Quantum phonons and the Peierls transition temperature

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The effect of quantum phonons on the Peierls transition temperature in a one-dimensional commensurate system is studied. The nonadiabatic effect due to finite phonon frequency $\omega_p>0$ are treated through an energy-dependent electron-phonon scattering function $\delta(k',k)$. By using the Green's-function perturbation theory we have shown that our theory gives a good description of the effect of quantum phonons: (i) There exists a critical electron-phonon coupling g_c^2. The Peierls transition temperature $T_p=0$ when the coupling $g^2<g_c^2$ and T_p increases with increasing $g^2>g_c^2$. (ii) The ratio $2\Delta/T_p$ could be much larger than the BCS value 3.527.

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I. INTRODUCTION

The Peierls instability and the related charge ordering or spin-Peierls phenomena in some quasi-one-dimensional systems have attracted a growing interest in these years.[1–3] The Peierls instability leads to a lattice distortion at wave vector $2k_F$ (k_F is the Fermi wave vector) in their lower temperature phases and the charge and/or spin degrees of freedom are coupled with the lattice displacement. Although the adiabatic approximation, that is, treating the lattice displacement as a static mean field, is usually used to deal with these systems,[1] there are several reasons that the nonadiabaticity of the electron-lattice interaction may play an important role:

(i) For many Peierls-distorted systems the zero-point motion of the lattice, $\delta u=\sqrt{\hbar/2M\omega_p}$ (ω_p is the phonon frequency with mass M), is comparable to the lattice distortion u_0 (Ref. 4) (e.g., for polyacetylene, $u_0\approx 0.03$ Å and $\delta u \approx 0.03$ Å). As the size of the gap 2Δ is proportional to u_0, lattice fluctuations should have an important effect on the electronic properties. The optical absorption coefficient $\alpha(\omega)$ calculated in the adiabatic mean-field approximation has an inverse-square-root singularity at $\omega=2\Delta$ and there is no absorption inside the gap. The observed absorption is quite different. The singularity is absent and, instead of it, there is a peak around $\omega=2\Delta$ with a significant tail below the peak.[5]

(ii) In some quasi-one-dimensional systems the phonon frequency may be of the same order of magnitude as the characteristic energy of the electrons; for example, in the inorganic spin-Peierls system $CuGeO_3$ the phonon frequency $\omega_p\approx 20$–30 K and the spin gap $\Delta\sim 23$ K.[6]

(iii) How to describe the finite temperature properties? The adiabatic theory predicts a higher Peierls transition temperature T_p ($2\Delta/T_p\sim 3.527$), but it does not agree with the experimental T_p ($2\Delta/T_p\sim 6$–10 in various experiments, or even larger).[7,8] Moreover, as the temperature increases the absorption spectrum broadens considerably. There is no accepted quantitative theory of the shape of the spectrum and its temperature dependence.[4]

(iv) The main theoretical approach which can be used to deal with the nonadiabaticity is the Migdal-Eliashberg theory, but, unfortunately, it may be broken down by the large nonadiabaticity $\omega_p/\Delta\sim 1$ and/or the low dimensionality.[9] As was shown by previous authors, the Migdal-Eliashberg theory cannot remove the inverse-square-root singularity of $\alpha(\omega)$ at $\omega=2\Delta$.[10,11]

We proposed to study the problem starting from the following Takayama-Lin-Liu-Maki (TLM) Hamiltonian for spinless electrons,[12]

$$H_e=\int dy\Psi^\dagger(y)\left(-iv_F\sigma_3\frac{\partial}{\partial y}+\varphi(y)\sigma_+ +\varphi^*(y)\sigma_-\right)\Psi(y), \tag{1}$$

which describes the low-energy properties of systems of Peierls instability (in the continuum limit). It may be the simplest model but contains the main physics of Peierls transition. Here $\sigma_\alpha(\alpha=1,2,3)$ and $\sigma_\pm=\frac{1}{2}(\sigma_1\pm\sigma_2)$ are Pauli matrices.

$$\Psi(y)=\begin{pmatrix}\psi_1(y)\\ \psi_2(y)\end{pmatrix} \tag{2}$$

is the spinor representation of Fermionic operators $\psi_1(y)$ and $\psi_2(y)$, which describe right and left movers, respectively. $\varphi(y)$ is the backscattering potential related to phonons,

$$\varphi(y)=\sqrt{\frac{\alpha^2\omega_p}{KN}}\sum_q (b^\dagger_{-q}+b_q)\exp(iqy). \tag{3}$$

N is the total number of unit cells, ω_p the phonon frequency with spring constant K, α the electron-phonon coupling constant, and b_q ($b^\dagger_{-q}$) the annihilation (creation) operator of the phonon mode q. We assume the commensurate case with a real backscattering potential $\varphi(y)=\varphi^*(y)$. Instead of the backscattering potential used by Ref. 4 which is a static but random one, here $\varphi(y)$ has its own dynamics which can be described by

$$H_p=\omega_p\sum_q b_q^\dagger b_q, \tag{4}$$

the harmonic Hamiltonian of phonons. The total Hamiltonian is $H=H_e+H_p$.

A spinless electron model is not so unphysical as one might consider at the beginning. It may be related to the spin-Peierls transition.[2,13] An XY spin chain with nearest-neighbor exchange and spin-lattice interaction is equivalent, through a Jordan-Wigner transformation together with the continuum approximation, to the spinless TLM model. Besides, both the strong correlation (for example, the double exchange model) and the strong magnetic field can lead to the consideration of only one spin component.

The theoretical analysis becomes difficult when the quantum phonons and the finite-temperature fluctuations are taken into account. Various methods have been used for the problem, such as the Monte Carlo simulation,[14–17] perturbation calculation,[18] Green's-function technique,[10,11] renormalization-group analysis,[19–21] variational method of the squeezed-polaronic wave function,[22] and a phenomenological random potential with Gaussian correlations.[4] Previously, one of us developed an approach to treat the lattice fluctuations due to finite phonon frequency $\omega_p>0$ through an energy-dependent electron-phonon scattering function $\delta(k',k)$.[23] In this work, we extend the approach to the study of effect of quantum phonons on the Peierls transition temperature and the ratio $2\Delta/T_p$. In our calculation some approximation to the self-energy of the Green's function will be used, which may be good when the phonon frequency ω_p is small: $\omega_p \ll \pi v_F$. Throughout this paper we put $\hbar=1$ and $k_B=1$.

II. THEORETICAL ANALYSIS

In momentum space the Hamiltonian reads

$$H=\sum_k v_F k\Psi^\dagger(k)\sigma_3\Psi(k)+\omega_p\sum_q b_q^\dagger b_q + \sqrt{\frac{\alpha^2\omega_p}{KN}}\sum_{k,q}(b_{-q}^\dagger+b_q)\Psi^\dagger(k+q)\sigma_1\Psi(k). \quad (5)$$

The last term in Eq. (5) describes the electron-phonon interaction: at the electron-phonon vertex an incoming electron with momentum k is scattered by the phonon into an outgoing one with momentum $k+q$. The momentum k is measured from the Fermi point $k=0$. A unitary transformation is used to take into account the electron-phonon correlation, $H'=\exp(S)H\exp(-S)$,

$$S=\sqrt{\frac{\alpha^2}{\omega_p KN}}\sum_{k,q}(b_{-q}^\dagger-b_q)\delta(k+q,k)\Psi^\dagger(k+q)\sigma_1\Psi(k). \quad (6)$$

Here a function $\delta(k',k)$ is introduced in S, which depends on the energies of incoming and outgoing electrons in the electron-phonon scattering process. It is defined as

$$\delta(k',k)=\frac{\omega_p}{\omega_p+v_F|k'+k|}, \quad (7)$$

and the reason for this definition will become clear later.

The total Hamiltonian H is divided as $H=H_0+H_1$, where H_1 is the last term in Eq. (5). Then the transformation can proceed order by order, The first-order terms in the transformed Hamiltonian H' are

$$H_1'=H_1+[S,H_0]=\sqrt{\frac{\alpha^2\omega_p}{KN}}\sum_{k,q}\frac{v_F}{\omega_p+v_F|2k+q|}\Psi^\dagger(k+q) \times\{[|2k+q|\sigma_1-i(2k+q)\sigma_2]b_{-q}^\dagger+[|2k+q|\sigma_1 +i(2k+q)\sigma_2]b_q\}\Psi(k), \quad (8)$$

where we have already used the functional form of $\delta(k',k)$. The second-order terms in H', which are diagonal in phonon operators, can be collected as follows:

$$H_2'=[S,H_1]+\frac{1}{2}[S,[S,H_0]]=\frac{\alpha^2}{KN}\sum_{k,q}\frac{v_F(2k+q)}{\omega_p} \times(b_{-q}^\dagger-b_q)(b_q^\dagger-b_{-q})\delta^2(k+q,k)\Psi^\dagger(k)\sigma_3\Psi(k) -\frac{\alpha^2}{KN}\sum_{k,k',q}[2-\delta(k'-q,k')]\delta(k+q,k)\Psi^\dagger \times(k+q)\sigma_1\Psi(k)\Psi^\dagger(k'-q)\sigma_1\Psi(k'). \quad (9)$$

We make a displacement transformation to H' to take into account the static phonon-staggered ordering, $\exp(R)H'\exp(-R)$,

$$R=-u_0\sqrt{\frac{KN}{4\omega_p}}(b_0^\dagger-b_0). \quad (10)$$

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

$$\exp(R)\varphi(y)\exp(-R)=\varphi(y)+\alpha u_0, \quad (11)$$

and u_0 is a variational parameter to describe the static phonon-staggered ordering. This transformation is to introduce a phonon-staggered potential $\Delta_0(k)$ for electrons,

$$H_0'=\sum_k v_F k\Psi^\dagger(k)\sigma_3\Psi(k)+\omega_p\sum_q b_q^\dagger b_q + \sum_k\Delta_0(k)\Psi^\dagger(k)\sigma_1\Psi(k)+\frac{Ku_0^2}{4}N, \quad (12)$$

$$\Delta_0(k)=\alpha u_0[1-\delta(k,k)]. \quad (13)$$

The equation to determine u_0 is

$$\alpha u_0=-\frac{2\alpha^2}{KN}\sum_k[1-\delta(k,k)]\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle, \quad (14)$$

where $\langle\cdots\rangle$ means the thermodynamical average.

All terms of order $O(\alpha^3)$ in H' will be neglected in what follows because $H'=H_0'+H_1'+H_2'$ becomes the exact Hamiltonian in both $\omega_p=0$ and $\omega_p\to\infty$ limits. When $\omega_p=0$, $\delta(k',k)=0$, and then $H_1'=0$, $H_2'=0$,

$$H'(\omega_p=0)=\sum_k v_F k\Psi^\dagger(k)\sigma_3\Psi(k)+\sum_k \alpha u_0\Psi^\dagger(k)\sigma_1\Psi(k)+\frac{Ku_0^2}{4}N. \quad (15)$$

This is equivalent to the original Hamiltonian H in adiabatic mean-field approximation. When $\omega_p\to\infty$, $\delta(k',k)=1$, and then $u_0=0$, $H_1'=0$,

$$H'(\omega_p\to\infty)=\sum_k v_F k\Psi^\dagger(k)\sigma_3\Psi(k)+\omega_p\sum_q b_q^\dagger b_q-\frac{\alpha^2}{KN}\sum_{k,k',q}\Psi^\dagger(k+q)\sigma_1\Psi(k)\times\Psi^\dagger(k'-q)\sigma_1\Psi(k'). \quad (16)$$

This is the exact Hamiltonian for $\omega_p\to\infty$ limit, which can be obtained through the functional integration method.[16]

The purpose of our transformation is to find a better way to divide the Hamiltonian into the unperturbed part and the perturbation. For the small $\omega_p\ll\pi v_F$ case we treat H_0' as the unperturbed part and $H_1'+H_2'$ the perturbation, because (i) $H_1'+H_2'\to 0$ as $\omega_p\to 0$, and (ii) by choosing the functional form of $\delta(k',k)$ in Eq. (7) the contribution of H_1' to the self-energy when $T=0$ is nearly zero (see below).

The perturbation treatment is through the conventional Green's-function theory. $G_0(k,ik_m)=[ik_m-v_Fk\sigma_3-\Delta_0(k)\sigma_1]^{-1}$ is the Green's function for H_0' and that for H', $G(k,ik_m)$, is related to $G_0(k,ik_m)$ via the Dyson equation. The second-order $[O(\alpha^2)]$ self-energy can be written as

$$\Sigma(k,ik_m)=ik_m\Sigma_0(k,ik_m)+[E(k)-v_Fk+\Sigma_3(k,ik_m)]\sigma_3+[\Delta(k)-\Delta_0(k)]\sigma_1. \quad (17)$$

Here $[E(k)-v_Fk]\sigma_3+[\Delta(k)-\Delta_0(k)]\sigma_1$ is the contribution of H_2'

$$E(k)=v_Fk-\frac{\alpha^2}{KN}\sum_{k'}\frac{v_F(k'+k)}{\omega_p}\coth\left(\frac{\omega_p}{2T}\right)\delta^2(k',k)+\frac{\alpha^2}{KN}\sum_{k'}[2-\delta(k',k)]\times\delta(k',k)\frac{v_Fk'}{W_0(k')}\tanh\left(\frac{W_0(k')}{2T}\right), \quad (18)$$

$$\Delta(k)=\alpha u_0[c-d\,\delta(k,k)], \quad (19)$$

$$c=1+\frac{\alpha^2}{KN}\sum_k \delta(k,k)\frac{\Delta_0(k)}{\alpha u_0 W_0(k)}\tanh\left(\frac{W_0(k)}{2T}\right), \quad (20)$$

$$d=1-\frac{\alpha^2}{KN}\sum_k [1-\delta(k,k)]\frac{\Delta_0(k)}{\alpha u_0 W_0(k)}\tanh\left(\frac{W_0(k)}{2T}\right). \quad (21)$$

$ik_m\Sigma_0(k,ik_m)$ and $\Sigma_3(k,ik_m)\sigma_3$ are contributions of H_1',

$$\Sigma_0(k,ik_m)=\frac{\alpha^2\omega_p}{KN}\sum_{k'}\frac{v_F^2(k+k')^2}{(\omega_p+v_F|k+k'|)^2}\times\left\{\left[1-\mathrm{sgn}(k+k')\frac{v_Fk'}{W_0(k')}\right]\times\frac{\coth\left(\frac{\omega_p}{2T}\right)+\tanh\left(\frac{W_0(k')}{2T}\right)}{(ik_m)^2-[\omega_p+W_0(k')]^2}+\left[1+\mathrm{sgn}(k+k')\frac{v_Fk'}{W_0(k')}\right]\times\frac{\coth\left(\frac{\omega_p}{2T}\right)-\tanh\left(\frac{W_0(k')}{2T}\right)}{(ik_m)^2-[\omega_p-W_0(k')]^2}\right\}, \quad (22)$$

$$\Sigma_3(k,ik_m)=\frac{\alpha^2\omega_p}{KN}\sum_{k'}\frac{v_F^2(k+k')^2}{(\omega_p+v_F|k+k'|)^2}\left\{\left[\mathrm{sgn}(k+k')-\frac{v_Fk'}{W_0(k')}\right]\frac{\omega_p+W_0(k')}{(ik_m)^2-[\omega_p+W_0(k')]^2}\times\left[\coth\left(\frac{\omega_p}{2T}\right)+\tanh\left(\frac{W_0(k')}{2T}\right)\right]+\left[\mathrm{sgn}(k+k')+\frac{v_Fk'}{W_0(k')}\right]\times\frac{\omega_p-W_0(k')}{(ik_m)^2-[\omega_p-W_0(k')]^2}\times\left[\coth\left(\frac{\omega_p}{2T}\right)-\tanh\left(\frac{W_0(k')}{2T}\right)\right]\right\}, \quad (23)$$

$$W_0(k)=\sqrt{v_F^2k^2+\Delta_0^2(k)}. \quad (24)$$

We note that the contribution of H_1' to the nondiagonal term [the prefactor of σ_1 in $\Sigma(k,ik_m)$] is zero and this is one of the reasons of choosing the form of $\delta(k',k)$ in Eq. (7). Besides, for $u_0=0$ and going to the Fermi point $k=0$,

$$\Sigma_0(0,ik_m)=\frac{\alpha^2\omega_p}{KN}\sum_{k'}\frac{2v_F^2k'^2}{(\omega_p+v_F|k'|)^2}\times\frac{\coth\left(\frac{\omega_p}{2T}\right)-\tanh\left(\frac{v_F|k'|)}{2T}\right)}{(ik_m)^2-(\omega_p-v_F|k'|)^2}, \quad (25)$$

$$\sigma(ik_m)=\lim_{k\to 0}\frac{\Sigma_3(k,ik_m)}{v_F k}=\left\{\frac{1}{v_F}\frac{d}{dk}\Sigma_3(k,ik_m)\right\}_{k\to 0}$$
$$=\frac{\alpha^2\omega_p}{KN}\sum_{k'}\left[\frac{d}{dk}\frac{2v_F(k+k')^2}{(\omega_p+v_F|k+k'|)^2}\right]_{k\to 0}$$
$$\times\mathrm{sgn}(k')\frac{\omega_p-W_0(k')}{(ik_m)^2-[\omega_p-W_0(k')]^2}$$
$$\times\left[\coth\left(\frac{\omega_p}{2T}\right)-\tanh\left(\frac{W_0(k')}{2T}\right)\right]. \quad (26)$$

It is easy to check that $\Sigma_0(0,ik_m)=0$ and $\sigma(ik_m)=0$ when $T=0$. This is another reason to choose the form of $\delta(k',k)$ in Eq. (7).

The thermodynamical average $\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle$ can be expressed as

$$\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle=\frac{1}{\beta}\sum_{k_m}\mathrm{Tr}[\sigma_1 G(k,ik_m)], \quad (27)$$

and then the equation to determine αu_0, Eq. (14), is

$$\alpha u_0=\frac{2\alpha^2}{KN}\sum_k[1-\delta(k,k)]\frac{1}{\beta}\sum_{k_m}\frac{2\Delta(k)}{k_m^2[1-\Sigma_0(k,ik_m)]^2+[E(k)+\Sigma_3(k,ik_m)]^2+\Delta^2(k)}. \quad (28)$$

Note that $k_m=(2m+1)\pi T$ and the summation over k_m is over the whole set of integers.

III. $T=0$ CASE

Let us discuss the $T=0$ case first. We make the approximation of taking the $k\to 0$ limit (at Fermi point): $\Sigma_0(k,ik_m)\approx\Sigma_0(0,ik_m)\approx 0$ and $\Sigma_3(k,ik_m)/v_F k\approx\sigma(ik_m)\approx 0$ [Eqs. (25) and (26)], which may be a good approximation when $\omega_p\ll\pi v_F$. Then the equation to determine u_0 is

$$1=\frac{2\alpha^2}{KN}\sum_k[1-\delta(k,k)]\frac{\Delta(k)}{\alpha u_0 W(k)}, \quad (29)$$

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

The density of states (DOS) $N(\omega)$ can be expressed by the retarded Green's function as follows:[24]

$$N(\omega)=-\frac{1}{\pi N}\sum_k\mathrm{Im}\,\mathrm{Tr}\,\tilde{G}^R(k,\omega), \quad (30)$$

where $\tilde{G}^R(k,\omega)=\tilde{G}(k,ik_m=\omega+i0^+)$ is the Green's function for the original Hamiltonian H,

$$\tilde{G}(k,ik_m)=-\int_0^\beta d\tau\langle T_\tau\Psi(k,\tau)\Psi^\dagger(k,0)\rangle\exp(i\tau k_m)$$
$$=-\int_0^\beta d\tau\exp(i\tau k_m)$$
$$\times\mathrm{Tr}[T_\tau e^{-\beta H}\Psi(k,\tau)\Psi^\dagger(k,0)]/\mathrm{Tr}(e^{-\beta H}). \quad (31)$$

$\Psi(k,\tau)=\exp(\tau H)\Psi(k)\exp(-\tau H)$ is in the Heisenberg representation. After the unitary transformation we have

$$\mathrm{Tr}[T_\tau e^{-\beta H}\Psi(k,\tau)\Psi^\dagger(k,0)]/\mathrm{Tr}(e^{-\beta H})$$
$$=\mathrm{Tr}[T_\tau e^{-\beta H'}\exp(\tau H')e^S\Psi(k)e^{-S}$$
$$\times\exp(-\tau H')e^S\Psi^\dagger(k)e^{-S}]/\mathrm{Tr}(e^{-\beta H'}). \quad (32)$$

The transformation of a single fermion operator can proceed as

$$e^S\Psi(k)e^{-S}=\Psi(k)+[S,\Psi(k)]+\frac{1}{2}[S,[S,\Psi(k)]]+O(\alpha^3)$$
$$=\Psi(k)-\sqrt{\frac{\alpha^2}{\omega_p KN}}\sum_q(b^\dagger_{-q}-b_q)\delta(k,k-q)$$
$$\times\sigma_1\Psi^\dagger(k-q)+\frac{\alpha^2}{2\omega_p KN}\sum_{q,q'}(b^\dagger_{-q}-b_q)$$
$$\times(b^\dagger_{-q'}-b_{q'})\delta(k-q,k-q-q')\delta(k,k-q)$$
$$\times\Psi(k-q-q'). \quad (33)$$

Then the Green's function reads (to the second order in α)

$$\tilde{G}(k,ik_m)=G(k,ik_m)-\frac{\alpha^2}{\omega_p KN}\sum_{k'}\delta^2(k,k')G(k,ik_m)$$
$$-\frac{\alpha^2}{\omega_p KN}\sum_q\delta^2(k,k-q)\frac{1}{\beta}\sum_{i\omega_n}\frac{2\omega_p}{(i\omega_n)^2-\omega_p^2}$$
$$\times G(k-q,ik_m-i\omega_n). \quad (34)$$

Here we can calculate the spectral function $A(k,\omega)$ for electrons,[24]

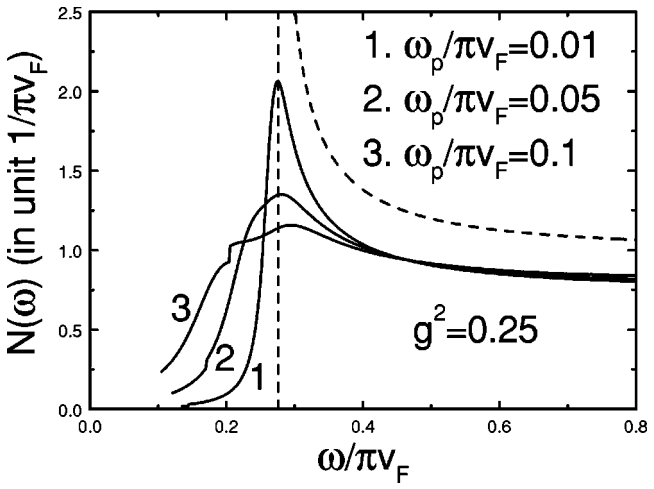

FIG. 1. The calculated DOS $N(\omega)$ for three different sets of parameters. The adiabatic result (dashed-line with $\omega_p=0$) is also shown.

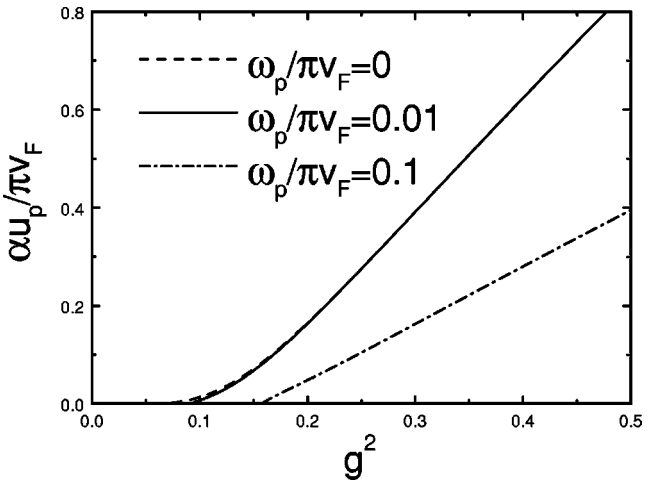

FIG. 2. The phonon-staggered ordering u_p as functions of the coupling constant g^2 for $\omega_p/\pi v_F=0$, 0.01, and 0.1. $g_c^2=0.0921$ when $\omega_p/\pi v_F=0.01$ and $g_c^2=0.1573$ when $\omega_p/\pi v_F=0.1$.

$$A(k,\omega)=-\frac{1}{\pi}\mathrm{Im\,Tr}\,\tilde{G}(k,\omega+i0^+)$$
$$=\left\{1-\frac{\alpha^2}{\omega_p KN}\sum_{k'}\delta^2(k,k')\right\}\{\delta[\omega-W(k)]$$
$$+\delta[\omega+W(k)]\}+\frac{\alpha^2}{\omega_p KN^2}\sum_{k'}\delta^2(k,k')$$
$$\times\{\delta[\omega-\omega_p-W(k')]+\delta[\omega+\omega_p+W(k')]\}. \tag{35}$$

One can easily check that

$$\int_{-\infty}^{\infty}d\omega A(k,\omega)=2, \tag{36}$$

the sum rule for the spectral function.

When $\omega>0$,

$$N(\omega)=\frac{1}{N}\sum_k\left[1-\frac{\alpha^2}{\omega_p KN}\sum_{k'}\delta^2(k,k')\right]\delta[\omega-W(k)]$$
$$+\frac{\alpha^2}{\omega_p KN^2}\sum_{k,k'}\delta^2(k,k')\delta[\omega-\omega_p-W(k')]. \tag{37}$$

The δ functions in integrations, $\delta[\omega-W(k)]$ and $\delta[\omega-\omega_p-W(k)]$, result in the fact that $N(\omega)=0$ when $\omega<\Delta(k=0)=\alpha u_0(c-d)$, which is the real gap. But what is the gap which can be measured through, say, the optical absorption spectra?

Figure 1 shows the DOS $N(\omega)$ for fixed $g^2=0.25$ with $\omega_p/\pi v_F=0.01$, 0.05, and 0.1, respectively, where $g^2=\alpha^2/\pi v_F K$ is the dimensionless coupling constant. For comparison, the adiabatic mean-field result is also shown where an inverse-square-root singularity exists at the gap edge [note that because of the linear k dependence $v_F k$ of the free fermion energy, the DOS $N_0(\omega)$ for $g^2=0$ is $1/\pi v_F$]. One can see that when $\omega_p>0$ there is a peak at $\omega=\omega_{peak}$ with a significant tail below the peak. The height of peak decreases but the width of it increases with increasing ω_p. $N(\omega)$ can be measured by the optical absorption (which measures the joint DOS) and in the observed absorption spectra of Peierls-distorted systems there is a peak with a significant tail below it.[1,4,5] Usually, the position of peak ω_{peak} is assigned as the gap, which is larger than the real gap $\Delta(k=0)=\alpha u_0(c-d)$ in our calculation.

When the frequency ω_p is small ($\omega_p/\pi v_F=0.01$ in Fig. 1), the peak in DOS is quite sharp with a tail going down to a small value: $N[\omega=\Delta(k=0)]\sim\omega_p/\alpha u_p$. For $\omega<\Delta(k=0)$ we have $N(\omega)=0$. The physical meaning of this result is that, because of the quantum lattice fluctuations, a finite gap still exists but its magnitude is reduced compared with the adiabatic mean-field value. For larger frequency ($\omega_p/\pi v_F=0.05$ and 0.1), the main peak is broadened and there is a small discontinuity at $\omega=\Delta(k=0)+\omega_p$. This discontinuity comes from the single-phonon sideband and if the finite lifetime of the phonon mode is taken into account the discontinuity would become a small peak.

Since u_0 is related to the static phonon-staggered ordering, we should define the phonon-staggered order parameter u_p,

$$\alpha u_p=\frac{1}{L}\int dy\left\langle\sqrt{\frac{\omega_p\alpha^2}{KN}}\sum_q(b_{-q}^\dagger+b_q)\exp(iqy)\right\rangle, \tag{38}$$

which can be measured by experiments or by Monte Carlo simulations. After performing the unitary transformations (6) and (10) we have ($T=0$)

$$\alpha u_p=\alpha u_0-\frac{2\alpha^2}{KN}\sum_k\delta(k,k)\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle$$
$$=-\frac{2\alpha^2}{KN}\sum_k\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle=\frac{2\alpha^2}{KN}\sum_k\frac{\Delta(k)}{W(k)}. \tag{39}$$

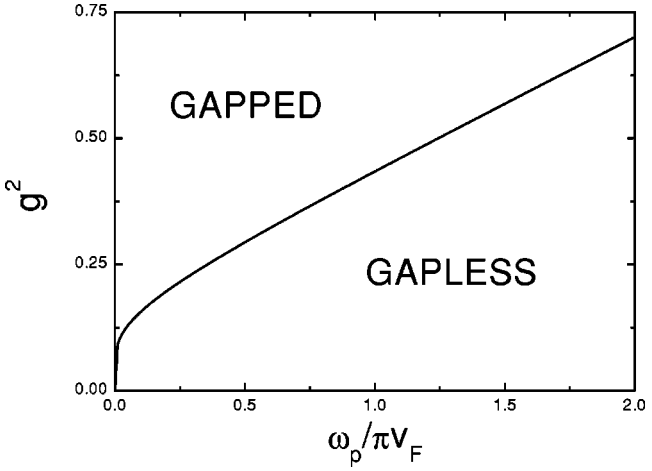

FIG. 3. The g^2 vs $\omega_p/\pi v_F$ phase diagram.

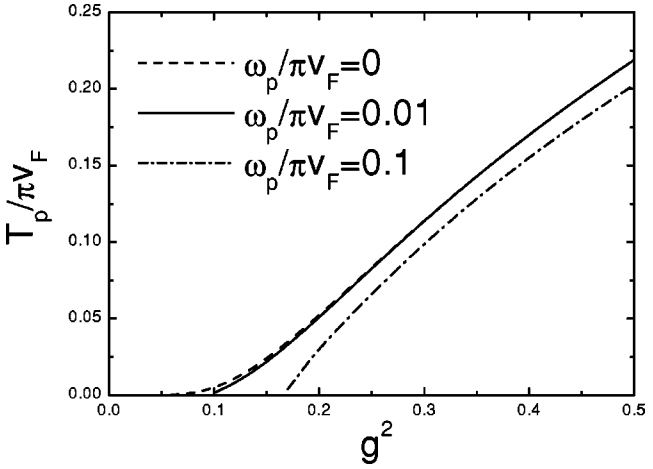

FIG. 4. The calculated Peierls transition temperature T_p as functions of g^2 for frequency $\omega_p/\pi v_F=0$, 0.01, and 0.1. g_c^2's are the same as those in Fig. 2.

Figure 2 shows the calculated αu_p as a function of g^2 for $\omega_p/\pi v_F=0$, 0.01, and 0.1, respectively. When $\omega_p=0$, the solution of Eq. (39) is

$$\alpha u_p=\alpha u_0=\pi v_F/\sinh\left(\frac{1}{2g^2}\right), \tag{40}$$

and the gap $\Delta=\alpha u_p=\omega_{peak}$. But when $\omega_p>0$ the gap $\Delta(k=0)$, the order parameter αu_p, and the peak position ω_{peak} are generally different from each other. However, when ω_p is small $\alpha u_p\approx\omega_{peak}$.

When $\omega_p>0$, there is a critical coupling constant g_c^2; $\Delta(k=0)=u_p=0$ when $g^2\leqslant g_c^2$. Figure 3 shows the phase diagram g_c^2 as a function of ω_p when $T=0$.

IV. CALCULATION OF T_p

For finite temperature, we also make the approximation of taking the $k\to 0$ limit (at Fermi point): $\Sigma_0(k,ik_m)\approx\Sigma_0(0,ik_m)$; besides, $\sigma(ik_m)=\Sigma_3(k,\omega)/v_Fk|_{k\to 0}$ is approximated as $\sigma(ik_m)\approx 0$ because $\sigma(ik_m)=0$ when $\omega_p=0$. These approximations should be good when $\omega_p\ll\pi v_F$.

The Peierls transition temperature T_p is determined by $u_0=0$ in Eq. (28),

$$1=\frac{2\alpha^2}{KN}\sum_k\left[1-\delta(k,k)\right]\frac{1}{\beta}\sum_{k_m}\frac{2[c-d\,\delta(k,k)]}{k_m^2Z^2(0,ik_m)+\rho^2(k)v_F^2k^2}, \tag{41}$$

where

$$\rho(k)=E(k)/v_Fk, \tag{42}$$
$$Z(0,ik_m)=1-\Sigma_0(0,ik_m).$$

When going to the adiabatic limit $\omega_p\to 0$, the gap at $T=0$ is $\Delta\approx 2\pi v_F\exp[-1/2g^2]$ if the coupling is weak. The equation for Peierls transition temperature T_p is

$$1=\frac{2\alpha^2}{KN}\sum_k\frac{1}{\beta}\sum_{k_m}\frac{2}{k_m^2Z_0^2(0,ik_m)+\rho_0^2v_F^2k^2}, \tag{43}$$

where

$$\rho_0=\rho(k=0)|_{\omega_p\to 0}=1-g^2\omega_p'\coth\left(\frac{\omega_p}{2T_p}\right), \tag{44}$$

$$\begin{aligned}Z_0(0,ik_m)&=Z(0,ik_m)|_{\omega_p\to 0}\\&=1+2g^2\omega_p'\coth\left(\frac{\omega_p}{2T_p}\right)\int_0^1\frac{dx}{(k_m/\pi v_F)^2+x^2}\\&=1+2g^2\omega_p'\coth\left(\frac{\omega_p}{2T_p}\right)\frac{\pi v_F}{k_m}\tan^{-1}\left(\frac{\pi v_F}{k_m}\right),\end{aligned} \tag{45}$$

$T_p'=T_p/\pi v_F$ and $\omega_p'=\omega_p/\pi v_F$. Let $\omega_p/\pi v_F\to 0$ and approximate $(\pi v_F/k_m)\tan^{-1}(\pi v_F/k_m)\approx\gamma$ (γ is a constant of order 1), we have $\rho_0=1-2g^2T_p'$ and $Z_0=1+4g^2\gamma T_p'$ and the solution of Eq. (43) is

$$T_p'=1.134\frac{\rho_0}{Z_0}\exp\left[-\frac{\rho_0Z_0}{2g^2}\right]. \tag{46}$$

Thus the ratio $2\Delta/T_p$ can be calculated as

$$\begin{aligned}\frac{2\Delta}{T_p}&=3.527\frac{Z_0}{\rho_0}\exp\left[-\frac{1-\rho_0Z_0}{2g^2}\right]\\&\approx 3.527+3.527[2\gamma-1+2g^2(2\gamma+1)]T_p'.\end{aligned} \tag{47}$$

Now we can see that $2\Delta/T_p\to 3.527$ at weak-coupling limit $g^2\to 0$ $(T_p'\to 0)$.

We note that when $\omega_p\to 0$ the lattice fluctuations are purely thermal fluctuations and their effect in our calculations is mainly contained in $Z_0(0,ik_m)$ [Eq. (45)]. From Eq. (45) one can see that the effect of thermal fluctuations is proportional to $\omega_p\coth(\omega_p/2T_p)$, which is the same as what was assumed in Ref. 4.

The numerical results for $\omega_p=0$ are shown in Figs. 4 and 5. For the weak-coupling limit, $T_p=1.134\pi v_F\exp[-1/2g^2]$, which is the typical BCS weak-coupling result. $2\Delta/T_p$ starts from the BCS value 3.527 and increases with increasing cou-

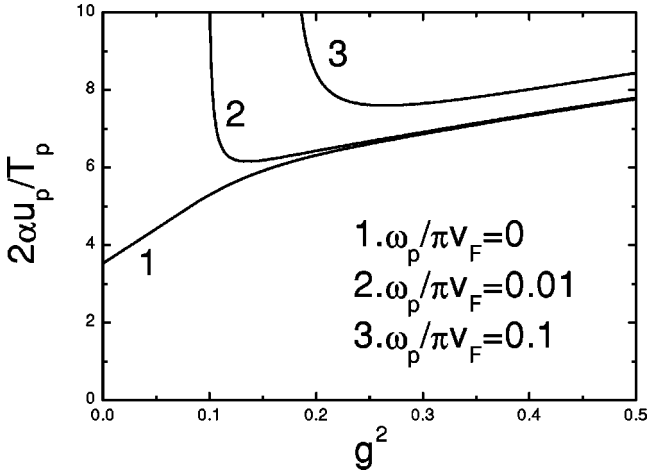

FIG. 5. The ratio $2\alpha u_p/T_p$ as functions of g^2 for frequency $\omega_p/\pi v_F=0$, 0.01, and 0.1.

pling g^2. The behaviors of T_p and $2\Delta/T_p$ are similar to those of the dynamical mean-field study of Blawid and Millis (they used the half filled spinless Holstein model).[7]

For general $\omega_p>0$ case, we have to solve Eq. (41) numerically. The results are also shown in Figs. 4 and 5 for $\omega_p/\pi v_F=0.01$ and 0.1 ($\omega_p \ll \pi v_F$). T_p vanishes for $g^2 < g_c^2$. In Fig. 5, instead of $2\Delta/T_p$, we show the ratio $2\alpha u_p/T_p$ because the real gap $\Delta(k=0)=\alpha u_0(c-d)$ is much smaller than both the peak position ω_{peak} and the ordering parameter αu_p, but $\omega_{peak}\approx\alpha u_p$ when $\omega_p \ll \pi v_F$. The ratio $2\alpha u_p/T_p$ goes to infinity when g^2 goes to g_c^2 ($g^2\to g_c^2$) from above. This is because T_p goes to zero faster than αu_p does when $g^2\to g_c^2$. One can see that the ratio is in the range around 5–10, larger than the BCS value 3.527. These results are in qualitative agreement with the dynamical mean-field study of Blawid and Millis for quantum phonons,[8] but they did not show the result for $2\Delta/T_p$.

We note that a larger ratio $2\alpha u_p/T_p$ comes from the following two points: (i) The zero-temperature Peierls distortion and gap parameter are only slightly reduced below the mean-field prediction when $\omega_p \ll \pi v_F$; (ii) but the fluctuations due to the thermal lattice motion can destroy the Peierls distortion at a temperature well below the mean-field transition temperature even if the phonon frequency is quite small.

V. SUMMARY AND DISCUSSION

The effect of quantum phonons on the Peierls transition temperature in a one-dimensional commensurate system is studied. The nonadiabatic effect due to finite phonon frequency $\omega_p>0$ are treated through an energy-dependent electron-phonon scattering function $\delta(k',k)$ and the functional dependence of it is determined by the perturbation theory, that is, the contribution of H_1' to the self-energy when $T=0$ is nearly zero. By using the Green's-function perturbation theory we have shown that our theory gives a good description of the effect of quantum phonons: (i) There exists a critical electron-phonon coupling g_c^2. The Peierls transition temperature $T_p=0$ when the coupling $g^2<g_c^2$ and T_p increases with increasing $g^2>g_c^2$. (ii) The ratio $2\Delta/T_p$ could be much larger than the BCS value 3.527.

Finally, we give a note on the physical meaning of $\delta(k',k)$ [Eq. (7)], which was introduced in the unitary transformation and plays an important role in our treatment. One can see that $\delta(k,k)=\omega_p/(\omega_p+2v_F|k|)$ has a peak at $k=0$, the Fermi point in our model system, and when $\omega_p/v_F \ll 1$ the peak is very sharp. This peak means that only those electrons near the Fermi point within a range of about $|k| \leqslant \omega_p/v_F$ can participate in the electron-phonon scattering and contribute to the reduction of the energy gap and the Peierls transition temperature compared with the adiabatic mean-field value [see Eq. (14)]. This fact is similar to that in the BCS theory[25] for superconductivity: only those electrons near the Fermi surface form Cooper pairs via a phonon-induced effective attraction.

ACKNOWLEDGMENTS

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