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2003 J. Phys. A: Math. Gen. 36 9405

(http://iopscience.iop.org/0305-4470/36/35/325)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 9405–9413 PII: S0305-4470(03)58992-2

Crossover between large and small polarons in many-electron system with on-site repulsion

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Received 30 January 2003, in final form 5 June 2003
Published 20 August 2003
Online at stacks.iop.org/JPhysA/36/9405

Abstract

An analytical approach has been developed for the electron–phonon coupling in the Holstein–Hubbard model. The Hubbard U is treated approximately by the slave-boson approach. We show that our approach is flexible and physically clear because it is based on perturbation theory. When the dimensionless ratio $\omega_p/2Dt$ is small, $\omega_p/2Dt \ll 1$, our result is similar to that of the Migdal–Eliashberg theory. When $\omega_p/2Dt > 1$, our result approaches that of the Lang–Firsov transformation and small polaron theory. We have calculated the effective mass of electrons at the Fermi surface to show that the new perturbation approach works well in the intermediate region where $\omega_p/2Dt \sim 1$.

PACS numbers: 71.38.+i, 64.60.Cn, 71.30.+h, 71.45.Lr

1. Introduction

Recently the polaronic behaviour of charge carriers in electron–phonon interacting systems with strong electron correlation has received considerable attention due to important classes of materials, such as the high-temperature superconductors [1, 2] and the colossal magnetoresistance manganites [3, 4]. As for the analytical studies of the electron–phonon interaction, usually the Migdal–Eliashberg (ME) theory [5] and the perturbation expansion are used for the region of lower phonon frequency $\omega_p \ll E_F$ (near-adiabatic case) where ω_p is the phonon frequency and E_F is the electron Fermi energy, and the small polaron theory with the strong-coupling expansion [6] is used for the region of lower Fermi energy $\omega_p \gg E_F$ (anti-adiabatic case) and strong coupling. However, how to treat the region between the two limits where the phonon energy is of the same order of magnitude as the Fermi energy, $\omega_p \sim E_F$, is still an open problem.

Among the models for correlated electrons coupled with phonons the Holstein–Hubbard model has been studied [7–10],

0305-4470/03/359405+09$30.00

$$H = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma}\left(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}\right) - \mu_0\sum_{\mathbf{j},\sigma}c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{j}\sigma} + \sum_{\mathbf{j}}\omega_p b^{\dagger}_{\mathbf{j}}b_{\mathbf{j}} + \sum_{\mathbf{j},\sigma}g\left(b^{\dagger}_{\mathbf{j}} + b_{\mathbf{j}}\right)\left(c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{j}\sigma} - \frac{n}{2}\right) + U\sum_{\mathbf{j}}n_{\mathbf{j}\uparrow}n_{\mathbf{j}\downarrow}. \tag{1}$$

The notation is usual (we put $\hbar = 1$ and $k_B = 1$). $n_{\mathbf{j}\sigma} = c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{j}\sigma}$ is the number operator and $n = \frac{1}{N}\sum_{\mathbf{j},\sigma}\langle n_{\mathbf{j}\sigma}\rangle$ is the number density of electrons with bare chemical potential μ_0 (N is the number of sites). Although there are many studies on the single-electron Holstein model, the research work on the many-polaron state is not sufficient and satisfied. Very recently, the many-polaron system was studied by Capone *et al* [9] using the exact diagonalization of small clusters, and by Millis and his co-workers [10] using the dynamical mean-field approximation.

In this work we propose a new perturbation approach to the many-electron Holstein–Hubbard model. We try to take advantage of both the variational and perturbation methods and the main procedure of the approach is as follows. H in (1) can be divided as $H = H_0 + V$ where V is the last term and may be treated as the perturbation. We try to find a better way to divide the Hamiltonian into an unperturbed part and perturbation by means of the unitary transformation: $\tilde{H} = \exp(S)H\exp(-S) = \tilde{H}_0 + \tilde{V}$. The unperturbed part $\tilde{H}_0 \neq H_0$ should be simple enough to solve 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.

2. Transformed Hamiltonian

In this paper the Hubbard U is treated approximately by the infinite-U slave-boson approach. The Holstein–Hubbard Hamiltonian can be approximated as

$$H = \sum_{\mathbf{k},\sigma}(z\epsilon_{\mathbf{k}} - \mu_0')c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}}\omega_p b^{\dagger}_{\mathbf{q}}b_{\mathbf{q}} + \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}g_{\mathbf{q}}\left(b^{\dagger}_{-\mathbf{q}} + b_{\mathbf{q}}\right)c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} + UdN \tag{2}$$

where d is the probability of double occupancy and z is the renormalization factor of the Hubbard U on the hopping. We have $z = 2(1-n)/(2-n)$ and $d = 0$ for the infinite-U slave-boson approach [11]. $\mu_0' \neq \mu_0$ is the renormalized chemical potential by the Hubbard U, $\epsilon_{\mathbf{k}} = -2t\sum_{\tau=1}^{D}\cos(k_\tau)$. Note that the $\mathbf{q} = 0$ phonon is not coupled with the electrons: $g_{\mathbf{q}} = g$ for $\mathbf{q} \neq 0$ and $g_0 = 0$.

H is an electron–phonon coupling system and we use the following two unitary transformations to treat the electron–phonon correlation. The first one is a polaronic transformation, $H' = \exp(S_1)H\exp(-S_1)$, where

$$S_1 = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}\frac{g_{\mathbf{q}}}{\omega_p}r_{\mathbf{q}}\left(b^{\dagger}_{-\mathbf{q}} - b_{\mathbf{q}}\right)c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}. \tag{3}$$

Here we introduce an electron–phonon correlation function $r_{\mathbf{q}}$ which is $\mathbf{q}$-dependent and its form will be determined later. The transformation can be done to the end and the result is

$$H' = H_0' + H_1' + H_2'$$
$$H_0' = \sum_{\mathbf{k},\sigma}(\eta z\epsilon_{\mathbf{k}} - \mu_0')c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}}\omega_p b^{\dagger}_{\mathbf{q}}b_{\mathbf{q}} + UdN \tag{4}$$

$$\eta = \exp\left\{-\frac{1}{N}\sum_{\mathbf{q}}\frac{g^2}{\omega_p^2}r_{\mathbf{q}}^2(1-\gamma_{\mathbf{q}})\right\} \qquad \gamma_{\mathbf{q}} = -\epsilon_{\mathbf{q}}/2Dt \tag{5}$$

$$H_1' = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g(1-r_{\mathbf{q}})\big(b_{-\mathbf{q}}^{\dagger}+b_{\mathbf{q}}\big)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$
$$-\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g\eta z r_{\mathbf{q}}\frac{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}{\omega_p}\big(b_{-\mathbf{q}}^{\dagger}-b_{\mathbf{q}}\big)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma} \tag{6}$$

$$H_2' = -tz\sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_{\sigma}\big(c_{\mathbf{i}\sigma}^{\dagger}c_{\mathbf{j}\sigma}+c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{i}\sigma}\big)\{\cosh[X_{\mathbf{i},\mathbf{j}}]-\eta\}$$
$$-tz\sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_{\sigma}\big(c_{\mathbf{i}\sigma}^{\dagger}c_{\mathbf{j}\sigma}-c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{i}\sigma}\big)\{\sinh[X_{\mathbf{i},\mathbf{j}}]-\eta X_{\mathbf{i},\mathbf{j}}\}$$
$$-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma,\sigma'}\frac{g_{\mathbf{q}}^2}{\omega_p}r_{\mathbf{q}}[2-r_{\mathbf{q}}]c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma}c_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger}c_{\mathbf{k}'\sigma'} \tag{7}$$

$$X_{\mathbf{i},\mathbf{j}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\frac{g}{\omega_p}r_{\mathbf{q}}\big(b_{-\mathbf{q}}^{\dagger}-b_{\mathbf{q}}\big)[\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{i}}-\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{j}}]. \tag{8}$$

Terms in H_2' are second order in g or higher. Up to now, the transformation has been done exactly and there is no approximation.

After the polaronic transformation, the first-order terms of $O(g)$ still exist in H_1'. We apply a further transformation to H' [12]: $H'' = \exp(S_2)H'\exp(-S_2)$, where the generator S_2 is

$$S_2 = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}\frac{g_{\mathbf{q}}}{\omega_p}\big(b_{-\mathbf{q}}^{\dagger}-b_{\mathbf{q}}\big)[\xi(\mathbf{k}+\mathbf{q},\mathbf{k})-r_{\mathbf{q}}]c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma} \tag{9}$$

$$\xi(\mathbf{k}+\mathbf{q},\mathbf{k}) = \frac{\omega_p}{\omega_p+\eta'(|\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|+|\epsilon_{\mathbf{k}}-\mu|)}. \tag{10}$$

μ is the real chemical potential, which may be different from the bare one, and $\eta' = \eta z$. Here a function $\xi(\mathbf{k}',\mathbf{k})$ is introduced. Note that $0 \leqslant \xi(\mathbf{k}',\mathbf{k}) \leqslant 1$ measures the intensity of the electron–phonon scattering process: $\xi(\mathbf{k}',\mathbf{k}) \sim 1$ if both the energies of the incoming and outgoing electrons $\epsilon_{\mathbf{k}+\mathbf{q}}$ and $\epsilon_{\mathbf{k}}$ are close to the chemical potential μ, and $\xi(\mathbf{k}',\mathbf{k}) \ll 1$ otherwise. The width of the region where $\xi(\mathbf{k}',\mathbf{k}) \sim 1$ is proportional to the phonon frequency ω_p. This is to say that only those electrons near the Fermi surface can be scattered by phonons intensively. The reason of choosing the form of $\xi(\mathbf{k}',\mathbf{k})$ in equation (10) will become clear later. The transformation can proceed order by order and till the second order of g,

$$H'' = \sum_{\mathbf{k},\sigma}(\eta'\epsilon_{\mathbf{k}}-\mu_0')c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}+\sum_{\mathbf{q}}\omega_p b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}+UdN$$
$$+\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g(1-\xi(\mathbf{k}+\mathbf{q},\mathbf{k}))\big(b_{-\mathbf{q}}^{\dagger}+b_{\mathbf{q}}\big)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$
$$-\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma}\frac{g}{\omega_p}\eta'(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})\xi(\mathbf{k}+\mathbf{q},\mathbf{k})\big(b_{-\mathbf{q}}^{\dagger}-b_{\mathbf{q}}\big)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$
$$-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} z\big(c_{\mathbf{i}\sigma}^{\dagger}c_{\mathbf{j}\sigma}+c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{i}\sigma}\big)\{\cosh[X_{\mathbf{i},\mathbf{j}}]-\eta\}$$
$$-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} z\big(c_{\mathbf{i}\sigma}^{\dagger}c_{\mathbf{j}\sigma}-c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{i}\sigma}\big)\{\sinh[X_{\mathbf{i},\mathbf{j}}]-\eta X_{\mathbf{i},\mathbf{j}}\}$$
$$-\frac{1}{2N}\sum_{\mathbf{k},\mathbf{q}}\sum_{\sigma}\frac{g^2}{\omega_p^2}\eta'(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}})\big(b_{-\mathbf{q}}^{\dagger}-b_{\mathbf{q}}\big)\big(b_{\mathbf{q}}^{\dagger}-b_{-\mathbf{q}}\big)$$

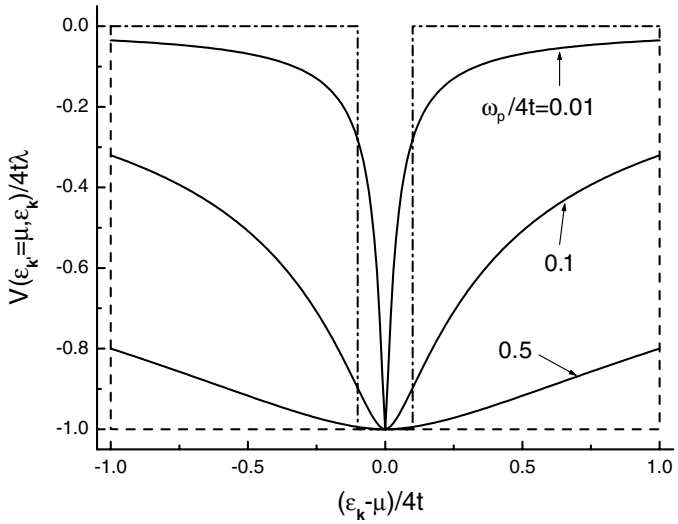

Figure 1. $V(\mathbf{k}+\mathbf{q},\mathbf{k})$ for $n = 0.6$, $\lambda = 0.5$ and $\omega_p/4t = 0.01$, 0.1 and 0.5, as well as $V_{\rm BCS}$ (dashed-dotted) and $V_{\rm LF}$ (dashed).

$$\times\left[\xi^2(\mathbf{k}+\mathbf{q},\mathbf{k})-r_{\mathbf{q}}^2\right]\left[c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}-c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right]$$
$$-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma,\sigma'}\frac{g_{\mathbf{q}}^2}{\omega_p}\xi(\mathbf{k}+\mathbf{q},\mathbf{k})[2-\xi(\mathbf{k}'-\mathbf{q},\mathbf{k}')]c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}. \tag{11}$$

All terms of higher order than g^2 will be omitted in the following treatment.

The phonon-induced interaction between electrons, the four-fermion term in H'', is

$$V(\mathbf{k}+\mathbf{q},\mathbf{k})=-g_{\mathbf{q}}^2\frac{\omega_p+2\eta'(|\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|+|\epsilon_{\mathbf{k}}-\mu|)}{(\omega_p+\eta'(|\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|+|\epsilon_{\mathbf{k}}-\mu|))^2}. \tag{12}$$

It should be compared with the BCS potential [13]

$$V_{\rm BCS}(\epsilon_{\mathbf{k}+\mathbf{q}},\epsilon_{\mathbf{k}})=\begin{cases}-g^2/\omega & |\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|,\ |\epsilon_{\mathbf{k}}-\mu|<\omega_p\\ 0 & |\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|,\ |\epsilon_{\mathbf{k}}-\mu|>\omega_p\end{cases} \tag{13}$$

and the Lang–Firsov potential for small polarons

$$V_{\rm LF}(\epsilon_{\mathbf{k}+\mathbf{q}},\epsilon_{\mathbf{k}})=-g^2/\omega_p,\ |\epsilon_{\mathbf{k}+\mathbf{q}}-\mu|,\ |\epsilon_{\mathbf{k}}-\mu|<E_F. \tag{14}$$

Figure 1 shows $V(\mathbf{k}+\mathbf{q},\mathbf{k})$ for $n = 0.6$, $\lambda = g^2/4t\omega_p = 0.5$ and $\omega_p/4t = 0.01$, 0.1 and 0.5, as well as $V_{\rm BCS}$ and $V_{\rm LF}$. One can see that for smaller phonon frequency, the induced potential has a sharp valley around the Fermi level $\epsilon_{\mathbf{k}} = \mu$, similar to the BCS potential which is a square well. For larger phonon frequency the valley becomes flatter and, finally, approaches that of the LF potential.

3. Perturbation treatment

The purpose of our transformation is to find a better way to divide the Hamiltonian into the unperturbed part and the perturbation. Up to the second order of g the unperturbed part H_0''

and the perturbation H_1'' of H'' are

$$H_0'' = \sum_{\mathbf{k},\sigma} \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)\left[c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} - \left\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\right\rangle\right] + \sum_{\mathbf{q}} \omega_p b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + E_g - \mu_0' nN \tag{15}$$

$$\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) = \eta'\epsilon_{\mathbf{k}} - \mu_0' + \frac{1}{N}\sum_{\mathbf{q}} \frac{g^2}{\omega_p^2}\eta'(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\left(\xi^2(\mathbf{k}+\mathbf{q},\mathbf{k}) - r_{\mathbf{q}}^2\right)$$
$$- \frac{1}{N}\sum_{\mathbf{k}'} \frac{g^2}{\omega_p}\xi(\mathbf{k}',\mathbf{k})[2 - \xi(\mathbf{k}',\mathbf{k})]\left(1 - 2\left\langle c_{\mathbf{k}'\sigma}^{\dagger} c_{\mathbf{k}'\sigma}\right\rangle\right) \tag{16}$$

$$E_g = \sum_{\mathbf{k},\sigma} \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)\left\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\right\rangle + UdN + 2V_0\left(\frac{n^2}{4} - d\right)N + \mu_0' nN$$
$$- \frac{1}{N}\sum_{\mathbf{k},\mathbf{q}}\sum_{\sigma} \frac{g^2}{\omega_p}\xi(\mathbf{k}+\mathbf{q},\mathbf{k})\left(1 - \left\langle c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q}\sigma}\right\rangle\right)\left\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\right\rangle \tag{17}$$

$$V_0 = \frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_p}\xi(\mathbf{k}+\mathbf{q},\mathbf{k})[2 - \xi(\mathbf{k}'-\mathbf{q},\mathbf{k}')] \tag{18}$$

$$H_1'' = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} g(1 - \xi(\mathbf{k}+\mathbf{q},\mathbf{k}))\left(b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}}\right)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}\sigma}$$
$$- \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g}{\omega_p}\eta'(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\xi(\mathbf{k}+\mathbf{q},\mathbf{k})\left(b_{-\mathbf{q}}^{\dagger} - b_{\mathbf{q}}\right)c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}\sigma}. \tag{19}$$

$\langle \ldots \rangle$ means an average over the ground state of H_0''. E_g is the ground state energy and the second-order contribution of the perturbation H_1'' to the ground state energy is

$$\Delta E_2 = \int_0^{\beta} \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \langle [H_1''(\tau_1) H_1''(\tau_2)]\rangle|_{T=0}$$
$$= -\frac{1}{2N}\sum_{\mathbf{k}',\mathbf{k}} \frac{\eta'^2 g^2}{[\omega_p + \eta'(|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)]^2}\{1 - \mathrm{sign}(\epsilon_{\mathbf{k}'} - \mu)\,\mathrm{sign}(\epsilon_{\mathbf{k}} - \mu)\}$$
$$\times \left\{[|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu| - (\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})]^2 \frac{1 + \mathrm{sign}(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})}{\omega_p + \rho(\epsilon_{\mathbf{k}'})(\epsilon_{\mathbf{k}'} - \mu) - \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)}\right.$$
$$\left. + [|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu| + (\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})]^2 \frac{1 - \mathrm{sign}(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})}{\omega_p - \rho(\epsilon_{\mathbf{k}'})(\epsilon_{\mathbf{k}'} - \mu) + \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)}\right\}$$
$$= 0 \tag{20}$$

because of the functional form of $\xi(\mathbf{k}+\mathbf{q},\mathbf{k})$ (equation (10)). 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 ($O(g)$) which are not exactly cancelled after the two unitary transformations are related to the higher lying excited states and should be irrelevant under renormalization [12].

Although the form of $\xi(\mathbf{k}+\mathbf{q},\mathbf{k})$ is already defined from the beginning (equation (10)), the form of $r_{\mathbf{q}}$ in the first transformation, equation (3), has not been determined. Note that $r_{\mathbf{q}}$ does not appear in E_g explicitly and E_g depends on $r_{\mathbf{q}}$ implicitly via η (equation (5)). Thus, we can determine the form of $r_{\mathbf{q}}^2$ by minimizing E_g:

$$r_{\mathbf{q}}^2 = -\frac{1}{1-\gamma_{\mathbf{q}}}\frac{1}{N}\sum_{\mathbf{k}} \frac{\omega_p^2(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}{[\omega_p + \eta_0 z(|\epsilon_{\mathbf{k}+\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)]^2}\left\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\right\rangle \Big/ \frac{1}{N}\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\left\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\right\rangle \tag{21}$$

where $0 \leqslant \eta_0 \leqslant 1$ is a parameter.

As g^2/ω_p is the polaronic binding energy independent of the ionic mass M, in the adiabatic limit $M \to \infty$ ($\omega_p = \sqrt{K/M} \to 0$, K is the spring constant) we have $r_{\mathbf{q}} = 0$ and $\eta = 1$. But in the anti-adiabatic limit $M \to 0$ ($\omega_p \to \infty$) it is easy to get $r_{\mathbf{q}} = 1$ and $\ln \eta = -g^2/\omega_p^2$. Besides, for the strong coupling limit $g/\omega_p \gg 1$, we have $\eta \ll 1$ and thus $r_{\mathbf{q}} \to 1$ and $\ln \eta \to -g^2/\omega_p^2$. These are consistent with the LF theory [6].

The electron Green function for the transformed Hamiltonian H'' can be derived from the Dyson equation

$$G(\mathbf{k}, \mathrm{i}k_m) = G_0(\mathbf{k}, \mathrm{i}k_m) + G_0(\mathbf{k}, \mathrm{i}k_m)\Sigma(\mathbf{k}, \mathrm{i}k_m)G(\mathbf{k}, \mathrm{i}k_m).$$

The second-order self-energy of H_1'' is ($T = 0$)

$$\begin{aligned}\Sigma(\mathbf{k}, \mathrm{i}k_m) = \frac{1}{N}\sum_{\mathbf{q}} & \frac{\eta'^2 g^2}{[\omega_p + \eta(|\epsilon_{\mathbf{k}-\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)]^2} \\ & \times \left\{ [|\epsilon_{\mathbf{k}-\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu| - (\epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}})]^2 \frac{\theta(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}{\mathrm{i}k_m - \omega_p - \rho(\epsilon_{\mathbf{k}-\mathbf{q}})(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)} \right. \\ & \left. + [|\epsilon_{\mathbf{k}-\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu| + (\epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}})]^2 \frac{\theta(\mu - \epsilon_{\mathbf{k}-\mathbf{q}})}{\mathrm{i}k_m - \omega_p + \rho(\epsilon_{\mathbf{k}-\mathbf{q}})(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)} \right\}. \end{aligned} \tag{22}$$

The renormalized chemical potential μ can be determined by

$$1 - n = \frac{1}{N}\sum_{\mathbf{k}} \mathrm{sign}(\epsilon_{\mathbf{k}} - \mu). \tag{23}$$

Obviously, $\Sigma(\epsilon_{\mathbf{k}} = \mu, \mathrm{i}k_m) = 0$ for $T = 0$. This is another reason for the choice of functional form of $\xi(\mathbf{k} + \mathbf{q}, \mathbf{k})$.

The quasi-particle energy determined as the pole of the Green function is

$$\begin{aligned} E_{\mathbf{k}} - \mu_0' &= \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) + \mathrm{Re}[\Sigma(\mathbf{k}, \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu))] \\ &= \eta'(\epsilon_{\mathbf{k}} - \mu) + (\eta'\mu - \mu_0') + \mathrm{Re}[\Sigma(\mathbf{k}, \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu))] \\ &\quad - \frac{1}{N}\sum_{\mathbf{k}'} \frac{g^2}{\omega_p}\xi(\mathbf{k}', \mathbf{k})[2 - \xi(\mathbf{k}', \mathbf{k})]\,\mathrm{sign}(\epsilon_{\mathbf{k}'} - \mu) \\ &\quad + \frac{1}{N}\sum_{\mathbf{q}} \frac{g^2}{\omega_p^2}\eta'(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\big(\xi^2(\mathbf{k} + \mathbf{q}, \mathbf{k}) - r_{\mathbf{q}}^2\big). \end{aligned} \tag{24}$$

The bare chemical potential μ_0' is determined by letting $\epsilon_{\mathbf{k}} = \mu$ in equation (24), which leads to

$$\begin{aligned}\mu_0' = \eta'(1 - \ln\eta)\mu &+ \frac{1}{N}\sum_{\mathbf{k}'} g^2 \frac{\eta'(\epsilon_{\mathbf{k}'} - \mu)}{(\omega_p + \eta'|\epsilon_{\mathbf{k}'} - \mu|)^2} \\ &- \frac{1}{N}\sum_{\mathbf{k}'} g^2 \frac{\omega_p + 2\eta'|\epsilon_{\mathbf{k}'} - \mu|}{(\omega_p + \eta'|\epsilon_{\mathbf{k}'} - \mu|)^2}\,\mathrm{sign}(\epsilon_{\mathbf{k}'} - \mu). \end{aligned} \tag{25}$$

The renormalized factor $\rho(\epsilon_{\mathbf{k}})$ is

$$\begin{aligned}\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) = \eta'(1 - \ln\eta)(\epsilon_{\mathbf{k}} - \mu) &- \frac{1}{N}\sum_{\mathbf{k}'} g^2 \\ &\times \left[\frac{\omega_p + 2\eta'(|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)}{[\omega_p + \eta'(|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)]^2} - \frac{\omega_p + 2\eta'|\epsilon_{\mathbf{k}'} - \mu|}{(\omega_p + \eta'|\epsilon_{\mathbf{k}'} - \mu|)^2} \right] \mathrm{sign}(\epsilon_{\mathbf{k}'} - \mu) \\ &+ \frac{1}{N}\sum_{\mathbf{k}'} g^2\eta' \left[\frac{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}}{[\omega_p + \eta'(|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)]^2} - \frac{\epsilon_{\mathbf{k}'} - \mu}{(\omega_p + \eta'|\epsilon_{\mathbf{k}'} - \mu|)^2} \right]. \end{aligned} \tag{26}$$

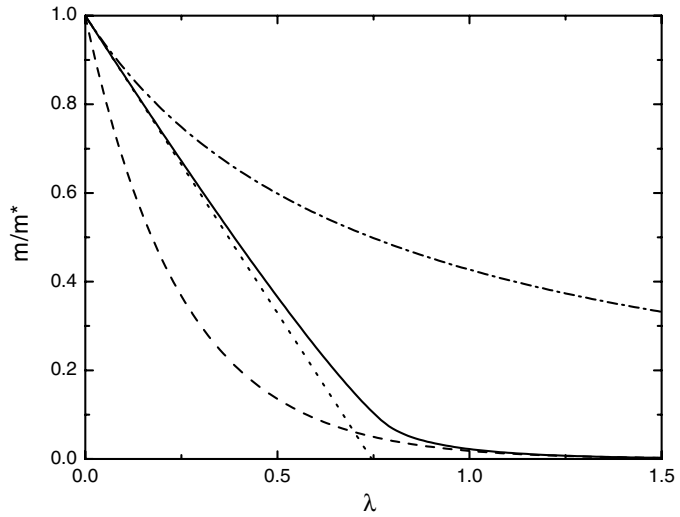

Figure 2. The effective mass m/m^* at Fermi surface in 2D as functions of the electron–phonon coupling λ, $n = 0.6$ and $\omega_p = t$. For comparison, $m/m^*_{\rm RS}$ (dotted), $m/m^*_{\rm ME}$ (dashed-dotted) and $m/m^*_{\rm LF}$ (dashed) are also shown.

The renormalization factor at the Fermi energy ($\epsilon_{\mathbf{k}} = \mu$), which is the mass renormalization factor m/m^*, is

$$m/m^* = \rho(\epsilon_{\mathbf{k}} = \mu) = \eta'(1 - \ln\,\eta) - \frac{1}{N}\sum_{\mathbf{k}'} \frac{g^2\eta'}{(\omega_p + \eta|\epsilon_{\mathbf{k}'} - \mu|)^2}. \tag{27}$$

This should be compared to the well-known mass renormalization factor of the ordinary perturbation theory (the Rayleigh–Schrodinger (RS) perturbation [14])

$$m/m^*_{\rm RS} = 1 - \frac{1}{N}\sum_{\mathbf{k}'} \frac{g^2}{(\omega_p + |\epsilon_{\mathbf{k}'} - \mu|)^2} \tag{28}$$

as well as to that of the ME theory (the same as that of the Brillouin–Wigner perturbation [14]),

$$m/m^*_{\rm ME} = 1 \Bigg/ \left(1 + \frac{1}{N}\sum_{\mathbf{k}'} \frac{g^2}{(\omega_p + |\epsilon_{\mathbf{k}'} - \mu|)^2}\right). \tag{29}$$

For the adiabatic limit $\omega_p \to 0$, $r_{\mathbf{q}} \to 0$ leads to $\eta \to 1$ and we can get $m/m^* = m/m^*_{\rm RS} = 1 - \lambda'$ and $m/m^*_{\rm ME} = 1/(1 + \lambda')$, where $\lambda' = 2g^2N(\epsilon_F)/z\omega_p$ and $N(\epsilon_F)/z$ is the DOS at the Fermi level. This result is the same for 1D, 2D and 3D.

For the anti-adiabatic limit $\omega_p \to \infty$ or for the strong coupling $\epsilon_p/\omega_p \gg 1$, we have $\eta \to \exp(-\epsilon_p/\omega_p)$. Then, we can get the LF result of the effective mass from equation (27): $m/m^*_{\rm LF} = \exp(-\epsilon_p/\omega_p)$.

For weak to intermediate electron–phonon coupling and finite phonon frequency, in figure 2 we show our calculation of the effective mass m/m^* at the Fermi surface in 2D as functions of the electron–phonon coupling $\lambda = g^2/4t\omega_p$ (with $n = 0.6$ and fixed phonon frequency $\omega_p = t$). For comparison, we also show $m/m^*_{\rm RS}$, $m/m^*_{\rm ME}$ and $m/m^*_{\rm LF}$. One can see that for weak coupling our results are nearly the same as those of the RS or ME theory; but for strong coupling they approach those of the LF theory.

4. Summary and discussion

An analytical approach has been developed for the many-electron Holstein–Hubbard model. Our approach is flexible and physically clear because it is based on the perturbation theory. When the dimensionless ratio $\omega_p/2Dt$ is small, $\omega_p/2Dt \ll 1$, our result is similar to that of the ME theory. When $\omega_p/2Dt > 1$, our result approaches that of the LF transformation and small polaron theory. We have calculated the Green function, the effective mass of electrons at the Fermi surface, to show that the new perturbation approach works well in the intermediate region where $\omega_p/2Dt \sim 1$.

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

The approach developed in this paper is based on two unitary transformations. 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, which is the main approximation we have made. Note that $r_{\mathbf{q}}$ introduced in the first transformation should be helpful for the convergence of the second transformation since the expansion parameter of the second transformation S_2 is, in fact, $g(\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}})/\omega_p$. This expansion parameter is quite small or even ~ 0 in the following four limiting cases:

(1) Adiabatic limit ($\omega_p = 0$): in this limit $r_{\mathbf{q}} = 0$, $\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) = 0$ (equation (10)), so we have $\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}} = 0$.
(2) Anti-adiabatic limit ($\omega_p \to \infty$): in this limit $r_{\mathbf{q}} = 1$ and $\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) = 1$, and we also have $\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}} = 0$.
(3) Strong coupling regime ($\epsilon_p/\omega_p \gg 1$): the narrowing factor η should be small enough ($\eta \to 0$) and then the difference $\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}}$ will also become small enough.
(4) Weak coupling regime ($\lambda \ll 1$): there should be no problem for the convergence of the second transformation.

Hence, we conclude that the two points which justify our perturbation approach are: (1) it can reproduce both the lower phonon frequency results of the ME theory and the higher frequency results of the LF theory; (2) in the intermediate region, $\omega_p/E_F \sim 1$ and/or $\epsilon_p/\omega_p \geqslant 1$, the expansion parameter $g(\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}})/\omega_p$ should be within the controllable region since we have $0 \leqslant \xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) \leqslant 1$, $0 \leqslant r_{\mathbf{q}} \leqslant 1$ and $|\xi(\mathbf{k}+\mathbf{q}, \mathbf{k}) - r_{\mathbf{q}}| < 1$.

Acknowledgment

This work was supported by the China National Natural Science Foundation (grant nos 10074044 and 90103022).

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