}}^{x}\rangle$ as the renormalization factor for bare tunneling matrix element Δ. Our result shows that, although the reduction of the tunneling matrix element by pseudospin-phonon interaction gets larger when $\alpha>0$, it is not so small as the theory of $\delta_{\mathbf{k}}\equiv 1$ predicts and the reduction is alleviated by introducing a $\mathbf{k}$-dependent $\delta_{\mathbf{k}}$.[10] In the disordered phase $T>T_c$ $\langle\sigma_{\mathbf{j}}^{x}\rangle>0$, but $T=T_c$ is a discontinuous point for $d\langle\sigma_{\mathbf{j}}^{x}\rangle/dT$.

IV. CONCLUSION

We have studied the long range order and phase transition in a simple cooperative Jahn-Teller system and show that, as a result of the competition between the intrasite pseudospin tunneling and the phonon-induced intersite pseudospin correlation, a phase transition to the pseudospin long range ordering phase may occur at some critical temperature. A new approach, based on a $\mathbf{k}$-dependent displacement transformation and then treating the transformed Hamiltonian in perturbation theory, has been proposed to deal with the nonadiabaticity and the retardation effect of the pseudospin-phonon interaction. The approach leads to correct results in both $M\to\infty$ and $M\to 0$ limits, as well as a smooth crossover between the limits. It has been pointed out that when $\omega_0/\Delta<2$ or $\omega_0/\alpha<2$ the retardation effect of the pseudospin-phonon interaction is quite important. The calculated renormalized tunneling matrix element, which is reduced by the pseudospin-phonon interaction, is not so small as the theory of $\delta_{\mathbf{k}}\equiv 1$ predicts, that is, the reduction is alleviated by introducing a $\mathbf{k}$-dependent $\delta_{\mathbf{k}}$.

Our treatment mainly depends on the perturbation theory. The purpose of the unitary transformation is to find a better way to divide the original Hamiltonian into unperturbed part and perturbation. We believe that our treatment has caught the main physics of the problem because (i) the perturbation $H_{I1}+H_{I2}$ [Eqs. (13) and (14)] is small in the meaning that its second order contributions to the free energy F, the order parameter $\langle\sigma_{\mathbf{j}}^{z}\rangle$, and the renormalization factor for tunneling $\langle\sigma_{\mathbf{j}}^{x}\rangle$ vanish when $T=0$ via properly choosing the form of $\delta_{\mathbf{k}}$ (18), η_0 (17), and σ_0 (28). (ii) In the mean field approximation the unperturbed part H_0 of the transformed Hamiltonian $\tilde{H}$ works well and the perturbation $H_{I1}+H_{I2}$ goes to zero in both $M\to\infty$ and $M\to 0$ limits. (iii) The mean field decoupling to the transformed Hamiltonian is justified since the phonon-induced pseudospin correlation is a long range one.

In this work we deal with a simplified model for the real copperative Jahn-Teller systems, so we do not compare our results with the experimental measurements. We will extend our approach to the real systems[7,8] in forthcoming publications.

ACKNOWLEDGMENTS

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