Long-range electron-phonon correlation and Peierls dimerization in the one-dimensional molecular-crystal model

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In this paper, we reexamine the effect of quantum lattice fluctuations in a half-filled quasi-one-dimensional electron-phonon coupling system by considering long-range electron-phonon correlation more precisely. Our results coincide with previous papers in the $\omega=0$ (adiabatic) and $\omega=\infty$ cases. We note that the off-site electron-phonon correlation plays an important role in the order-disorder transition of the spinless case. But in the spin-$\frac{1}{2}$ case, the Peierls dimerization always exists. The effect of the off-site electron-phonon correlation is slight. Our results are in good agreement with Monte Carlo simulations, and the small squeezed-polaron approach is the special case of our method.

I. INTRODUCTION

Studies of lattice instabilities in quasi-one-dimensional electron-phonon systems have a long history[1-7] since Peierls' pioneering work,[6] and in recent years the question of whether the Peierls dimerization can survive the quantum lattice fluctuations if the ionic mass is lower than some critical value has been of wide interest among theorists and experimentalists. In theoretical studies,[8-20] particular attention has been paid to the Holstein[23] model, because it is perhaps the simplest model for an electron-phonon system but contains the main physics. In the adiabatic limit (phonon frequency $\omega=0$) the ground-state properties of the model are easily obtained in mean-field theory by freezing out the lattice distortion and determining it self-consistently from the minimization of the total elastic plus electronic energy.[6,7] In contrast, the Lang-Firsov transformation[24] followed by an average over the phonon vacuum state can be used in the $\omega=\infty$ limit, where the Peierls dimerization disappears. The difficulty is how to treat the intermediate region where $\hbar\omega$ is of the same order of magnitude as the electronic bandwidth $W=4t$ and the nonadiabaticity plays an important role. Several papers have studied this difficulty: Hirsch and Fradkin's[9] strong-coupling expansion and Monte Carlo simulations in the general case, Bourbonnais and Caron's[10] functional intergral approach coupled to a renormalization-group procedure, Hirsch's[11] one-dimensional molecular-crystal model with Coulomb interaction, Takahashi's[12] adiabatic quantum Monte Carlo method, Z. B. Su and Yu's[13] consideration of the transition between multielectron states under the theory of relaxation and multiphonon processes, Z. B. Su, Wang, and Yu's[14] Green's function technique, W. P. Su's[18] Monte Carlo method, and Schmeltzer's[20] renormalization group in the $1/N$ expansion.

Zheng, Feinberg, and Avignon[8] proposed a small squeezed-polaron[21,22] approach to investigate the effect of quantum lattice fluctuations on the Peierls dimerization in a half-filled one-dimensional Holstein model. The nonadiabatic effects due to finite phonon frequency $\omega\neq0$ are treated through a variational polaron wave function, in which only the on-site electron-phonon correlation is taken into account. Thus we shall call this approach the small squeezed-polaron (SSP) one.

In this paper, we reconsider the SSP approach and take into account both the on-site and the off-site electron-phonon correlations. We shall show by our results that the long-range electron-phonon correlation cannot be neglected in the intermediate region where $\hbar\omega$ is of the same order of magnitude as $W=4t$.

This paper is organized as follows. In Sec. II, we give the theoretical analysis of the Holstein model in the spinless and spin-$\frac{1}{2}$ cases. Section III contains the definitions of some interesting quantities and the numerical calculation of these quantities in the limits ($\omega=0,\infty$) and the general case. The discussion of our results is in Sec. IV, which gives some comparisons with other papers. Some details of theoretical derivations are in the Appendix.

II. THEORETICAL ANALYSIS

A. Spinless case

Our starting Hamiltonian is the one-dimensional molecular-crystal model[9] (Holstein model):

$$H=\sum_l (b_l^\dagger b_l+\tfrac{1}{2})\hbar\omega-\sum_l \lambda\sqrt{\hbar/2M\omega}(b_l^\dagger+b_l)(n_l-\tfrac{1}{2}) -t\sum_l (c_l^\dagger c_{l+1}+c_{l+1}^\dagger c_l)\,, \tag{1}$$

where $\omega=\sqrt{K/M}$, K is the elastic constant, M is the mass, λ is the electron-phonon coupling, t is the hopping integral, $c_l^\dagger$ and c_l are the creation and annihilation operators of an electron at site l, $n_l=c_l^\dagger c_l$ is the number operator of the electron, and $b_l^\dagger$ and b_l are the creation and annihilation operators of a localized phonon at site l. The total number of electrons is $N/2$ in the case of half filling, where N is the number of sites.

In the following text, three unitary transformations are used. The first unitary transformation is a modified

Lang-Firsov transformation, which introduces the q-dependent function δ_q. q is the wave vector.

$$S_1=-\sum_{l,l'} g\delta_{l-l'}(b_{l'}^{\dagger}-b_{l'})(n_l-\tfrac{1}{2})$$
$$=-\frac{1}{\sqrt{N}}\sum_{l,q} g\delta_q e^{iql}(b_q^{\dagger}-b_{-q})(n_l-\tfrac{1}{2})\ . \tag{2}$$

Here $\delta_{l-l'}$ clearly represents the electron-phonon correlation between sites l and l', and δ_q is the Fourier transformation to $\delta_{l-l'}$: $\delta_q=(1/N)\sum_{l-l'} e^{-iq(l-l')}\delta_{l-l'}$. Thus δ_q describes both the on-site and the off-site electron-phonon correlation, $\delta_{-q}=\delta_q$. b_q and $b_q^{\dagger}$ are in the momentum representation, $g^2=\epsilon_p/\hbar\omega$, and $\epsilon_p=\lambda^2/2K$. ϵ_p is the polaron binding energy.[23–25] Thus

$$H_1=\exp(S_1)H\exp(-S_1)$$
$$=\sum_q (b_q^{\dagger}b_q+\tfrac{1}{2})\hbar\omega-\frac{1}{\sqrt{N}}\sum_{l,q}\lambda\sqrt{\hbar/2M\omega}e^{-iql}(1-\delta_q)(b_{-q}^{\dagger}+b_q)(n_l-\tfrac{1}{2})$$
$$+\frac{1}{N}\sum_{l,l',q} g\lambda\sqrt{\hbar/2M\omega}e^{-iq(l-l')}(\delta_q^2-2\delta_q)(n_l-\tfrac{1}{2})(n_{l'}-\tfrac{1}{2})$$
$$-t\sum_l\left\{c_l^{\dagger}c_{l+1}\exp\left[-\frac{1}{\sqrt{N}}\sum_q g\delta_q e^{igl}(b_q^{\dagger}-b_{-q})\right]\exp\left[\frac{1}{\sqrt{N}}\sum_q g\delta_q e^{iq(l+1)}(b_q^{\dagger}-b_{-q})\right]+\text{H.c.}\right\}, \tag{3}$$

In order to increase the possibility of polaron tunneling and offset the polaronic narrowing effect[23] on the bandwidth which is produced by Lang-Firsov transformation and energetically unfavorable to many-polaron system, we introduce the second unitary transformation, the squeezing transformation,[21,22]

$$S_2=-\sum_q \alpha_q(b_q^{\dagger}b_{-q}^{\dagger}-b_q b_{-q})\ , \tag{4}$$

where $\{\alpha_q\}$ is a q-dependent function.

Thus

$$H_2=\exp(S_2)H_1\exp(-S_2)$$
$$=H_0+H'\ . \tag{5}$$

$$H_0=\frac{\hbar\omega}{2}\sum_q(\tau_q^2+\tau_q^{-2})(b_q^{\dagger}b_q+\tfrac{1}{2})-\frac{\lambda^2}{8K}(\delta_0^2-2\delta_0)N-2\rho t\sum_k c_k^{\dagger}c_k\cos k\ ,$$

$$H'=-\frac{\hbar\omega}{4}\sum_q(\tau_q^2-\tau_q^{-2})(b_q^{\dagger}b_{-q}^{\dagger}+b_q b_{-q})-\frac{1}{\sqrt{N}}\sum_{q,k}\lambda\sqrt{\hbar/2M\omega}(1-\delta_q)\tau_q^{-1}(c_k^{\dagger}c_{k-q}b_{-q}^{\dagger}+c_k^{\dagger}c_{k-q}b_q)$$
$$+\frac{\lambda}{2}\sqrt{N}\sqrt{\hbar/2M\omega}(1-\delta_0)\tau_0^{-1}(b_0^{\dagger}+b_0)+\frac{1}{N}\sum_{q,k,k'}\frac{\lambda^2}{2K}(\delta_q^2-2\delta_q)c_{k+q}^{\dagger}c_k c_{k'-q}^{\dagger}c_{k'}$$
$$-\frac{1}{N}\sum_{l,k,k'} t\left[e^{i(k-k')l}e^{-ik'}c_k^{\dagger}c_{k'}\left\{\exp\left[-\frac{1}{\sqrt{N}}\sum_q g\delta_q\tau_q e^{iql}(b_q^{\dagger}-b_{-q})\right]\right.\right.$$
$$\left.\left.\times\exp\left[\frac{1}{\sqrt{N}}\sum_q g\delta_q\tau_q e^{iq(l+1)}(b_q^{\dagger}-b_{-q})\right]-\rho\right\}+\text{H.c.}\right], \tag{6}$$

where $c_k^{\dagger}$ and c_k are the electron operators in the momentum representation. $\tau_q=\exp(-2\alpha_q)$, the second q-dependent function, is in the range of $0<\tau_q<1$.

$$\rho=\exp\left[-\frac{1}{N}\sum_q 2g^2\delta_q^2\tau_q^2\sin^2\frac{q}{2}\right] \tag{7}$$

is the narrowing factor to bandwidth $W=4t$, $0<\rho<1$. When $\delta_q=1$ and $\tau_q=1$ for any q,

$$\rho=\rho_0=\exp\left[-\frac{1}{N}\sum_q 2g^2\sin^2\frac{q}{2}\right],$$

which is the Holstein narrowing factor.[23]

The ground state $|G\rangle$ of H_0 is the direct product of a Fermi sea $|\text{FS}\rangle$ and a phonon vacuum state $|\text{ph},0\rangle$, $|G\rangle=|\text{FS}\rangle|\text{ph},0\rangle$.

H' is considered as the perturbation to H_0 and the first-order perturbation $\langle G|H'|G\rangle$ is zero. We note that the first term in H' is the two-phonon one, which generates a different type of coherent lattice state, the two-phonon state.[21,22]

In our method, $\{\delta_q\}$ and $\{\tau_q\}$ are two q-dependent functions and how to determine them is the central problem of this paper. In Eq. (5) H_2 is separated into H_0 and H', which is considered as a perturbation to H_0. We choose $\{\delta_q\}$ and $\{\tau_q\}$ to make the matrix elements of H'

between the ground state and lowest-lying excited states of H_0 be zero or minimized.

The lowest-lying excited states of H_0 are

$$|1\rangle = b_q^\dagger b_{-q}^\dagger |G\rangle ,$$
$$|2\rangle = c_{k+q}^\dagger c_k b_{-q}^\dagger |G\rangle , \tag{8}$$

where $|k+q|>\pi/2$ and $|k|<\pi/2$. $\{\delta_q\}$ and $\{\tau_q\}$ are determined to let

$$\langle G|H'|1\rangle = 0 , \tag{9}$$
$$\langle G|H'|2\rangle = 0 . \tag{10}$$

We obtain the following equations:

$$\delta_q = \frac{1}{1+4(t/\hbar\omega)\tau_q^2\rho|\sin(k+q/2)||\sin q/2|} ,$$
$$\tau_q^4 = \frac{1}{1+16(t/\hbar\omega)g^2\delta_q^2\rho(1/N)\sum_k \langle \mathrm{FS}|c_k^\dagger c_k|\mathrm{FS}\rangle \cos k \sin^2 q/2} . \tag{11}$$

We note that in the one-electron situation the electron is at the bottom of conduction band and then $k=0$ in the excited state $|2\rangle$. Thus we obtain the functional form of δ_q:

$$\delta_q = \frac{1}{1+4(t/\hbar\omega)\rho \sin^2 q/2}$$

with $\tau_q^4=1$, which is the same as that of Wagner and Kongeter.[5]

But we consider the many-electron situation in this paper. Note that δ_q is a function of q only and cannot satisfy Eq. (10) for any k. So we have to replace $\tau_q^2\rho|\sin(k+q/2)|$ with a parameter $1/\Phi$, which is determined to minimize the energy of the ground state. Thus we have

$$\delta_q = \frac{1}{1+4(t/\hbar\omega\Phi)|\sin q/2|} ,$$
$$\tau_q^4 = \frac{1}{1+16(t/\hbar\omega)(1/\pi)g^2\delta_q^2\rho \sin^2 q/2} , \tag{12}$$
$$\rho = \exp\left[-\frac{1}{\pi}\int_0^\pi dq\, 2g^2\delta_q^2\tau_q^2 \sin^2\frac{q}{2}\right] .$$

It is apparent that $\delta_0=1, \tau_0=1$, and δ_q, τ_q are monotonically decreasing functions of q.

We believe that $\{\delta_q\}$ and $\{\tau_q\}$, determined by the above method, can describe the long-range electron-phonon correlation in the one-dimensional molecular-crystal model better.

The third unitary transformation is

$$S_3 = -\sum_l (-1)^l m_0 \sqrt{M\omega/2\hbar}(b_l^\dagger - b_l) . \tag{13}$$

$$\begin{aligned} H_3 &= \exp(S_3) H_2 \exp(-S_3) \\ &= \frac{\hbar\omega}{2}\sum_q (\tau_q^2+\tau_q^{-2})(b_q^\dagger b_q + \tfrac{1}{2}) - \frac{\hbar\omega}{4}\sum_q (\tau_q^2-\tau_q^{-2})(b_q^\dagger b_{-q}^\dagger + b_q b_{-q}) + \frac{K}{2}m_0^2 N \\ &\quad - \frac{\lambda^2}{8K}(\delta_0^2-2\delta_0) - m_0\lambda(1-\delta_\pi)\sum_k c_k^\dagger c_{k-\pi} + m_0\hbar\omega\sqrt{M\omega/2\hbar}\sqrt{N}\,\tau_\pi^{-1}(b_\pi^\dagger + b_\pi) \\ &\quad - \frac{1}{\sqrt{N}}\sum_{q,k}\lambda\sqrt{\hbar/2M\omega}(1-\delta_q)\tau_q^{-1}(c_k^\dagger c_{k-q} b_{-q}^\dagger + c_k^\dagger c_{k-q} b_q) \\ &\quad + \frac{\lambda}{2}\sqrt{N}\sqrt{\hbar/2M\omega}(1-\delta_0)\tau_0^{-1}(b_0^\dagger + b_0) + \frac{1}{N}\sum_{q,k,k'}\frac{\lambda^2}{2K}(\delta_q^2-2\delta_q)c_{k+q}^\dagger c_k c_{k'-q}^\dagger c_{k'} \\ &\quad - \frac{1}{N}\sum_{l,k,k'} t\left\{e^{i(k-k')l}e^{-ik'}c_k^\dagger c_{k'} \exp\left[-\frac{1}{\sqrt{N}}\sum_q g\delta_q\tau_q e^{iql}(b_q^\dagger - b_{-q})\right]\right. \\ &\qquad \left. \times \exp\left[\frac{1}{\sqrt{N}}\sum_q g\delta_q\tau_q e^{iq(l+1)}(b_q^\dagger - b_{-q})\right] + \mathrm{H.c.}\right\} , \end{aligned} \tag{14}$$

where the parameter m_0 measures the phonon staggered ordering.[8] This transformation changes the original point of the localized phonon mode to $(-1)^l m_0$. In other words, the system is in a phonon-staggered-ordering state (dimerization state) as long as $m_0\neq 0$. When $\delta_q=1$ for all q, m_0 approaches zero. That is, the polaronic effect suppresses the phonon staggered ordering. In the general case $0<\delta_q<1$, we expect that there will be a nonzero dimerization, but reduced by the polaron effect, that is, by the quantum fluctuations of phonons.

Our method with two q-dependent functions $\{\delta_q\}$ and $\{\tau_q\}$ is different from the SSP approach of Ref. 8. In the SSP approach, the squeezed polaron is treated as an absolutely small one, which means that the lattice motion is influenced by the on-site electron-phonon correlation only and has nothing to do with the electrons at other sites. In fact, the vibrations of all lattice sites are correlated by the tunneling of the electrons and an electron will influence the motion of the lattice at neighboring sites. Thus we think that our method, taking into account the long-range electron-phonon correlation by q-dependent δ_q and τ_q^2, is reasonable. In this paper, we also calculate the "size" of the polaron.

At this point, we average H_3 over the vacuum state $|\mathrm{ph},0\rangle$ of the transformed phonon subsystem. The effective Hamiltonian for the electron subsystem.

$$
\begin{aligned}
H_{\mathrm{eff}} &= \langle \mathrm{ph},0|H_3|\mathrm{ph},0\rangle \\
&= \frac{\hbar\omega}{4}\sum_q(\tau_q^2+\tau_q^{-2})+\frac{K}{2}m_0^2N+\frac{\lambda^2}{8K}(2\delta_0-\delta_0^2)N-\frac{\lambda^2}{4K}\sum_q(2\delta_q-\delta_q^2)-m_0\lambda(1-\delta_\pi)\sum_k c_k^\dagger c_{k-\pi} \\
&\quad -2\rho t\sum_k c_k^\dagger c_k\cos k+\frac{1}{N}\sum_{q,k,k'}\frac{\lambda^2}{2K}\left[\delta_q^2-2\delta_q-\frac{1}{N}\sum_{q'}(\delta_{q'}^2-2\delta_{q'})\right]c_{k+q}^\dagger c_k c_{k'-q}^\dagger c_{k'} \,. \qquad (15)
\end{aligned}
$$

If we set $\delta_q=\delta$ and $\tau_q=\tau$ for every q, H_{eff} becomes

$$
H_{\mathrm{eff}}=\frac{\hbar\omega}{4}(\tau^2+\tau^{-2})N+\frac{K}{2}m_0^2N-(2\delta-\delta^2)\frac{\lambda^2}{8K}N-m_0\lambda(1-\delta)\sum_k c_k^\dagger c_{k-\pi}-2\rho t\sum_k c_k^\dagger c_k\cos k \,, \qquad (16)
$$

which is the same as the SSP approach. This means that the SSP approach is just a special case of ours.

The effective Hamiltonian Eq. (15) is more difficult to solve because of the four-fermion term. We use the self-consistent-field approximation, decoupling the four-fermion term, and the Bogoliubov transformation, diagonalizing the other terms. The details are listed in the Appendix. The ground-state energy is

$$
\begin{aligned}
E_g(\delta_q,\tau_q)/N &= \frac{\hbar\omega}{4\pi}\int_0^\pi dq(\tau_q^2+\tau_q^{-2})+\frac{\lambda^2}{8K}V_0+\frac{\lambda^2}{2K}(1+V_0)m_e^2 \\
&\quad -\frac{1}{\pi}\int_0^{\pi/2}dk\left[4\rho^2t^2\cos^2k+\left[(1+V_0)\frac{\lambda^2}{K}m_e\right]^2\right]^{1/2} \\
&\quad -\frac{\lambda^2}{4K}\frac{1}{4\pi^2}\int_0^\pi dk'\int_0^\pi dk(\delta_{k'-k}^2-2\delta_{k'-k}+\delta_{k'+k}^2-2\delta_{k'+k}) \\
&\qquad \times\frac{2\rho t\cos k'}{\sqrt{4\rho^2t^2\cos^2k'+[(1+V_0)(\lambda^2/K)m_e]^2}} \\
&\qquad \times\frac{2\rho t\cos k}{\sqrt{4\rho^2t^2\cos^2k+[(1+V_0)(\lambda^2/K)m_e]^2}} \,, \qquad (17)
\end{aligned}
$$

where

$$
V_0=\frac{1}{\pi}\int_0^\pi dq(\delta_q^2-2\delta_q) \,.
$$

m_e, the charge-density-wave[6] (CDW) ordering parameter, is determined self-consistently by

$$
m_e=\frac{1}{N}\sum_l(-1)^l\langle n_l\rangle=\frac{1}{\pi}\int_0^{\pi/2}dk\frac{(1+V_0)(\lambda^2/K)m_e}{\sqrt{4\rho^2t^2\cos^2k+[(1+V_0)(\lambda^2/K)m_e]^2}} \,, \qquad (18)
$$

where $\langle\cdots\rangle$ means the averaging over the ground state of H_{eff}; and

$$
m_0=\frac{\lambda(1-\delta_\pi)}{K}m_e \,. \qquad (19)
$$

B. Spin-$\frac{1}{2}$ case

In the spin-$\frac{1}{2}$ case, the total number of electrons is N in the case of half filling. The Hamiltonian[9] is

$$
H=\sum_l(b_l^\dagger b_l+\tfrac{1}{2})\hbar\omega-t\sum_{l,\sigma}(c_{l,\sigma}^\dagger c_{l+1,\sigma}+c_{l+1,\sigma}^\dagger c_{l,\sigma})-\sum_{l,\sigma}\lambda\sqrt{\hbar/2M\omega}(b_l^\dagger+b_l)(n_{l,\sigma}-\tfrac{1}{2}) \,, \qquad (20)
$$

in which the phonon creation and annihilation operators have been used and σ is the spin index.

Three unitary transformations, which are similar to those in the spinless case, are used.

$$
\begin{aligned}
H_3 &= \exp(S_3)\exp(S_2)\exp(S_1) H \exp(-S_1)\exp(-S_2)\exp(-S_3) \\
&= \frac{\hbar\omega}{2}\sum_q (\tau_q^2+\tau_q^{-2})(b_q^\dagger b_q+\tfrac{1}{2}) - \frac{\lambda^2}{2K}(\delta_0^2-2\delta_0)N - m_0\lambda(1-\delta_\pi)\sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k-\pi,\sigma} \\
&\quad + \frac{K}{2}m_0^2 N - \frac{\hbar\omega}{4}\sum_q (\tau_q^2-\tau_q^{-2})(b_q^\dagger b_{-q}^\dagger + b_q b_{-q}) + m_0\hbar\omega\sqrt{M\omega/2\hbar}\sqrt{N}\,\tau_\pi^{-1}(b_\pi^\dagger + b_\pi) \\
&\quad - \frac{1}{\sqrt{N}}\sum_{q,k,\sigma} \lambda\sqrt{\hbar/2M\omega}(1-\delta_q)\tau_q^{-1}(c_{k,\sigma}^\dagger c_{k-q,\sigma} b_{-q}^\dagger + c_{k,\sigma}^\dagger c_{k-q,\sigma} b_q) \\
&\quad + \frac{\lambda}{2}\sqrt{\hbar/2M\omega}\sqrt{N}(1-\delta_0)\tau_0^{-1}(b_0^\dagger + b_0) + \frac{1}{N}\sum_q \frac{\lambda^2}{2K}(\delta_q^2-2\delta_q)\sum_{k,\sigma,k',\sigma'} c_{k+q,\sigma}^\dagger c_{k,\sigma} c_{k'-q,\sigma'}^\dagger c_{k',\sigma'} \\
&\quad - \frac{1}{N}\sum_l t\left\{\sum_{k,k',\sigma} e^{i(k-k')l} e^{-ik'} c_{k,\sigma}^\dagger c_{k',\sigma} \exp\left[-\frac{1}{\sqrt{N}}\sum_q g e^{iql}\delta_q\tau_q(b_q^\dagger - b_{-q})\right]\right. \\
&\qquad \left. \times \exp\left[\frac{1}{\sqrt{N}}\sum_q g e^{iq(l+1)}\delta_q\tau_q(b_q^\dagger - b_{-q})\right] + \text{H.c.}\right\} .
\end{aligned} \tag{21}
$$

Two q-dependent functions $\{\delta_q\}$ and $\{\tau_q\}$, which are determined by the same method as in the spinless case, satisfy the following equations:

$$
\begin{aligned}
\delta_q &= \frac{1}{1+4(t/\hbar\omega\Phi)|\sin q/2|} , \\
\tau_q^4 &= \frac{1}{1+32(t/\hbar\omega)(1/\pi)g^2\delta_q^2\rho\sin^2 q/2} , \\
\rho &= \exp\left[-\frac{1}{N}\sum_q 2g^2\delta_q^2\tau_q^2\sin^2\frac{q}{2}\right] .
\end{aligned} \tag{22}
$$

From averaging H_3 over the vacuum state $|\text{ph},0\rangle$ of the transformed phonon subsystem, we obtain an effective Hamiltonian for the electron subsystem,

$$
\begin{aligned}
H_{\text{eff}} &= \langle \text{ph},0|H_3|\text{ph},0\rangle \\
&= \frac{\hbar\omega}{4}\sum_q (\tau_q^2+\tau_q^{-2}) + \frac{K}{2}m_0^2 N - \frac{\lambda^2}{2K}(\delta_0^2-2\delta_0)N + \frac{\lambda^2}{2K}\sum_q (\delta_q^2-2\delta_q) \\
&\quad - m_0\lambda(1-\delta_\pi)\sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k-\pi,\sigma} + \frac{1}{N}\sum_{q,l}\frac{\lambda^2}{N}(\delta_q^2-2\delta_q) n_{l,\uparrow} n_{l,\downarrow} - 2\rho t\sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma}\cos k \\
&\quad + \frac{1}{N}\sum_{q,k,k',\sigma,\sigma'}\frac{\lambda^2}{2K}\left[\delta_q^2-2\delta_q-\frac{1}{N}\sum_{q'}(\delta_{q'}^2-2\delta_{q'})\right] c_{k-q,\sigma}^\dagger c_{k,\sigma} c_{k'+q,\sigma'}^\dagger c_{k',\sigma'} .
\end{aligned} \tag{23}
$$

The sixth term is decoupled as Zheng, Feinberg, and Avignon[8] have done:

$$
c_{l,\uparrow}^\dagger c_{l,\uparrow} c_{l,\downarrow}^\dagger c_{l,\downarrow} \approx c_{l,\uparrow}^\dagger c_{l,\uparrow}\langle c_{l,\downarrow}^\dagger c_{l,\downarrow}\rangle + \langle c_{l,\uparrow}^\dagger c_{l,\uparrow}\rangle c_{l,\downarrow}^\dagger c_{l,\downarrow} - \langle c_{l,\uparrow}^\dagger c_{l,\uparrow}\rangle\langle c_{l,\downarrow}^\dagger c_{l,\downarrow}\rangle , \tag{24}
$$

$$
\langle c_{l,\sigma}^\dagger c_{l,\sigma}\rangle = \frac{1}{2} + (-1)^l\frac{m_e}{2} , \tag{25}
$$

$$
m_e = \frac{1}{N}\sum_{l,\sigma}(-1)^l\langle c_{l,\sigma}^\dagger c_{l,\sigma}\rangle , \tag{26}
$$

where m_e is the charge-density-wave ordering parameter. Using the same method as in the spinless case, we get the result

$$E_g(\delta_q,\tau_q)/N=\frac{\hbar\omega}{4\pi}\int_0^{\pi}dq(\tau_q^2+\tau_q^{-2})+\frac{\lambda^2}{4K}[V_0+(2+V_0)m_e^2]$$
$$-\frac{2}{\pi}\int_0^{\pi/2}dk\left\{4\rho^2t^2\cos^2k+\left[\left[1+\frac{V_0}{2}\right]\frac{\lambda^2}{K}m_e\right]^2\right\}^{1/2}$$
$$-\frac{\lambda^2}{2K}\frac{1}{4\pi^2}\int_0^{\pi}dk'\int_0^{\pi}dk(\delta_{k'-k}^2-2\delta_{k'-k}+\delta_{k'+k}^2-2\delta_{k'+k})$$
$$\times\frac{2\rho t\cos k'}{\sqrt{4\rho^2t^2\cos k'+[(1+V_0/2)(\lambda^2/K)m_e]^2}}$$
$$\times\frac{2\rho t\cos k}{\sqrt{4\rho^2t^2\cos^2k+[(1+V_0/2)(\lambda^2/K)m_e]^2}}\ , \tag{27}$$

where

$$V_0=\frac{1}{\pi}\int_0^{\pi}dq(\delta_q^2-2\delta_q)\ , \tag{28}$$

$$m_e=\frac{2}{\pi}\int_0^{\pi/2}dk\frac{(1+V_0/2)(\lambda^2/K)m_e}{\sqrt{4\rho^2t^2\cos^2k+[(1+V_0/2)(\lambda^2/K)m_e]^2}}\ . \tag{29}$$

We also get

$$m_0=\frac{\lambda(1-\delta_\pi)}{K}m_e\ . \tag{30}$$

We find the result of the SSP approach is a special case of our result, just as in the spinless case. But in this paper we do not consider the superconducting singlet pairing parameter.

III. NUMERICAL CALCULATIONS

First, we define some interesting quantities. The phonon-staggered ordering parameter m_p is

$$m_p=\frac{1}{N}\sum_l(-1)^l\langle q_l\rangle\ , \tag{31}$$

where q_l is the position operator of the lattice

$$m_p=m_0+\frac{\lambda}{K}\delta_\pi m_e$$
$$=\frac{\lambda}{K}m_e \tag{32}$$

for the spinless case and

$$m_p=m_0+\frac{\lambda}{K}\delta_\pi m_e$$
$$=\frac{\lambda}{K}m_e \tag{33}$$

for the spin-$\frac{1}{2}$ case. The contribution of the polaron effect is included in m_p, apart from the static staggered ordering parameter m_0.

We also consider the "size" of the polaron R. As we have said, the polaron in our approach is not an absolutely small one as in the SSP approach. Because $\{\delta_q\}$ represents the dynamical distortion of the lattice when electrons move, we use $\{\delta_q\}$ to define the size of the polaron R, using the anti-Fourier transformation to $\{\delta_q\}$,

$$\delta_l=\frac{1}{\pi}\int_0^{\pi}dq\ e^{iql}\delta_q\ , \tag{34}$$

which represents the displacement of the lattice at site l, when an electron is at the origin. Thus, the "size" of a polaron R is defined as

$$\delta_R=\delta_0/10\ . \tag{35}$$

$\omega=0$ limit

In the $\omega=0$ limit, we find that $\delta_q=0$ $(q\neq0)$, $\delta_0=1$, and $\tau_q^2=1$ for both spinless $(n=1)$ and spin-$\frac{1}{2}$ $(n=2)$ cases. So in this limit

$$E_g/N=\frac{K}{2}m_0^2-\frac{n}{\pi}\int_0^{\pi/2}(4t^2\cos^2k+m_0^2\lambda^2)^{1/2}dk\ , \tag{36}$$

$$1=\frac{\lambda^2n}{\pi K}\int_0^{\pi/2}(4t^2\cos^2k+m_0^2\lambda^2)^{-1/2}dk\ , \tag{37}$$

which is the same as that of the SSP approach and mean-field theory.[7] The $\omega=0$ limit is the adiabatic limit at which Eqs. (1) and (20) can be solved exactly, and the solution is Eqs. (36) and (37). In this limit, the system is dimerized for arbitrary electron-phonon coupling constant λ.

$\omega=\infty$ limit

When $\omega=\infty,\rho=1$ for both spinless and spin-$\frac{1}{2}$ case. Thus we find $\delta_q=1,\tau_q=1$ for every q. In other words, there is no squeezing effect and dimerization for any λ. Our results in this limit become those of the SSP approach.

General ω case

Equations (1) and (20), as far as the ground-state properties are concerned, are defined by two parameters, the phonon frequency ω and electron-phonon coupling constant λ (or $J=\lambda^2/2Kt$), which are chosen as the same values as in previous papers for comparison with them. The transfer intergal t of the electron can be set to equal 1 by redefining the overall energy scale.[9] The force con-

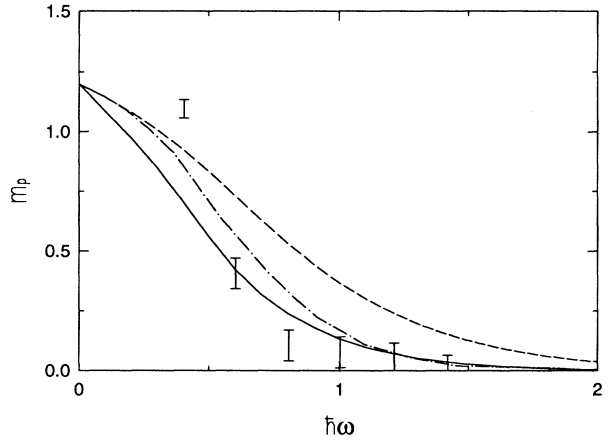

FIG. 1. m_p vs $\hbar\omega$ relation in the spinless case and $J=1.62$. The short-dashed line represents m_p for the SSP approach (Ref. 8); dot-dashed line, result of Bourbonnais and Caron (Ref. 10); error bar, Monte Carlo simulations (Ref. 9). See text for details.

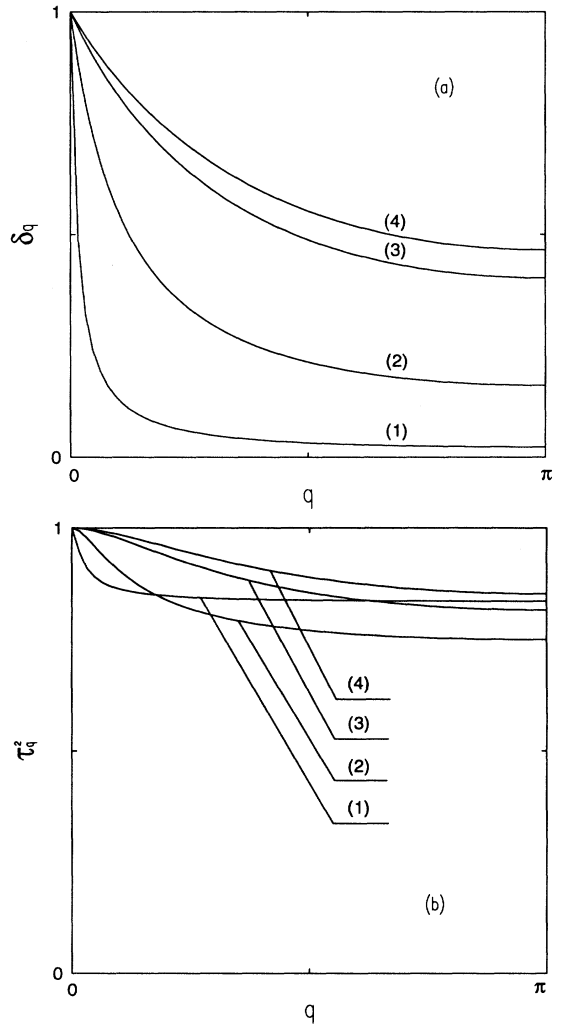

FIG. 2. (a) δ_q vs q relations in the spinless case and $J=1.62$, $\hbar\omega=0.1$ (1), 0.5 (2), 1.5 (3), and 2.0 (4), respectively. (b) τ_q^2 vs q relations in the spinless case and $J=1.62$, $\hbar\omega=0.1$ (1), 0.5 (2), 1.5 (3), and 2.0 (4), respectively.

stant K is chosen to be 0.25 throughout this paper for comparison with previous work.

1. Spinless case

In Fig. 1, we plot the phonon staggered ordering parameter m_p as a function of $\hbar\omega$ in the case of $J=1.62$. For comparison, the results by other methods are plotted. All curves coincide at $\omega=0$, where Eq. (1) can be solved exactly. In the intermediate case, our result is much smaller than that of the SSP approach. This means that the polaronic effect is strong in that case, after considering the off-site effect more precisely. Our result is in good agreement with Monte Carlo simulations[9] and the results of Bourbonnais and Caron[10] using a functional integral approach coupled to a renormalization-group procedure. When ω becomes larger, these results become the same.

In Fig. 2(a), as an example, we plot δ_q versus q relations in the case of $J=1.62$ and $\hbar\omega=0.1, 0.5, 1.5, 2.0$, respectively. All of them are monotonically decreasing functions of q. On the other hand, with increase of ω, the polaronic effect increased.

In Fig. 2(b), as an example, we plot τ_q^2 versus q relations in the case of $J=1.62$ and $\hbar\omega=0.1, 0.5, 1.5, 2.0$, respectively. All of them are monotonically decreasing functions of q. On the other hand, with the increase of ω, τ_π^2 decreased at first and then increased.

Figure 3 shows the dimerization ordering parameter m_e and narrowing factor ρ versus $\hbar\omega$ relations in the case of $J=4$. For comparison, the short-dashed and dot-dashed lines represent those of the SSP approach. The narrowing factor ρ becomes larger in our method. The critical ω of the order-disorder transition, in which m_e decreases sharply, is at a smaller value. m_e is smaller, which is the same as Fig. 1.

In Fig. 4, we plot the functional dependence of the phonon staggered ordering m_p and narrowing factor ρ on λ in the case of $\hbar\omega=2$. Also, as a comparison, the result

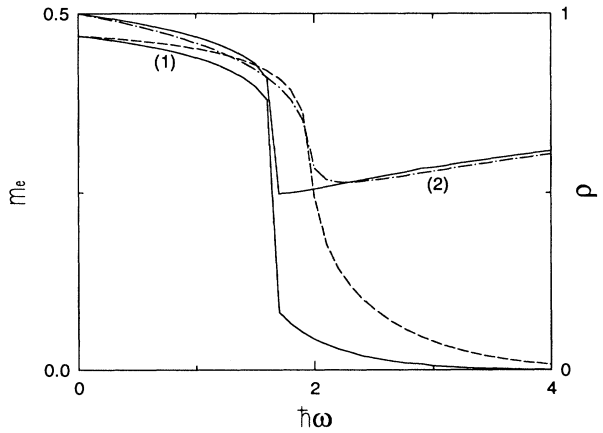

FIG. 3. m_e (1) and ρ (2) vs $\hbar\omega$ relations in the spinless case and $J=4.0$. Short-dashed and dot-dashed lines represent the results of the SSP approach (Ref. 8) for m_e and ρ, respectively.

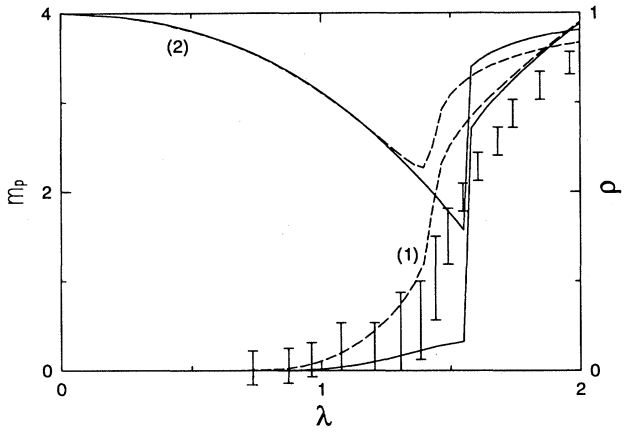

FIG. 4. m_p (1) and ρ (2) vs λ relations in the spinless case and $\hbar\omega=2.0$. Short-dashed lines represent the results of the SSP approach (Ref. 8). Error bar, Monte Carlo simulations (Ref. 9).

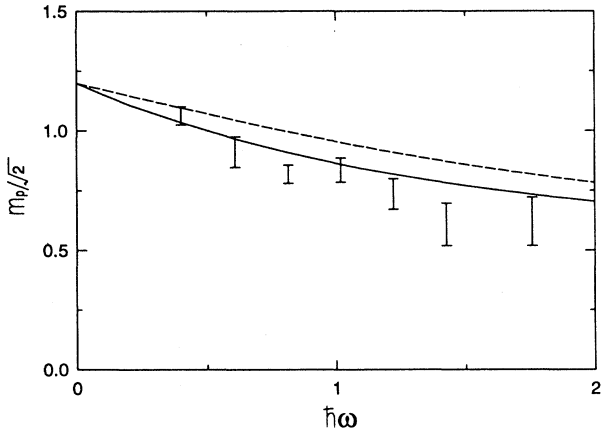

FIG. 6. $m_p/\sqrt{2}$ vs $\hbar\omega$ relation in the spin-$\frac{1}{2}$ case for $J=0.81$. Short-dashed line, the SSP approach (Ref. 8); error bar, Monte Carlo simulations (Ref. 9).

of the SSP approach is plotted. The results of these two methods are the same at large and small λ. The difference is in the intermediate region, in which m_p is much smaller and increases more rapidly at larger λ. This means that the role of off-site effects cannot be neglected in this region. Our result is in agreement with Monte Carlo simulations.

Figure 5 shows the "size" of the polaron R as a function of $\hbar\omega$ in the case of $j=4.0, 1.62, 1.0$, respectively. R becomes infinity in the $\omega=0$ limit, which means there is no polaronic effect because dimerization suppresses the polaronic effect completely. With increase of ω, the role of the polaronic effect gets stronger rapidly, which results in a sharp decrease of the polaronic "size" R. We also find that the electron-phonon coupling constant J, the weaker the polaronic effect.

2. *Spin-$\frac{1}{2}$ case*

In Fig. 6, the relation between m_p and $\hbar\omega$ is plotted in the case of $J=0.81$. For comparison, the short-dashed

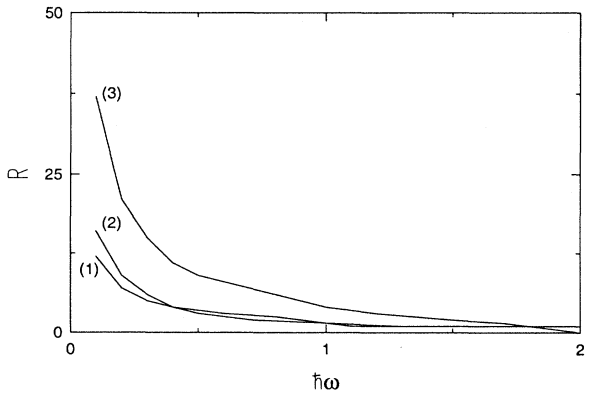

FIG. 5. Curves (1), (2), and (3) represent relations between R and $\hbar\omega$ in the spinless case and $J=1.0$, 1.62, and 4.0, respectively.

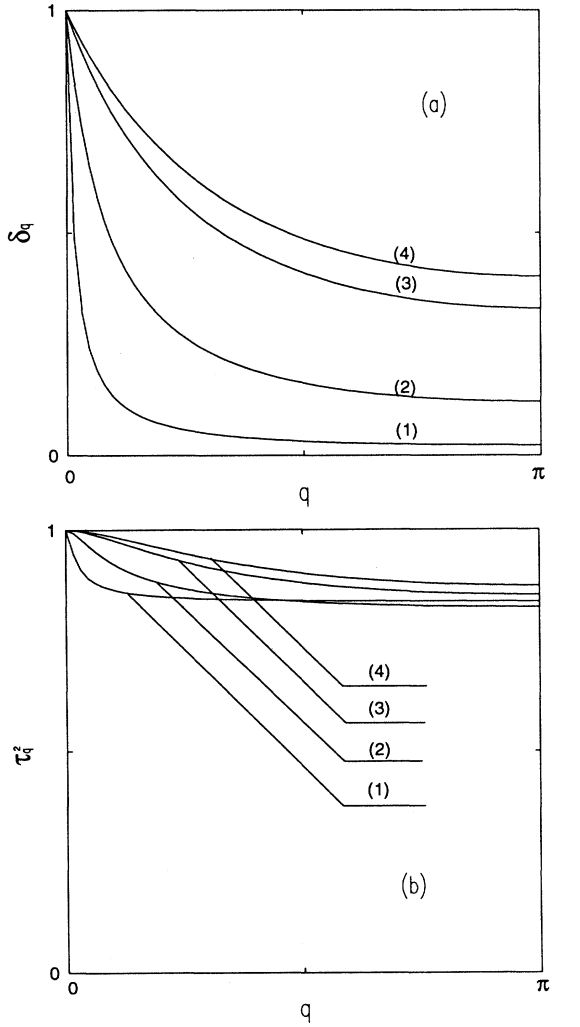

FIG. 7. (a) δ_q vs q relations in the spin-$\frac{1}{2}$ case and $J=0.81$, $\hbar\omega=0.1$ (1), 0.5 (2), 1.5 (3), and 2.0 (4), respectively. (b) τ_q^2 vs q relations in the spin-$\frac{1}{2}$ care and $J=0.81$, $\hbar\omega=0.1$ (1), 0.5 (2), 1.5 (3), and 2.0 (4), respectively.

line represents the result of the SSP approach, and the result of Monte Carlo simulations is also plotted. m_p is smaller than the SSP approach. The difference is smaller, compared with the spinless case, because there always exists a CDW state in the spin-$\frac{1}{2}$ case. Our result is in good agreement with Monte Carlo simulations.

Figure 7(a) shows δ_q as a function of mode q in the case of $J=0.81$ and $\hbar\omega=0.1,0.5,1.5,2.0$, respectively. We also note that the polaronic effect increased with increase of ω. Compared with the spinless case, δ_q is smaller, which corresponds to a slight polaronic effect.

Figure 7(b) shows τ_q^2 as a function of mode q in the case of $J=0.81$ and $\hbar\omega=0.1,0.5,1.5,2.0$, respectively. We also note that τ_π^2 decreased at first and then increased with increase of ω.

Figure 8 shows the CDW ordering parameter m_e and narrowing parameter ρ versus $\hbar\omega$ relations in the case of $J=2$. The dimerization ordering m_e falls slowly and is slightly smaller than that of the SSP approach shown as the short-dashed line. There is no order-disorder transition. ρ is the same as in the SSP approach.

We plot the dimerization parameter m_p and narrowing parameter ρ as functions of the electron-phonon coupling constant λ in the case of $\hbar\omega=2.0$ in Fig. 9. The short-dashed and dot-dashed lines are the results of the SSP approach. Our result is in good agreement with that of the SSP approach, except that there is a slight difference in the intermediate region.

Figure 10 is the polaronic "size" R as a function of $\hbar\omega$ in the case of $J=0.81$ and 2.0, respectively. The features of the polaronic "size" are similar to those in the spinless case.

IV. SUMMARY AND DISCUSSION

We have studied the properties of quasi-one-dimensional half-filled electron-phonon coupling systems

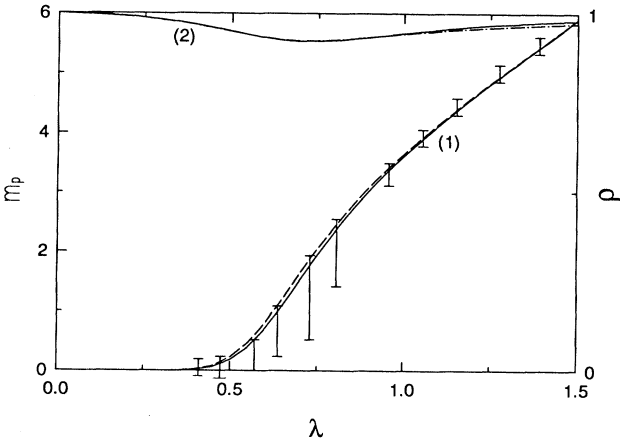

FIG. 9. m_p (1) and ρ (2) vs λ relations in the spin-$\frac{1}{2}$ case and $\hbar\omega=2.0$. Short-dashed and dot-dashed lines represent the results of the SSP approach (Ref. 8) for m_p and ρ, respectively. Error bar, Monte Carlo simulations (Ref. 9).

in the ground state by reconsidering the SSP approach. Two q-dependent functions δ_q and τ_q are introduced to take into account both the on-site and the off-site electron-phonon correlations, because the lattice motion is influenced by not only the on-site electron but also the off-site ones due to the tunneling of electrons. How to determine the functional forms of δ_q and τ_q is the central problem of this paper. By comparison between our result and previous works,[8-10] we note that our method (the details can be seen in Sec. II) is effective. As we have said, the SSP approach is actually a special case of our method. Thus these two methods become the same at $\omega=0$ and ∞ (the details can be seen in Sec. III). In the general case, a difference occurs, especially in the intermediate range where $\hbar\omega$ is of the same order of magnitude as the electronic bandwidth $W=4t$. Our results are

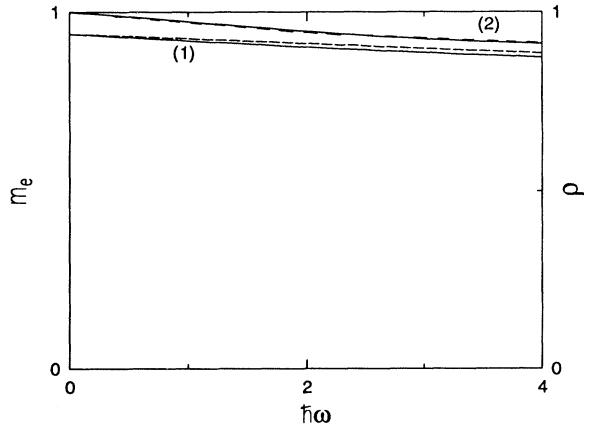

FIG. 8. m_e (1) and ρ (2) vs $\hbar\omega$ relations in the spin-$\frac{1}{2}$ case and $J=2.0$. Short-dashed lines represent the results of the SSP approach (Ref. 8).

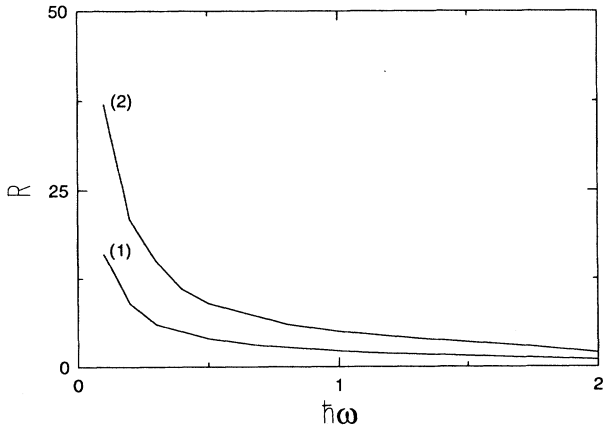

FIG. 10. Curves (1) and (2) represent the relations between R and $\hbar\omega$ in the spin-$\frac{1}{2}$ case and $J=0.81$ and 2.0, respectively.

in good agreement with those of Monte Carlo simulations and renormalization-group analysis. In this paper, we also estimate the "size" of a polaron, which represents the range of the dynamical distortion of the lattice.

In the spinless case, there is an order-disorder transition depending on the value of ω. After considering the long-range electron-phonon correlation carefully, the dimerization is reduced by a larger amount comparted with that of the SSP approach, especially in the intermediate region, and the transition point is changed to smaller ω or larger J. These features mean that the role of long-range electron-phonon correlation, which is almost neglected in the SSP approach, becomes important in the intermediate region.

In the spin-$\frac{1}{2}$ case, the long-range order dominates, for arbitrary ω. There is no order-disorder transition. The order parameter is slightly reduced by the quantum lattice fluctuations. The difference between the SSP approach and ours can be neglected, though the order parameter is a little bit smaller.

In the calculation, we find that the ground-state energy, not plotted in this paper, is almost the same as in the SSP approach. We note that the off-site electron-phonon correlation is important to the order-disorder transition in the spinless case. In contrast, the role of the off-site electron-phonon correlation is slight in the spin-$\frac{1}{2}$ case, because there exists dimerization for arbitrary ω and no obvious competition between the phonon staggered ordering and the polaronic effect.

ACKNOWLEDGMENTS

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APPENDIX

In the Appendix, we give the details of the decoupling four-fermion term in Eq. (15). Because we only take interest in the properties of the CDW case, the last term in Eq. (15) is zero, except for $q=0$, π, and $k'-k$.

Thus $H_{\rm eff}$ becomes

$$
\begin{aligned}
H_{\rm eff}=&\frac{\hbar\omega}{4}\sum_q(\tau_q^2+\tau_q^{-2})+\frac{K}{2}m_0^2N-\frac{\lambda^2}{8K}\sum_q(2\delta_q-\delta_q^2)-m_0\lambda(1-\delta_\pi)\sum_k c_k^\dagger c_{k-\pi}-2\rho t\sum_k c_k^\dagger c_k\cos k\\
&+\frac{1}{N}\sum_{k,k'}\frac{\lambda^2}{2K}\left[\delta_\pi^2-2\delta_\pi-\frac{1}{N}\sum_q(\delta_{q'}^2-2\delta_{q'})\right]c_{k-\pi}^\dagger c_k c_{k'-\pi}^\dagger c_{k'}\\
&-\frac{1}{N}\sum_{k,k'}\frac{\lambda^2}{2K}\left[\delta_{k-k'}^2-2\delta_{k-k'}-\frac{1}{N}\sum_{q'}(\delta_{q'}^2-2\delta_{q'})\right]c_k^\dagger c_k c_{k'}^\dagger c_{k'}\ .
\end{aligned}
\tag{A1}
$$

The last two terms are decoupled as follows:

$$
\begin{aligned}
&c_{k-\pi}^\dagger c_k c_{k'-\pi}^\dagger c_{k'}\approx\langle c_{k-\pi}^\dagger c_k\rangle c_{k'-\pi}^\dagger c_{k'}+c_{k-\pi}^\dagger c_k\langle c_{k'-\pi}^\dagger c_{k'}\rangle-\langle c_{k-\pi}^\dagger c_k\rangle\langle c_{k'-\pi}^\dagger c_{k'}\rangle\ ,\\
&c_k^\dagger c_k c_{k'}^\dagger c_{k'}\approx\langle c_k^\dagger c_k\rangle\langle c_{k'}^\dagger c_{k'}\rangle\ ,
\end{aligned}
\tag{A2}
$$

where $\langle\cdots\rangle$ means the averaging over the ground state of $H_{\rm eff}$, which should be determined self-consistently. We note that the charge-density-wave ordering parameter m_e is

$$
m_e=\frac{1}{N}\sum_k c_{k-\pi}^\dagger c_k\ . \tag{A3}
$$

Now, introducing the Bogoliubov transformation for $k>0$,

$$
\begin{aligned}
&\beta_{1k}=x_k c_k+y_k c_{k-\pi}\ ,\\
&\beta_{2k}=y_k c_k-x_k c_{k-\pi}\ ,\\
&x_k^2+y_k^2=1\ .
\end{aligned}
\tag{A4}
$$

After letting the nondiagonal terms $\beta_{1k}^\dagger\beta_{2k}$ and $\beta_{2k}^\dagger\beta_{1k}$ disappear, we get

$$
\begin{aligned}
&x_k=\cos\theta_k\ ,\\
&y_k=\sin\theta_k\ ,\\
&\tan 2\theta_k=-\frac{m_0\lambda(1-\delta_\pi)-(\lambda^2/K)[\delta_\pi^2-2\delta_\pi-(1/N)\sum_{q'}(\delta_{q'}^2-2\delta_{q'})]m_e}{2\rho t\cos k}\ .
\end{aligned}
\tag{A5}
$$

Here, we define the energy gap

$$\Delta = m_0\lambda(1-\delta_\pi) - \frac{\lambda^2}{K}\left[\delta_\pi^2 - 2\delta_\pi - \frac{1}{N}\sum_{q'}(\delta_{q'}^2 - 2\delta_{q'})\right] m_e \ .$$

Then

$$\langle c_k^\dagger c_k \rangle = \frac{1}{2}\left[1 + \frac{2\rho t\cos k}{\sqrt{4\rho^2 t^2\cos^2 k + \Delta^2}}\right] , \tag{A6}$$

$$m_e = \frac{1}{\pi}\int_0^{\pi/2} dk \frac{\Delta}{\sqrt{4\rho^2 t^2\cos^2 k + \Delta^2}} \ . \tag{A7}$$

Thus H_{eff} becomes

$$\begin{aligned} H_{\text{eff}} = {} & \frac{\hbar\omega}{4} N \sum_q (\tau_q^2 + \tau_q^{-2}) - \frac{\lambda^2}{2K} N \left[\delta_\pi^2 - 2\delta_\pi - \frac{1}{N}\sum_{q'}(\delta_{q'}^2 - 2\delta_{q'})\right] m_e^2 \\ & - \sum_{k>0} \sqrt{4\rho^2 t^2\cos^2 k + \Delta^2}\,(\beta_{1k}^\dagger \beta_{1k} - \beta_{2k}^\dagger \beta_{2k}) + \frac{\lambda^2}{8K}\sum_q (\delta_q^2 - 2\delta_q) + \frac{K}{2} m_0^2 N \\ & - \frac{\lambda^2}{4K}\frac{1}{N}\sum_{k'>0}\sum_{k>0} (\delta_{k'-k}^2 - 2\delta_{k'-k} + \delta_{k'+k}^2 - 2\delta_{k'+k}) \frac{2\rho t\cos k'}{\sqrt{4\rho^2 t^2\cos^2 k' + \Delta^2}} \frac{2\rho t\cos k}{\sqrt{4\rho^2 t^2\cos^2 k + \Delta^2}} \ . \end{aligned} \tag{A8}$$

Therefore, the ground state $|g\rangle$ of H_{eff} should satisfy

$$\beta_{1k}^\dagger |g\rangle = \beta_{2k}|g\rangle = 0 \ . \tag{A9}$$

m_0 can easily be derived for the ground state,

$$m_0 = \frac{\lambda(1-\delta_\pi)}{K} m_e \ . \tag{A10}$$

So we obtain the ground-state energy

$$\begin{aligned} E_g(\delta_q, \tau_q)/N = {} & \frac{\hbar\omega}{4}\frac{1}{\pi}\int_0^\pi dq(\tau_q^2 + \tau_q^{-2}) + \frac{\lambda^2}{8K} V_0 + \frac{\lambda^2}{2K}(1+V_0) m_e^2 \\ & - \frac{1}{\pi}\int_0^{\pi/2} dk \left[4\rho^2 t^2\cos^2 k + \left[(1+V_0)\frac{\lambda^2}{K} m_e\right]^2\right]^{1/2} \\ & - \frac{\lambda^2}{4K}\frac{1}{4\pi^2}\int_0^\pi dk' \int_0^\pi dk (\delta_{k'-k}^2 - 2\delta_{k'-k} + \delta_{k'+k}^2 - 2\delta_{k'+k}) \\ & \times \frac{2\rho t\cos k'}{\sqrt{4\rho^2 t^2\cos^2 k' + [(1+V_0)(\lambda^2/K) m_e]^2}} \\ & \times \frac{2\rho t\cos k}{\sqrt{4\rho^2 t^2\cos^2 k + [(1+V_0)(\lambda^2/K) m_e]^2}} \ , \end{aligned} \tag{A11}$$

where

$$V_0 = \frac{1}{\pi}\int_0^\pi dq(\delta_q^2 - 2\delta_q) \ .$$

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