Quantum lattice fluctuations in the ground state of an *XY* spin-Peierls chain

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An analytical approach, based on the unitary transformation method, has been developed to study the effect of quantum lattice fluctuations on the ground state of an *XY* spin-Peierls chain, which is equivalent to the spinless Su-Schrieffer-Heeger model in half-filling after the Jordan-Wigner transformation. We show that when the spin-phonon coupling constant $\alpha^2/4K$ decreases or the phonon frequency ω_π increases, the lattice dimerization and the gap in the fermion spectrum decrease gradually. At some critical value $(\alpha^2/4K)_c$ or $\omega_{\pi c}$, the system becomes gapless and the lattice dimerization disappears. This can be attributed to the fact that the ground state fails to develop the spin-Peierls long-range order because of the quantum lattice fluctuations. [S0163-1829(97)03545-5]

I. INTRODUCTION

Recently the physics of quasi-one-dimensional spin-Peierls systems has attracted considerable interests of both theoretists and experimentalists because of the discovery of a spin-Peierls transition at $T_{SP}\approx 14$ K in the cuprate compound $CuGeO_3$.[1] Below T_{SP} the lattice is dimerized[2] and a spin gap has been observed.[3]

From the theoretical viewpoint the quasi-one-dimensional spin-Peierls system can be described by the Heisenberg antiferromagnetic chain coupled with lattice phonons. Within the adiabatic approximation, that is, treating the phonon degrees of freedom classically, Bray *et al.*[4] and Cross and Fisher[5] treated this type of model systems and uncovered some interesting physics. But the nonadiabatic effect related to the finite phonon frequency, which tends to decrease the Peierls transition temperature and the order parameter, was not taken into account. Very recently, Caron and Moukouri[6] suggested studying the effect of quantum lattice fluctuations in the spin-Peierls system by starting from an *XY* spin chain in which the phonons interact with the spins by modifying the magnetic interaction,

$$H=\sum_l [J+\alpha(u_l-u_{l-1})]\{S_l^X S_{l+1}^X+S_l^Y S_{l+1}^Y\} + \sum_l \left(\frac{1}{2M}p_l^2+\frac{K}{2}(u_l-u_{l+1})^2\right). \quad (1)$$

Here, S_l^X and S_L^Y are the spin-$\frac{1}{2}$ operators on site l, $J>0$ is the usual antiferromagnetic exchange energy, α is the spin-phonon coupling constant, u_l and p_l are the displacement and momentum operators of the magnetic ion on site l. M is the mass of the magnetic ion and K the spring constant. By using the Jordan-Wigner transformation[7]

$$S_l^+=f_l^\dagger \exp\left(i\pi\sum_{n<l} f_n^\dagger f_n\right),$$

$$S_l^-=f_l \exp\left(-i\pi\sum_{n<l} f_n^\dagger f_n\right),$$

$$S_l^Z=f_l^\dagger f_l-\frac{1}{2}, \quad (2)$$

where $f_l^\dagger$ and f_l are spinless fermion operators, we can get

$$H=-\frac{1}{2}\sum_l [J+\alpha(u_l-u_{l+1})](f_l^\dagger f_{l+1}+f_{l+1}^\dagger f_l) + \sum_l \left(\frac{1}{2M}p_l^2+\frac{K}{2}(u_l-u_{l+1})^2\right). \quad (3)$$

This is a Hamiltonian for Jordan-Wigner fermions in a half-filled band. Note that it is the spinless version of the Su-Schrieffer-Heeger model[8] which was introduced in the studies of properties of a quasi-one-dimensional electron-phonon system such as polyacetylene. As pointed out by Caron and Moukouri, this may be the simplest model but contains the essential elements for a spin-Peierls system. In this work we start from this model.

Within the adiabatic approximation the model can be solved easily. In the half-filled case the system undergoes a Peierls instability and the ground state is dimerized with an energy gap 2Δ at the Fermi points $k=\pm\pi/2$.[8] The theoretical analysis becomes much more difficult when the quantum lattice fluctuations are taken into account. Fradkin and Hirsch[9] have calculated the electronic and lattice structure of the half-filled SSH model by the Monte Carlo simulations, and concluded that for spinless fermions quantum lattice fluctuations destroy the Peierls dimerization for a small coupling constant if the ionic mass is finite. Caron and Moukouri[6] calculated the $T=0$ K phase diagram of the system by using the density matrix renormalization group (DMRG) method. Their results showed a power-law dependence of the critical spin-phonon coupling on the phonon frequency for the onset of a spin gap. They also observed a classical quantum crossover when the spin-Peierls gap 2Δ is of order ω_π.

In this work, we use the unitary transformation to take into account the fermion-phonon correlation[10] and show that when $\omega_\pi > 0$ there may exist a static dimerization of the lattice but the quantum lattice fluctuations play a very important role. When the spin-phonon coupling constant $\alpha^2/4K$ decreases or the phonon frequency ω_π increases the lattice dimerization and the spin gap decrease gradually. At some critical value $(\alpha^2/4K)_c$ or $\omega_{\pi c}$, the dimerization disappears and the system becomes gapless. This can be attributed to the fact that the ground state fails to develop a spin-Peierls long-range order because of the quantum lattice fluctuations. Throughout this paper we put $\hbar = 1$ and $k_B = 1$.

II. THEORETICAL ANALYSIS

In Hamiltonian (3) the operators of the latttice modes, u_l and p_l, can be expanded by using the phonon creation and annihilation operators,

$$u_l = \sum_q \sqrt{\frac{1}{2MN\omega_q}} (b^\dagger_{-q} + b_q)\exp(iql), \tag{4}$$

$$p_l = i\sum_q \sqrt{\frac{M\omega_q}{2N}} (b^\dagger_{-q} - b_q)\exp(iql). \tag{5}$$

N is the total number of sites. $\omega_q^2 = (4K/M)\sin^2(q/2)$. Then H becomes

$$H = \sum_k \epsilon_k f^\dagger_k f_k + \sum_q \omega_q b^\dagger_q b_q + \frac{1}{\sqrt{N}} \sum_{k,q} g(k+q,k)(b^\dagger_{-q} + b_q) f^\dagger_{k+q} f_k, \tag{6}$$

where $\epsilon_k = -J\cos(k)$ is the band function. The coupling function $g(k+q,k)$ is

$$g(k+q,k) = -i\alpha\sqrt{\frac{1}{2M\omega_q}}\,[\sin k - \sin(k+q)]. \tag{7}$$

In order to take into account the fermion-phonon correlation a unitary transformation is applied to H,

$$H' = \exp(S) H \exp(-S), \tag{8}$$

where the generator S is

$$S = \frac{1}{\sqrt{N}} \sum_{k,q} \frac{g(k+q,k)}{\omega_q} (b^\dagger_{-q} - b_q)\,\delta(k+q,k) f^\dagger_{k+q} f_k. \tag{9}$$

Here we introduce a function $\delta(k',k)$ which is a function of the energies of the incoming and outgoing fermions in the fermion-phonon scattering process. The form of $\delta(k',k)$ will be defined later. We divide the original Hamiltonian into $H = H^0 + H^1$, where H^0 contains the first two terms and H^1 the last term. Then the transformation can proceed order by order,

$$H' = H^0 + H^1 + [S,H^0] + [S,H^1] + \frac{1}{2}[[H^0,S],S] + O(\alpha^3).$$

The first-order terms in H' are

$$H^1 + [S,H^0] = \frac{1}{\sqrt{N}} \sum_{k,q} g(k+q,k)(b^\dagger_{-q} + b_q) f^\dagger_{k+q} f_k - \frac{1}{\sqrt{N}} \sum_{k,q} g(k+q,k)\,\delta(k+q,k)(b^\dagger_{-q} + b_q) f^\dagger_{k+q} f_k + \frac{1}{\sqrt{N}} \sum_{k,q} \frac{g(k+q,k)}{\omega_q} (\epsilon_k - \epsilon_{k+q})\,\delta(k+q,k)(b^\dagger_{-q} - b_q) f^\dagger_{k+q} f_k. \tag{10}$$

Now we can choose the functional form of $\delta(k+q,k)$ to make the contribution of these first-order terms as small as possible. Note that the ground state $|g_0\rangle$ of H^0, the noninteracting system, is a direct product of a filled Fermi sea $|\mathrm{FS}\rangle$ and a phonon vacuum state $|\mathrm{ph},0\rangle$:

$$|g_0\rangle = |\mathrm{FS}\rangle|\mathrm{ph},0\rangle. \tag{11}$$

Applying the first-order terms on $|g_0\rangle$ we get

$$(H^1 + [S,H^0])|g_0\rangle = \frac{1}{\sqrt{N}} \sum_{k,q} g(k+q,k) b^\dagger_{-q} f^\dagger_{k+q} f_k \left(1 - \delta(k+q,k) + \frac{\epsilon_k - \epsilon_{k+q}}{\omega_q}\,\delta(k+q,k)\right)|g_0\rangle, \tag{12}$$

since $b_q|\mathrm{ph},0\rangle = 0$. As the band is half-filled the Fermi energy $\epsilon_F = 0$. Thus $f^\dagger_{k+q} f_k|\mathrm{FS}\rangle \neq 0$ only if $\epsilon_{k+q} \geq 0$ and $\epsilon_k \leq 0$. So, if we choose

$$\delta(k+q,k) = 1/(1 + |\epsilon_{k+q} - \epsilon_k|/\omega_q), \tag{13}$$

we have

$$(H^1+[S,H^0])|g_0\rangle=0. \tag{14}$$

We believe that this form of $\delta(k',k)$ makes the contribution of first-order terms as small as possible. The second-order terms in H' can be collected as follows:

$$\begin{aligned}[S,H^1]+\frac{1}{2}[[H^0,S],S]=&\frac{1}{2N}\sum_{q,q'}\sum_{k,k'}\frac{g(k+q,k)g(k'+q',k')}{\omega_q\omega_{q'}}(b^\dagger_{-q}-b_q)(b^\dagger_{-q'}-b_{q'})(\epsilon_{k+q}-\epsilon_k)\delta(k+q,k)\delta(k'+q',k')\\
&\times[f^\dagger_{k+q}f_{k'}\delta_{k'+q',k}-f^\dagger_{k'+q'}f_k\delta_{k+q,k'}]+\frac{1}{2N}\sum_{q,q'}\sum_{k,k'}\frac{g(k+q,k)g(k'+q',k')}{\omega_q}(b^\dagger_{-q}-b_q)\\
&\times(b^\dagger_{-q'}+b_{q'})[2\delta(k+q,k)-\delta(k+q,k)\delta(k'+q',k')][f^\dagger_{k+q}f_{k'}\delta_{k'+q',k}-f^\dagger_{k'+q'}f_k\delta_{k+q,k'}]\\
&-\frac{1}{N}\sum_q\sum_{k,k'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}[2\delta(k+q,k)-\delta(k+q,k)\delta(k'-q,k')]f^\dagger_{k+q}f_kf^\dagger_{k'-q}f_{k'}.\end{aligned} \tag{15}$$

$\delta_{k'+q',k}$ is the Kronecker δ symbol. All terms of higher order than α^2 will be omitted in the following treatment.

Then we make a displacement transformation to H' to take into account the static phonon-staggered ordering,

$$\widetilde{H}=\exp(R)H'\exp(-R). \tag{16}$$

Here

$$R=-\sum_l(-1)^l u_0\sqrt{\frac{M\omega_\pi}{2}}(b^\dagger_l-b_l) \tag{17}$$

and $\exp(R)$ is a displacement operator:

$$\exp(R)u_l\exp(-R)=(-1)^l u_0+\sum_q\sqrt{\frac{1}{2MN\omega_q}}(b^\dagger_{-q}+b_q)\exp(iql). \tag{18}$$

If the ground state of H is $|g\rangle$, then the ground state of $\widetilde{H}$ is $|g'\rangle:|g\rangle=\exp(-S)\exp(-R)|g'\rangle$. We assume that for $|g'\rangle$ the fermions and phonons can be decoupled: $|g'\rangle\approx|fe\rangle|ph,0\rangle$, where $|fe\rangle$ is the ground state for fermions. After averaging $\widetilde{H}$ over the phonon vacuum state we get an effective Hamiltonian for the fermions,

$$\begin{aligned}H_{\rm eff}=\langle{\rm ph},0|\widetilde{H}|{\rm ph},0\rangle=&2Ku_0^2N+\sum_k E_0(k)f^\dagger_kf_k+\sum_{k>0}i\Delta_0(k)(f^\dagger_kf_{k-\pi}-f^\dagger_{k-\pi}f_k)\\
&-\frac{1}{N}\sum_q\sum_{k,k'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}\delta(k+q,k)[2-\delta(k'-q,k')]f^\dagger_{k+q}f_kf^\dagger_{k'-q}f_{k'},\end{aligned} \tag{19}$$

where

$$E_0(k)=\epsilon_k-\frac{1}{N}\sum_{k'}(\epsilon_k-\epsilon_{k'})\frac{|g(k',k)|^2}{\omega^2_{k'-k}}\delta^2(k',k), \tag{20}$$

$$\Delta_0(k)=2\alpha u_0\sin(k)[1-\delta(k,k-\pi)]. \tag{21}$$

We find by means of the variational principle

$$u_0=-\frac{i}{4KN}\sum_{k>0}2\alpha\sin(k)[1-\delta(k,k-\pi)]\langle fe|f^\dagger_kf_{k-\pi}-f^\dagger_{k-\pi}f_k|fe\rangle. \tag{22}$$

We note that in the adiabatic limit where $\omega_\pi=0$ one has $\delta(k',k)=0$ and $H_{\rm eff}$ goes back to the adiabatic mean-field Hamiltonian,

$$H_{\rm eff}(\omega_\pi=0)=2Ku_0^2N+\sum_k\epsilon_kf^\dagger_kf_k+\sum_{k>0}i2\alpha u_0\sin(k)(f^\dagger_kf_{k-\pi}-f^\dagger_{k-\pi}f_k). \tag{23}$$

On the other hand, in the antiadiabatic limit where $\omega_\pi\to\infty$, we have $u_0=0$, $\delta(k',k)=1$, and $H_{\rm eff}$ becomes

$$H_{\rm eff}(\omega_\pi\to\infty)=\sum_k \epsilon_k f_k^\dagger f_k-\frac{1}{N}\sum_q\sum_{k,k'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}f_{k+q}^\dagger f_k f_{k'-q}^\dagger f_{k'}. \tag{24}$$

Returning to the real space, this Hamiltonian is

$$H_{\rm eff}(\omega_\pi\to\infty)=-\frac{J}{2}\sum_l (f_l^\dagger f_{l+1}+f_{l+1}^\dagger f_l)+\frac{\alpha^2}{4K}\sum_l (f_l^\dagger f_l f_{l+1}^\dagger f_{l+1}-f_l^\dagger f_l). \tag{25}$$

This is the antiferromagnetic XXZ model (through Jordan-Wigner transformation).[9] It can be solved exactly and there exists a transition point at $\alpha^2/4K=J$.[11] Thus our effective Hamiltonian works well in these two limits. When $0<\omega_\pi<\infty$, we have $0<\delta(k',k)<1$ and our effective Hamiltonian $H_{\rm eff}$ is complicated and evolves from the adiabatic limit to the antiadiabatic limit.

The last term in $H_{\rm eff}$ is a four-fermion interaction. As we are dealing with a one-dimensional system, how to treat the four-fermion interaction is a difficult problem. Since the case for the small ω_π, $\omega_\pi<2J$, is very different from that for the large ω_π, $\omega_\pi>2J$, we treat $H_{\rm eff}$ in these two cases with different methods.

III. $\omega_\pi<2J$

In this case we let $H_{\rm eff}=H_{\rm eff}^0+H_{\rm eff}'$, where

$$H_{\rm eff}^0=2Ku_0^2N+\sum_k E_0(k)f_k^\dagger f_k+\sum_{k>0} i\Delta_0(k)(f_k^\dagger f_{k-\pi}-f_{k-\pi}^\dagger f_k) \tag{26}$$

contains a gap term (so it describes an insulating state). $H_{\rm eff}^0$ will be treated as an unperturbed Hamiltonian. $H_{\rm eff}'$ contains all four-fermion terms and will be treated as a perturbation since it is small at least for $\omega_\pi\ll 2J$ ($H_{\rm eff}'=0$ when $\omega_\pi/2J=0$). Usually people think that for the fermionic metallic state in one dimension the perturbation theory is not suitable for treating the four-fermion interaction.[12] But for the gapped state (insulating state) I believe the perturbation theory is still a good one. In this work, the perturbative results will be justified by the good agreement with the DMRG results of Caron and Moukouri.[6]

The four-fermion terms can be rewritten as

$$\begin{aligned}H_{\rm eff}'=&-\frac{1}{N}\sum_{q\neq 0}\sum_{k,k'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}\delta(k+q,k)[2-\delta(k'-q,k')](f_{k+q}^\dagger f_k-f_{k+q-\pi}^\dagger f_{k-\pi})(f_{k'-q}^\dagger f_{k'}-f_{k'-q-\pi}^\dagger f_{k'-\pi})\\&+\frac{1}{N}\sum_q\sum_{k,k'}\frac{g(k+q,k-\pi)g(k'-q,k'-\pi)}{\omega_{q-\pi}}\delta(k+q,k-\pi)[2-\delta(k'-q,k'-\pi)](f_{k+q}^\dagger f_{k-\pi}f_{k'-q-\pi}^\dagger f_{k'}\\&+f_{k+q-\pi}^\dagger f_k f_{k'-q}^\dagger f_{k'-\pi})-\frac{1}{N}\sum_q\sum_{k,k'}\frac{g(k+q,k-\pi)g(k'-q,k'-\pi)}{\omega_{q-\pi}}\delta(k+q,k-\pi)[2-\delta(k'-q,k'-\pi)]\\&\times(f_{k+q}^\dagger f_{k-\pi}f_{k'-q}^\dagger f_{k'-\pi}+f_{k+q-\pi}^\dagger f_k f_{k'-q-\pi}^\dagger f_{k'}).\end{aligned} \tag{27}$$

In these terms we have the constraints

$$k+q>0,\quad k>0,\quad k'-q>0,\quad k'>0.$$

We can distinguish between different physical processes. The first term in Eq. (27) is the forward scattering one (g_2 and g_4 terms in the g-ology language),[13] the second is the back scattering one (g_1 term), and the last is the Umklapp scattering one (g_3 term). $q\neq 0$ in the first term means that there are no phonons of $q=0$.

We use the Green's function method to implement the perturbation treatment.[14] It is more convenient to work within a two-component representation,

$$\Psi_k=\begin{pmatrix} f_k \\ f_{k-\pi}\end{pmatrix}, \tag{28}$$

in which $k>0$. Thus the Hamiltonian becomes

$$H_{\rm eff}^0=2Ku_0^2N+\sum_{k>0}E_0(k)\Psi_k^\dagger\sigma_z\Psi_k+\sum_{k>0}i\Delta_0(k)\Psi_k^\dagger i\sigma_y\Psi_k, \tag{29}$$

$$H'_{\rm eff}=-\frac{1}{N}\sum_{q\neq 0}\sum_{k,k'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}\delta(k+q,k)[2-\delta(k'-q,k')]\Psi^{\dagger}_{k+q}\sigma_z\Psi_k\Psi^{\dagger}_{k'-q}\sigma_z\Psi_{k'}$$
$$-\frac{1}{2N}\sum_{q}\sum_{k,k'}\frac{g(k+q,k-\pi)g(k'-q,k'-\pi)}{\omega_{q-\pi}}\delta(k+q,k-\pi)[2-\delta(k'-q,k'-\pi)]$$
$$\times(\Psi^{\dagger}_{k+q}i\sigma_y\Psi_k\Psi^{\dagger}_{k'-q}i\sigma_y\Psi_{k'}-\Psi^{\dagger}_{k+q}\sigma_x\Psi_k\Psi^{\dagger}_{k'-q}\sigma_x\Psi_{k'})-\frac{1}{2N}\sum_{q}\sum_{k,k'}\frac{g(k+q,k-\pi)g(k'-q,k'-\pi)}{\omega_{q-\pi}}$$
$$\times\delta(k+q,k-\pi)[2-\delta(k'-q,k'-\pi)](\Psi^{\dagger}_{k+q}i\sigma_y\Psi_k\Psi^{\dagger}_{k'-q}i\sigma_y\Psi_{k'}+\Psi^{\dagger}_{k+q}\sigma_x\Psi_k\Psi^{\dagger}_{k'-q}\sigma_x\Psi_{k'}). \tag{30}$$

σ_β ($\beta=x,y,z$) is the Pauli matrix. The matrix Green's function is defined as (the temperature Green's function is used and at the end $T\to 0$)

$$G(k,\tau)=-\langle T_\tau\Psi_k(\tau)\Psi^{\dagger}_k(0)\rangle=T\sum_n \exp(-i\omega_n\tau)G(k,\omega_n). \tag{31}$$

The Dyson equation is

$$G(k,\omega_n)=G_0(k,\omega_n)+G_0(k,\omega_n)\Sigma(k,\omega_n)G(k,\omega_n), \tag{32}$$

where

$$G_0(k,\omega_n)=\{i\omega_n-E_0(k)\sigma_z+\Delta_0(k)\sigma_y\}^{-1} \tag{33}$$

is the unperturbed Green's function. The self-energy $\Sigma(k,\omega_n)$ can be calculated by the perturbation theory,[14]

$$\Sigma(k,\omega_n)=-\frac{T}{N}\sum_{k'>0}\sum_{m}\frac{g(k,k-\pi)g(k',k'-\pi)}{\omega_\pi}[\delta(k)+\delta(k')-\delta(k)\delta(k')]\{\mathrm{Tr}[i\sigma_yG_0(k',\omega_m)]i\sigma_y$$
$$+\mathrm{Tr}[\sigma_xG_0(k',\omega_m)]\sigma_x\}+\frac{T}{N}\sum_{k'>0}\sum_{m}\frac{|g(k',k)|^2}{\omega_{k'-k}}\delta(k',k)[2-\delta(k,k')]\{G_0(k',\omega_m)+\sigma_zG_0(k',\omega_m)\sigma_z\}$$
$$+\frac{T}{N}\sum_{k'>0}\sum_{m}\frac{g(k',k-\pi)g(k,k'-\pi)}{\omega_{k'-k-\pi}}\delta(k',k-\pi)[2-\delta(k,k'-\pi)]\{i\sigma_yG_0(k',\omega_m)i\sigma_y-\sigma_xG_0(k',\omega_m)\sigma_x\}. \tag{34}$$

Here $\delta(k)=\delta(k,k-\pi)$ and $\mathrm{Tr}[\cdots]$ is the trace of $\cdots$. When making the perturbation calculation we have taken into account the fact that the forward and back scattering term contribute nothing to the ''charge'' gap.[12] Then, by using the Dyson equation we can get

$$G(k,\omega_n)=\{i\omega_n-E(k)\sigma_z+\Delta(k)\sigma_y\}^{-1}. \tag{35}$$

From $G(k,\omega_n)$ the fermionic spectrum in the gapped state can be derived

$$W(k)=\sqrt{E^2(k)+\Delta^2(k)}. \tag{36}$$

The renormalized band function is

$$E(k)=E_0(k)-\frac{1}{N}\sum_{k'>0}\frac{\alpha^2}{2K}\left[\cos^2\left(\frac{k'+k}{2}\right)\delta(k',k)[2-\delta(k',k)]\right.$$
$$\left.-\sin^2\left(\frac{k'+k}{2}\right)\delta(k'-\pi,k)[2-\delta(k'-\pi,k)]\right]\frac{E_0(k')}{\sqrt{E_0^2(k')+\Delta_0^2(k')}}. \tag{37}$$

The gap function is

$$\Delta(k)=2\alpha u_0\sin(k)[c-d\,\delta(k)], \tag{38}$$

where

$$c=1+\frac{1}{N}\sum_{k>0}\frac{\alpha^2}{2K}\sin(k)\delta(k)\frac{\Delta_0(k)}{2\alpha u_0\sqrt{E_0^2(k)+\Delta_0^2(k)}}, \tag{39}$$

$$d=1-\frac{1}{N}\sum_{k>0}\ \frac{\alpha^2}{2K}\sin(k)[1-\delta(k)]\ \frac{\Delta_0(k)}{2\alpha u_0\sqrt{E_0^2(k)+\Delta_0^2(k)}}. \tag{40}$$

The equation to determine u_0 is

$$1=\frac{2}{N}\sum_{k>0}\ \frac{\alpha^2}{2K}\sin(k)[1-\delta(k)]\ \frac{\Delta(k)}{2\alpha u_0 W(k)}. \tag{41}$$

In the nonadiabatic case u_0 is a variational parameter and cannot be measured by experiment or Monte Carlo simulations. The quantity which can be measured is m_p,

$$\begin{aligned} m_p&=\frac{1}{N}\sum_l\ \langle(-1)^l u_l\rangle=\frac{1}{N}\sum_l\ (-1)^l\sum_q\ \sqrt{\frac{1}{2MN\omega_q}}\,\langle g|(b_{-q}^{\dagger}+b_q)e^{iql}|g\rangle \\ &=\frac{1}{N}\sum_l\ (-1)^l\sum_q\ \sqrt{\frac{1}{2MN\omega_q}}\,\langle g'|e^R e^S(b_{-q}^{\dagger}+b_q)e^{iql}e^{-S}e^{-R}|g'\rangle \\ &=u_0-\frac{1}{N}\sum_{k>0}\ \sqrt{\frac{2}{M\omega_\pi}}\frac{g(k,k-\pi)}{\omega_\pi}\,\delta(k)\langle fe|\Psi_k i\sigma_y\Psi_k|fe\rangle \\ &=\frac{u_0}{N}\sum_{k>0}\ \frac{\alpha^2}{K}\sin(k)\ \frac{\Delta(k)}{2\alpha u_0 W(k)}. \end{aligned} \tag{42}$$

These are basic equations for the $\omega_\pi<2J$ case. If $\omega_\pi=0$ we have $\delta(k',k)=0$ and $c=1$, Eq. (41) becomes the same as that in the adiabatic theory. In our theory $\delta(k)$ has a sharp peak at the Fermi point and, since

$$1-\delta(k)=\frac{2J|\cos(k)|}{\omega_\pi+2J|\cos(k)|}, \tag{43}$$

the logarithmic singularity in the integration of Eq. (41) in the adiabatic case is removed by the factor $1-\delta(k)$ as long as the ratio ω_π/J is finite.

Comparing Eq. (38) with that in the adiabatic case, $\Delta(k)=2\alpha u_0\sin(k)$, we have the gap in the nonadiabatic case,

$$\Delta=\Delta(\pi/2)=2\alpha u_0(c-d). \tag{44}$$

This is the true gap in the fermionic spectrum. Figure 1 shows the density of states (DOS) of fermions,

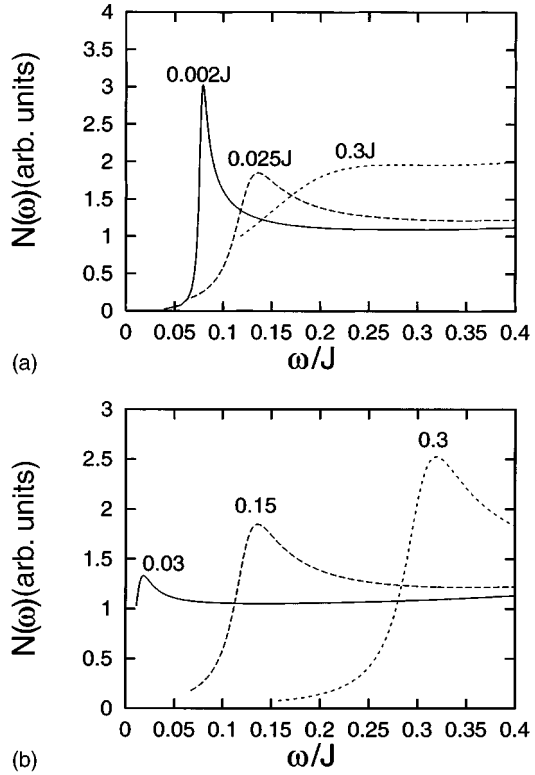

FIG. 1. The density of states of fermions for (a) $g^2-g_c^2=0.15$ with $\omega_\pi=0.002J$, $0.025J$, and $0.3J$, and (b) $\omega_\pi=0.025J$ with $g^2-g_c^2=0.03$, 0.15, and 0.3.

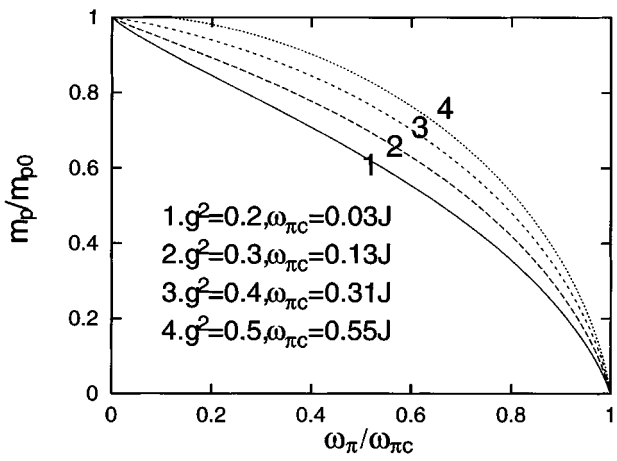

FIG. 2. The normalized dimerization parameter m_p/m_{p0} as functions of the normalized phonon frequency $\omega_\pi/\omega_{\pi c}$ for $g^2=0.2$ (curve 1), 0.3 (2), 0.4 (3), and 0.5 (4).

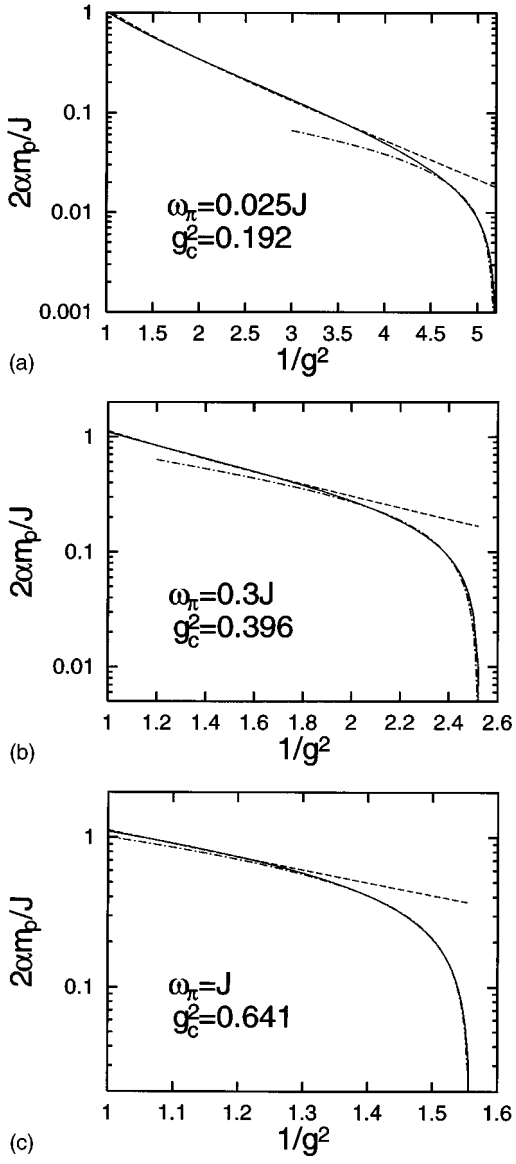

FIG. 3. The dimerization parameter $2\alpha m_p/J$ as functions of the coupling constant g^2 in the cases of (a) $\omega_\pi=0.025J$, (b) $0.3J$, and (c) J. The solid lines are results of our theory, the dashed lines are fitted results of Eq. (46), and the dash-dotted lines are fitted results of Eq. (47).

$$N(\omega)=\frac{1}{N}\sum_k \delta[\omega-\sqrt{E^2(k)+\Delta^2(k)}], \tag{45}$$

for some ω_π and $g^2=\alpha^2/4KJ$ values. One can see that a nonzero DOS starts from the gap edge and, for smaller values of ω_π/J, there is a peak above the gap edge with a significant tail between it and the true gap edge. The inverse-square-root singularity at the gap edge in the adiabatic case[8] disappears.

The adiabatic theory predicts a ratio $\Delta/\alpha m_p=2$.[6,8,9] But our calculations show that $\Delta/\alpha m_p$ is around or smaller than 1 when $\omega_\pi>0$. The DMRG results of Caron and Moukouri[6] is similar to ours. This fact seems to indicate that there might be a discontinuous transition of the ratio between $\omega_\pi=0$ and $\omega_\pi>0$. But if we use the peak position in the DOS, $\omega_{\rm peak}$, to calculate the ratio $\omega_{\rm peak}/\alpha m_p$ there will be no discontinuity

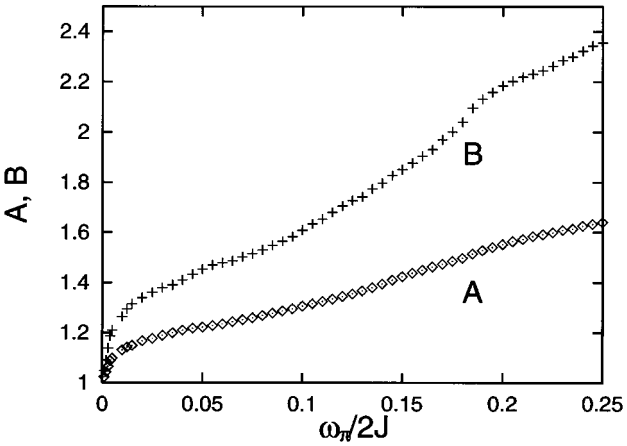

FIG. 4. The values of fitting parameters A and B in Eq. (46).

because, for smaller ω_π, $\omega_{\rm peak}\approx 2\Delta$. From an experimental view point, when $\omega_\pi/J\ll 1$, detection of the true gap may be difficult and could be misinterpreted.

We list some of our numerical results in following figures. Note that the fermion-phonon coupling α used in this work is different from that of Caron and Moukouri[6] (theirs is denoted as $\alpha_{\rm c.m.}$): $\alpha=\alpha_{\rm c.m.}\sqrt{2M\omega_\pi}$. Besides, they used dispersionless phonons with frequency $\omega_{\rm c.m.}$ and we assume $\omega_{\rm c.m.}=\omega_\pi$. Thus we have the relation $\alpha_{\rm c.m.}^2/J^2=g^2\omega_\pi/2J$.

Figure 2 shows the normalized dimerization parameter m_p/m_{p0} (m_{p0} is the adiabatic value when $\omega_\pi=0$) as functions of the normalized phonon frequency $\omega_\pi/\omega_{\pi c}$ ($\omega_{\pi c}$ is the critical frequency of the transition) for several coupling constant g^2 values. It is obvious that quantum lattice fluctuations reduce the dimerization gradually as ω_π increases. The behavior is not universal with respect to different g^2. For smaller g^2, it is easier to reduce the long-range dimerization order than for larger one. In the figure the corresponding values of the critical frequency $\omega_{\pi c}$ are listed.

Figure 3 shows the dimerization parameter $2\alpha m_p/J$ as functions of the coupling constant g^2 in the cases of $\omega_\pi=0.025J$, $0.3J$, and J. As pointed out by Caron and Moukouri,[6] there exists a classical-quantum crossover when $2\alpha m_p\sim\omega_\pi$. For the classical region where $2\alpha m_p>\omega_\pi$ the behavior of the dimerization m_p as a function of g^2 can be described by the form of an adiabatic mean-field solution,

$$\frac{1}{g^2}=\frac{4}{A\pi}\left(1-\frac{4\alpha^2m_p^2}{J^2B^2}\right)^{-1}\left(K\left[1-\frac{4\alpha^2m_p^2}{J^2B^2}\right]-E\left[1-\frac{4\alpha^2m_p^2}{J^2B^2}\right]\right), \tag{46}$$

but the mean-field parameters are renormalized by the quantum lattice fluctuations. In Eq. (46) $E[m]$ and $K[m]$ are first- and second-type complete elliptic functions. A and B are fitting parameters and in the adiabatic case $A=1$ and $B=1$. In Fig. 4 we show the fitted values of A and B for $\omega_\pi\leqslant 0.5J$. Both A and B increase with increasing ω_π, however, in our case $A<B$ but in Caron and Moukouri's work $A>B$.

For the quantum region where $2\alpha m_p<\omega_\pi$ we use the form

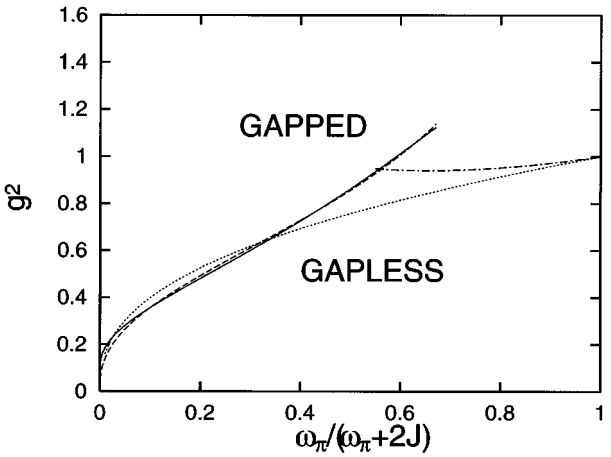

FIG. 5. The phase diagram. See text for details.

$$\frac{2\alpha m_p}{J}\propto(g^2-g_c^2)^{0.5}\exp[-b(g^2-g_c^2)^{-0.5}] \tag{47}$$

to fit our calculations, where b is a fitting parameter. We find that the form used by Caron and Moukouri,[6]

$$\frac{2\alpha m_p}{J}\propto(g^2-g_c^2)^{-0.5}\exp[-b(g^2-g_c^2)^{-0.5}], \tag{48}$$

is not good for fitting our calculations compared with the form of Eq. (47). We believe this is because of the retardation effect of the spin-phonon interaction.

Figure 5 shows the phase diagram. We use $\omega_\pi/(\omega_\pi+2J)$, instead of ω_π, as the variable because it goes to 1 when $\omega_\pi\to\infty$. The solid line is the result of this section. The dashed line is

$$g_c^2=0.857\,125\left[\frac{\omega_\pi}{2J}\right]^{0.4}. \tag{49}$$

We can see that a power law is quite good to fit our calculations. The power-law relationship $g_c^2\sim\omega_\pi^{0.4}$ is the result of Caron and Moukouri[6] [they showed $(\alpha_{\text{c.m.}}^2)_c\sim\omega_{\text{c.m.}}^{1.4}$ and we have the relation $\alpha_{\text{c.m.}}^2/J^2=g^2\omega_\pi/2J$ and $\omega_{\text{c.m.}}=\omega_\pi$].

IV. $\omega_\pi>2J$

In this case H_{eff} can be rewritten as

$$H_{\text{eff}}=2Ku_0^2N+\sum_k\rho_0\epsilon_k f_k^\dagger f_k-\frac{1}{N}\sum_q\sum_{k,k'}\frac{\alpha^2V}{2K}\cos(k+q/2)\cos(k'-q/2)f_{k+q}^\dagger f_k f_{k'-q}^\dagger f_{k'}+\sum_k[E_0(k)-\rho_0\epsilon_k]f_k^\dagger f_k$$
$$+\sum_{k>0}i\Delta_0(k)(f_k^\dagger f_{k-\pi}-f_{k-\pi}^\dagger f_k)-\frac{1}{N}\sum_q\sum_{k,k'}\frac{\alpha^2}{2K}\cos(k+q/2)\cos(k'-q/2)$$
$$\times\{\delta(k+q,k)[2-\delta(k'-q,k')]-V\}f_{k+q}^\dagger f_k f_{k'-q}^\dagger f_{k'}, \tag{50}$$

where

$$-J\rho_0=\frac{2}{N}\sum_k\cos(k)E_0(k), \tag{51}$$

$$V=\frac{4}{N^3}\sum_q\sum_{k,k'}\cos^2(k+q/2)\cos^2(k'-q/2)\,\delta(k+q,k)[2-\delta(k'-q,k')]. \tag{52}$$

One can show that $\rho_0\leqslant1$ and $V\leqslant1$. When $\omega_\pi>2J$, u_0 is a small quantity and the last three terms can be treated as perturbation because they go to zero when $\omega_\pi\to\infty$. The unperturbed Hamiltonian is

$$H_{\text{eff}}^0=\sum_k\rho_0\epsilon_k f_k^\dagger f_k-\frac{1}{N}\sum_q\sum_{k,k'}\frac{\alpha^2V}{2K}\cos(k+q/2)\cos(k'-q/2)f_{k+q}^\dagger f_k f_{k'-q}^\dagger f_{k'}$$
$$=-\frac{1}{2}J\rho_0\sum_l(f_l^\dagger f_{l+1}+f_{l+1}^\dagger f_l)+\frac{\alpha^2V}{4K}\sum_l(f_l^\dagger f_l f_{l+1}^\dagger f_{l+1}-f_l^\dagger f_l). \tag{53}$$

It is the antiferromagnetic XXZ model with $J_X=J_Y=J\rho_0$ and $J_Z=\alpha^2V/4K$. This means that, because of the spin-phonon coupling, when $\omega_\pi>2J$ we can get an effective XXZ model as the unperturbed Hamiltonian with a phonon-induced Z interaction $\alpha^2V/4K$ and the XY magnetic interaction being renormalized by a factor ρ_0. The result of Yang and Yang[11] shows that there exists a transition point at $J_X=J_Y=J_Z$, that is, at

$$\alpha^2V/4K=J\rho_0. \tag{54}$$

The transition points determined by this equation are shown in Fig. 5 by the dash-dotted line. The dotted line is a fit by

$$g_c^2=\left[\frac{\omega_\pi}{\omega_\pi+2J}\right]^{0.4}. \tag{55}$$

One can see that, although the formula is very simple, the interpolated result is, at least, qualitatively correct. Note that the powerlaw of Eq. (49) cannot be used for the whole range $0<\omega_\pi<\infty$ because it leads to $g_c^2\to\infty$ when $\omega_\pi\to\infty$.

V. CONCLUSIONS

An analytical approach has been developed to study the effect of quantum lattice fluctuations on the ground state of an XY spin-Peierls chain, which is equivalent to the spinless Su-Schrieffer-Heeger model in half-filling after the Jordan-Wigner transformation. We have shown that when the spin-phonon coupling constant g^2 decreases or the phonon frequency ω_π increases the lattice dimerization m_p and the gap function $\Delta(k)$ in the fermionic spectrum decreases gradually. At some critical value g_c^2 or $\omega_{\pi c}$, the system becomes gapless and the lattice dimerization disappears. This can be attributed to the fact that the ground state fails to develop the spin-Peierls long-range order because of the quantum lattice fluctuations. A phase diagram in the $g^2\sim\omega_\pi$ plane is derived.

From our work we can see that the main effect of quantum lattice fluctuations is twofold. One is to lower the effective dimerization potential seen by Jordan-Wigner fermions, as is represented by the factor $1-\delta(k)$ in Eq. (41). The other is to induce a four-fermion interaction term. In this work the standard perturbation approach is used to treat the interaction term.

In our model system, quantum lattice fluctuations compete with the long-range dimerization order and the physical properties of the system should be determined by this competition. When $2\alpha m_p>\omega_\pi$ the long-range dimerization order dominates and the system is in the classical region. In this region the behavior of the dimerization m_p can be described by the form of an adiabatic mean-field solution but the mean-field parameters are renormalized by the quantum lattice fluctuations. For the quantum region where $2\alpha m_p<\omega_\pi$ the behavior of m_p can be described by an exponential function of $(g^2-g_c^2)^{-0.5}$ which is similar to, but different from, the fitting formula of Caron and Moukouri.[6] We believe that this type of difference comes from the retardation effect of the spin-phonon coupling.

In this work we mainly concentrated on the long-range ordering phase, where $m_p>0$ and there is a gap in the fermionic spectrum, and the phase transition point. The properties of the disordered phase with gapless fermions are also of interest because the disordered phase should be a Luttinger liquid with fermion-phonon interaction. This will be the topic of next work.

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