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Polaronic behavior in single- and many-electron Holstein model: A new perturbation approach

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Abstract. A new perturbation approach is developed for single- and many-electron Holstein model in one-, two-, and three-dimension. The results show that this approach has a good agreement with the Migdal theory in the adiabatic regime when the coupling is moderate ($\lambda < 1$), but with the Lang-Firsov theory in the antiadiabatic regime ($\omega_0/W \gg 1$). In the intermediate region, our approach can describe the transition from a large-polaron Fermi-liquid to the small-polaron, and this transition may be discontinuous in adiabatic regime, which means a phase transition appears in many-electron system. In single-electron case, we eliminate the abrupt transition using the degenerate perturbation theory, and the calculated ground state energy and effective mass are successfully compared with those of previous authors. Besides, the method has the advantage of requiring little computational effort.

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1 Introduction

Recently the polaronic behavior of charge carriers in electron-phonon interacting systems has received considerable attention due to important classes of materials, such as the high-temperature superconductors [1] and the colossal magnetoresistance manganites [2]. Among the models for electron-phonon coupling systems the Holstein model may be the simplest one but contains the main physics. The Hamiltonian of it is

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} (c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) - \mu_0 \sum_{\mathbf{j},\sigma} c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{j}} \omega_0 b^\dagger_{\mathbf{j}} b_{\mathbf{j}} + g \sum_{\mathbf{j}\sigma} (c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma} - n)(b^\dagger_{\mathbf{j}} + b_{\mathbf{j}}). \quad (1)$$

The first summation is over nearest-neighbors. Here $b^\dagger_{\mathbf{j}}$ ($b_{\mathbf{j}}$) is the creation (annihilation) operator of local phonon mode on site $\mathbf{j}$ with frequency ω_0, $c^\dagger_{\mathbf{j}\sigma}$ ($c_{\mathbf{j}\sigma}$) is the creation (annihilation) operator of an electron on site $\mathbf{j}$ with spin σ. t is the hopping integral and g the electron-phonon coupling constant. $n = \langle c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma}\rangle$ is the number density of electrons with bare chemical potential μ_0. There are two commonly used dimensionless parameters, the adiabaticity ratio $\gamma = \omega_0/W$ ($W = 2dt$ is half-band width, where d is the dimension), and the electron-phonon coupling strength $\lambda = E_p/W$, where $E_p = g^2/\omega_0$ is the polaronic binding energy. An additional dimensionless parameter is E_p/ω_0.

The model has motivated many studies since Holstein's pioneering work in 1959 [3]. The perturbation treatments, starting either from the free-electron limit (weak coupling limit) or from the atomic limit (strong coupling expansions), fail to describe the dressing effect in the intermediate region. The variational ansatz, based on various choices of trial wave functions, are expected to give reliable results only for ground state properties. In recent years, numerical methods, such as the Monte Carlo simulations [4], the density matrix renormalization group analysis [5], and the exact diagonalization of small clusters [6], have been used for studies of the Holstein model with special attention to the single polaron problem. Furthermore, the dynamical mean-field theory of the model, which becomes exact in the limit of infinite-dimension, has been established for the single-electron case [7].

For many-electron case, a reliable approach is crucial due to the failure of the standard approximations; in fact, as pointed out by Alexandrov *et al.* [8], the Migdal approximation is valid only for a weakly coupled adiabatic system, while the Lang-Firsov's canonical transformation treatment [9] could not be suitable far from the antiadiabatic limit. Migdal-Eliashberg(ME) theory gives a description without instability (where the Fermi-liquid description may break down) at any value of the coupling constant λ. The Lang-Firsov(LF) transformation together with the small polaron approximation [1,9] cannot lead to those results which can be obtained *via* the ME approach.

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In this work we propose a new perturbation approach to the single- and many-electron Holstein model for one-, two- and three-dimensions. We try to utilize the advantages of both the variational and perturbation methods and the main idea of the approach is as follows. In the weak coupling perturbation theory, H in (1) can be divided as $H = H_0 + V$ where V is the last term and treated as the perturbation. We try to find a better way to divide the Hamiltonian into unperturbed part and perturbation by means of the unitary transformation: $\tilde{H} = \exp(S)H\exp(-S) = \tilde{H}_0 + \tilde{V}$. $\tilde{H}_0$ should be simple enough to be solved exactly and, at the same time, contains the main physics of the coupling system. $\tilde{V}$ should be small in the meaning that the matrix elements of $\tilde{V}$ between different eigenstates of $\tilde{H}_0$ are as small as possible. Besides, the ground state average of the transformed Hamiltonian $\tilde{H}_0$ is minimized by a variational ansatz.

This paper is organized as follows. In the next section we introduce our approach. The method will be applied to many-electron case and the results are summarized in Section 3. In Section 4, we solve the single polaron problem and compare the results with those of previous authors to show that our approach is well in reproducing the ground state energy and the effective mass of single polaron. Section 5 is devoted to a summary.

2 The method

2.1 The q-dependent transformation

A $\mathbf{q}$-dependent transformation is applied to H, $H' = \exp(S_1)H\exp(-S_1)$, where

$$\begin{aligned} S_1 &= \frac{1}{\sqrt{N}}\sum_{\mathbf{j},\mathbf{q},\sigma}\frac{g}{\omega_0}r_{\mathbf{q}}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{j}}(b^\dagger_{-\mathbf{q}} - b_{\mathbf{q}})(c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{j}\sigma} - n) \\ &= \sum_{\mathbf{i},\mathbf{j},\sigma}\frac{g}{\omega_0}r(\mathbf{i}-\mathbf{j})(b^\dagger_{\mathbf{j}} - b_{\mathbf{j}})(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma} - n). \end{aligned} \tag{2}$$

N is the total number of sites. Here we introduce a displacement function $r_{\mathbf{q}}$ which is $\mathbf{q}$-dependent and its form will be determined later. The non-local electron-phonon correlation $r(\mathbf{i}-\mathbf{j})$ is related to $r_{\mathbf{q}}$ by a Fourier transformation: $r(\mathbf{i}-\mathbf{j}) = \frac{1}{N}\sum_{\mathbf{q}}\exp[\mathrm{i}\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})]r_{\mathbf{q}}$. For the small polaron the lattice deformation accompanied it is confined to the site where the electron sits, so $r_{\mathbf{q}} = 1$, $r(\mathbf{i}-\mathbf{j}) = \delta_{\mathbf{i},\mathbf{j}}$, and the transformation (2) becomes the Lang-Firsov transformation [9–11]. For general case, $r(\mathbf{i}-\mathbf{j}) \neq 0$ when $\mathbf{i} \neq \mathbf{j}$ and it may be a measure of the intersite electron-phonon correlation.

The transformation can be done to the end and terms after transformation can be collected as follows:

$$\begin{aligned} H' &= H'_0 + H'_1 + H'_2, \\ H'_0 &= \sum_{\mathbf{k},\sigma}(\eta\epsilon_{\mathbf{k}} - \mu_0)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_q \omega_0 b^\dagger_{\mathbf{q}}b_{\mathbf{q}}, \end{aligned} \tag{3}$$

$$\eta = \exp\left\{-\frac{1}{N}\sum_{\mathbf{q}}\frac{g^2}{\omega_0^2}r_{\mathbf{q}}^2(1-\gamma_{\mathbf{q}})\right\}, \tag{4}$$

$$\begin{aligned} H'_1 = &\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g(1-r_{\mathbf{q}})(b^\dagger_{-\mathbf{q}} + b_{\mathbf{q}})c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} \\ &- \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g\eta r_{\mathbf{q}}\frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{\omega_0}(b^\dagger_{-\mathbf{q}} - b_{\mathbf{q}})c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}, \end{aligned} \tag{5}$$

$$\begin{aligned} H'_2 = &-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle,\sigma}(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma})\{\cosh[X_{\mathbf{i},\mathbf{j}}] - \eta\} \\ &- t\sum_{\langle\mathbf{i},\mathbf{j}\rangle,\sigma}(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} - c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma})\{\sinh[X_{\mathbf{i},\mathbf{j}}] - \eta X_{\mathbf{i},\mathbf{j}}\} \\ &- \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'}\sum_{\mathbf{q}(\neq\mathbf{0})}\frac{g^2}{\omega_0}r_{\mathbf{q}}(2-r_{\mathbf{q}})c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}, \end{aligned} \tag{6}$$

$$X_{\mathbf{i},\mathbf{j}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\frac{g}{\omega_0}r_{\mathbf{q}}\left(b^\dagger_{-\mathbf{q}} - b_{\mathbf{q}}\right)\left[\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{i}} - \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{j}}\right]. \tag{7}$$

Terms in H'_2 are second order in g or higher. $\gamma_{\mathbf{k}} = \frac{1}{d}\sum_{\tau=1}^{d}\cos(k_\tau)$ and $\epsilon_{\mathbf{k}} = -2dt\gamma_{\mathbf{k}}$.

In single electron case, in order to eliminate the second order contribution of H'_1 to the self-energy of ground state, we can let $r_{\mathbf{q}} = \frac{\omega_0}{\omega_0 + \eta(\epsilon_{\mathbf{q}} - \epsilon_0)}$, which is the same as that of the Lee-Low-Pines(LLP) method.

2.2 The energy-dependent transformation

For many-electron case, the conduction band is filled to the Fermi level and, therefore, the second order contribution of H'_1 to the ground state energy will not vanish no matter how we choose the form of r_q. So we use another unitary transformation [11] to take into account the contribution of H'_1: $H'' = \exp(S_2)(H'_0 + H'_1 + H'_2)\exp(-S_2)$, where

$$S_2 = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}\frac{g}{\omega_0}(b^\dagger_{-\mathbf{q}} - b_{\mathbf{q}})[\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}]c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}. \tag{8}$$

Here a function $\delta(\mathbf{k}',\mathbf{k})$, which is a function of the energies of incoming and outgoing electrons in the electron-phonon scattering process, is introduced. The form of $\delta(\mathbf{k}',\mathbf{k})$ will be determined later. The transformation can proceed order by order and the result is:

$$H''_0 = \sum_{\mathbf{k},\sigma}\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_q \omega_0 b^\dagger_{\mathbf{q}}b_{\mathbf{q}}, \tag{9}$$

$$\begin{aligned} \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) = &\eta\epsilon_{\mathbf{k}} - \mu_0 - \frac{1}{N}\sum_{\mathbf{k}'}\frac{g^2}{\omega_0}\delta(\mathbf{k}',\mathbf{k}) \\ &\times [2 - \delta(\mathbf{k}',\mathbf{k})]\mathrm{sgn}(\epsilon_{\mathbf{k}'} - \mu) \\ &+ \frac{1}{N}\sum_{\mathbf{q}}\frac{g^2}{\omega_0^2}\eta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \\ &\times \left(\delta^2(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}^2\right), \end{aligned} \tag{10}$$

where μ is the renormalized chemical potential.

$$\begin{aligned}H_1'' &= H_1' + [S_2, H_0'] = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g[1-\delta(\mathbf{k}+\mathbf{q},\mathbf{k})] \\ &\times(b^\dagger_{-\mathbf{q}} + b_{\mathbf{q}})c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} - \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}\frac{g}{\omega_0} \\ &\times\eta(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})\delta(\mathbf{k}+\mathbf{q},\mathbf{k})(b^\dagger_{-\mathbf{q}} - b_{\mathbf{q}})c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}, \quad (11)\end{aligned}$$

$$\begin{aligned}H_2'' &= \sum_{\mathbf{k},\sigma}(\eta\epsilon_{\mathbf{k}} - \mu_0 - \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}}-\mu))c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + H_2' \\ &+[S_2, H_1'] + \frac{1}{2}[S_2,[S_2,H_0']] \\ &= -t\sum_{\langle\mathbf{i},\mathbf{j}\rangle,\sigma}(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma})\{\cosh[X_{\mathbf{i},\mathbf{j}}] - \eta\} \\ &-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle,\sigma}(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} - c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma})\{\sinh[X_{\mathbf{i},\mathbf{j}}] - \eta X_{\mathbf{i},\mathbf{j}}\} \\ &+\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\sigma}\frac{g^2}{\omega_0}\delta(\mathbf{k}',\mathbf{k})[2-\delta(\mathbf{k}',\mathbf{k})]\mathrm{sgn}(\epsilon_{\mathbf{k}'}-\mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \\ &-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'}\sum_{\mathbf{q}(\neq\mathbf{0})}\frac{g^2}{\omega_0}\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) \\ &\times[2-\delta(\mathbf{k}'-\mathbf{q},\mathbf{k}')]c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}. \quad (12)\end{aligned}$$

All terms of higher order than g^2 will be omitted in the following treatment. Note that $r_{\mathbf{q}}$ should be helpful for the convergence of the second transformation since the generator S_2 depends on the difference $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}$.

The free energy can be calculated by the following perturbation expansion in the electron-phonon coupling g [12],

$$\begin{aligned}-\beta(F-F_0) &= -\int_0^\beta \mathrm{d}\tau\langle H_1''(\tau)\rangle_0 \\ &+\int_0^\beta \mathrm{d}\tau_1\int_0^{\tau_1}\mathrm{d}\tau_2\,\langle[H_1''(\tau_1)H_1''(\tau_2)]\rangle_0 \\ &-\int_0^\beta \mathrm{d}\tau\langle H_2''(\tau)\rangle_0 + O(g^3), \quad (13)\end{aligned}$$

$$F_0 = -T\ln\mathrm{Tr}\exp[-H_0''/T] + \mu_0 N, \quad \beta = 1/T, \quad (14)$$

where $H''(\tau) = \exp(H_0''\tau)H''\exp(-H_0''\tau)$ is in the interaction picture and

$$\langle\ldots\rangle_0 = \mathrm{Tr}\{\exp(-\beta H_0'')[\ldots]\}/\mathrm{Tr}\exp(-\beta H_0'').$$

Obviously one can see that the first term on the right side of (13) is zero because of the linear form of phonon operators in H_1''. The second term, which is the second order contribution of H_1'', is not zero in general. However, we can choose the functional form of $\delta(\mathbf{k}+\mathbf{q},\mathbf{k})$,

$$\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) = \omega_0/(\omega_0 + \eta|\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}|), \quad (15)$$

so that

$$\int_0^\beta \mathrm{d}\tau_1\int_0^{\tau_1}\mathrm{d}\tau_2\langle[H_1''(\tau_1)H_1''(\tau_2)]\rangle_0 = 0, \quad (16)$$

when $T = 0$ (ground state). This is nothing but making the matrix element of H_1'' between the ground state and the lowest-lying excited states of H_0'' vanishing. Thus the first order terms H_1'' which are not exactly cancelled after the two unitary transformations are related to the higher lying excited states and should be irrelevant under renormalization.

The electron Green's function can be derived from the Dyson's equation

$$G(\mathbf{k},\omega) = G_0(\mathbf{k},\omega) + G_0(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega). \quad (17)$$

The second order self-energy of H_1'' is

$$\begin{aligned}\Sigma(\mathbf{k},\omega) &= \frac{1}{N}\sum_{\mathbf{q}}\frac{\eta^2 g^2}{(\omega_0 + \eta|\epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}}|)^2} \\ &\times\left\{[|\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}| - (\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}})]^2\frac{n(\omega_0)+1-f(\epsilon_{\mathbf{k}-\mathbf{q}})}{\omega-\omega_0-\rho(\epsilon_{\mathbf{k}-\mathbf{q}})(\epsilon_{\mathbf{k}-\mathbf{q}}-\mu)}\right. \\ &\left.+[|\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}| + (\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}})]^2\frac{n(\omega_0)+f(\epsilon_{\mathbf{k}-\mathbf{q}})}{\omega+\omega_0-\rho(\epsilon_{\mathbf{k}-\mathbf{q}})(\epsilon_{\mathbf{k}-\mathbf{q}}-\mu)}\right\}, \quad (18)\end{aligned}$$

where $n(\omega_0) = 1/(\exp(\beta\omega_0) - 1)$ and $f(\epsilon_{\mathbf{k}}) = 1/(\exp[\beta\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)] + 1)$. The renormalized chemical potential μ can be determined by

$$1 - n = \frac{1}{N}\sum_{\mathbf{k}}\mathrm{sgn}(\epsilon_{\mathbf{k}} - \mu). \quad (19)$$

When $T = 0$, we have $n(\omega_0) = 0$ and $f(\epsilon_{\mathbf{k}})$ is a step function, and then, $\Sigma(\epsilon_{\mathbf{k}} = \mu, \omega) = 0$. This is the reason for the choice of the functional form of $\delta(\mathbf{k}+\mathbf{q},\mathbf{k})$. For comparison, the ordinary second order self-energy is

$$\begin{aligned}\Sigma_o(\mathbf{k},\omega) &= \frac{1}{N}\sum_{\mathbf{q}(\neq\mathbf{0})} g^2\left\{\frac{n(\omega_0)+1-f_o(\epsilon_{\mathbf{k}-\mathbf{q}})}{\omega-\omega_0-\epsilon_{\mathbf{k}-\mathbf{q}}+\mu}\right. \\ &\left.+\frac{n(\omega_0)+f_o(\epsilon_{\mathbf{k}-\mathbf{q}})}{\omega+\omega_0-\epsilon_{\mathbf{k}-\mathbf{q}}+\mu}\right\}, \quad (20)\end{aligned}$$

where $f_o(\epsilon_{\mathbf{k}}) = 1/(\exp[\beta(\epsilon_{\mathbf{k}} - \mu)] + 1)$. We have $\Sigma_o(\epsilon_{\mathbf{k}} = \mu, \omega) \neq 0$.

3 Many-electron case

The quasi-particle energy $E_{\mathbf{k}}$ should include the total self-energy in the second order in g. The contribution from H_2'', which can be calculated easily with the Hatree-Fock approximation, is zero. The contribution from H_1'' is the real part of equation (18), $\mathrm{Re}[\Sigma(\mathbf{k}, E_{\mathbf{k}} - \mu_0)]$, which should be zero at the Fermi surface when $T = 0$ according to the preceding discussion. Thus, the quasi-particle energy $E_{\mathbf{k}}$, determined as the pole of the Green's function, is

$$E_{\mathbf{k}} - \mu_0 = \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) + \mathrm{Re}[\Sigma(\mathbf{k}, E_{\mathbf{k}} - \mu_0)]. \quad (21)$$

The renormalized chemical potential μ is already determined by equation (19). The bare one is then determined by

$$\mu_0 = E_{\mathbf{k}}|_{\epsilon_{\mathbf{k}}=\mu}, \quad (22)$$

which leads to

$$\mu_0 = \eta(1-\ln\eta)\mu - \frac{1}{N}\sum_{\mathbf{k}'} g^2 \frac{\omega_0 + 2\eta|\epsilon_{\mathbf{k}'} - \mu|}{(\omega_0 + \eta|\epsilon_{\mathbf{k}'} - \mu|)^2} \times \mathrm{sgn}(\epsilon_{\mathbf{k}'} - \mu) + \frac{1}{N}\sum_{\mathbf{k}'} g^2 \frac{\eta(\epsilon_{\mathbf{k}'} - \mu)}{(\omega_0 + \eta|\epsilon_{\mathbf{k}'} - \mu|)^2} \cdot \quad (23)$$

Now we can get the effective mass of the electrons at the Fermi surface when $T = 0$,

$$\frac{m}{m^*} = \rho(\epsilon_{\mathbf{k}} = \mu) = \eta\left\{1 - \ln\eta - \frac{1}{N}\sum_{\mathbf{k}} \frac{g^2}{(\omega_0 + \eta|\epsilon_{\mathbf{k}} - \mu|)^2}\right\} \cdot \quad (24)$$

The ground state energy can be derived from equations (13) and (14) ($T = 0$). The contribution of H_1'' is zero and the contribution from other terms in H_0'' and H_2'' can be collected as follows:

$$E_g = \sum_{\mathbf{k},\sigma} \eta(1-\ln\eta)\epsilon_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_0 + \frac{1}{N}\sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g^2}{\omega_0^2}\eta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\delta^2(\mathbf{k}+\mathbf{q},\mathbf{k})\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_0 - \frac{1}{N}\sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g_{\mathbf{q}}^2}{\omega_0}\delta(\mathbf{k}+\mathbf{q},\mathbf{k})[2 - \delta(\mathbf{k},\mathbf{k}+\mathbf{q})] \times \langle c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}\rangle_0 \langle c_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}\rangle_0. \quad (25)$$

Although the form of $\delta(\mathbf{k}+\mathbf{q},\mathbf{k})$ is already determined, the form of $r_{\mathbf{q}}$ in S_1 has not been determined. Note that $r_{\mathbf{q}}$ dose not appear in E_g explicitly and E_g depends on $r_{\mathbf{q}}$ implicitly *via* η. Thus, we can variationally determine the value of η by differentiation:

$$\ln\eta = \frac{\frac{1}{N}\sum_{\mathbf{k},\mathbf{q},\sigma} g^2 \frac{2\eta|\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}|^2 + (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})(\omega_0 - \eta|\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}|)}{(\omega_0 + \eta|\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}|)^3}}{\sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_0} \times \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\right\rangle_0 \left\langle c_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}\right\rangle_0 \cdot \quad (26)$$

The summation for the momentum k and q could be simplified as an integral over the energy by using the DOS (density of state) of energy band. We calculate the effective mass of electrons at the Fermi surface with the DOS of tight-binding approximation (TBA) model.

At the weak coupling limit $\lambda \ll 1$, the solution of equation (26) is $\eta \approx 1$, and then $\rho \to (1 - \frac{1}{N}\sum_{\mathbf{k}} \frac{g^2}{(\omega_0 + |\epsilon_{\mathbf{k}} - \mu|)^2})$. This is similar to the result of ME theory

$$m/m^* = \left(1 + \frac{1}{N}\sum_{\mathbf{k}} \frac{g^2}{(\omega_0 + |\epsilon_{\mathbf{k}} - \mu|)^2}\right)^{-1} \cdot$$

In the strong coupling regime $E_p/\omega_0 \gg 1$, we have solution $\eta = \exp\left[-\frac{E_p}{\omega_0}\right]$ and thus the effective mass is the same as that of the Lang-Firsov approach,

$$\rho(\epsilon_{\mathbf{k}} = \mu) = \exp\left[-\frac{E_p}{\omega_0}\right].$$

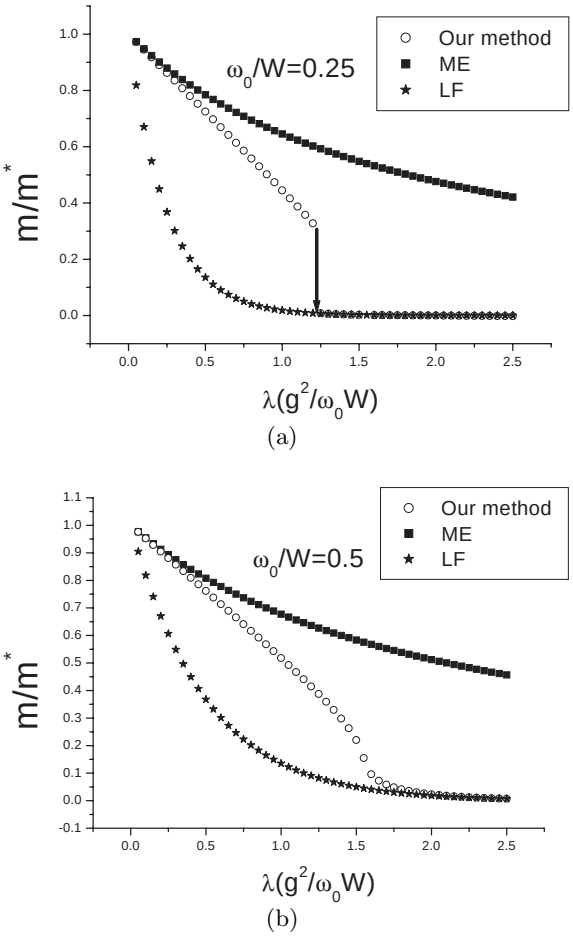

Fig. 1. The effective mass of electrons at the Fermi surface with different adiabaticity ratio ω_0/W in 2D. The renormalized chemical potential $\mu = -0.8$ (in this paper, μ is in unit of half bandwidth W).

In Figures 1 and 2, we report the effective mass of electrons at the Fermi surface obtained within our approach (Eq. (24)) in two-dimension together with the results of ME and LF approach. Our approach recovers the ME or LF result in different regions and it gives the transition in between. In Figure 1, we show the effective mass as a function of the coupling strength with fixed adiabaticity ratio. We find that there is an intermediate-coupling region ($1.0 < \lambda < 1.5$) where both ME theory and LF theory do not work well and a discontinuous transition appears in this region when the adiabaticity ratio is small enough. In Figure 2, we show the variation of the effective mass from adiabatic to antiadiabatic region with fixed ratio E_p/ω_0. With increasing binding energy, the adiabatic region shrinks and the difference of the effective mass between large and small polaron increases. When the binding energy exceeds a critical value, the effective mass changes

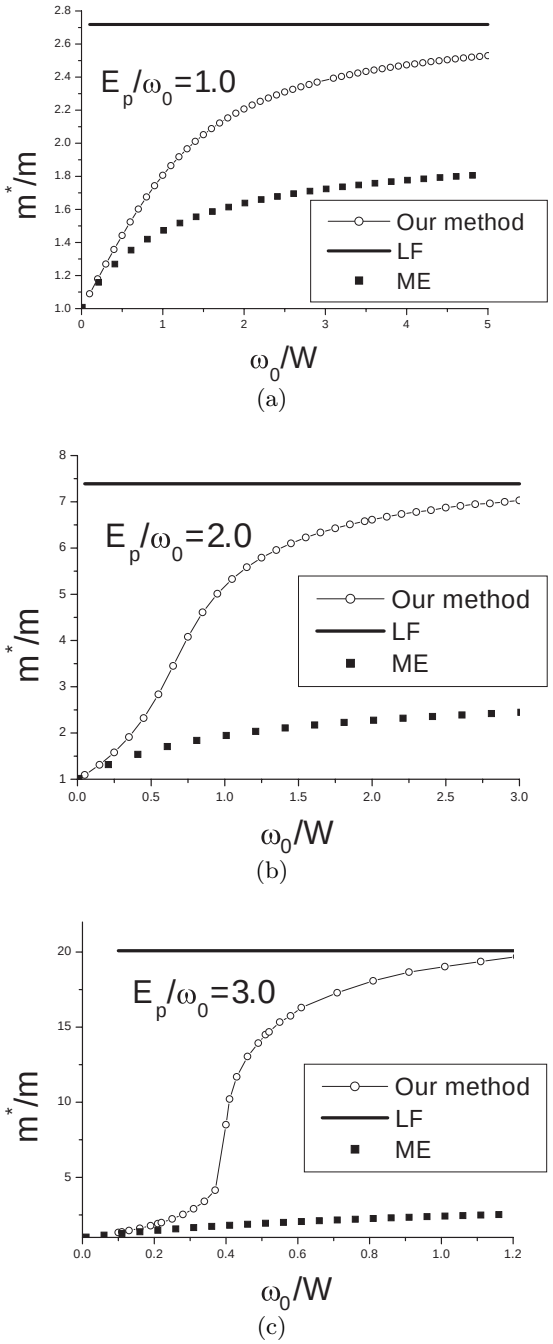

Fig. 2. The effective mass of electrons at the Fermi surface with different E_p/ω_0 in 2D. The chemical potential $\mu = -0.5$.

discontinuously to an enormous value with increasing ratio $\frac{\omega_0}{W}$. In the materials with narrow band($\frac{\omega_0}{W} \sim 0.8$ for doped C_{60}, ~ 0.2 for cuprates and ~ 0.15 for manganites), if the ratio of polaronic binding energy to phonon frequency $\frac{E_p}{\omega_0} > 3$ ($\frac{E_p}{\omega_0} > 5$ for Jahn-Teller(JT) distortion in manganites), the strong electron-phonon coupling will lead to the formation of a many-electron "self-trapped" state.

The electron-phonon correlation function $\chi(\mathbf{i}-\mathbf{j})$ can be defined as

$$\chi(\mathbf{i}-\mathbf{j}) = \frac{\langle (b_{\mathbf{j}}^\dagger + b_{\mathbf{j}}) c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0}{A} = \frac{\mathrm{Tr}\{\exp(-\beta H)(b_{\mathbf{j}}^\dagger + b_{\mathbf{j}}) c_{\mathbf{i}}^\dagger c_{\mathbf{i}}\}}{A \mathrm{Tr}\exp(-\beta H)}$$
$$= \frac{\mathrm{Tr}\{\exp(-\beta H'')\mathrm{e}^{S_2}\mathrm{e}^{S_1}(b_{\mathbf{j}}^\dagger + b_{\mathbf{j}}) c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \mathrm{e}^{-S_1}\mathrm{e}^{-S_2}\}}{A \mathrm{Tr}\exp(-\beta H'')}. \quad (27)$$

$\chi(\mathbf{i}-\mathbf{j})$ indicates the strength of the electron-induced lattice distortion and its spatial extent, where $A = \sum_j \langle (b_{\mathbf{j}}^\dagger + b_{\mathbf{j}}) c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0$ is a normalization factor. After some calculations we get (all terms of order $O(g^3)$ are neglected)

$$\begin{aligned} A \times \chi(\mathbf{i}-\mathbf{j}) &= -\frac{2}{N} \sum_{\mathbf{k}} \sum_{\mathbf{q}(\neq \mathbf{0})} \frac{g}{\omega_0} \delta(\mathbf{k}-\mathbf{q}, \mathbf{k}) \\ &\quad \times \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{j}} \langle c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0 \\ &= -\frac{2}{N} \sum_{\mathbf{k},\mathbf{q}} \frac{g}{\omega_0} (\delta(\mathbf{k}-\mathbf{q}, \mathbf{k}) - \phi_{\mathbf{q}}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{j}} \\ &\quad \times \langle c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0 - \frac{2}{N} \sum_{\mathbf{k},\mathbf{q}} \frac{g}{\omega_0} \phi_{\mathbf{q}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{j}} \\ &\quad \times \langle c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0 + \frac{2}{N} \sum_{\mathbf{k}} \frac{g}{\omega_0} \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} c_{\mathbf{i}}^\dagger c_{\mathbf{i}} \rangle_0. \end{aligned} \quad (28)$$

where $\phi_{\mathbf{q}} = \frac{1}{N} \sum_{\mathbf{k}} \delta(\mathbf{k}-\mathbf{q}, \mathbf{k})$.

4 Single-electron case

In this section, our approach is used to treat the single electron problem. We compare our results with previous ones to show that our approach is quite well in reproducing the ground state energy and the effective mass of single polaron. For single electron case, the renormalized chemical potential $\mu = -2dt$ in the case of cosine energy band $\epsilon_{\mathbf{k}} = -2dt\gamma_{\mathbf{k}}$. Then equations (21, 24), and (27) become:

$$\begin{aligned} E_{\mathbf{k}} &= \eta(1 - \ln\eta)\epsilon_{\mathbf{k}} + \mathrm{Re}[\Sigma(\mathbf{k}, E_{\mathbf{k}} - \mu_0)] \\ &\quad - \frac{1}{N} \sum_{\mathbf{k}'} \frac{g^2}{\omega_0} \delta(\mathbf{k}', \mathbf{k})[2 - \delta(\mathbf{k}', \mathbf{k})] \\ &\quad + \frac{1}{N} \sum_{\mathbf{q}} \frac{g^2}{\omega_0^2} \eta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \delta^2(\mathbf{k}+\mathbf{q}, \mathbf{k}), \end{aligned} \quad (29)$$

$$\rho(\epsilon_{\mathbf{k}} = \mu) = \eta \left\{ 1 - \ln\eta - \frac{1}{N} \sum_{\mathbf{k}} \frac{g^2}{(\omega_0 + \eta|\epsilon_{\mathbf{k}} + 2dt|)^2} \right\}, \quad (30)$$

$$\chi(\mathbf{i}-\mathbf{j}) = \frac{1}{N} \sum_{q} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \delta(\mathbf{0}, \mathbf{q}). \quad (31)$$

η can be determined by the variational method and equation (26) becomes:

$$\ln \eta = -\frac{1}{N} \sum_q \frac{g^2(1-\gamma_{\mathbf{q}})}{(\omega_0 + \eta|\epsilon_{\mathbf{q}} + 2dt|)^2}. \quad (32)$$

which is the same as the LLP approach. However, as the form of $r_{\mathbf{q}}$ in S_1 is not determined from the beginning and the ground state energy E_g depends on $r_{\mathbf{q}}$ implicitly *via* η, for the single-polaron problem we would use another variational ansatz to determine η.

For the single-polaron case it has been proved that the discontinuous transition between the large and small polaron may be an artifact and come from the variational ansatz [13]. From the mathematical view point, the discontinuous transition comes from the fact that equation (32) has more than one solution (corresponding to different minimums of E_g) when the adiabaticity ratio is small. In order to remove the discontinuous transition and make it a continuous one, we utilize the degenerate perturbation theory: Let the real ground state be a superposition of the near-degenerate solutions of equation (32).

In the intermediate-coupling region, where two near-degenerate variational ground states ($|\psi_s\rangle$ and $|\psi_l\rangle$) coexist, we suppose that the real ground state $|\psi\rangle$ is the linear superposition of these two states:

$$|\psi\rangle = \frac{A|\psi_s\rangle + B|\psi_l\rangle}{\sqrt{A^2 + B^2 + 2ABS}}. \quad (33)$$

where S is the overlap factor of the two wave functions $|\psi_s\rangle$ and $|\psi_l\rangle$

$$S = \frac{\langle\psi_s|\psi_l\rangle + \text{h.c.}}{2}. \quad (34)$$

In equation (33) A and B are two additional variational parameters that provide the relative weight of $|\psi_s\rangle$ and $|\psi_l\rangle$. The procedure of minimization of the quantity $\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$ with respect to A and B gives the polaron energy

$$E = \frac{E_m - SE_c - \sqrt{(E_m - SE_c)^2 - (1-S^2)(E_l E_s - E_c^2)}}{1-S^2}, \quad (35)$$

and the ratio

$$\frac{A}{B} = \frac{E_c - ES}{E - E_l}. \quad (36)$$

Here, $E_m = (E_l + E_s)/2$ and $E_c = (\langle\psi_l|H|\psi_s\rangle + \text{h.c.})/2$. E_l and E_s are the energy of $|\psi_s\rangle$ and $|\psi_l\rangle$. Finally the overlap factor and the matrix element of the Hamiltonian between the two solutions $|\psi_s\rangle$ and $|\psi_l\rangle$ are,

$$S = \langle\psi_l|\psi_s\rangle = \exp\left(-\frac{1}{2N}\sum_{\mathbf{q}} \frac{g^2}{\omega_0^2}(r_q^s - r_q^l)^2\right), \quad (37)$$

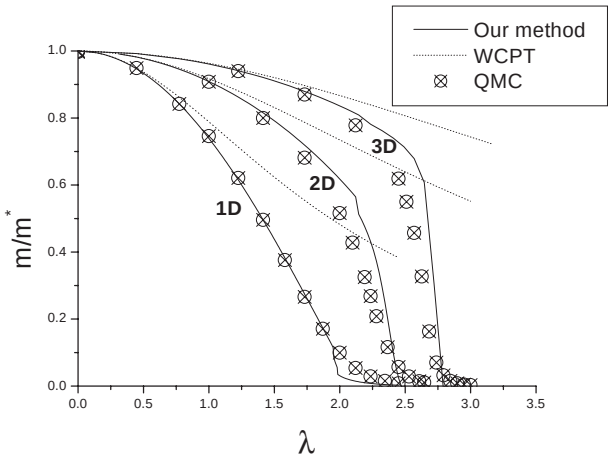

Fig. 3. Single-polaron effective mass m/m^*. The adiabaticity ratio ω_0/W for 1D is 0.5, for 2D is 0.25 and for 3D is 0.167. OMC data are kindly provided by Kornilovitch. The results of Weak Coupling Perturbation theory that predicts the effective mass as $m/m^* = (1 + \sum_q \frac{g^2}{(\omega_0 + \epsilon_{\mathbf{q}} + 2dt)^2})^{-1}$ are also shown for comparison.

Table 1. Polaron ground state energies (in unit of t) at $k = 0$ in 1D, 2D and 3D for $\lambda = 0.5$ and $\omega_0/W = 1.0$.

	1D	2D	3D
L.C. Ku	−2.469685	−4.814736	−7.162395
This work	−2.455992	−4.792187	−7.132117

and

$$\langle\psi_l|H|\psi_s\rangle = -2t \exp\left(-\frac{1}{2N}\sum_{\mathbf{q}} \frac{g^2}{\omega_0^2}|r_q^s - r_q^l e^{-iq}|^2\right) - \frac{g^2}{\omega_0} S \sum_q (r_q^s + r_q^l - r_q^s r_q^l). \quad (38)$$

Here, $r_q^s = \frac{\omega_0}{\omega_0 + \eta_s(\epsilon_{\mathbf{q}} + 2dt)}$ and $r_q^l = \frac{\omega_0}{\omega_0 + \eta_l(\epsilon_{\mathbf{q}} + 2dt)}$, where η_s and η_l are two solutions of equation (32). We redefine the quantity η:

$$\eta = \frac{A^2\eta_l + B^2\eta_s + 2AB\exp\left(-\frac{1}{2N}\sum_{\mathbf{q}} \frac{g^2}{\omega_0^2}|r_q^s - r_q^l e^{-iq}|^2\right)}{A^2 + B^2 + 2ABS}. \quad (39)$$

Now we can describe the polaronic effect more properly in the intermediate-coupling region.

Figure 3 shows the effective mass of the single-polaron case for 1D, 2D and 3D. For comparison, the data from the quantum Monte Carlo simulations and those of the weak coupling perturbation theory (WCPT) are also shown. Obviously our approach works well in the weak- and intermediate-coupling case, especially in the nonadiabatic regime. Table 1 compares our results with those of Ku's variational method [15] for intermediate coupling. We note that our approach gives reasonably accurate results for ground state energy and the fractional error is about 0.5%.

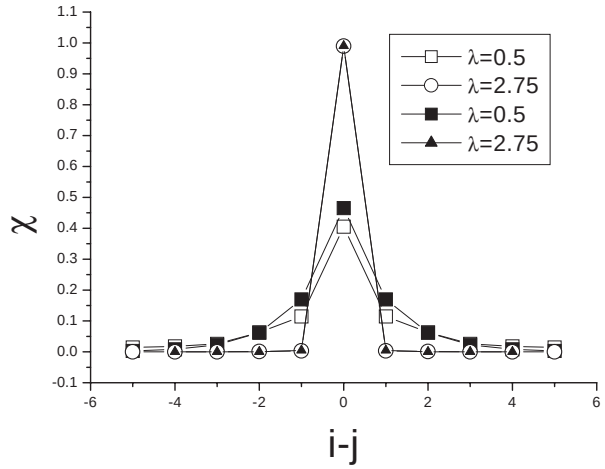

Fig. 4. The electron-lattice correlation $\chi(i-j)$ as a function of $(i-j)$ for 1D when $\omega_0/W = 0.5$, $\lambda = 0.5$ and $\lambda = 2.75$. The hollow symbols are for many-electron case ($\mu = -0.2$) and the solid ones are for single-electron case.

As an approach that could be easily extended to the many-electron case, the accuracy of these results is satisfying.

Figure 4 shows the electron-lattice correlation function $\chi(i-j)$ for moderate coupling ($\lambda = 0.5$) and strong coupling ($\lambda = 2.75$) for both the single- and many-electron systems. In strong coupling case, the lattice deformation is confined to the site where the electron sits, which indicates that our method can provide a quantitative picture of the "self-trapped" state. From equation (31) we see that in the single-electron case the correlation function is just $r(i-j)$ that used in the $\mathbf{q}$-dependent transformation S_1.

To describe the polaronic state at different $\mathbf{k}$ the energy band distortion, calculated according to equation (29), is plotted for different parameters in Figure 5 for 1D and 2D. The band is suppressed from above because of the polaronic effect.

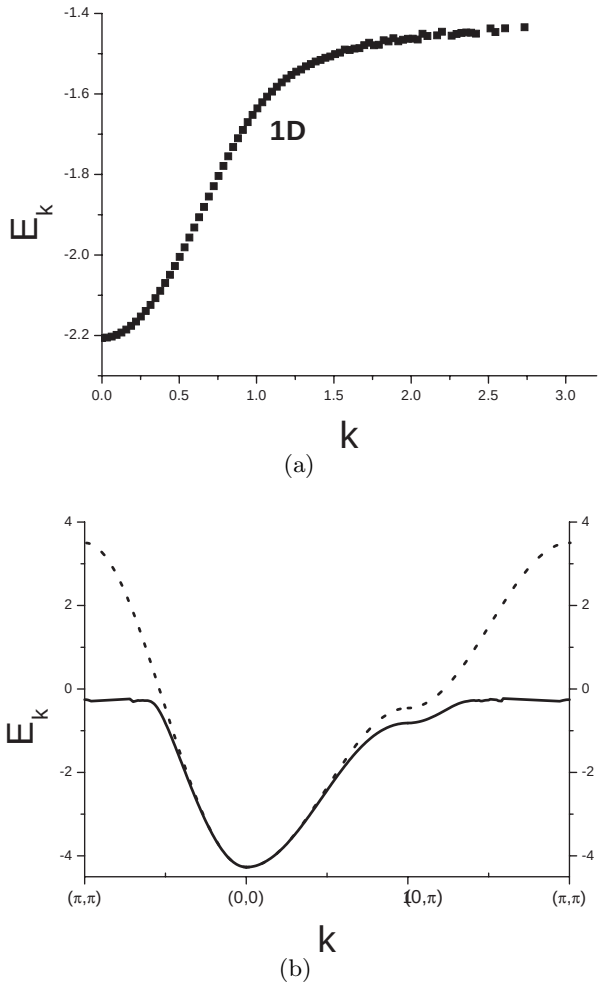

Fig. 5. Polaronic band structure (in unit of t) (a) for 1D with $\omega_0/W = 0.4$ and $\lambda = 0.25$; (b) for 2D with $\omega_0/W = 1.0$ and $\lambda = 0.125$, The dotted curve gives the free electron dispersion $\epsilon_{\mathbf{k}}$.

5 Summary and discussion

A new perturbation approach is developed for single- and many-electron Holstein model in one-, two-, and three-dimension. The results show that this approach has a good agreement with the ME theory in the adiabatic regime when the coupling is moderate ($\lambda < 1$) but with the LF theory in the antiadiabatic regime ($\omega_0/W \gg 1$). In the intermediate region, our approach can describe the transition from a large-polaron Fermi-liquid to the small-polaron, and this transition may be discontinuous in adiabatic regime, which means a phase transition appears in many-electron system. In single-electron case, we eliminate the abrupt transition using the degenerate perturbation theory, and the calculated ground state energy and effective mass are successfully compared with those of previous authors.

The purpose of our unitary transformations is to find a better way to divide the Hamiltonian into the unperturbed part and the perturbation. In this work the transformed H'' is divided into two part: The unperturbed part is H_0'' and the perturbation $H_1'' + H_2''$. We believe that the unperturbed part H_0'' contains the main physics of the coupling system because the effect of the first order terms in H'' (H_1'') is eliminated in the lowest order of perturbation by introducing a function $\delta(\mathbf{k}+\mathbf{q},\mathbf{k})$.

In our approach, the first transformation is done to the end and after the transformation all terms have been collected. The second transformation cannot be done to the end and we stop after the second order. The expansion parameter of the second transformation S_2 is, in fact, $\frac{g}{\omega_0}(\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}})$. This expansion parameter is quite small or even ~ 0 in the following four limiting cases:

1. Adiabatic limit ($\omega_0 = 0$): at this limit $r_{\mathbf{q}} = 0$, $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) = 0$ (Eq. (15)), so we have $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}} = 0$.

2. Antiadiabatic limit ($\omega_0 \to \infty$): at this limit $r_{\mathbf{q}} = 1$ and $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) = 1$ (Eq. (15)), and we also have $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}} = 0$.

3. Strong coupling regime ($E_p/\omega_0 \gg 1$): the narrowing factor η, derived from equation (26), should be small

enough ($\eta \to 0$) and then the difference $\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}$ will become small enough also.

4. Weak coupling regime ($\lambda \ll 1$): there should be no problem for the convergence of the second transformation.

Hence, we believe that in the intermediate region, $\omega_0/W \sim 1$ and/or $E_p/\omega_0 \geq 1$, the expansion parameter $\frac{g}{\omega_0}(\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}})$ should be within the controllable region since we have $0 \leq \delta(\mathbf{k}+\mathbf{q},\mathbf{k}) \leq 1$, $0 \leq r_{\mathbf{q}} \leq 1$ and $|\delta(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}| < 1$.

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