Quantum lattice fluctuations in a model electron-phonon system

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Abstract

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 a model electron-phonon system. To study nonadiabatic case, the Green’s function method is used to implement the perturbation treatment. The phase diagram and the density of states of fermions are obtained. We show that when electron-phonon coupling constant $\alpha^2/K$ decreases or phonon frequency $\omega_\pi$ increases the lattice dimerization and the gap in the fermion spectrum decrease gradually. At some critical value the system becomes gapless and the lattice dimerization disappears. The inverse-square-root singularity of the density of states at the gap edge in the adiabatic case disappears because of the nonadiabatic effect, which is consistent with the measurement of optical conductivity in quasi-one-dimensional systems.

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1 Introduction

The physical and chemical properties of materials with a quasi-one-dimensional charge-density-wave (CDW) state, for example, the halogen-bridged mixed-valence transition-metal complexes and the conducting polymers, have been the subject of intense study in recent years, because of their intrinsically interesting properties and important technological applications [1, 2]. Among the models for one-dimensional systems the Holstein model[3] and Su-Schrieffer-Heeger (SSH) model[4] are the two typical electron-phonon coupling Hamiltonian studied by many previous authors. The Holstein model is for the on-site electron-phonon interaction with dispersionless phonons coupled with electron density operator, while the SSH model is for the on-bond electron-phonon interaction.

In this work we deal with another one-dimensional electron-phonon coupling model, the simplified one band Hamiltonian for the halogen-bridged mixed-valence transition-metal complexes [5, 6, 7],

\[ H = \sum_l \left( \frac{1}{2M} P_l^2 + \frac{1}{2} K u_l^2 \right) - \sum_{l,s} t_0 (c_{l,s}^\dagger c_{l+1,s} + c_{l+1,s}^\dagger c_{l,s}) + \sum_{l,s} \alpha (u_l - u_{l+1}) c_{l,s}^\dagger c_{l,s} \]  \hspace{1cm} (1)


where \( c_{l,s}^\dagger \) and \( c_{l,s} \) are the creation and annihilation operators of electrons at site \( l \) with spin \( s \), \( u_l \) (with conjugated momentum \( p_l \)) is the displacement of the \( l \) ion, \( t_0 \) is the supertransfer energy of electrons between neighboring two orbitals, \( \alpha \) is the electron-phonon coupling constant, \( K \) is the elastic constant and \( M \) the mass of ions (throughout this paper we set \( \hbar = k_B = 1 \)). We will show that, at least for the spinless case, this model is the same as the Holstein model in the adiabatic limit (\( M \to \infty \)) but may be similar to the SSH model in the antiadiabatic limit (\( M \to 0 \)).

Within the adiabatic mean-field approximation, that is, treating the phonon degrees of freedom classically, the model can be solved easily. In the half-filled-band case, the system undergoes a Peierls instability and the ground state is dimerized with an energy gap at the Fermi points \( k = \pm \pi/2 \). However, this approach is questionable and it has been shown that the quantum lattice fluctuations must be taken into account to satisfactorily describe some physical properties of quasi-one-dimensional systems[8]. Generally speaking, the quantum lattice fluctuations may decrease the CDW order parameter[10, 11]. As the density of states (DOS) is concerned, the results of adiabatic approximation have inverse-square-root
singularity at the gap edge. By considering the quantum lattice fluctuations, the singularity at the gap edge may disappear\[12]. The relationship between Peierls distortion and phonon frequency in the range from $\omega_\pi = 0$ to $\omega_\pi \to \infty$ should be studied for understanding the physical properties of electron-phonon interactions in nonadiabatic case.

In Hamiltonian (1) the operators of lattice modes, $u_l$ and $p_l$, can be expanded by the phonon creation and annihilation operators $b_{-q}$ and $b_q$, and after Fourier transformation the $H$ becomes

$$H = \sum_q \omega_\pi \left( b_q^\dagger b_q + \frac{1}{2} \right) + \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} + \sum_{q,k,s} \frac{1}{\sqrt{N}} \frac{g(q)(b_q + b_{-q})}{\omega_\pi} c_{k+q,s}^\dagger c_{k,s},$$

where $\epsilon_k = -2t_0 \cos k$ is the bare band function, $N$ is the total number of sites. The dispersionless phonon frequency $\omega_\pi = \sqrt{K/M}$ and the coupling function $g(q) = \alpha \sqrt{1/2M \omega_\pi}[1 - \exp(iq)].$

2 Effective Hamiltonian

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

$$H' = \exp(S)H \exp(-S),$$

where the generator $S$ is

$$S = \frac{1}{\sqrt{N}} \sum_{q,k,s} \frac{g(q)}{\omega_\pi} (b_{-q}^\dagger b_q - b_q) \delta(k + q, k) c_{k+q,s}^\dagger c_{k,s}. \quad (4)$$

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. We divide the original Hamiltonian into $H = H^0 + H^1$, where $H^0$ contains the first two terms of $H$ and $H^1$ the last term. Then the unitary transformation can proceed order by order,

$$H' = H^0 + H^1 + [S, H^0] + [S, H^1] + \frac{1}{2} [S, [S, H^0]] + O(\alpha^3). \quad (5)$$

The first-order terms in $H'$ are

$$H^1 + [S, H^0] = \frac{1}{\sqrt{N}} \sum_{q,k,s} g(q)(b_{-q}^\dagger b_q + b_q) c_{k+q,s}^\dagger c_{k,s}$$
This is nothing but making the matrix element of $H$ only if $\epsilon$ if we choose $H$, under renormalization \[13\]. The second-order terms in $\phi$ after the transformation, are related to the higher-lying excited states and should be irrele-

\[\delta \]

Note that the ground state $|g\rangle$ of $H^0$, the non-interacting system, is a direct product of a filled fermi-sea $|FS\rangle$ and a phonon vacuum state $|ph, 0\rangle$ \[13\]:

\[|g\rangle = |FS\rangle |ph, 0\rangle. \quad (7)\]

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

\[\langle H^1 + [S, H^0]|g\rangle = \frac{1}{\sqrt{N}} \sum_{q,k,s} g(q)b_{q,k+s}c_{k,s} \left[ 1 - \delta(k + q, k) \left( 1 - \frac{\epsilon_k - \epsilon_{k+q}}{\omega} \right) \right]|g\rangle \quad (8)\]

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

\[\langle H^1 + [S, H^0]|g\rangle = 0, \quad (9)\]

if we choose

\[\delta(k + q, k) = 1/(1 + |\epsilon_{k+q} - \epsilon_k|/\omega). \quad (10)\]

This is nothing but making the matrix element of $H^1 + [S, H^0]$ between $|g\rangle$ and the lowest-lying excited states vanishing. Thus the first-order terms, which are not exactly canceled after the transformation, are related to the higher-lying excited states and should be irrelevant under renormalization \[13\]. The second-order terms in $H'$ can be collected as follows:

\[\langle S, H' \rangle + \frac{1}{2}\langle [S, [S, H^0]] \rangle \]

\[= \frac{1}{2N} \sum_{q,k,s,q',k'} \frac{g(q)g(q')}{\omega} \delta(k + q, k) \left[ 2 - \delta(k' + q', k') \right] (b_{q,k+s}^\dagger b_{q', k'}^\dagger + b_{q'}^\dagger b_{q,k+s}^\dagger - b_q^\dagger b_{q'} b_{q'}^\dagger b_q) \]

\[\times \left( c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'} \delta_{k,k'+q'} - c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'+q'}^\dagger \delta_{k,k'} \delta_{k,k'+q'}^\dagger \right) \]

\[+ \frac{1}{2N} \sum_{q,k,s,q',k'} \frac{g(q)g(q')}{\omega^2} \delta(k + q, k) \delta(k' + q', k') (\epsilon_{k'} - \epsilon_{k'+q'}) (b_{q,k+s}^\dagger b_{q'} b_{q'}^\dagger b_{q,k+s} - b_q^\dagger b_{q'} b_{q'}^\dagger b_{q,q,k+s}) \]

\[\times \left( c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'+q'}^\dagger \delta_{k,k'} + c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'+q'}^\dagger \delta_{k,k'} \delta_{k,k'+q'}^\dagger \right) \]

\[= \frac{1}{2N} \sum_{q,k,s,q',k'} \frac{g(q)g(-q)}{\omega} \delta(k + q, k) \left[ 2 - \delta(k' - q, k') \right] (c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'+q'}^\dagger \delta_{k,k'} + c_{k+s}^\dagger c_{k+s}^\dagger \delta_{k,k'+q'}^\dagger \delta_{k,k'} \delta_{k,k'+q'}^\dagger \right). \quad (11)\]

$\delta_{k,k+q}$ is the Kronecker $\delta$ symbol. All terms of higher order than $\alpha^2$ will be omitted in the following treatment.
For the dimerized state, the neighboring atoms move in opposite directions. To take into account the static phonon-staggered ordering\[12\], we make a displacement transformation to $H'$

$$
\tilde{H} = \exp(R)H'\exp(-R).
$$

(12)

Here

$$
R = -\sum_l (-1)^l u_0 \sqrt{\frac{M\omega}{2}} (b^+_l - b_l),
$$

(13)

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

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

(14)

Applying the transformation on phonon annihilation operator, we get

$$
\exp(R)b_q \exp(-R) = b_q + u_0 \sqrt{\frac{NM\omega}{2}} \delta_{\pi,q}.
$$

(15)

If the ground state of $H$ is $|g\rangle$, then the ground state of $\tilde{H}$ 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 $\tilde{H}$ over the phonon vacuum state we get an effective Hamiltonian for the fermions,

$$
H_{eff} = \langle ph,0|\tilde{H}|ph,0\rangle
$$

$$
= \frac{1}{2} Ku_0^2 N + \sum_{k,s} E_0(k)c^+_k c_{k,s} + \sum_{k>0,s} \Delta_0(k)(c^+_k c_{k,-\pi,s} c_{k,s} + c^+_k c_{k-\pi,s} c_{k,s})
$$

$$
- \frac{1}{N} \sum_{q,k,s,k',s'} \frac{g(q)g(-q)}{\omega_\pi} \delta(k+q,k)[2 - \delta(k'-q,k')] c^+_{k+q,s} c_{k,s} c^+_{k'-q,s} c_{k',s'},
$$

(16)

where

$$
E_0(k) = \epsilon_k - \frac{1}{N} \sum_{k'} \frac{g(k'-k)g(k-k')}{\omega_\pi^2} \delta(k',k) \delta(k,k') (\epsilon_k - \epsilon_{k'}),
$$

(17)

$$
\Delta_0(k) = 2\alpha u_0 [1 - \delta(k-\pi,k)].
$$

(18)

We find by means of the variational principle that the dimerized lattice displacement ordering parameter is

$$
u_0 = -\frac{1}{KN} \sum_{k>0,s} 2\alpha [1 - \delta(k-\pi,k)] \langle fe |(c^+_k c_{k,s} + c^+_k c_{k-\pi,s}) |fe\rangle.
$$

(19)
Note that in the adiabatic limit where $\omega_\pi = 0$ one has $\delta(k', k) = 0$ and $H_{eff}$ goes back to the adiabatic mean-field Hamiltonian,

$$H_{eff}(\omega_\pi = 0) = \frac{1}{2} KNu_0^2 + \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} + \sum_{k>0,s} 2\alpha u_0 (c_{k-\pi,s}^\dagger c_{k,s} + c_{k,s}^\dagger c_{k-\pi,s}). \quad (20)$$

This is the same as the adiabatic mean-field Hamiltonian for the dimerized Holstein model\[13\].

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

$$H_{eff}(\omega_\pi \to \infty) = \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} - \frac{1}{N} \sum_{k,k', q,s,s'} \frac{g(q)g(-q)}{\omega_\pi} c_{k+q,s} c_{k,s}^\dagger c_{k'-q,s'}^\dagger c_{k',s'}. \quad (21)$$

Returning to the real space, this Hamiltonian is

$$H_{eff}(\omega_\pi \to \infty) = -t_0 \sum_{l,s} (c_{l+1,s}^\dagger c_{l,s} + c_{l,s}^\dagger c_{l+1,s}) - \frac{\alpha^2}{K} \sum_{l,s,s'} c_{l,s}^\dagger c_{l,s} c_{l,s'}^\dagger c_{l,s'} + \frac{\alpha^2}{K} \sum_{l,s,s'} c_{l,s}^\dagger c_{l,s} c_{l+1,s'}^\dagger c_{l+1,s'}. \quad (22)$$

For the spinless case, the on-site interaction disappears because of the Pauli principle and this is the antiferromagnetic XXZ model (through Jordan-Wigner transformation)\[11\]. The situation is very similar to the spinless SSH mode in the large $\omega_\pi$ limit \[4\]. XXZ model can be solved exactly and there exists a transition point at $\alpha^2/2K = t_0$\[14\]. For the spin-$\frac{1}{2}$ case, (22) is the negative-$U$ extended Hubbard model with $V = -U$.

Our effective Hamiltonian works well in the $\omega_\pi = 0$ and $\omega_\pi \to \infty$ limits and, furthermore, for the spinless case $H_{eff}$ can be solved exactly in both limits. In this work we concentrate on the nonadiabatic effect due to finite phonon frequency $\omega_\pi$ in the spinless case because we have the exact solutions in the two limits. The last term in $H_{eff}$ 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 $\omega_\pi$, $\omega_\pi \leq 2t_0$, is very different from that for the large $\omega_\pi$, $\omega_\pi > 2t_0$, we treat $H_{eff}$ in these two cases with different methods.

\section{$\omega_\pi < 2t_0$}

In this case the four-fermion term goes to zero as $\omega_\pi \to 0$, so it can be treated as a perturbation and the unperturbed Hamiltonian is

$$H_{eff}^0 = \frac{1}{2} Ku_0^2 N + \sum_k E_0(k)c_k^\dagger c_k + \sum_{k>0} \Delta_0(k)(c_{k-\pi}^\dagger c_k + c_k^\dagger c_{k-\pi}). \quad (23)$$
The four-fermion term can be re-written as

\[ H'_{\text{eff}} = \frac{1}{N} \sum_{q>0,k>0,k'>0} \frac{g(q)g(-q)}{\omega_{\pi}} \delta(k + q, k)[2 - \delta(k' - q, k')] \times (c^\dagger_{k+q}c_k + c^\dagger_{k+q-\pi}c_{k-\pi})(c^\dagger_{k'q}c_{k'} + c^\dagger_{k'-q-\pi}c_{k'-\pi}) \]

\[ -\frac{1}{N} \sum_{q>0,k>0,k'>0} \frac{g(q - \pi)g(\pi - q)}{\omega_{\pi}} \delta(k + q, k - \pi)[2 - \delta(k' - q, k' - \pi)] \times (c^\dagger_{k+q}c_{k-\pi}c^\dagger_{k'-q-\pi}c_{k'} + c^\dagger_{k+q}c_kc^\dagger_{k'-q}c_{k'-\pi}) \]

\[ -\frac{1}{N} \sum_{q>0,k>0,k'>0} \frac{g(q - \pi)g(\pi - q)}{\omega_{\pi}} \delta(k + q, k - \pi)[2 - \delta(k' - q, k' - \pi)] \times (c^\dagger_{k+q-\pi}c^\dagger_{k'-q-\pi}c_{k'} + c^\dagger_{k+q}c_{k-\pi}c^\dagger_{k'-q}c_{k'-\pi}). \] (24)

We can distinguish between different physical processes. The first term in Eq.(24) is the forward scattering one, the second is the backward scattering one, and the last is the Umklapp scattering one. We use the Green’s function method to implement the perturbation treatment and it is more convenient to work within a two-component representation,

\[ \Psi_k = \begin{pmatrix} c_k \\ c_{k-\pi} \end{pmatrix}, \quad k > 0. \] (25)

Thus we have

\[ \begin{cases} 
\Psi^\dagger_k \sigma_z \Psi_k = c^\dagger_k c_k - c^\dagger_{k-\pi} c_{k-\pi} \\
\Psi^\dagger_k \sigma_x \Psi_k = c^\dagger_k c_{k-\pi} + c^\dagger_{k-\pi} c_k \\
\Psi^\dagger_k i \sigma_y \Psi_k = c^\dagger_k c_{k-\pi} - c^\dagger_{k-\pi} c_k 
\end{cases} \] (26)

and the Hamiltonian becomes

\[ H'_{\text{eff}} = \frac{1}{2} Ku_0 N + \sum_{k>0} E_0(k) \Psi^\dagger_k \sigma_z \Psi_k + \sum_{k>0} \Delta_0(k) \Psi^\dagger_k \sigma_x \Psi_k, \] (27)

\[ H'_{\text{eff}} = -\frac{1}{N} \sum_{q>0,k>0,k'>0} \frac{g(q)g(-q)}{\omega_{\pi}} \delta(k + q, k)[2 - \delta(k' - q, k')] \Psi^\dagger_{k+q} \Psi_k \Psi^\dagger_{k'-q} \Psi_{k'} \]

\[ + \frac{1}{2N} \sum_{q>0,k>0,k'>0} \frac{g(q - \pi)g(\pi - q)}{\omega_{\pi}} \delta(k + q, k - \pi)[2 - \delta(k' - q, k' - \pi)] \times (\Psi^\dagger_{k+q} i \sigma_y \Psi_k \Psi^\dagger_{k'-q} i \sigma_y \Psi_{k'} - \Psi^\dagger_{k+q} \sigma_x \Psi_k \Psi^\dagger_{k'-q} \sigma_x \Psi_{k'}) \]

\[ -\frac{1}{2N} \sum_{q>0,k>0,k'>0} \frac{g(q - \pi)g(\pi - q)}{\omega_{\pi}} \delta(k + q, k - \pi)[2 - \delta(k' - q, k' - \pi)] \times (\Psi^\dagger_{k+q} i \sigma_y \Psi_k \Psi^\dagger_{k'-q} i \sigma_y \Psi_{k'} + \Psi^\dagger_{k+q} \sigma_x \Psi_k \Psi^\dagger_{k'-q} \sigma_x \Psi_{k'}). \] (28)
\( \sigma_\beta (\beta = x, y, z) \) is the Pauli matrix. The matrix Green's function is defined as (the temperature Green's function is used and at the end let \( T \rightarrow 0 \))

\[
G(k, \tau) = - \langle T_\tau \Psi_k(\tau) \Psi_k^\dagger(0) \rangle = \frac{1}{\beta} \sum_n \exp(-i\omega_n \tau) G(k, \omega_n). \tag{29}
\]

The Dyson equation is

\[
G(k, \omega_n) = G_0(k, \omega_n) + G_0(k, \omega_n) \Sigma^*(k, \omega_n) G(k, \omega_n), \tag{30}
\]

where

\[
G_0(k, \omega_n) = \{i\omega_n - E_0(k)\sigma_z - \Delta_0(k)\sigma_x\}^{-1}, \tag{31}
\]

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

\[
\Sigma^*(k, \omega_n) = T \sum_{k'} \sum_{m} \frac{g(k' - k)g(k - k')}{\omega_\pi} \delta(k', k)[2 - \delta(k, k')] \\
\times \{G_0(k', \omega_m) + T_r[\sigma_z G_0(k', \omega_m)]\sigma_z\} \\
- \frac{T}{N} \sum_{k'} \sum_{m} \frac{g(k' - k - \pi)g(\pi - k' + k)}{\omega_\pi} \delta(k', k - \pi)[2 - \delta(k, k' - \pi)] \\
\times \{i\sigma_y G_0(k', \omega_m)i\sigma_y - \sigma_x G_0(k', \omega_m)\sigma_x\} \\
+ \frac{T}{N} \sum_{k'} \sum_{m} \frac{g(-\pi)g(\pi)}{\omega_\pi} [\delta(k, k - \pi) + \delta(k', k' - \pi) - \delta(k, k - \pi)\delta(k', k' - \pi)] \\
\times \{T_r[i\sigma_y G_0(k', \omega_m)]i\sigma_y + T_r[\sigma_x G_0(k', \omega_m)]\sigma_x\}. \tag{32}
\]

In the perturbation calculation we have taken into account the fact that the forward and backward scattering terms contribute nothing to the "charge" gap \([13, 16]\). From Eq.\( (32) \) one can get that \( \Sigma^*(k, \omega_n) \) is irrelative to \( \omega_n \), therefore the spectrum structure of \( G(k, \omega_n) \) should be

\[
G(k, \omega_n) = \{i\omega_n - E(k)\sigma_z - \Delta(k)\sigma_x\}^{-1}. \tag{33}
\]

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

\[
W(k) = \sqrt{E^2(k) + \Delta^2(k)}. \tag{34}
\]
The renormalized band function and the gap function are

\[ E(k) = E_0(k) - \frac{2\alpha^2}{KN} \sum_{k'>0} \left\{ \sin^2 \left( \frac{k' - k}{2} \right) \delta(k', k)[2 - \delta(k', k)] - \cos^2 \left( \frac{k' - k}{2} \right) \delta(k' - \pi, k)[2 - \delta(k' - \pi, k)] \right\} \frac{E_0(k')}{\sqrt{E_0^2(k') + \Delta_0^2(k')}} , \]

(35)

\[ \Delta(k) = 2\alpha u_0[c - d\delta(k - \pi, k)]. \]

(36)

Where

\[ c = 1 + \frac{2\alpha^2}{KN} \sum_{k>0} \delta(k - \pi, k) \frac{\Delta_0(k)}{2\alpha u_0 \sqrt{E_0^2(k) + \Delta_0^2(k)}} , \]

(37)

\[ d = 1 - \frac{2\alpha^2}{KN} \sum_{k>0} [1 - \delta(k - \pi, k)] \frac{\Delta_0(k)}{2\alpha u_0 \sqrt{E_0^2(k) + \Delta_0^2(k)}} . \]

(38)

The equation to determine \( u_0 \) is

\[ 1 = \frac{4\alpha^2}{KN} \sum_{k>0} [1 - \delta(k - \pi, k)] \frac{\Delta(k)}{2\alpha u_0 W(k)} . \]

(39)

In nonadiabatic case \( u_0 \) is a variational parameter and cannot be measured by experiment or Monte Carlo simulation. The quantity which can be measured is the phonon-staggered ordering parameter \( m_p \),

\[ m_p = \frac{1}{N} \sum_{l} (-1)^l < u_l > = \frac{1}{N} \sum_{l} \sum_{q} (-1)^l \sqrt{\frac{1}{2MN\omega_\pi}} \exp(iql) < b_{l-q}^\dagger + b_q > = u_0 - \frac{2\alpha}{KN} \sum_{k} \delta(k - \pi, k) < c_{k-\pi}^\dagger c_k > = \frac{2\alpha}{KN} \sum_{k>0} < fe| \Psi_k^\dagger \sigma_x \Psi_k | fe > = \frac{2\alpha}{KN} \sum_{k>0} \Delta(k) W(k) . \]

(40)

These are basic equations for the \( \omega_\pi < 2t_0 \) case. If \( \omega_\pi = 0 \) we have \( \delta(k', k) = 0 \) and \( c = 1 \), Eq.(35) becomes the same as that in the adiabatic theory.

Fig.1 shows the phonon-staggered ordering parameter \( \alpha m_p / t_0 \) as function of the electron-phonon coupling constant \( \alpha^2/Kt_0 \) in the cases of \( \omega_\pi / t_0 = 0.3 \) and 0.5. As shown in the figure, the dimerization parameter \( \alpha m_p / t_0 \) increases as the electron-phonon coupling constant \( \alpha^2/Kt_0 \) increases but decreases as the phonon frequency \( \omega_\pi / t_0 \) increases. Fig.2 shows the
normalized phonon-staggered ordering 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 value when \(m_p = 0\)) in the cases of \(\alpha^2/Kt_0 = 0.5\) and 1.0. As shown in the figure, the dimerization parameter \(m_p\) decreases as the phonon frequency \(\omega_\pi\) increases but increases as the electron-phonon coupling constant \(\alpha^2/Kt_0\) increases, which indicates that the nonadiabatic effect is to reduce the dimerization ordering parameters.

Comparing Eq.(36) with that in the adiabatic case, \(\Delta(k) = 2\alpha u_0\), we have the gap in the nonadiabatic case,

\[
\Delta = \Delta(\pi/2) = 2\alpha u_0[c - d].
\]

This is the true gap in the fermionic spectrum.

From Eq.(39), let \(u_0 = 0\), we get the self-consistent equation of phase transition points in the \(\alpha^2/K \sim \omega_\pi\) plane,

\[
1 = \frac{4\alpha^2}{KN} \sum_{k>0} [1 - \delta(k - \pi, k)] \frac{c - d\delta(k - \pi, k)}{|E(k)|},
\]

The density of states(DOS) of fermions is

\[
N(\omega) = \frac{1}{N} \sum_k \delta \left( \omega - \sqrt{E^2(k) + \Delta^2(k)} \right) \\
= \frac{1}{2\pi} \left( \frac{d}{dk} \sqrt{E^2(k) + \Delta^2(k)} \bigg|_{k=f(\omega)} \right)^{-1}, \tag{43}
\]

where, \(k = f(\omega)\) is the inverse function of \(\omega = \sqrt{E^2(k) + \Delta^2(k)}\). Fig.3 shows the density of states(DOS) of fermions for some values of phonon frequency \(\omega_\pi\). One can see that a nonzero DOS starts from the gap edge and, for small values of \(\omega_\pi\), there is a peak with a significant tail below it. The inverse-square-root singularity at the gap edge in the adiabatic case[4] disappears.

\section{**4** \(\omega_\pi > 2t_0\)}

In this case \(H_{eff}\) can be re-written as

\[
H_{eff} = \frac{1}{2} Ku_0^2 N + \sum_k E_0(k)c_k^\dagger c_k + \sum_{k>0} \Delta_0(k)(c_{k-\pi}^\dagger c_k + c_k^\dagger c_{k-\pi}) \\
- \frac{1}{N} \sum_{q,k,k'} \frac{g(q)g(-q)}{\omega_\pi} \delta(k + q, k)[2 - \delta(k' - q, k')] c_k^\dagger c_{k+q} c_{k'-q}^\dagger c_{k'}. \tag{44}
\]
According to Eq.(22), when $\omega_\pi \to \infty$, the effective Hamiltonian includes only electron-electron interactions of on-site and nearest-neighbor. Therefore, we treat the terms of on-site and nearest-neighbor interactions as the unperturbed Hamiltonian and the others as perturbation because they go to zero when $\omega_\pi \to \infty$. In real space, the unperturbed Hamiltonian is

$$H^0_{\text{eff}} = \frac{1}{2} Ku_0^2 N - t_0[1 - F(\omega_\pi)] \sum_l (c^\dagger_{l+1} c_l + c^\dagger_l c_{l+1}) + V_1 \sum_l c^\dagger_l c_l c^\dagger_{l+1} c_{l+1},$$

where

$$V_1 = -\frac{2}{N^3} \sum_{q,k,k'} |g(q)|^2 \frac{\cos q}{\omega_\pi} \delta(k + q, k)[2 - \delta(k' - q, k')].$$

$$F(\omega_\pi) = \frac{\omega_\pi}{(2\pi)^2} \frac{2\alpha^2}{K} \int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dk' \frac{(1 - \cos k \cos k')(\cos k - \cos k') \cos k}{\omega_\pi + 2t_0|\cos k - \cos k'|^2}.$$  

(45) is the antiferromagnetic XXZ model and can be solved exactly [11]. The result of Yang-Yang shows that there exists a transition point at $V_1 = 2t_0[1 - F(\omega_\pi)]$. (48)

This equation determines the diagram of phase transition in the case of $\omega_\pi > 2t_0$. Fig.4 shows the phase diagram. We use $\omega_\pi/(\omega_\pi + 2t_0)$, instead of $\omega_\pi$, as the variable because it goes to 1 when $\omega_\pi \to \infty$. The solid line is the result of Eq.(42) and the dashed line is the result obtained from Eq.(48). The dashed-dotted line is the result of equation

$$\frac{\alpha^2}{K} \sim \left(\frac{\omega_\pi}{\omega_\pi + 2t_0}\right)^{0.4}.$$  

One can see that, although the formula is very simple, the interpolated result is, at least, qualitatively correct.

5 Conclusions

The effects of quantum lattice fluctuations on the ground state of a model electron-phonon system are studied through an analytical approach. Our results show that when the electron-phonon coupling constant $\alpha^2/K$ decreases or the phonon frequency $\omega_\pi$ increases the lattice
dimerization and the gap in the fermion spectrum decrease gradually. At some critical value, the system becomes gapless and the lattice dimerization disappears. A phase diagram in the $\alpha^2/K \sim \omega_\pi$ plane and the density of states of fermions are derived. The inverse-square-root singularity of DOS at the gap edge in the adiabatic case disappears because of the nonadiabatic effect, which is consistent with the measurement of optical conductivity in quasi-one-dimensional systems.

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Figure Caption

Fig.1 The dimerization parameter $\alpha m_p/t_0$ as function of the electron-phonon coupling constant $f = \alpha^2/Kt_0$ for $\omega_\pi/t_0 = 0.3$ and 0.5.

Fig.2 The normalized dimerization parameter $m_p/m_{p0}$ as functions of the normalized phonon frequency $\omega_\pi/\omega_{\pi c}$ in the cases of $f = 0.5$ and 1.0.

Fig.3 The density of states (DOS) of fermions for $\alpha^2/Kt_0 = 0.4$ with $\omega_\pi/t_0 = 0.001$ and 0.01.

Fig.4 The phase diagram from Eq.(42), Eq.(48) and Eq.(49).