Nonquasiparticle behavior in momentum-dependent spectral functions of the many-electron Frohlich model

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(Received 15 May 2007; revised manuscript received 29 July 2007; published 5 September 2007)

We have developed a new approach, starting from the Frohlich Hamiltonian and by means of the unitary transformation with the perturbation treatment, to deal with the momentum-dependent spectral functions (MDSF) of electron-phonon coupling system. The approach takes care of the fact that only those electrons near the Fermi surface within a layer of width ω_{ph} (phonon frequency) are scattered by phonons strongly. Our results show that the MDSF is mainly composed of two parts: the zero-phonon part and the one-phonon one. When the bare electron energy $\epsilon_{\mathbf{k}}$ is close to the Fermi energy E_F, $|\epsilon_{\mathbf{k}} - E_F| \simeq \omega_{ph}$, the one-phonon part is quite significant and the MDSF shows a two-headed peak. However, for $|\epsilon_{\mathbf{k}} - E_F| \gg \omega_{ph}$, the one-phonon part disappears gradually and the MDSF shows a single broad peak. Our calculation for MDSF is qualitatively in agreement with recent measurement of angle-resolved photoemission spectroscopy on the Be(0001) surface and $Bi_2Sr_2CaCu_2O_8$. Besides, the two-headed structure of MDSF indicates the "hybridization" between electrons and phonons.

I. INTRODUCTION

The quasiparticle (QP) description of the electronic structure in metallic state is a basic problem of solid state physics, which can now be measured by angle-resolved photoemission spectroscopy (ARPES) with high resolution. This is a rapidly developing area and there are many new discoveries including some direct and clear evidences for the important role played by the electron-phonon (e-ph) interaction in metallic systems.[1–10]

Generally speaking, the ARPES describes the following process:[10] an incident photon creates an emitted electron together with a hole under the Fermi level with net momentum zero and total energy conserved. The energy of emitted electron and its parallel component of momentum are measured by ARPES. If the holes are free from any interaction, at each momentum $\mathbf{k}$, the ARPES would consist of a δ-function peak corresponding to the bare QP energy $\omega = \epsilon_{\mathbf{k}} - \mu$ ($\epsilon_{\mathbf{k}}$ is the noninteracting one-electron energy and μ is the chemical potential). The electron-electron, electron-phonon, and electron-impurity interaction may lead to a dressed QP picture and the corresponding ARPES consists of a single Lorentzian peak at each momentum $\mathbf{k}$. The width of the peak is the inverse lifetime of the hole excitation due to the interaction.

According to recent experimental results, it has become clear that in some strong e-ph interacting systems, the ARPES evolve quite drastically as the momentum changes from Fermi surface to the states deep in the Fermi sea. It is now well known that the ARPES on the Be(0001) surface takes sharp two-headed asymmetric structure at around k_F, while it becomes a broad peak away from Fermi surface by more than two or three times of the phonon energy.[1–3,7] Furthermore, similar spectral evolution was also found in the conduction plane of $Bi_2Sr_2CaCu_2O_8$ under various doping levels.[4,9] These experiments tell us that a QP picture for electrons close to the Fermi surface within a layer of the width of

two or three times of the phonon energy may not be valid when the e-ph interaction is strong. This spectral evolution from the two-headed structure to the broad peak, or from a two-peak nonquasiparticle state to a short lifetime QP one, is a basic problem of the e-ph coupling.[11] However, its origin seems beyond the conventional approximation theories. Thus, the problem how e-ph interaction dominates the spectral shape has now emerged as a new challenge for the theory of solid state physics.

Theoretical studies of e-ph interaction already have a long history starting from the Frohlich's pioneering work.[12] For the many-electron system coupled with phonons, the Migdal-Eliashberg (ME) theory[13–15] has been used to calculate the dressed QP structures and corresponding physical properties. In some cases, systematic theoretical methods have been devised to take into account high order corrections, which are not included in the ordinary second-order perturbation theory. However, the existing theories seem to be not so successful to clarify the measured ARPES since it spans the whole momentum region from the Fermi surface down to the states deep in the Fermi sea.

In this work, we present a theoretical approach to calculate the momentum-dependent spectral function (MDSF) of many-electron systems with e-ph interaction, which is usually denoted as $A(\mathbf{k}, \omega)$.[16] The main purpose of this paper is to clarify the impact of e-ph interaction on the spectral evolution. We consider a many-electron Frohlich model,[12] which has been studied extensively with various interests by perturbative and nonperturbative methods. In this work, we will focus mainly on the metallic phase and try to clarify the evolution of MDSF from a two-peak nonquasiparticle structure for electrons near the Fermi surface to a wide single-peak structure for holes deep in the Fermi sea. Throughout this paper, we set $\hbar = 1$ and $k_B = 1$.

II. UNITARY TRANSFORMATION AND PERTURBATION

We start from the many-electron Frohlich model,

$$H = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu_0) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$$

$$+ \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} g_{\mathbf{q}} (b_{-\mathbf{q}}^\dagger + b_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}, \qquad (1)$$

where $c_{\mathbf{k}\sigma}^\dagger$ and $b_{\mathbf{q}}^\dagger$ ($c_{\mathbf{k}\sigma}$ and $b_{\mathbf{q}}$) are creation (annihilation) operators of electrons (with spin σ) and phonons, respectively. $\epsilon_{\mathbf{k}}$ is the bare electron energy, μ_0 the bare chemical potential, $\omega_{\mathbf{q}}$ the phonon frequency, and $g_{\mathbf{q}}$ the e-ph coupling. The electron-phonon correlation in H is treated by means of the following unitary transformation: $H' = \exp(S)H\exp(-S)$, where the generator S is

$$S = \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g_{\mathbf{q}}}{\omega_{\mathbf{q}}} (b_{-\mathbf{q}}^\dagger - b_{\mathbf{q}}) \xi(\mathbf{k}+\mathbf{q},\mathbf{k}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}, \qquad (2)$$

$$\xi(\mathbf{k}+\mathbf{q},\mathbf{k}) = \frac{\omega_{\mathbf{q}}}{\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}+\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu|}. \qquad (3)$$

μ is the real chemical potential, which may be different from the bare one μ_0. Here, a function $\xi(\mathbf{k}',\mathbf{k})$ is introduced. Note that $0 \leq \xi(\mathbf{k}',\mathbf{k}) \leq 1$ 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 $\epsilon_{\mathbf{k}'}$ and $\epsilon_{\mathbf{k}}$ are close to the chemical potential μ; $\xi(\mathbf{k}',\mathbf{k}) \ll 1$ otherwise. The width of the region where $\xi(\mathbf{k}',\mathbf{k}) \sim 1$ is proportional to the phonon frequency $\omega_{\mathbf{q}}$. This is similar to the Bardeen-Cooper-Schrieffer theory of superconductivity[17] that only those electrons near the Fermi surface within a layer of width ω_{ph} (phonon frequency) contribute to the pairing. The transformation can proceed order by order and we collect all terms to the second order of $g_{\mathbf{q}}$,

$$H' = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu_0) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$$

$$+ \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} g_{\mathbf{q}} [1 - \xi(\mathbf{k}+\mathbf{q},\mathbf{k})] (b_{-\mathbf{q}}^\dagger + b_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$- \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g_{\mathbf{q}}}{\omega_{\mathbf{q}}} (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \xi(\mathbf{k}+\mathbf{q},\mathbf{k}) (b_{-\mathbf{q}}^\dagger - b_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$- \frac{1}{2N} \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2} (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}) (b_{-\mathbf{q}}^\dagger - b_{\mathbf{q}}) (b_{\mathbf{q}}^\dagger - b_{-\mathbf{q}}) \xi^2(\mathbf{k}$$

$$+ \mathbf{q},\mathbf{k}) [c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} - c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}] - \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\sigma,\sigma'} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}} \xi(\mathbf{k}+\mathbf{q},\mathbf{k})$$

$$\times [2 - \xi(\mathbf{k}'-\mathbf{q},\mathbf{k}')] c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma} c_{\mathbf{k}'-\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}'\sigma'}. \qquad (4)$$

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 $g_{\mathbf{q}}$, the unperturbed part H_0' and the perturbation H_1' are

$$H_0' = \sum_{\mathbf{k},\sigma} \rho(\epsilon_{\mathbf{k}}) (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + E_0, \qquad (5)$$

$$\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) = \epsilon_{\mathbf{k}} - \mu_0 + \frac{1}{N} \sum_{\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2} (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \coth\left(\frac{\omega_{\mathbf{q}}}{2T}\right)$$

$$\times \xi^2(\mathbf{k}+\mathbf{q},\mathbf{k}) - \frac{1}{N} \sum_{\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}} \xi(\mathbf{k}+\mathbf{q},\mathbf{k})$$

$$\times [2 - \xi(\mathbf{k}+\mathbf{q},\mathbf{k})] \tanh\left(\frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \mu}{2T}\right), \qquad (6)$$

$$H_1' = \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} g_{\mathbf{q}} [1 - \xi(\mathbf{k}+\mathbf{q},\mathbf{k})] (b_{-\mathbf{q}}^\dagger + b_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$- \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} \frac{g_{\mathbf{q}}}{\omega_{\mathbf{q}}} (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \xi(\mathbf{k}+\mathbf{q},\mathbf{k}) (b_{-\mathbf{q}}^\dagger - b_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}. \qquad (7)$$

E_0 is an unimportant number which plays no role in following calculations. The other terms of H' are collected in H_2', $H_2' = H' - H_0' - H_1'$. One can check that $\langle H_2' \rangle = 0$, where $\langle \cdots \rangle$ means an average over the thermodynamic ensemble of H_0'. Besides, H_2' contributes nothing to the Green's function (GF) in the order $O(g_{\mathbf{q}}^2)$. So, in what follows, we omit the effect of H_2'. The physics after the unitary transformation is contained in the Hamiltonian $H' \approx H_0' + H_1'$.

We shall treat H_0' as the unperturbed part, since it can be solved exactly, and H_1' the perturbation. The contribution of H_1' may be small since the second-order contribution of H_1' to the ground state energy is zero,[16]

$$\Delta E_2 = \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \langle [H_1'(\tau_1) H_1'(\tau_2)] \rangle |_{T=0}$$

$$= -\frac{1}{N} \sum_{\mathbf{q},\mathbf{k}} \frac{g_{\mathbf{q}}^2}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}+\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)^2}$$

$$\times [1 - \text{sign}(\epsilon_{\mathbf{k}+\mathbf{q}} - \mu)\text{sign}(\epsilon_{\mathbf{k}} - \mu)] \left\{ (|\epsilon_{\mathbf{k}+\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} \right. $$

$$- \mu| - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}})^2 \frac{\theta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}{\omega_{\mathbf{q}} + (\epsilon_{\mathbf{k}+\mathbf{q}} - \mu) - (\epsilon_{\mathbf{k}} - \mu)}$$

$$+ (|\epsilon_{\mathbf{k}+\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu| + \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})^2$$

$$\left. \times \frac{\theta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}})}{\omega_{\mathbf{q}} - (\epsilon_{\mathbf{k}+\mathbf{q}} - \mu) + (\epsilon_{\mathbf{k}} - \mu)} \right\} = 0, \qquad (8)$$

because of the functional form of $\xi(\mathbf{k}+\mathbf{q},\mathbf{k})$. This is nothing but makes the matrix element of H_1' between the ground state and the lowest-lying excited states of H_0' vanish. Thus, the first order terms $[O(g_{\mathbf{q}})]$ which are not exactly canceled after the unitary transformation are related to the higher-lying excited states and should be irrelevant under renormalization.

The Green's function of H_0' is

$$\tilde{G}_0(\mathbf{k},\omega) = 1/[\omega - \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)]. \qquad (9)$$

The real chemical potential μ is determined by

$$1 - n = \frac{1}{N}\sum_{\mathbf{k}} \tanh[(\epsilon_{\mathbf{k}} - \mu)/2T], \qquad (10)$$

where n is the band filling. The bare μ_0 is then determined by letting $\epsilon_{\mathbf{k}} = \mu$ in Eq. (6). Thus, the renormalization factor $\rho(\epsilon_{\mathbf{k}})$ is

$$\rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu)$$

$$= \epsilon_{\mathbf{k}} - \mu - \frac{1}{N}\sum_{\mathbf{k}'} g_{\mathbf{q}}^2 \left[\frac{\omega_{\mathbf{q}} + 2(|\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)^2} \right.$$

$$\left. - \frac{\omega_{\mathbf{q}} + 2|\epsilon_{\mathbf{k}'} - \mu|}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu|)^2} \right] \tanh\left(\frac{\epsilon_{\mathbf{k}'} - \mu}{2T}\right)$$

$$+ \frac{1}{N}\sum_{\mathbf{k}'} g_{\mathbf{q}}^2 \left[\frac{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu| + |\epsilon_{\mathbf{k}} - \mu|)^2} \right.$$

$$\left. - \frac{\epsilon_{\mathbf{k}'} - \mu}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu|)^2} \right] \coth\left(\frac{\omega_{\mathbf{q}}}{2T}\right). \qquad (11)$$

The Green's function of H' can be derived from Dyson's equation,

$$\widetilde{G}(\mathbf{k},\omega) = \widetilde{G}_0(\mathbf{k},\omega) + \widetilde{G}_0(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)\widetilde{G}(\mathbf{k},\omega), \qquad (12)$$

where $\Sigma(\mathbf{k},\omega)$ is the self-energy. The contribution of H'_1 to the self-energy [to the order $O(g_{\mathbf{q}}^2)$] is

$$\Sigma(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2} \xi^2(\mathbf{k}-\mathbf{q},\mathbf{k}) \left[(|\epsilon_{\mathbf{k}-\mathbf{q}} - \mu| + |\epsilon_{\mathbf{k}} - \mu| \right.$$

$$- \epsilon_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{k}})^2 \frac{n(\omega_{\mathbf{q}}) + 1 - f(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}{\omega - \omega_{\mathbf{q}} - (\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)} + (|\epsilon_{\mathbf{k}-\mathbf{q}} - \mu|$$

$$\left. + |\epsilon_{\mathbf{k}} - \mu| + \epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}})^2 \frac{n(\omega_{\mathbf{q}}) + f(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}{\omega + \omega_{\mathbf{q}} - (\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)} \right], \quad (13)$$

where $n(\omega_{\mathbf{q}}) = 1/[\exp(\beta\omega_{\mathbf{q}}) - 1]$ and $f(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu) = 1/\{\exp[\beta(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)] + 1\}$. Note that, when $T=0$ $[n(\omega_{\mathbf{q}})=0]$, the self-energy at the Fermi surface, $\epsilon_{\mathbf{k}} = \mu$, is $\Sigma(\epsilon_{\mathbf{k}} = \mu, \omega) = 0$. This is to say that we have diagonalized the electron-phonon Hamiltonian at least for the terms up to second order of $g_{\mathbf{q}}$ at the Fermi surface. The self-energy in our theory is a function of both $\epsilon_{\mathbf{k}}$ and ω, in contrast to the ME theory where it is a function of ω only at least for the Einstein phonons.

The spectrum of elementary excitations in the normal state is the solution of

$$\omega = \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) + \Sigma(\epsilon_{\mathbf{k}},\omega), \qquad (14)$$

so the mass renormalization at the Fermi surface ($T=0$) is

$$\frac{m}{m^*} = \left[\rho(\epsilon_{\mathbf{k}}) + \frac{\partial}{\partial \epsilon_{\mathbf{k}}} \Sigma(\mathbf{k},\omega) \right] \Big/ \left[1 - \frac{\partial}{\partial \omega} \Sigma(\mathbf{k},\omega) \right]\Big|_{\omega=0,\epsilon_{\mathbf{k}}=\mu}$$

$$= \rho(\epsilon_{\mathbf{k}} = \mu) = 1 - \frac{1}{N}\sum_{\mathbf{k}'} \frac{g_{\mathbf{q}}^2}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu|)^2}. \qquad (15)$$

Equations (8), (13), and (15) are three main reasons for the choice of the functional form of $\xi(\mathbf{k}+\mathbf{q},\mathbf{k})$ in Eq. (3).

III. SPECTRAL FUNCTION

The solution of Dyson's equation [Eq. (12)] is

$$\widetilde{G}(\mathbf{k},\omega) = \frac{1}{\omega - \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) - \Sigma(\mathbf{k},\omega)}. \qquad (16)$$

The spectral function of $\widetilde{G}(\mathbf{k},\omega)$ is

$$\widetilde{A}(\mathbf{k},\omega)$$

$$= -\frac{1}{\pi} \operatorname{Im} \widetilde{G}(\mathbf{k},\omega)$$

$$= -\frac{1}{\pi} \frac{\operatorname{Im}\Sigma(\mathbf{k},\omega)}{[\omega - \rho(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \mu) - \operatorname{Re}\Sigma(\mathbf{k},\omega)]^2 + [\operatorname{Im}\Sigma(\mathbf{k},\omega)]^2}. \qquad (17)$$

Since $\widetilde{G}(\mathbf{k},\omega)$ is GF for the transformed H', we have to take into account the effect of the unitary transformation when calculating the Green's function for the original Hamiltonian H, which can be defined as

$$G(\mathbf{k},\tau) = -\operatorname{Tr}[T_{\tau}\exp(-\beta H)c_{\mathbf{k}\sigma}(\tau)c_{\mathbf{k}\sigma}^{\dagger}]/Z, \qquad (18)$$

where $Z = \operatorname{Tr}[\exp(-\beta H)]$. After the transformation, we have

$$G(\mathbf{k},\tau) = -\operatorname{Tr}(T_{\tau}e^{-\beta H'}e^{H'\tau}e^{S}c_{\mathbf{k}\sigma}e^{-S}e^{-H'\tau}e^{S}c_{\mathbf{k}\sigma}^{\dagger}e^{-S})/Z. \qquad (19)$$

The transformation of a single fermion operator can proceed as

$$e^{S}c_{\mathbf{k}\sigma}e^{-S} = c_{\mathbf{k}\sigma} - \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} \frac{g_{\mathbf{q}}}{\omega_{\mathbf{q}}}\xi(\mathbf{k},\mathbf{k}-\mathbf{q})(b_{-q}^{\dagger} - b_{\mathbf{q}})c_{\mathbf{k}-\mathbf{q}\sigma}$$

$$+ \frac{1}{2N}\sum_{\mathbf{q},\mathbf{q}'} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi(\mathbf{k},\mathbf{k}-\mathbf{q})\xi(\mathbf{k}-\mathbf{q},k-\mathbf{q}-\mathbf{q}')$$

$$\times (b_{-\mathbf{q}}^{\dagger} - b_{\mathbf{q}})(b_{-\mathbf{q}'}^{\dagger} - b_{\mathbf{q}'})c_{\mathbf{k}-\mathbf{q}-\mathbf{q}'\sigma}. \qquad (20)$$

Thus, the original Green's function [to the second order $O(g_{\mathbf{q}}^2)$] can be expressed as a sum of the coherent part (zero phonon) $G(\mathbf{k},ik_m)_0$ and the incoherent part $G(\mathbf{k},ik_m)_1$ (one phonon),

$$G(\mathbf{k},ik_m) = G(\mathbf{k},ik_m)_0 + G(\mathbf{k},ik_m)_1, \qquad (21)$$

$$G(\mathbf{k},ik_m)_0 = \left[1 - \frac{1}{N}\sum_{\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})\coth\left(\frac{\omega_{\mathbf{q}}}{2T}\right) \right]\widetilde{G}(\mathbf{k},ik_m), \qquad (22)$$

$$G(\mathbf{k},ik_m)_1 = \frac{1}{N}\sum_{\mathbf{q}} \frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})\frac{1}{\beta}\sum_{\omega_n} \frac{2\omega_{\mathbf{q}}}{\omega_n^2 + \omega_{\mathbf{q}}^2}$$

$$\times \widetilde{G}(\mathbf{k}-\mathbf{q},ik_m - i\omega_n), \qquad (23)$$

where $\widetilde{G}(\mathbf{k},ik_m)$ and $\widetilde{G}(\mathbf{k}-\mathbf{q},ik_m - i\omega_n)$ are GF of H' [Eq. (16)]. The MDSF $A(\mathbf{k},\omega) = -\frac{1}{\pi}\operatorname{Im} G(\mathbf{k},\omega)$ may also be expressed as a sum of the zero-phonon part and the one-phonon part,
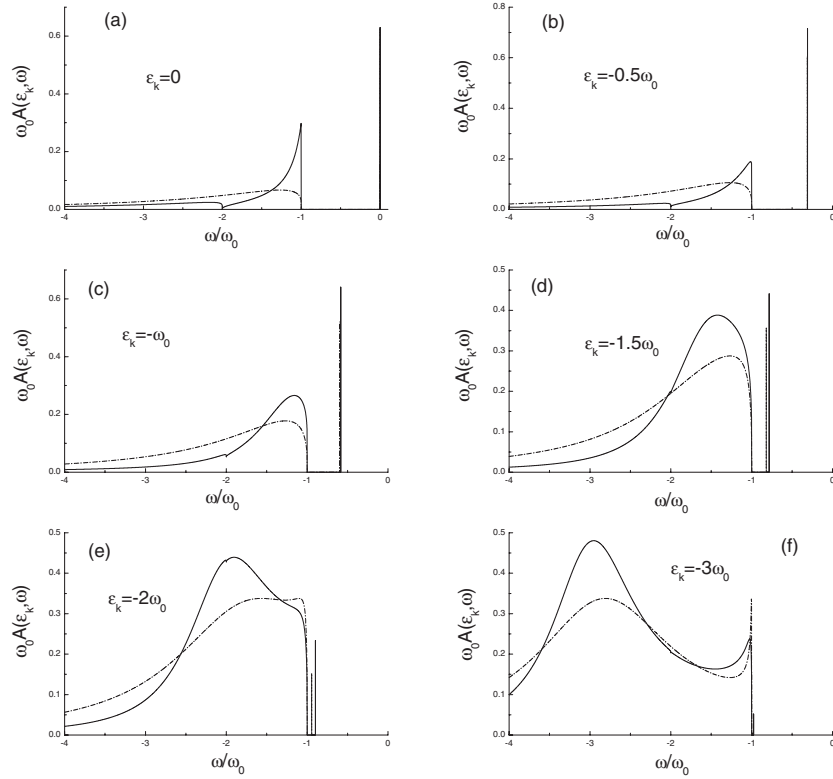
FIG. 1. The calculated MDSF (solid lines) with Einstein phonons are compared with those of the ME theory (dashed lines). $\epsilon_{\mathbf{k}}=$(a) 0, (b) $-0.5\omega_0$, (c) $-\omega_0$, (d) $-1.5\omega_0$, (e) $-2\omega_0$, (f) $-3\omega_0$. Temperature $T=0$, $\omega_D/2D=0.01$, $\lambda=0.378$ for our calculations and $\lambda_{ME}=0.6$ for those of the ME theory. The vertical lines are to indicate the position of the δ-function peak with the height to its weight (area of the peak).

$$A(\mathbf{k},\omega) = A(\mathbf{k},\omega)_0 + A(\mathbf{k},\omega)_1, \qquad (24)$$

$$A(\mathbf{k},\omega)_0 = \left[1 - \frac{1}{N}\sum_{\mathbf{q}}\frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})\coth\left(\frac{\omega_{\mathbf{q}}}{2T}\right)\right]\widetilde{A}(\mathbf{k},\omega),$$
$$(25)$$

$$A(\mathbf{k},\omega)_1 = \frac{1}{N}\sum_{\mathbf{q}}\frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})\{[n(\omega_{\mathbf{q}}) + 1 - f(\omega - \omega_{\mathbf{q}})]$$

$$\times \widetilde{A}(\mathbf{k}-\mathbf{q},\omega - \omega_{\mathbf{q}}) + [n(\omega_{\mathbf{q}}) + f(\omega + \omega_{\mathbf{q}})]$$

$$\times \widetilde{A}(\mathbf{k}-\mathbf{q},\omega + \omega_{\mathbf{q}})\}. \qquad (26)$$

Since $\widetilde{A}(\mathbf{k},\omega)$ is the spectral function for H', we have $\int d\omega\widetilde{A}(\mathbf{k},\omega)=1$. So,

$$\int d\omega A(\mathbf{k},\omega)_0 = \left[1 - \frac{1}{N}\sum_{\mathbf{q}}\frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})\coth\left(\frac{\omega_{\mathbf{q}}}{2T}\right)\right],$$
$$(27)$$

$$\int d\omega A(\mathbf{k},\omega)_1 = \frac{1}{N}\sum_{\mathbf{q}}\frac{g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}^2}\xi^2(\mathbf{k},\mathbf{k}-\mathbf{q})[n(\omega_{\mathbf{q}}) + 1 + n(\omega_{\mathbf{q}})],$$
$$(28)$$

and $\int d\omega A(\mathbf{k},\omega)=1$, which is the sum rule for the original spectral function. Because of the sum rule, it is easy to see

that, for increasing coupling, the spectral weight moves from $A(\mathbf{k},\omega)_0$ to $A(\mathbf{k},\omega)_1$.

These results should be compared with the ME theory in the second-order perturbation. The solution of Dyson's equation in ME theory is

$$G_{ME}(\mathbf{k},\omega) = \frac{1}{\omega - (\epsilon_{\mathbf{k}} - \mu) - \Sigma_{ME}(\mathbf{k},\omega)}. \qquad (29)$$

The self-energy in ME theory is

$$\Sigma_{ME}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}}g_{\mathbf{q}}^2\left\{\frac{n(\omega_{\mathbf{q}}) + 1 - f(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}{\omega - \omega_{\mathbf{q}} - (\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}\right.$$

$$\left. + \frac{n(\omega_{\mathbf{q}}) + f(\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}{\omega + \omega_{\mathbf{q}} - (\epsilon_{\mathbf{k}-\mathbf{q}} - \mu)}\right\}. \qquad (30)$$

The mass renormalization at the Fermi surface ($T=0$) is

$$\frac{m}{m_{ME}^*} = \left[1 + \frac{\partial}{\partial\epsilon_{\mathbf{k}}}\Sigma_{ME}(\mathbf{k},\omega)\right]\Bigg/$$

$$\left[1 - \frac{\partial}{\partial\omega}\Sigma_{ME}(\mathbf{k},\omega)\right]\Bigg|_{\omega=0,\epsilon_{\mathbf{k}}=\mu}$$

$$= \left[1 + \frac{1}{N}\sum_{\mathbf{k}'}\frac{g_{\mathbf{q}}^2}{(\omega_{\mathbf{q}} + |\epsilon_{\mathbf{k}'} - \mu|)^2}\right]^{-1}. \qquad (31)$$

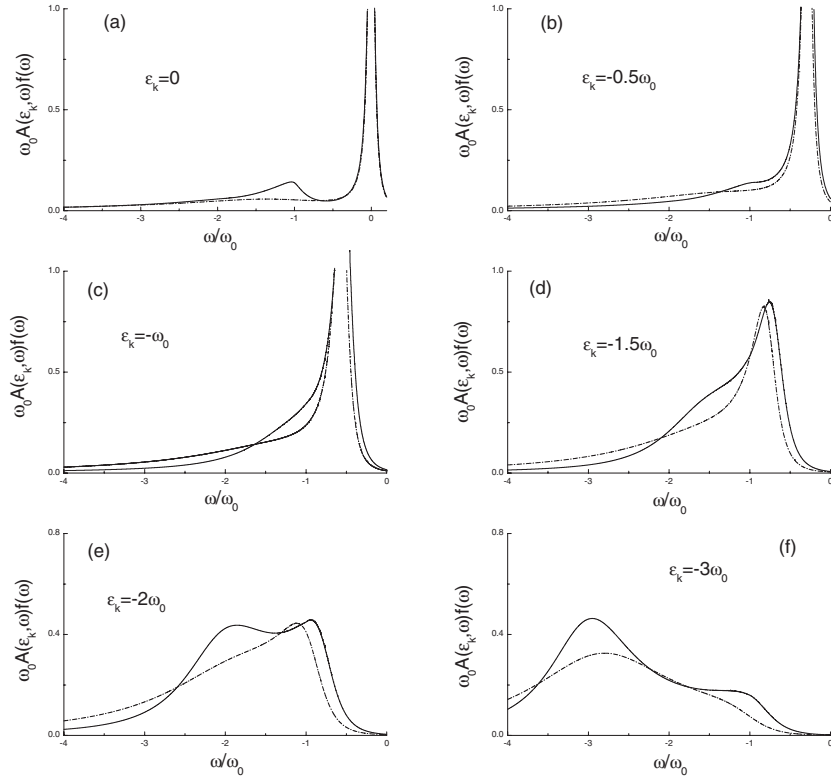Compared with Eq. (15), one can see that our renormalized

FIG. 2. The calculated MDSFs multiplied by the Fermi function (solid lines) with Einstein phonons are compared with those of the ME theory (dashed lines). $\epsilon_{\mathbf{k}}=$(a) 0, (b) $-0.5\omega_0$, (c) $-\omega_0$, (d) $-1.5\omega_0$, (e) $-2\omega_0$, (f) $-3\omega_0$. $\omega_0/2D=0.01$, temperature $T=0.25\omega_0$, $\lambda=0.378$ for our calculations and $\lambda_{ME}=0.6$ for those of the ME theory.

mass m^* [Eq. (15)] is the same as m^*_{ME} for weak electron-phonon coupling $g_{\mathbf{q}}/\omega_{\mathbf{q}} \ll 1$.

The MDSF of $G_{ME}(\mathbf{k},\omega)$ is

$A_{ME}(\mathbf{k},\omega)$

$= -\dfrac{1}{\pi} \operatorname{Im} G_{ME}(\mathbf{k},\omega)$

$= -\dfrac{1}{\pi} \dfrac{\operatorname{Im} \Sigma_{ME}(\mathbf{k},\omega)}{[\omega - (\epsilon_{\mathbf{k}} - \mu) - \operatorname{Re} \Sigma_{ME}(\mathbf{k},\omega)]^2 + [\operatorname{Im} \Sigma_{ME}(\mathbf{k},\omega)]^2}.$

(32)

IV. NUMERICAL CALCULATIONS AND DISCUSSIONS

For numerical calculations, one needs the information about the band structure $\epsilon_{\mathbf{k}}$, the phonon spectrum $\omega_{\mathbf{q}}$, and the coupling $g_{\mathbf{q}}$. We follow the procedure of Eliashberg theory and introduce the Eliashberg function $\alpha^2 F(\Omega)$,

$$\dfrac{N(\epsilon)}{N(\mu)} \alpha^2 F(\Omega) = \dfrac{1}{N} \sum_{\mathbf{q}} \delta(\epsilon - \epsilon_{\mathbf{k}-\mathbf{q}}) g_{\mathbf{q}}^2 \delta(\Omega - \omega_{\mathbf{q}}). \quad (33)$$

$N(\epsilon)$ is the density of state (DOS) of bare electrons and $N(\mu)$ that at the Fermi level. $\delta(\cdots)$ is the δ function. In numerical calculations, for simplicity but without loss of main physics, we assume a symmetrical band structure from the bottom $-D$ to the top D with $\mu=0$ and constant DOS $N(\epsilon) \approx N(\mu)$. Then,

Eqs. (11), (13), (15), (25), and (26) can be rewritten as

$$\rho(\epsilon_{\mathbf{k}}) = 1 - \int d\epsilon \int d\Omega \alpha^2 F(\Omega) \coth\left(\dfrac{\Omega}{2T}\right) \dfrac{1}{(\Omega + |\epsilon| + |\epsilon_{\mathbf{k}}|)^2},$$
(34)

$$\Sigma(\epsilon_{\mathbf{k}},\omega) = \int d\epsilon \int d\Omega \dfrac{\alpha^2 F(\Omega)}{(\Omega + |\epsilon| + |\epsilon_{\mathbf{k}}|)^2}$$

$$\times \left[(|\epsilon| + |\epsilon_{\mathbf{k}}| - \epsilon + \epsilon_{\mathbf{k}})^2 \dfrac{n(\Omega) + 1 - f(\epsilon)}{\omega - \Omega - \epsilon} \right.$$

$$\left. + (|\epsilon| + |\epsilon_{\mathbf{k}}| + \epsilon - \epsilon_{\mathbf{k}})^2 \dfrac{n(\Omega) + f(\epsilon)}{\omega + \Omega - \epsilon} \right], \quad (35)$$

$$\dfrac{m}{m^*} = \rho(\epsilon_{\mathbf{k}} = 0) = 1 - \int d\epsilon \int d\Omega \alpha^2 F(\Omega) \dfrac{1}{(\Omega + |\epsilon|)^2},$$
(36)

$$A(\epsilon_{\mathbf{k}},\omega)_0 = \rho(\epsilon_{\mathbf{k}}) \widetilde{A}(\epsilon_{\mathbf{k}},\omega), \quad (37)$$

$$A(\epsilon_{\mathbf{k}},\omega)_1 = \int d\epsilon \int d\Omega \dfrac{\alpha^2 F(\Omega)}{(\Omega + |\epsilon| + |\epsilon_{\mathbf{k}}|)^2}$$

$$\times \{[n(\Omega) + 1 - f(\omega - \Omega)] \widetilde{A}(\epsilon, \omega - \Omega)$$

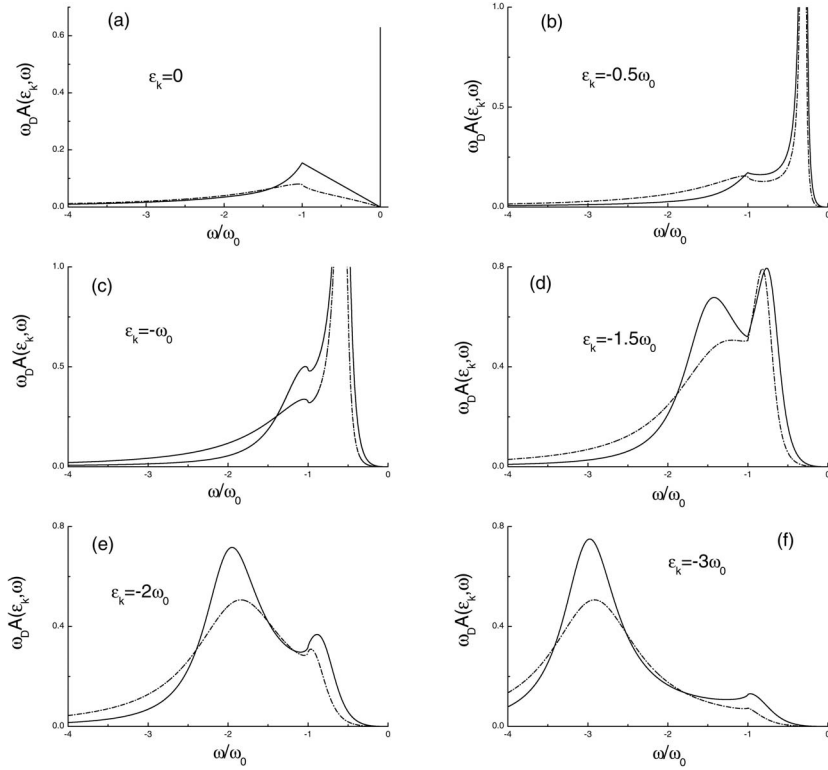$$+ [n(\Omega) + f(\omega + \Omega)] \widetilde{A}(\epsilon, \omega + \Omega)\}, \quad (38)$$

FIG. 3. (Color online) The calculated MDSFs (solid lines) with Debye phonons are compared with those of the ME theory (dashed lines). $\epsilon_{\mathbf{k}}=$(a) 0, (b) $-0.5\omega_D$, (c) $-\omega_D$, (d) $-1.5\omega_D$, (e) $-2\omega_D$, (f) $-3\omega_D$. Temperature $T=0$, $\omega_D/2D=0.01$, $\lambda=0.377$ for our calculations and $\lambda_{ME}=0.6$ for those of the ME theory. The vertical lines in (a) are to indicate the position of the δ-function peak with the height to its weight (area of the peak). Here, the height is 0.628, the same for our calculation and that of ME theory because of the different coupling λ and λ_{ME}.

where the integration over ϵ is from the bottom of the band, $-D$ to the top D. For ME theory in the second-order perturbation,

$$\Sigma_{ME}(\omega) = \int d\epsilon \int d\Omega \alpha^2 F(\Omega) \left[\frac{n(\Omega)+1-f(\epsilon)}{\omega-\Omega-\epsilon} \right.$$

$$\left. + \frac{n(\Omega)+f(\epsilon)}{\omega+\Omega-\epsilon} \right], \tag{39}$$

$$\frac{m}{m^*_{ME}} = \left[1 + \int d\epsilon \int d\Omega \alpha^2 F(\Omega) \frac{1}{(\Omega+|\epsilon|)^2} \right]^{-1}, \tag{40}$$

$A_{ME}(\mathbf{k},\omega)$

$$= -\frac{1}{\pi} \frac{\operatorname{Im} \Sigma_{ME}(\omega)}{[\omega-(\epsilon_{\mathbf{k}}-\mu)-\operatorname{Re}\Sigma_{ME}(\omega)]^2 + [\operatorname{Im}\Sigma_{ME}(\omega)]^2}. \tag{41}$$

In ME theory, the second-order self-energy $\Sigma_{ME}(\omega)$ does not depend on the momentum or the bare QP energy $\epsilon_{\mathbf{k}}$ and the spectral function $A_{ME}(\mathbf{k},\omega)$ depends on the bare QP energy $\epsilon_{\mathbf{k}}$ via the term $[\omega-(\epsilon_{\mathbf{k}}-\mu)-\operatorname{Re}\Sigma_{ME}(\omega)]$ in denominator. In our theory, however, $\Sigma(\epsilon_{\mathbf{k}},\omega)$ is $\epsilon_{\mathbf{k}}$ dependent and $\Sigma(\epsilon_{\mathbf{k}},\omega)=0$ for $\epsilon_{\mathbf{k}}=\mu$ and $T=0$. Besides, both $A(\epsilon_{\mathbf{k}},\omega)_0$ and $A(\epsilon_{\mathbf{k}},\omega)_1$ are functions of the bare QP energy $\epsilon_{\mathbf{k}}$.

The input for numerical calculations is the Eliashberg function $\alpha^2 F(\Omega)$. We consider two typical ones: (1) Einstein

phonons with $\alpha^2 F(\Omega)=\frac{1}{2}\lambda\omega_0\delta(\Omega-\omega_0)$ and (2) Debye phonons in three-dimensions with $\alpha^2 F(\Omega)=\lambda(\Omega/\omega_D)^2$ ($0<\Omega<\omega_D$). In these spectra, $\lambda=\int d\Omega \alpha^2 F(\Omega)/\Omega$ is the electron-phonon coupling. Then, we can calculate the mass renormalization by Eqs. (36) and (40). For Einstein phonons,

$$m/m^* = 1 - \frac{\lambda D}{\omega_0+D}, \tag{42}$$

$$m/m^*_{ME} = \left(1 + \frac{\lambda_{ME}D}{\omega_0+D} \right)^{-1}. \tag{43}$$

For Debye phonons,

$$m/m^* = 1 - \frac{2\lambda D}{\omega_D} \left(1 - \frac{D}{\omega_D} \ln\frac{\omega_D+D}{D} \right), \tag{44}$$

$$m/m^*_{ME} = \left[1 + \frac{2\lambda_{ME}D}{\omega_D} \left(1 - \frac{D}{\omega_D} \ln\frac{\omega_D+D}{D} \right) \right]^{-1}. \tag{45}$$

For adiabatic limit $\omega_0 \to 0$ or $\omega_D \to 0$, we can get $m/m^*=1-\lambda$ and $m/m^*_{ME}=1/(1+\lambda_{ME})$. Here, we use different notations for coupling constant, λ and λ_{ME}, of our theory and ME theory, respectively, because when we compare our calculations with those of ME theory, we shall make $m/m^*=m/m^*_{ME}$ with different input parameters λ or λ_{ME}.

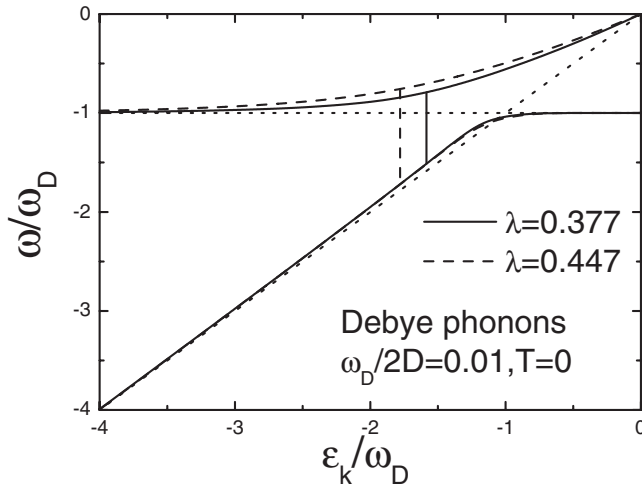Figure 1 shows our calculated MDSF with Einstein phonons for temperature $T=0$, $\omega_0/2D=0.01$, and coupling

FIG. 4. The peak position ω_{peak} versus $\epsilon_{\mathbf{k}}$ relations for λ =0.377 (solid lines) and λ=0.447 (dashed line). Debye phonons with temperature T=0, $\omega_D/2D$=0.01. The vertical line indicates the value of $\epsilon_{\mathbf{k}}$ at which the peak height for upper branch and that for lower branch are equal with each other.

FIG. 5. The proposed dispersion relation $\omega \sim \epsilon_{\mathbf{k}}$ derived from Fig. 4.

λ=0.378. For comparison, the dashed lines are results of ME theory with the same parameters but λ_{ME}=0.6. Because of the Einstein phonons, at T=0, the peak within the range $|\omega| < \omega_0$ is a δ function and we use a vertical line to indicate the position of this peak with its height to the weight of the peak (area of the peak). When $\epsilon_{\mathbf{k}}$=0 [Fig. 1(a)], $A(\epsilon_{\mathbf{k}} =0,\omega)_0$ is a δ-function peak at ω=0 (with height 0.63) but the peak at around $\omega=-\omega_0$ comes from $A(\epsilon_{\mathbf{k}}=0,\omega)_1$. The δ-function peak of $A_{ME}(\epsilon_{\mathbf{k}}=0,\omega)$ is the same as our $A(\epsilon_{\mathbf{k}} =0,\omega)_0$, but it has a much weaker peak at around $\omega=-\omega_0$ than that of $A(\epsilon_{\mathbf{k}}=0,\omega)_1$. When $\epsilon_{\mathbf{k}}<0$, the contributions from $A(\epsilon_{\mathbf{k}},\omega)_0$ and $A(\epsilon_{\mathbf{k}},\omega)_1$ are mixed with each other and the total ARPES is composed of two parts: one is a δ-function peak within the range $|\omega| < \omega_0$ which is of a decreasing weight with increasing $|\epsilon_{\mathbf{k}}|$, and the other is a finite peak at around $\omega=-\omega_0$ for $\epsilon_{\mathbf{k}} \geqslant -\omega_0$ but for $\epsilon_{\mathbf{k}} < -\omega_0$ the position of it goes down with expanding width (weight of the peak). The spectra of $A_{ME}(\epsilon_{\mathbf{k}},\omega)$ is also composed of two parts: a δ-function peak within the range $|\omega| < \omega_0$ and a finite peak with lower height but wider width compared with our calculation.

For finite temperature, the δ-function peak within the range $|\omega| < \omega_0$ in Fig. 1 becomes a Lorentzian peak with finite height and width. Figure 2 shows our calculated MDSF multiplied by the Fermi function, $A(\epsilon_{\mathbf{k}},\omega)f(\omega)$, with Einstein phonons for temperature T=0.25ω_0, $\omega_0/2D$=0.01, and coupling λ=0.378. For comparison, the dashed lines are results of ME theory with the same parameters but λ_{ME}=0.6. For $\epsilon_{\mathbf{k}}$=0 [Fig. 2(a)], the spectrum has a strong peak at ω_{peak} =0 with height $A(\epsilon_{\mathbf{k}}=0,\omega_{peak})f(0)$=2.26 together with a small peak at around $\omega=-\omega_0$. $A_{ME}(\epsilon_{\mathbf{k}}=0,\omega)f(\omega)$ has a similar peak at ω_{peak}=0 with height 2.31 but without the second peak at around $\omega=-\omega_0$. In Figs. 2(b) and 2(c), the spectrum has a main peak within the range $|\omega| < \omega_0$ with a small shoulder at around $\omega=-\omega_0$. In Fig. 2(d) ($\epsilon_{\mathbf{k}}=-1.5\omega_0$), the main peak at $\omega_{peak} > -\omega_0$ becomes weaker [compared with that in
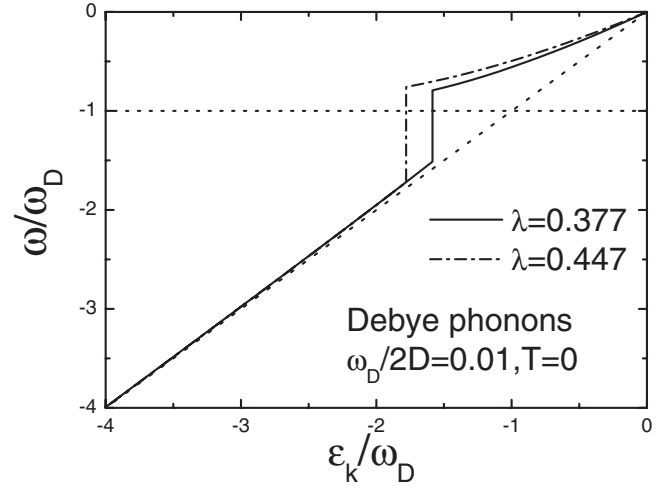
(a), (b), and (c)], but there is a larger shoulder at around ω =$-1.5\omega_0$. Figure 2(e) ($\epsilon_{\mathbf{k}}=-2\omega_0$) shows clearly a two-headed structure of nearly the same height, with one peak at around $\omega=-\omega_0$ and the other at around $\omega=-2\omega_0$. The main peak of Fig. 2(f) ($\epsilon_{\mathbf{k}}=-3\omega_0$) is at around $\omega=-3\omega_0$ and there is a larger shoulder at around $\omega=-\omega_0$. For comparison, the spectra of ME theory do not show the two-headed structure or the main peak plus shoulder structure in the finite temperature case.

The Einstein phonons may not be good to model the practical e-ph interaction because the phonon may have finite dispersion and lifetime. We use Debye phonons to model the Eliashberg function $\alpha^2F(\Omega)$ and show in Fig. 3 our calculated MDSF for temperature T=0, $\omega_D/2D$=0.01, and coupling λ=0.377. For comparison, the dashed lines are results of ME theory with the same parameters but λ_{ME}=0.6. Figure 3(a) is the MDSF for $\epsilon_{\mathbf{k}}$=0, where the δ-function peak at ω=0 (with height 0.628) comes from $A(\epsilon_{\mathbf{k}}=0,\omega)_0$ but the peak at around $\omega=-\omega_D$ comes from $A(\epsilon_{\mathbf{k}}=0,\omega)_1$. The δ-function peak of $A_{ME}(\epsilon_{\mathbf{k}}=0,\omega)$ is the same as our $A(\epsilon_{\mathbf{k}} =0,\omega)_0$, but it has a much weaker peak at around $\omega=-\omega_D$ than that of $A(\epsilon_{\mathbf{k}}=0,\omega)_1$. When $\epsilon_{\mathbf{k}}<0$, the contributions from $A(\epsilon_{\mathbf{k}},\omega)_0$ and $A(\epsilon_{\mathbf{k}},\omega)_1$ are mixed with each other; however, one can see clearly that there is a two-headed structure with one peak nearly fixed at around $\omega=-\omega_D$ but the position of another peak going down with decreasing $\epsilon_{\mathbf{k}}$. For comparison, the two-headed structure in the spectra of ME theory is not so evident, especially for the case of $\epsilon_{\mathbf{k}}<-\omega_D$ where the second weaker peak nearly disappears.

The relative weight of the two peaks in Fig. 3 changes continuously with changing $\epsilon_{\mathbf{k}}$ and it may be explained by a "hybridization" between electrons and phonons. Figure 4 shows the peak position ω_{peak} versus $\epsilon_{\mathbf{k}}$ relations for λ =0.377 (solid lines) and λ=0.447 (dashed line) for Debye phonons with temperature T=0 and $\omega_D/2D$=0.01. Here, we have two branches for the $\omega_{peak} \sim \epsilon_{\mathbf{k}}$ relation, the upper branch for $\omega \geqslant -\omega_D$ and the lower branch for $\omega \leqslant -\omega_D$. The upper branch is electronlike with larger weight for $\epsilon_{\mathbf{k}} >$ $-1.585\omega_D$ (λ=0.377) and becomes phononlike for $\epsilon_{\mathbf{k}} <$

$-1.585\omega_D$ with smaller weight. The lower branch is phonon-like with smaller weight for $\epsilon_\mathbf{k} > -1.585\omega_D$ ($\lambda=0.377$) and becomes electronlike for $\epsilon_\mathbf{k} < -1.585\omega_D$ with larger weight. The vertical line indicates the value of $\epsilon_\mathbf{k}=-1.585\omega_D$ at which the peak weight for the upper branch and that for the lower branch are equal with each other. The dashed line is for a stronger coupling $\lambda=0.447$ with the similar hybridization behavior but the value of $\epsilon_\mathbf{k}=-1.78\omega_D$ at which the upper and lower branches are of the same weight.

If we delete the phononlike part of the upper and lower branches in Fig. 4, the left electronlike part of the curves is shown in Fig. 5. The curve may be treated as our proposed dispersion relation $\omega \sim \epsilon_\mathbf{k}$, which is quite similar to the kink structure of the dispersion relation determined by ARPES observation.[4,7,9]

V. SUMMARY AND DISCUSSIONS

We have developed an analytical approach, starting from the Frohlich Hamiltonian and by means of the unitary transformation with the perturbation treatment, to deal with the momentum-dependent spectral function of electron-phonon coupling system. The approach takes care of the fact that only those electrons near the Fermi surface within a layer of width ω_{ph} (phonon frequency: $\omega_{ph}=\omega_D$ for Debye phonons and $\omega_{ph}=\omega_0$ for Einstein phonons) are scattered by phonons strongly. Our results show that the MDSF is mainly composed of two parts: the zero-phonon part and the one-phonon one. When the bare electron energy $\epsilon_\mathbf{k}$ is close to the Fermi energy μ, $\epsilon_\mathbf{k}-\mu \simeq -\omega_{ph}$, the one-phonon part is quite significant and the MDSF shows a two-headed peak. However, for $\epsilon_\mathbf{k}-\mu \ll -\omega_{ph}$, the one-phonon part disappears gradually and the MDSF shows a single broad peak. These results qualitatively agree with recent experiments of ARPES on the Be(0001) surface and Bi2212.

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