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Effect of lattice fluctuations on the quantum phase transition in a one-dimensional commensurate system

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Abstract. The effect of quantum lattice fluctuations on the properties of quantum phase transition in a one-dimensional commensurate system near and at criticality is studied. The nonadiabatic effect due to finite phonon frequency $\omega_{\rm p} > 0$ are treated through an energy-dependent electron-phonon scattering function introduced in a unitary transformation. By using the Green's function perturbation theory we have shown that our theory gives a good description of the effect of quantum lattice fluctuations: (1) At the criticality, when the coupling constant g^2 decreases or the phonon frequency $\omega_{\rm p}$ increases the lattice distortion and the gap in the fermionic spectrum decreases gradually; at some critical value $g_{\rm c}^2$ or $(\omega_{\rm p})_{\rm c}$, the system becomes gapless and the lattice distortion disappears. (2) The calculated density of states do not have the inverse-square-root singularity but have a peak with a significant tail below the peak. (3) At the criticality our approach successfully describes the classical-quantum crossover. In the classical region the adiabatic mean-field parameters may strongly be renormalized by nonadiabatic corrections, and in the quantum region the phase transition is of the signature of a Kosterlitz-Thouless transition. (4) Away from the criticality the critical exponents for the energy gap and the ordering parameter have been calculated.

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1 Introduction

Recently, there is a growing interest in the quantum phase transitions of some low-dimensional models of interacting fermions, which are phase transitions at zero temperature as some parameter is varied. It has been proposed that a quantum critical point plays an important role in high-$T_{\rm c}$ superconductivity [1].

Theoretical studies of quantum phase transitions in the presence of quenched (time-independent) disorder have been done by several authors. Fisher [2] performed an exhaustive study of the effect of randomness on the transverse field Ising spin chain to undergo a quantum phase transition. McKenzie [3] proposed to study the following Hamiltonian,

$$H_{\rm s}=\int {\rm d}y\Psi^{\dagger}(y)\left(-{\rm i}v_{\rm F}\sigma_3\frac{\partial}{\partial y}+V(y)\sigma_{+}+V^{*}(y)\sigma_{-}\right)\Psi(y), \tag{1}$$

which describes the low-energy properties of quantum phase transitions in the random XY spin chains (in continuum limit). In (1) $\sigma_\alpha(\alpha=1,2,3)$ and $\sigma_{\pm}=\frac{1}{2}(\sigma_1\pm{\rm i}\sigma_2)$ are Pauli matrices.

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

is the spinor representation of the fermionic field satisfying the anti-commutation relations. $V(y)$ is the back scattering potential. For the pure spin system without disorder, $V(y)=V_0$ is a constant where V_0 is a measure of the deviation from criticality. McKenzie assumed a Gaussian correlation $\langle V(x)V(y)\rangle = V_0^2+\gamma\delta(x-y)$ to describe the randomness.

In this paper we propose to study the effect of lattice fluctuations on the low-energy properties of quantum phase transitions starting from the Hamiltonian (1) with $V(y)=V_0+\varphi(y)$, where $\varphi(y)$ is an operator proportional to the local lattice displacement

$$\varphi(y)=\sqrt{\frac{\alpha^2\omega_{\rm p}}{KN}}\sum_q(b_{-q}^{\dagger}+b_q)\exp({\rm i}qy). \tag{3}$$

N is the total number of unit cells, $\omega_{\rm p}$ is the phonon frequency with spring constant K, α is the fermion-phonon coupling constant, and $b_q(b_{-q}^{\dagger})$ is the annihilation (creation) operator of the phonon mode q. Here we assume the commensurate case with a real back scattering potential $V(y)=V^{*}(y)$. Roughly speaking, in some sense the

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effect of lattice fluctuations are similar to that of the randomness. But the former have their own dynamics which can be described by

$$H_{\rm p} = \omega_{\rm p} \sum_q b_q^\dagger b_q, \tag{4}$$

the harmonic Hamiltonian of phonons. The total Hamiltonian is $H = H_{\rm s} + H_{\rm p}$.

H is of the same form as the non-degenerate ($V_0 \neq 0$) Takayama-Lin-Liu-Maki (TLM) Hamiltonian [4] for spinless electrons, which is the continuum version of the Su-Schrieffer-Heeger (SSH) model [5] describing the physics of quasi-one-dimensional polymers where the phonons interact with the electrons by modifying the electron hopping matrix elements. McKenzie *et al.* [6] treated H as the model Hamiltonian for studying the effect of lattice fluctuations on the energy gap and the optical absorption spectra of quasi-one-dimensional systems, such as polyacetylene, $K_{0.3}MoO_3$, and the halogen-bridged metal complexes. Generally speaking, H can be used to describe: (1) the low-energy properties of quantum phase transitions in the XY spin chains (in continuum limit) where the lattice fluctuations play the role of dynamical randomness, and (2) the Peierls instabilities with degenerate ($V_0 = 0$) and non-degenerate ($V_0 \neq 0$) ground state.

The theoretical analysis becomes difficult when the quantum lattice fluctuations are taken into account. Various methods have been used for the problem, such as the Monte Carlo simulation [7–10], perturbation calculation [11], Green's function technique [12,13], renormalization group analysis [14–16], variational method of the squeezed-polaronic wave-function [17], a phenomenological random potential with Gaussian correlations [6]. Previously, one of us developed a new approach to treat the lattice fluctuations due to finite phonon frequency $\omega_{\rm p} > 0$ through an energy-dependent electron-phonon scattering function $\delta(k', k)$ introduced in the unitary transformation [18]. In this work, we extend this approach to the study of effect of lattice fluctuations on the quantum phase transition in the model system $H = H_{\rm s} + H_{\rm p}$.

Throughout this paper we put $\hbar = 1$ and $k_{\rm B} = 1$.

2 Theoretical analysis

In momentum space the Hamiltonian reads

$$H = \sum_k v_{\rm F} k \Psi^\dagger(k)\sigma_3\Psi(k) + \sum_k V_0 \Psi^\dagger(k)\sigma_1\Psi(k) + \omega_{\rm p}\sum_q b_q^\dagger b_q + \sqrt{\frac{\alpha^2\omega_{\rm p}}{KN}}\sum_{k,q}(b_{-q}^\dagger + b_q)\Psi^\dagger(k+q)\sigma_1\Psi(k). \tag{5}$$

The last term in (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 fermion-phonon correlation, $H' = \exp(S) H \exp(-S)$,

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

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

$$\delta(k', k) = \frac{\omega_{\rm p}}{\omega_{\rm p} + v_{\rm F}|k' + k|}, \tag{7}$$

and the reason of this definition will become clear later.

The total Hamiltonian H is divided as $H = H_0 + H_1$, where H_1 is the fermion-phonon interaction. Then the transformation can proceed order by order,

$$H' = H_0 + H_1 + [S, H_0] + [S, H_1] + \frac{1}{2}[S, [S, H_0]] + O(\alpha^3).$$

The first order terms in the transformed Hamiltonian H' are

$$H_1' = H_1 + [S, H_0] = \sqrt{\frac{\alpha^2\omega_{\rm p}}{KN}}\sum_{k,q}\frac{v_{\rm F}}{\omega_{\rm p} + v_{\rm F}|2k+q|}\Psi^\dagger(k+q) \times \Big\{\Big[|2k+q|\sigma_1 - {\rm i}(2k+q)\sigma_2\Big]b_{-q}^\dagger + \Big[|2k+q|\sigma_1 + {\rm i}(2k+q)\sigma_2)b_q\Big]\Big\}\Psi(k), \tag{8}$$

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:

$$\begin{aligned} H_2' &= [S, H_1] + \frac{1}{2}[S, [S, H_0]] \\ &= \frac{\alpha^2}{KN}\sum_{k,q}\frac{v_{\rm F}(2k+q)}{\omega_{\rm p}}(b_{-q}^\dagger - b_q)(b_q^\dagger - b_{-q}) \\ &\quad\times\delta^2(k+q,k)\Psi^\dagger(k)\sigma_3\Psi(k) \\ &\quad -\frac{\alpha^2}{KN}\sum_{k,k',q}\Big[2 - \delta(k'-q,k')\Big]\delta(k+q,k) \\ &\quad\times\Psi^\dagger(k+q)\sigma_1\Psi(k)\Psi^\dagger(k'-q)\sigma_1\Psi(k'). \end{aligned} \tag{9}$$

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

$$R = -u_0\sqrt{\frac{KN}{4\omega_{\rm p}}}(b_0^\dagger - b_0). \tag{10}$$

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

$$\exp(R)\varphi(y)\exp(-R) = \varphi(y) + \alpha u_0, \tag{11}$$

and u_0 is a variational parameter to describe the static lattice distortion. This transformation is to introduce a distortion potential $\Delta_0(k)$ for fermions,

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

$$\Delta_0(k) = V_0 + \alpha u_0[1-\delta(k,k)]. \quad (13)$$

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 $\langle ...\rangle$ 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 $\omega_{\rm p} = 0$ and $\omega_{\rm p} \to \infty$ limits. When $\omega_{\rm p} = 0$, $\delta(k',k) = 0$, and then $H_1' = 0$, $H_2' = 0$,

$$H'(\omega_{\rm p}=0) = \sum_k v_{\rm F} k\Psi^\dagger(k)\sigma_3\Psi(k) + \sum_k [V_0+\alpha u_0]\,\Psi^\dagger(k)\sigma_1\Psi(k) + \frac{Ku_0^2}{4}N. \quad (15)$$

This is equivalent to the original Hamiltonian H in adiabatic approximation. When $\omega_{\rm p} \to \infty$, $\delta(k',k) = 1$, and then $u_0 = 0$, $H_1' = 0$,

$$H'(\omega_{\rm p}\to\infty) = \sum_k v_{\rm F} k\Psi^\dagger(k)\sigma_3\Psi(k) + \omega_{\rm p}\sum_q b_q^\dagger b_q + \sum_k V_0\Psi^\dagger(k)\sigma_1\Psi(k) - \frac{\alpha^2}{KN}\sum_{k,k',q}\Psi^\dagger(k+q)\sigma_1\Psi(k)\Psi^\dagger(k'-q)\sigma_1\Psi(k'). \quad (16)$$

This is the exact Hamiltonian for $\omega_{\rm p} \to \infty$ limit, which can be obtained through the functional integration method [9].

3 $\omega_{\rm p} < \pi v_{\rm F}$ case

The purpose of our transformation is to find a better way to divide the Hamiltonian into the unperturbed part and the perturbation. For the $\omega_{\rm p} < \pi v_{\rm F}$ case we treat H_0' as the unperturbed part and $H_1' + H_2'$ the perturbation, because (1)$H_1' + H_2' \to 0$ as $\omega_{\rm p} \to 0$ and (2) by choosing the functional form of $\delta(k',k)$ in equation (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. $G_0(k,{\rm i}k_m) = [{\rm i}k_m - v_{\rm F}k\sigma_3 - \Delta_0(k)\sigma_1]^{-1}$ is the Green's function for H_0' and that for H', $G(k,{\rm i}k_m)$, is related to $G_0(k,{\rm i}k_m)$ *via* the Dyson equation. The second order ($O(\alpha^2)$) self-energy can be written as:

$$\Sigma(k,{\rm i}k_m) = {\rm i}k_m\Sigma_0(k,{\rm i}k_m) + (E(k) - v_{\rm F}k + \Sigma_3(k,{\rm i}k_m))\,\sigma_3 + (\Delta(k) - \Delta_0(k))\,\sigma_1. \quad (17)$$

Here $(E(k) - v_{\rm F}k)\,\sigma_3 + (\Delta(k) - \Delta_0(k))\,\sigma_1$ is the contribution of H_2'

$$E(k) = v_{\rm F}k - \frac{\alpha^2}{KN}\sum_{k'}\frac{v_{\rm F}(k'+k)}{\omega_{\rm p}}\delta^2(k',k) + \frac{\alpha^2}{KN}\sum_{k'}[2-\delta(k',k)]\delta(k',k)\frac{v_{\rm F}k'}{W_0(k')}, \quad (18)$$

$$\Delta(k) = c - d\delta(k,k), \quad (19)$$

$$c = V_0 + \alpha u_0 + \frac{\alpha^2}{KN}\sum_k \delta(k,k)\frac{\Delta_0(k)}{W_0(k)}, \quad (20)$$

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

${\rm i}k_m\Sigma_0(k,{\rm i}k_m)$ and $\Sigma_3(k,{\rm i}k_m)\sigma_3$ are contributions of H_1'. When $T = 0$,

$$\Sigma_0(k,{\rm i}k_m) = \frac{\alpha^2\omega_{\rm p}}{KN}\sum_{k'}\frac{2v_{\rm F}^2(k+k')^2}{(\omega_{\rm p}+v_{\rm F}|k+k'|)^2}\times\left[1-{\rm sign}(k+k')\frac{v_{\rm F}k'}{W_0(k')}\right]\times\frac{1}{({\rm i}k_m)^2-(\omega_{\rm p}+W_0(k'))^2}, \quad (22)$$

$$\Sigma_3(k,{\rm i}k_m) = \frac{\alpha^2\omega_{\rm p}}{KN}\sum_{k'}\frac{2v_{\rm F}^2(k+k')^2}{(\omega_{\rm p}+v_{\rm F}|k+k'|)^2}\times\left[{\rm sign}(k+k') - \frac{v_{\rm F}k'}{W_0(k')}\right]\times\frac{\omega_{\rm p}+W_0(k')}{({\rm i}k_m)^2-(\omega_{\rm p}+W_0(k'))^2}, \quad (23)$$

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

We note that the contribution of H_1' to the non-diagonal term (the prefactor of σ_1 in $\Sigma(k,{\rm i}k_m)$) is zero. Besides, when $T = 0$, $V_0 = 0$, $u_0 = 0$, and at the Fermi point $k = 0$, we have $\Sigma_0(k = 0,{\rm i}k_m) = 0$ and $\Sigma_3(k = 0,{\rm i}k_m) = 0$. These are the reasons of choosing the form of $\delta(k',k)$ in equation (7).

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

$$\langle\Psi^\dagger(k)\sigma_1\Psi(k)\rangle = \frac{1}{\beta}\sum_{{\rm i}k_m}{\rm Tr}\left[\sigma_1 G(k,{\rm i}k_m)\right], \quad (25)$$

and then the equation to determine αu_0, equation (14), is (when $T = 0$)

$$\alpha u_0 = \frac{2\alpha^2}{KN}\sum_k [1-\delta(k,k)]\frac{\Delta(k)}{W(k)}, \quad (26)$$

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

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

$$\rho(\omega) = -\frac{1}{\pi N} \sum_k \mathrm{Im}\mathrm{Tr}\tilde{G}^R(k,\omega), \tag{27}$$

where $\tilde{G}^R(k,\omega) = \tilde{G}(k, \mathrm{i}k_m = \omega + \mathrm{i}0^+)$ is the Green's function for the original Hamiltonian H,

$$\begin{aligned}\tilde{G}(k,\mathrm{i}k_m) =& -\int_0^\beta \mathrm{d}\tau \left\langle T_\tau \Psi(k,\tau)\Psi^\dagger(k,0)\right\rangle \exp(\mathrm{i}\tau k_m) \\ =& -\int_0^\beta \mathrm{d}\tau \exp(\mathrm{i}\tau k_m) \\ & \times \mathrm{Tr}\left(T_\tau \mathrm{e}^{-\beta H}\Psi(k,\tau)\Psi^\dagger(k,0)\right)/\mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right). \end{aligned} \tag{28}$$

$\beta = 1/T$ and $\Psi(k,\tau) = \exp(\tau H)\Psi(k)\exp(-\tau H)$ is in the Heisenberg representation. After the unitary transformation

$$\begin{aligned} & \mathrm{Tr}\left(T_\tau \mathrm{e}^{-\beta H}\Psi(k,\tau)\Psi^\dagger(k,0)\right)/\mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) \\ =& \mathrm{Tr}\left(T_\tau \mathrm{e}^{-\beta H'}\exp(\tau H')\mathrm{e}^S\Psi(k)\mathrm{e}^{-S}\right. \\ & \left.\times \exp(-\tau H')\mathrm{e}^S\Psi^\dagger(k)\mathrm{e}^{-S}\right)/\mathrm{Tr}\left(\mathrm{e}^{-\beta H'}\right). \end{aligned} \tag{29}$$

The transformation of a single fermion operator can proceed as

$$\begin{aligned} \mathrm{e}^S\Psi(k)\mathrm{e}^{-S} =& \Psi(k) + [S,\Psi(k)] + \frac{1}{2}[S,[S,\Psi(k)]] + O(\alpha^3) \\ =& \Psi(k) - \sqrt{\frac{\alpha^2}{\omega_\mathrm{p} KN}}\sum_q (b^\dagger_{-q} - b_q)\delta(k,k-q)\sigma_1\Psi^\dagger(k-q) \\ & + \frac{\alpha^2}{\omega_\mathrm{p} KN}\sum_{q,q'}(b^\dagger_{-q} - b_q)(b^\dagger_{-q'} - b_{q'})\delta(k-q,k-q-q') \\ & \times\delta(k,k-q)\Psi(k-q-q'). \end{aligned} \tag{30}$$

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

$$\begin{aligned} \tilde{G}(k,\mathrm{i}k_m) =& G(k,\mathrm{i}k_m) - \frac{\alpha^2}{\omega_\mathrm{p} KN}\sum_{k'}\delta^2(k,k')G(k,\mathrm{i}k_m) \\ & - \frac{\alpha^2}{\omega_\mathrm{p} KN}\sum_q \delta^2(k,k-q)\frac{1}{\beta} \\ & \times \sum_{\mathrm{i}\omega_n}\frac{2\omega_\mathrm{p}}{(\mathrm{i}\omega_n)^2 - \omega_\mathrm{p}^2}G(k-q,\mathrm{i}k_m - \mathrm{i}\omega_n). \end{aligned} \tag{31}$$

When $T = 0$ and $\omega > 0$,

$$\begin{aligned} \rho(\omega) =& \frac{1}{N}\sum_k \left[1 - \frac{\alpha^2}{\omega_\mathrm{p} KN}\sum_{k'}\delta^2(k,k')\right]\delta(\omega - W(k)) \\ & + \frac{\alpha^2}{\omega_\mathrm{p} KN^2}\sum_{k,k'}\delta^2(k,k')\delta(\omega - \omega_\mathrm{p} - W(k')). \end{aligned} \tag{32}$$

It is easy to check that $\int_0^\infty \mathrm{d}\omega\rho(\omega) = 1$, the normalization of DOS. The δ-functions in integrations, $\delta(\omega - W(k))$ and $\delta(\omega - \omega_\mathrm{p} - W(k))$, result in the fact that $\rho(\omega) = 0$ when $\omega < \Delta(k=0) = c - d$, which is the gap.

Since u_0 is related to the static lattice distortion, we should define the ordering parameter u_p,

$$\alpha u_\mathrm{p} = \frac{1}{L}\int \mathrm{d}y \left\langle \sqrt{\frac{\omega_\mathrm{p}\alpha^2}{KN}}\sum_q (b^\dagger_{-q} + b_q)\exp(\mathrm{i}qy)\right\rangle, \tag{33}$$

which can be measured by experiments or by Monte Carlo simulations. After performing the unitary transformations (6) and (11),

$$\begin{aligned} \alpha u_\mathrm{p} =& \alpha u_0 - \frac{2\alpha^2}{KN}\sum_k \delta(k,k)\left\langle \Psi^\dagger(k)\sigma_1\Psi(k)\right\rangle \\ =& -\frac{2\alpha^2}{KN}\sum_k \left\langle \Psi^\dagger(k)\sigma_1\Psi(k)\right\rangle. \end{aligned} \tag{34}$$

At criticality ($V_0 = 0$), equation (26) becomes

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

where $\Delta(k) = \alpha u_0(c' - d'\delta(k,k))$ and

$$\begin{aligned} c' =& 1 + \frac{\alpha^2}{KN}\sum_k \delta(k,k)\frac{1-\delta(k,k)}{W_0(k)}, \\ d' =& 1 - \frac{\alpha^2}{KN}\sum_k [1-\delta(k,k)]\frac{1-\delta(k,k)}{W_0(k)}. \end{aligned}$$

We note that, since $1 - \delta(k,k) = 2v_\mathrm{F}|k|/(\omega_\mathrm{p} + 2v_\mathrm{F}|k|)$, the logarithmic singularity in the integration when $u_0 \to 0$ and $\omega_\mathrm{p} = 0$ is removed by the factor $1 - \delta(k,k)$ as long as the ratio $\omega_\mathrm{p}/v_\mathrm{F}$ is finite. This means that when $V_0 = 0$ the system undergoes a phase transition from the gapped phase ($u_0 \neq 0$) to the gapless one ($u_0 = 0$) when the dimensionless coupling constant $g^2 = \alpha^2/\pi v_\mathrm{F} K$ decreases across the critical coupling g_c^2. This result is the same as that of reference [8], but different from those of references [13] and [18].

Figure 1 is the g^2 *vs.* $\omega_\mathrm{p}/(\omega_\mathrm{p} + \pi v_\mathrm{F})$ phase diagram when $V_0 = 0$. The solid line is the phase boundary between the gapped and gapless phases determined by the condition $u_0 = 0$. From the line one can obtain the critical coupling g_c^2 for fixed ω_p, or the critical frequency $(\omega_\mathrm{p})_\mathrm{c}$ for fixed g^2. The dashed line is the phase boundary which will be determined in next section for the $\omega > \pi v_\mathrm{F}$ case.

Figure 2a shows the calculated DOS $\rho(\omega)$ *versus* $\omega/\pi v_\mathrm{F}$ relations for three different sets of parameters at criticality ($V_0 = 0$), Curve 1 is the case near the critical point (for $\omega_\mathrm{p}/\pi v_\mathrm{F} = 0.01$, $g_\mathrm{c}^2 = 0.0921$) and it is similar to the DOS of free fermions (note that because of the linear k-dependence $v_\mathrm{F}k$ of the free fermion energy, the DOS $\rho_0(\omega)$ for $g^2 = 0$ is $1/\pi v_\mathrm{F}$) except the small gap and two peaks just above the gap (the second peak is the phonon side-band). Curve 3 is the case far away from the critical point ($g^2 - g_\mathrm{c}^2 = 0.1$). For comparison, the adiabatic

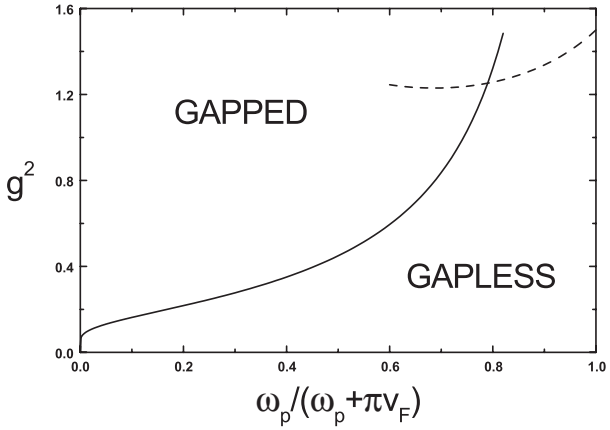

Fig. 1. The g^2 *vs.* $\omega_{\rm p}/(\omega_{\rm p}+\pi v_{\rm F})$ phase diagram for the case at criticality ($V_0 = 0$). See text for details.

result (the dashed-line with $\omega_{\rm p} = 0$ and $g^2 = 0.1921$) is also shown which has an inverse-square-root singularity at $\omega/\omega_{\rm peak} = 1$. For finite $\omega_{\rm p}$, the singularity is absent and there is a significant tail below the peak. The gap is $\Delta(k = 0) = c - d$, which is non-zero but lower than the peak. Curve 2 is the case with larger phonon frequency ($\omega_{\rm p}/\pi v_{\rm F} = 0.1$ for which $g_{\rm c}^2 = 0.1573$). One can see that the separation between the main peak and the phonon side-band is nearly $\omega_{\rm p}/\pi v_{\rm F} = 0.1$.

Figure 2b compares $\rho(\omega)$ *versus* $\omega/\pi v_{\rm F}$ relations between the cases of $V_0 = 0$ and $V_0 > 0$. Curve 1 is in the gapless phase (for $V_0 = 0$ and $\omega_{\rm p}/\pi v_{\rm F} = 0.05$, $g_{\rm c}^2 = 0.1297$). Away from the criticality ($V_0 > 0$) the system becomes gapped with a peak above the gap. For comparison, the adiabatic result (the dashed-line with $\omega_{\rm p} = 0$, $g^2 = 0.1$, and $V_0/\pi v_{\rm F} = 0.1$) is also shown which has an inverse-square-root singularity at $\omega/\omega_{\rm peak} = 1$. Curve 2 and curve 3 are generally the same, except that the size of the gap and the peak height increases with increasing V_0. The small peak which is a little bit higher than the main peak is the phonon side-band.

We note that, qualitatively, our calculated DOS's in Figure 2 are similar to those of McKenzie *et al.* [6], especially for smaller $\omega_{\rm p}$ and larger $g^2 > g_{\rm c}^2$ (curve 3 in Fig. 2a) or larger $V_0 > 0$ (curve 3 in Fig. 2b). The singularity at the gap edge (which may appear in the adiabatic mean-field approximation) is absent and, instead of the singularity, there is a peak with a significant tail below the peak. Main difference between ours and those of McKenzie *et al.* [6] is the second weak peak accompanied the main one in our DOS's which is the dynamical effect of phonons.

At criticality ($V_0 = 0$) there exists a classical-quantum crossover around $\alpha u_{\rm p} \sim \omega_{\rm p}$. Figure 3 shows the ordering parameter $\alpha u_{\rm p}$ as functions of the coupling constant g^2 for different values of $\omega_{\rm p}$. For the classical region where $\alpha u_{\rm p} > \omega_{\rm p}$ the behavior of $\alpha u_{\rm p}$ can be described by the form of an adiabatic mean-field solution,

$$\alpha u_{\rm p}/\pi v_{\rm F} = \frac{A_2}{\sinh\left(A_1/2g^2\right)}, \tag{35}$$

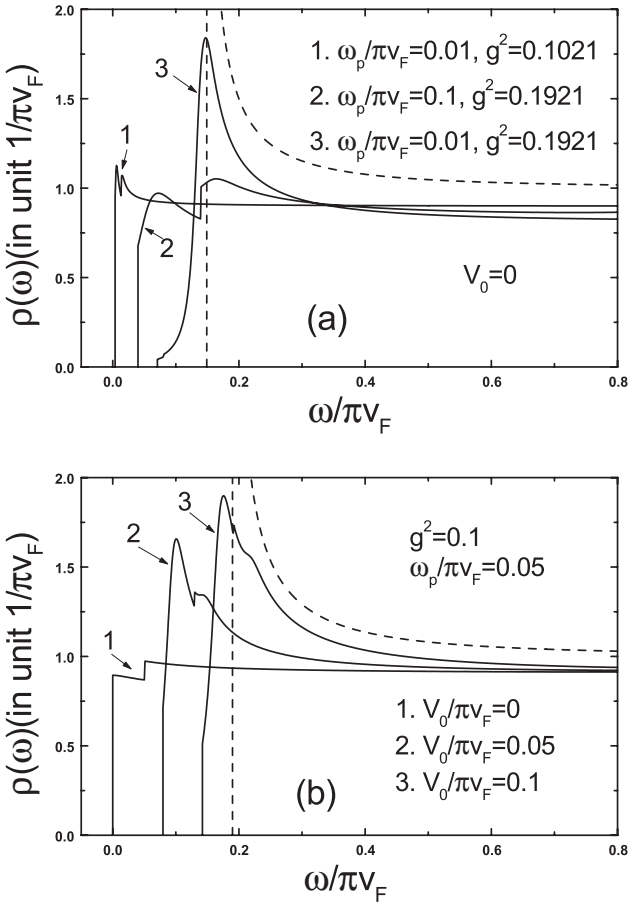

Fig. 2. (a) The calculated DOS $\rho(\omega)$ *versus* $\omega/\pi v_{\rm F}$ relations for three different sets of parameters at criticality ($V_0 = 0$). The adiabatic result (dashed-line with $\omega_{\rm p} = 0$, $g^2 = 0.1921$) is also shown. (b) $\rho(\omega)$ *versus* $\omega/\pi v_{\rm F}$ relations for the cases of $V_0 = 0$ and $V_0 > 0$. The adiabatic result (dashed-line with $\omega_{\rm p} = 0$, $g^2 = 0.1$, and $V_0/\pi v_{\rm F} = 0.1$) is also shown.

but the mean-field parameters ($A_1 = A_2 = 1$ when $\omega_{\rm p} = 0$) are renormalized by the quantum lattice fluctuations. In calculations A_1 and A_2 are treated as fitting parameters and we found $A_2 > A_1 > 0$ when $\omega_{\rm p} > 0$, which means that in the classical region $\alpha u_{\rm p} > \omega_{\rm p}$ the adiabatic mean-field parameters are strongly renormalized by nonadiabatic corrections. The fitting results are shown in Figure 3 with dotted-lines. For the quantum region where $\alpha u_{\rm p} < \omega_{\rm p}$ we use the form

$$\alpha u_{\rm p}/\pi v_{\rm F} = B_1\sqrt{g^2 - g_{\rm c}^2}\exp\left[-\frac{B_2}{\sqrt{g^2 - g_{\rm c}^2}}\right] \tag{36}$$

to fit our calculations, where B_1 and B_2 are fitting parameters. The fitting results are shown in Figure 3 with dashed-lines. Note that equation (36) is of the similar form as that of the Kosterlitz-Thouless (KT) transition [8,9,16].

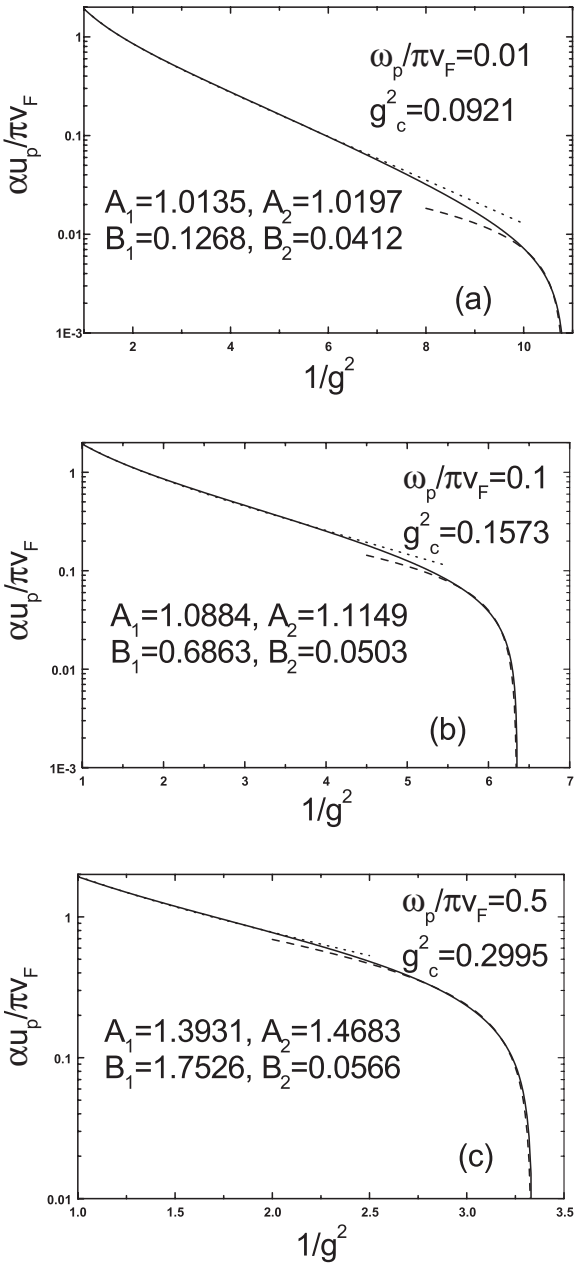

Fig. 3. The lattice distortion $u_{\rm p}$ as functions of the coupling constant g^2 at criticality ($V_0 = 0$) for $\omega_{\rm p} = 0.01$ (a), 0.1 (b), and 0.5 (c). The solid lines are results of our theory, the dotted-lines are fitted results of equation (35), and the dashed-lines are fitted results of equation (36). The calculated fitting parameters are shown in the figures.

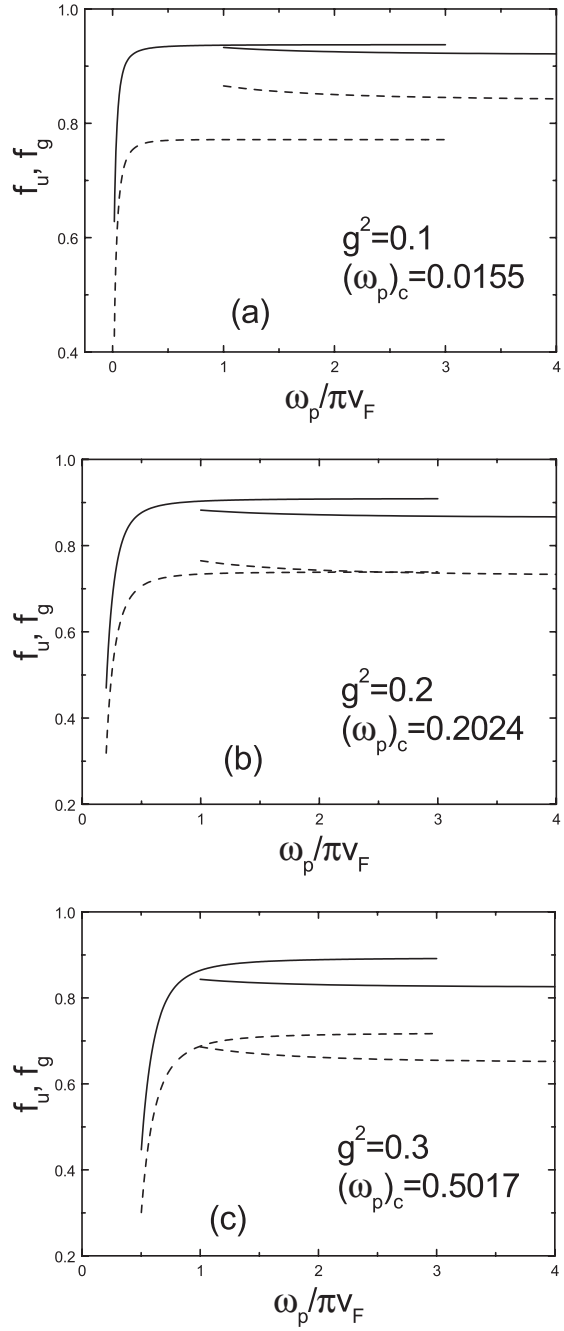

Fig. 4. The calculated critical exponents as functions of $\omega_{\rm p} > (\omega_{\rm p})_{\rm c}$ for coupling constant $g^2 = 0.1$ (a) ($f_g^\infty = 0.9198$, $f_u^\infty = 0.8397$), 0.2 (b) ($f_g^\infty = 0.8659$, $f_u^\infty = 0.7318$), and 0.3 (c) ($f_g^\infty = 0.8268$, $f_u^\infty = 0.6537$). The solid lines are for f_g and the dashed-lines for f_u. In every figure the two curves at left side are the results of Section 3 and the two at right side those of Section 4.

As V_0 is a measure of the deviation from criticality, for fixed g^2 and $\omega_{\rm p} > (\omega_{\rm p})_{\rm c}$ the gap and $\alpha u_{\rm p}$ *versus* V_0 relations should satisfy some power laws (for small V_0):

$$\text{gap} \propto (V_0)^{f_g}, \tag{37}$$

$$u_{\rm p} \propto (V_0)^{f_u}. \tag{38}$$

f_g and f_u are critical exponents and we determine them through fitting calculations. The fitted results for f_g and f_u as functions of $\omega_{\rm p} > (\omega_{\rm p})_{\rm c}$ are shown in Figure 4 for fixed coupling constant $g^2 = 0.1$, 0.2, and 0.3, respectively. When $\omega_{\rm p} > (\omega_{\rm p})_{\rm c}$ both critical exponents go up very quickly and reach a saturated value when $\omega_{\rm p}/\pi v_{\rm F} \geq 1$.

4 $\omega_{\rm p} > \pi v_{\rm F}$ case

In the $\omega_{\rm p} \to \infty$ limit (where $\delta(k',k)=1$), the transformed Hamiltonian (16), which is exact, reads (the phonon energy is not taken into account)

$$\begin{aligned} H' = & -{\rm i}v_{\rm F}\int {\rm d}y \left(\psi_1^\dagger(y)\frac{\partial}{\partial y}\psi_1(y) - \psi_2^\dagger(y)\frac{\partial}{\partial y}\psi_2(y)\right) \\ & +V_0\int {\rm d}y \left(\psi_1^\dagger(y)\psi_2(y)+\psi_2^\dagger(y)\psi_1(y)\right) \\ & -\frac{\alpha^2}{K}\int {\rm d}y \left[\psi_1^\dagger(y)\psi_2(y)+\psi_2^\dagger(y)\psi_1(y)\right]^2. \end{aligned} \tag{39}$$

It can be bosonized in the conventional way [19]:

$$\begin{aligned} H' = & \frac{v_{\rm F}}{2}\sqrt{1+2g^2}\int {\rm d}y \left[\Pi^2(y)+\left(\frac{\partial\varphi(y)}{\partial y}\right)^2\right] \\ & -\frac{V_0}{\pi\epsilon}\int {\rm d}y\cos\left[B\varphi(y)\right] - \frac{\alpha^2}{2K\pi^2\epsilon^2}\int {\rm d}y\cos\left[2B\varphi(y)\right], \end{aligned} \tag{40}$$

where $B^2 = 4\pi/\sqrt{1+2g^2}$. This is a two-frequency sine-Gordon (s-G) model and there is no exact solution for general case [20]. But we can discuss some regions of parameters which are of interest in our problem. For $V_0 = 0$, H' becomes single-frequency s-G model and it is well-known that the gapless-gapped phase transition point is at $B_{\rm c}^2 = 2\pi$ where $g_{\rm c}^2 = 3/2$. For $V_0 > 0$ but $g^2 < 3/2$, the last term in (40) is irrelevant[20] and the relation between gap (or mass) and V_0 is

$$\text{gap} \propto (V_0)^{f_g^\infty},\ f_g^\infty = 1/\left(2-\frac{B^2}{4\pi}\right). \tag{41}$$

The relation between u_p and V_0 can be derived from equation (34). Since

$$\begin{aligned} \sum_k \Psi^\dagger(k)\sigma_1\Psi(k) &= \int {\rm d}y \left(\psi_1^\dagger(y)\psi_2(y)+\psi_2^\dagger(y)\psi_1(y)\right) \\ &\sim \int {\rm d}y\cos\left[B\varphi(y)\right], \end{aligned}$$

we have [19]

$$u_{\rm p} \propto (V_0)^{f_u^\infty},\ f_u^\infty = \frac{B^2}{4\pi}/\left(2-\frac{B^2}{4\pi}\right). \tag{42}$$

The values of f_u^∞ and f_g^∞ are listed in Figure 4 for $g^2 = 0.1$, 0.2, and 0.3, respectively.

For the region $\infty > \omega_{\rm p} > \pi v_{\rm F}$, $H' = H_0' + H_1' + H_2'$ should be re-divided into the unperturbed part and perturbation: $H' = H_0^\infty + H_I^\infty$,

$$\begin{aligned} H_0^\infty = & -{\rm i}v_{\rm F}\eta\int {\rm d}y \left(\psi_1^\dagger(y)\frac{\partial}{\partial y}\psi_1(y) - \psi_2^\dagger(y)\frac{\partial}{\partial y}\psi_2(y)\right) \\ & +V_0\int {\rm d}y \left(\psi_1^\dagger(y)\psi_2(y)+\psi_2^\dagger(y)\psi_1(y)\right) \\ & -\frac{\alpha^2}{K}r\int {\rm d}y \left[\psi_1^\dagger(y)\psi_2(y)+\psi_2^\dagger(y)\psi_1(y)\right]^2, \end{aligned} \tag{43}$$

$$\begin{aligned} H_I^\infty = & \sum_k \left[v_{\rm F}(1-\eta)k - \frac{\alpha^2}{KN}\sum_{k'}\frac{v_{\rm F}(k'+k)}{\omega_{\rm p}}\delta^2(k',k)\right] \\ & \times\Psi^\dagger(k)\sigma_3\Psi(k) + \sum_k \alpha u_0(1-\delta(k,k))\Psi^\dagger(k)\sigma_1\Psi(k) \\ & +\frac{Ku_0^2}{4}N - \frac{\alpha^2}{KN}\sum_{k,k',q}\Big([2-\delta(k'-q,k')]\delta(k+q,k)-r\Big) \\ & \times\Psi^\dagger(k+q)\sigma_1\Psi(k)\Psi^\dagger(k'-q)\sigma_1\Psi(k') \end{aligned} \tag{44}$$

where

$$\eta = 1 - \frac{\alpha^2}{KN^2}\sum_{k,k'}\frac{k'+k}{\omega_p k}\delta^2(k',k), \tag{45}$$

$$r = \frac{1}{N^3}\sum_{k,k',q}[2-\delta(k'-q,k')]\delta(k+q,k). \tag{46}$$

When $\omega_{\rm p} \to \infty$, $H_{\rm I}^\infty \to 0$. So we can treat $H_{\rm I}^\infty$ as perturbation for $\omega_{\rm p} > \pi v_{\rm F}$. The unperturbed part, after bosonization, is

$$\begin{aligned} H_0^\infty = & \frac{v_{\rm F}\eta}{2}\sqrt{1+2g^2\frac{r}{\eta}}\int {\rm d}y \left[\Pi^2(y)+\left(\frac{\partial\varphi(y)}{\partial y}\right)^2\right] \\ & -\frac{V_0}{\pi\epsilon}\int {\rm d}y\cos\left[B'\varphi(y)\right] - \frac{\alpha^2 r}{2K\pi^2\epsilon^2}\int {\rm d}y\cos\left[2B'\varphi(y)\right], \end{aligned} \tag{47}$$

where $B'^2 = 4\pi/\sqrt{1+2g^2r/\eta}$ (Note that $B' \to B$ when $\omega_{\rm p} \to \infty$.) When $V_0 = 0$, the phase boundary between the gapped and gapless phases is at $B_{\rm c}'^2 = 2\pi$, that is, $g^2 r/\eta = 3/2$. The g^2 *vs.* $\omega_{\rm p}$ relation is shown in Figure 1 by the dashed line. Note that r and η are functions of g^2 and $\omega_{\rm p}$.

For $V_0 > 0$ but $g^2 r/\eta < 3/2$, the last term in H_0^∞ is irrelevant. The relation between gap (or mass) and V_0 is

$$\text{gap} \propto (V_0)^{f_g},\ f_g = 1/\left(2-\frac{B'^2}{4\pi}\right) \tag{48}$$

and that for $u_{\rm p}$ is

$$u_{\rm p} \propto (V_0)^{f_u},\ f_u = \frac{B'^2}{4\pi}/\left(2-\frac{B'^2}{4\pi}\right). \tag{49}$$

It is easy to check that $f_g \to f_g^\infty$ and $f_u \to f_u^\infty$ when $\omega_p \to \infty$. The two curves at right side in every figure of Figure 4 show the exponents as functions of $\omega_{\rm p}$ for $g^2 = 0.1$, 0.2, and 0.3, respectively. Generally speaking, the results of this section and those of last section cannot be connected smoothly. But there exists a common property that when $\omega_{\rm p}/\pi v_{\rm F} \geq 1$ the critical exponents are nearly constants.

5 Summary and discussion

We have studied the effect of quantum lattice fluctuations on the low-energy properties of quantum phase transition in a one-dimensional commensurate system. An energy-dependent electron-phonon scattering function $\delta(k',k)$ is

introduced in the unitary transformation 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 lattice fluctuations: (1) At criticality ($V_0 = 0$), when the constant g^2 decreases or the phonon frequency $\omega_{\rm p}$ increases the lattice distortion and the gap in the fermionic spectrum decreases gradually; and at some critical value $g_{\rm c}^2$ or $(\omega_{\rm p})_{\rm c}$, the system becomes gapless and the lattice distortion disappears. A phase diagram is derived. (2) The calculated DOS do not have the inverse-square-root singularity but have a peak with a significant tail below the peak. (3) Our approach successfully describes the classical-quantum crossover around $\alpha u_{\rm p} \sim \omega_{\rm p}$ when $V_0 = 0$. In the classical region $\alpha u_{\rm p} > \omega_{\rm p}$ the adiabatic mean-field parameters are strongly renormalized by nonadiabatic corrections, and in the quantum region $\alpha u_{\rm p} < \omega_{\rm p}$ the phase transition is of the signature of a KT transition. (4) For $\omega_{\rm p} > (\omega_{\rm p})_{\rm c}$ the critical exponents for gap and the $u_{\rm p}$ have been calculated,

In Section 2 we point out that the transformed Hamiltonian H' becomes exact for both $\omega_{\rm p} = 0$ and $\omega_{\rm p} \to \infty$ limit. Here we show that H' is also perturbatively exact for $\omega_{\rm p}/\pi v_{\rm F} \ll 1$ and $\omega_{\rm p}/\pi v_{\rm F} \gg 1$ as follows. When $V_0 = 0$ and $u_0 = 0$ the renormalization factor of the band function $\tau(k) = E(k)/\pi v_{\rm F}$ ($E(k)$ is the renormalized band equation (18)) at the Fermi point $k \to 0$ is correctly described in leading order in $\omega_{\rm p}$ or $1/\omega_{\rm p}$:

$$\tau(0) = \lim_{k\to 0}\frac{E(k)}{\pi v_{\rm F}} = 1 - \frac{\alpha^2\omega_{\rm p}}{KN}\sum_{k'>0}\frac{2}{(\omega_{\rm p} + v_{\rm F}k')^2}$$
$$= 1 - \frac{\alpha^2}{K(\omega_{\rm p} + \pi v_{\rm F})}. \qquad (50)$$

When $\omega_{\rm p} \ll \pi v_{\rm F}$, $\tau(0) = 1 - \alpha^2/\pi v_{\rm F}K$, which is similar to the renormalization factor $1/(1+\lambda)$ in the Migdal-Eliashberg theory (in our work DOS is a constant $1/\pi v_{\rm F}$ for $V_0 = 0$ and $\alpha = 0$). When $\omega_{\rm p} \gg \pi v_{\rm F}$, $\tau(0) = 1 - \alpha^2/\omega_{\rm p}K$, which is the same as the mass renormalization factor in the small polaron theory.

In this work we are mainly concerned with the gapped phase which is semiconducting. Voit and Schulz [21] studied the gapless metallic phase of the one-dimensional electron-phonon coupling system starting from the similar Hamiltonian $H = H_{\rm s} + H_{\rm p}$ (Eqs. (1) and (4)) with $V_0 = 0$. Here we try to compare our result for the case of $V_0 = 0$ and $u_0 = 0$ (thus there is no gap) with that of Voit and Schulz [21]. Our renormalization factor $\tau(0) = 1 - \alpha^2/K(\omega_{\rm p} + \pi v_{\rm F})$ is the ratio between the renormalized Fermi velocity $v_{\rm F}^R$ and the bare one $v_{\rm F}$, which was also calculated by Voit and Schulz [21]. Briefly speaking, our $\tau(0)$ correctly describes the behavior of $v_{\rm F}^R/v_{\rm F}$ as a function of $g^2 = \alpha^2/\pi v_{\rm F}K$ when g^2 is small.

The approach developed in this paper is based on the unitary transformations (6) and (10), and the main approximation we made is the omitting of higher order terms after the transformation. The approximation becomes bad one when the electron-phonon interaction is quite strong ($g^2 > 1$). So our approach is good for the weak- to intermediate-coupling case but cannot be used to treat the strong-coupling electron-phonon system, for example, the self trapping case.

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 $\delta(k, k) = \omega_{\rm p}/(\omega_{\rm p} + 2v_{\rm F}|k|)$ has a peak at $k = 0$, the Fermi point in our model system, and when $\omega_{\rm p}/v_{\rm F} \ll 1$ the peak is very sharp. This peak means that only those electrons near the Fermi point within a range of about $\omega_{\rm p}/v_{\rm F}$ can participate in the electron-phonon scattering and contribute to the reduction of the energy gap compared with the adiabatic value (see Eq. (14)). This fact is similar to that in the Bardeen-Cooper-Schrieffer theory [22] for superconductivity: only those electrons near the Fermi surface form Cooper pairs *via* a phonon-induced effective attraction.

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