Self-consistent theory of phonon renormalization and electron-phonon coupling near a two-dimensional Kohn singularity

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We show that the usual expression for evaluating electron-phonon coupling and the phonon linewidth in two-dimensional metals with a cylindrical Fermi surface cannot be applied near the wave vector corresponding to the Kohn singularity. Instead, the Dyson equation for phonons has to be solved self-consistently. If a self-consistent procedure is properly followed, there is no divergency in either the coupling constant or the phonon linewidth near the offending wave vectors, in contrast to the standard expression.

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INTRODUCTION

First principles calculations of the phonon spectra and electron-phonon coupling in MgB_2 (see Ref. 1 for a review) have determined that the interaction mainly responsible for superconductivity in this material is coupling of small-q, high-energy optical phonons of a particular symmetry with approximately parabolic nearly two-dimensional hole bands forming practically perfect circular cylinders occupying only a small fraction of the Brillouin zone. It was realized early enough[2] that the case of an *ideal* two-dimensional (2D) cylinder leads to a divergency in the calculated phonon linewidth at the 2D Kohn singularity, $q=2k_F$, which presents serious difficulties in calculating the electron-phonon coupling function. One option that was exploited was to use an analytical integration for the wave vectors comparable with or smaller than $2k_F$,[2,3] and a numerical one for the larger vectors.

It was also pointed out[1,4] that this singularity gets stronger when the Fermi surface gets smaller, while the integrated electron-phonon coupling (for 2D parabolic bands) does not change. While a perfectly cylindrical Fermi surface is an idealized construction, deviations may be quite small, it seems, on the first glance, unphysical that all phonons with $|\mathbf{q}|=2k_F$ have infinite linewidth. Note that the problem is not specific for MgB_2: it occurs in doped graphenes such as CaC_6 and, YbC_6,[5] and, in fact, in any 2D material sporting Kohn singularities. In particular, the hypothetical hexagonal LiB, a subject of substantial recent interest, has σ bands that are even more 2D that those in MgB_2 (Ref. 6) and the described problem is even more pronounced.

This intuition is correct. In this paper, we show that close to a Kohn anomaly, standard formulas for calculating electron-phonon interaction (EPI) become incorrect and new, self-consistent expressions replace them. These expressions have no singularities, and exhibit a much more natural, reasonably smooth, $\mathbf{q}$ dependence of the phonon self-energy.

To start with, we shall remind the readers of the standard formalism. We first define the retarded phonon Green function

$$D^{\alpha\beta}(\mathbf{q},t) \equiv -i\theta(t)\langle[u^{\alpha}_{\mathbf{q}}(t)u^{\beta}_{-\mathbf{q}}(0)]\rangle,$$

where $[\ldots]$ is a commutator and $\langle\ldots\rangle$ denotes statistical averaging. The displacement operator $u^{\alpha}_{\mathbf{q}}$ in the α direction can be expressed via the phonon eigenvectors $e_{\mathbf{q}\nu}$ and frequencies squared $\omega^2_{\mathbf{q}\nu}$:

$$\mathbf{u}_{\mathbf{q}} = \sum_{\nu}\left(\frac{1}{2M\omega_{\mathbf{q}\nu}}\right)\mathbf{e}_{\mathbf{q}\nu}(a_{\mathbf{q}\nu}+a^{\dagger}_{-\mathbf{q}\nu}). \tag{1}$$

For simplicity, a primitive lattice with a single kind of ions with a single mass M will be considered below. Also, atomic (hartree) units will be used throughout the paper. In this case, the "bare" phonon Green function has a form

$$D_0(\mathbf{q},\omega) = \frac{1}{2M\omega_{\mathbf{q}0}}\left[\frac{1}{\omega-\omega_{\mathbf{q}0}+i\delta}-\frac{1}{\omega+\omega_{\mathbf{q}0}+i\delta}\right], \tag{2}$$

where $\omega_{\mathbf{q}0}$ is the bare phonon frequency, before accounting for electron-phonon coupling (screening by electrons). Without losing generality, it can be assumed to be $\mathbf{q}$ independent, $\omega_{\mathbf{q}0}=\omega_0$. Correspondingly, the full Green function is

$$D(\mathbf{q},\omega) = \frac{1}{2M\omega_{\mathbf{q}}}\left[\frac{1}{\omega-\omega_{\mathbf{q}}+i\Gamma_{\mathbf{q}}}-\frac{1}{\omega+\omega_{\mathbf{q}}+i\Gamma_{\mathbf{q}}}\right], \tag{3}$$

where $\omega_{\mathbf{q}}$ is the renormalized (observable) frequency, and $\Gamma_{\mathbf{q}}$ is damping (phonon linewidth) due to EPI.[7]

The Dyson equation reads

$$D^{-1}(\mathbf{q},\omega) = D_0^{-1}(\mathbf{q},\omega) - \Pi(\mathbf{q},\omega), \tag{4}$$

where the polarization operator in the lowest approximation (as usual, the Migdal theorem[8] allows neglecting the vertex corrections) along the real frequency axis at $T=0$ has a form (a is the lattice constant in the plane)

$$\Pi(\mathbf{q},\omega) = -2i\int |g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}}|^2 G_0\left(\mathbf{k}+\frac{\mathbf{q}}{2},\varepsilon+\frac{\omega}{2}\right) \times G_0\left(\mathbf{k}-\frac{\mathbf{q}}{2},\varepsilon-\frac{\omega}{2}\right)\frac{a^2d^2k}{(2\pi)^2}\frac{d\varepsilon}{2\pi}. \tag{5}$$

Here, $g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}}$ is the bare electron-ion scattering matrix element (the commonly used EPI matrix element differs in that the potential gradient is replaced by the derivatives with respect to the normal phonon coordinates)

$$g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}} = \frac{1}{a^2}\int_{a^2} \psi^*_{\mathbf{k}+\mathbf{q}}(\mathbf{r})\,\nabla\, V(\mathbf{r})\,\psi_{\mathbf{k}}(\mathbf{r})d^2r, \tag{6}$$

where

$$G_0(\mathbf{k},\varepsilon) = \frac{1}{\varepsilon - \varepsilon_0(\mathbf{k}) + i\delta\,\mathrm{sign}(k-k_F)} \tag{7}$$

is the bare electron Green function, and $\varepsilon_0(\mathbf{k})=(k_x^2+k_y^2-k_F^2)/2m$. The *renormalized* phonon frequency and the phonon *linewidth* $\Gamma_\mathbf{q}$ are determined by the *pole* of the phonon Green function $D(\mathbf{q},\omega)$ or

$$D^{-1}(\mathbf{q},\omega_\mathbf{q}+i\Gamma_\mathbf{q}) \equiv D_0^{-1}(\mathbf{q},\omega_\mathbf{q}+i\Gamma_\mathbf{q}) - \Pi(\mathbf{q},\omega_\mathbf{q}+i\Gamma_\mathbf{q}) = 0$$

[note that in the experiment, the phonon linewidth is usually defined as the half-width of the peak in $\mathrm{Im}\,D(\mathbf{q},\omega)$, which differs from our definition by terms of the order $(\Gamma/\omega)^4$]. This leads to

$$\omega_\mathbf{q}^2 = \omega_0^2 + \frac{1}{M}\,\mathrm{Re}\,\Pi(\mathbf{q},\omega_\mathbf{q}+i\Gamma_\mathbf{q}) + \Gamma_\mathbf{q}^2 \tag{8}$$

and

$$\Gamma_\mathbf{q} = -\frac{1}{2M\omega_\mathbf{q}}\,\mathrm{Im}\,\Pi(\mathbf{q},\omega_\mathbf{q}+i\Gamma_\mathbf{q}). \tag{9}$$

The next standard step, following Ref. 9, is to expand the polarization operator

$$\Pi(\mathbf{q},\omega+i\delta) = -2\sum_\mathbf{k} |g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}}|^2 \frac{n_\mathbf{k}-n_{\mathbf{k}+\mathbf{q}}}{\varepsilon_0(\mathbf{k}+\mathbf{q})-\varepsilon_0(\mathbf{k})-\omega-i\delta} \tag{10}$$

to first order in frequency just above the real axis of the complex frequency ω. In this case,

$$\omega^2_{app\mathbf{q}} = \frac{1}{M}\Pi(\mathbf{q},0)\left[1+O\left(\frac{\omega_0^2}{\varepsilon_F^2}\right)\right] \tag{11}$$

and

$$\Gamma^{app}_\mathbf{q} = -\frac{1}{2M}\left.\frac{d\,\mathrm{Im}\,\Pi(\mathbf{q},\omega)}{d\omega}\right|_{\omega=0} \equiv \frac{\pi}{M}\sum_\mathbf{k} |g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}}|^2 \delta[\varepsilon_0(\mathbf{k}+\mathbf{q})]\delta[\varepsilon_0(\mathbf{k})], \tag{12}$$

where the factor $(n_\mathbf{k}-n_{\mathbf{k}+\mathbf{q}})\delta[\varepsilon_0(\mathbf{k}+\mathbf{q})-\varepsilon_0(\mathbf{k})-\omega]$ has been changed to $-\omega\delta[\varepsilon_0(\mathbf{k}+\mathbf{q})]\delta[\varepsilon_0(\mathbf{k})]$. According to Ref. 10, "Except for extremely pathological energy bands, it is an excellent approximation." Unfortunately, MgB_2 and some other recently discovered superconductors are examples where the energy bands are, in some aspects, pathological. Formally, expression (12) for a 2D system is divergent near a Kohn anomaly $q\to 2k_F$, and we have $\Gamma_\mathbf{q} \geqslant \omega_\mathbf{q}$, i.e., phonons are not well defined quasiparticles. To describe electron-phonon interaction in these systems, we have to calculate the polarization operator $\Pi(\mathbf{q},Z)$ for a complex frequency Z and solve Eqs. (8) and (9).

I. COMPLEX POLARIZATION OPERATOR

Let us consider a model with a cylindrical Fermi surface of radius k_F, whose electrons interact with an optical phonon with a bare frequency ω_0, and a momentum-independent matrix element g^0 (we also neglect possible warping of the Fermi-surface cylinder, cf. Ref. 11). In this case, the imaginary part of Eq. (10) reads

$$\mathrm{Im}\,\Pi(\mathbf{q},\omega+i\delta) = -2\pi|g^0|^2\sum_\mathbf{k}\{\theta[\varepsilon_0(\mathbf{k}+\mathbf{q})]-\theta[\varepsilon_0(\mathbf{k})]\} \times\delta[\varepsilon_0(\mathbf{k}+\mathbf{q})-\varepsilon_0(\mathbf{k})-\omega]$$

or

$$\mathrm{Im}\,\Pi(\mathbf{q},\omega) = -\frac{m|g^0|^2}{2\pi a^2 q}\int_{\max\{k_F,m\omega/q+q/2\}}^{\sqrt{k_F^2+2m\omega}} \times\mathrm{Re}\,\frac{dk}{\sqrt{1-(q/2k+m\omega/kq)^2}} = -\frac{m|g^0|^2}{\pi a^2 Q}[\mathrm{Re}\,\sqrt{1-(Q-\Omega)^2} - \mathrm{Re}\,\sqrt{1-(Q+\Omega)^2}], \tag{13}$$

where $Q=q/2k_F$ and $\Omega=\omega/qv_F$ (v_F is the Fermi velocity).

To find the polarization operator for a complex frequency $Z=\omega+i\gamma$, we use the Hilbert transformation

$$\Pi(\mathbf{q},Z) = \frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{dE}{E-Z}\,\mathrm{Im}\,\Pi(\mathbf{q},E).$$

The result is

$$\Pi(\mathbf{q},Z) = -\frac{m|g^0|^2}{\pi a^2 Q}\int_C dxdy\frac{x}{-(Z/4\varepsilon_F)^2/Q^2+x^2}, \tag{14}$$

where $\varepsilon_F=k_F^2/2m$, $x=k_x/k_F$, $y=k_y/k_F$, and $N(0)=m/2\pi a^2$ is the density of states at the Fermi level, per spin. The integration is performed over the range $(x-Q)^2+y^2<1$. The substitution $x-Q=r\cos\varphi$ and $y=r\sin\varphi$ leads to

$$\int_C dxdy \Rightarrow \int_0^1 rdr\int_0^{2\pi} d\varphi,$$

$$\Pi(\mathbf{q},Z) = -\frac{m|g^0|^2}{2\pi a^2}\left[2-\left(1-\frac{Z}{4\varepsilon_F Q^2}\right)\sqrt{1-\left(Q-\frac{Z}{4\varepsilon_F Q}\right)^{-2}} - \{Z\to -Z\}\right]. \tag{15}$$

The branches of the square roots are chosen so as to get the correct behavior $\Pi\propto q^2V_F^2/\omega^2$ at large frequencies ω ($\omega=\mathrm{Re}\,Z$). For a 2D system for $\Pi(\mathbf{q},\omega)$ on the real frequency axis, one can write:[12–15]

$$\mathrm{Re}\,\Pi(\mathbf{q},\omega+i\delta)=-\frac{m|g^0|^2}{2\pi a^2 Q}[2Q-(Q-\Omega)\mathrm{Re}\,\sqrt{1-(Q-\Omega)^{-2}}-(Q+\Omega)\mathrm{Re}\,\sqrt{1-(Q+\Omega)^{-2}}],$$

$$\mathrm{Im}\,\Pi(\mathbf{q},\omega+i\delta)=-\frac{m|g^0|^2}{2\pi a^2 Q}[\mathrm{Re}\,\sqrt{1-(Q-\Omega)^2}-\mathrm{Re}\,\sqrt{1-(Q+\Omega)^2}]. \quad (16)$$

A three-dimensional (3D) plot of the functions (16) can be found, for instance, in Ref. 16. Note that while the expression for real frequencies [Eq. (16)] has been published multiple times, we have not found in the literature the general expression for an arbitrary complex frequency argument [Eq. (15)].

First, we see that the imaginary part is finite for all values of the wave vector q and vanishes inside the Landau-damping cone $q<\omega/v_F$ [more exactly, at $Q<(\omega/4\varepsilon_F)-(\omega/4\varepsilon_F)^2$]. It has two maxima: one is rather small, $\mathrm{Im}\,\Pi(\omega)\simeq -m|g^0|^2\sqrt{\omega/4\varepsilon_F}/\pi a^2$, at $Q\simeq 1-(\omega/4\varepsilon_F)$, while the other has an antiadiabatical behavior, $\mathrm{Im}\,\Pi(\omega)\simeq -m|g^0|^2\sqrt{2\varepsilon_F/\omega}/\pi a^2$, and occurs at a very low frequency $Q\simeq(\omega/4\varepsilon_F)+(\omega/4\varepsilon_F)^2$.

However, if we expand the polarization operator at small frequencies, we recover a standard result (see, e.g., Refs. 2 and 4)

$$\Pi_{app}(\mathbf{q},\omega+i\delta)\simeq -\frac{m|g^0|^2}{\pi a^2}\left[1+\frac{i\omega/4\varepsilon_F}{Q\sqrt{1-Q^2}}\theta(1-Q)-\sqrt{1-\frac{1}{Q^2}}\theta(Q-1)\right], \quad (17)$$

where the imaginary part diverges at $q\to 0$ and $q\to 2k_F$. The real part of Eq. (16) practically coincides with the real part of Eq. (17) except inside the Landau-damping region.

At $\omega\to 0$ and finite $\mathbf{q}$, we get

$$\mathrm{Im}\,\Pi_{app}(\mathbf{q},\omega)\simeq -\frac{\omega}{4\varepsilon_F}\frac{m|g^0|^2}{\pi a^2}\frac{\theta(1-Q)}{Q\sqrt{1-Q^2}}. \quad (18)$$

In the opposite limit, $\mathrm{Im}\,\Pi(\mathbf{q},\omega)\equiv 0$ for $q\leqslant m\omega/\sqrt{k_F^2-m\omega}$. For the real part, one can set $\omega=0$ in Eq. (17):

$$\mathrm{Re}\,\Pi(\mathbf{q},0)=-2|g^0|^2\sum_{\mathbf{k}}\theta(|\mathbf{k}|-k_F)\theta(k_F-|\mathbf{k}+\mathbf{q}|)\times\frac{1}{\varepsilon_0(\mathbf{k}+\mathbf{q})-\varepsilon_0(\mathbf{k})}.$$

In this case,

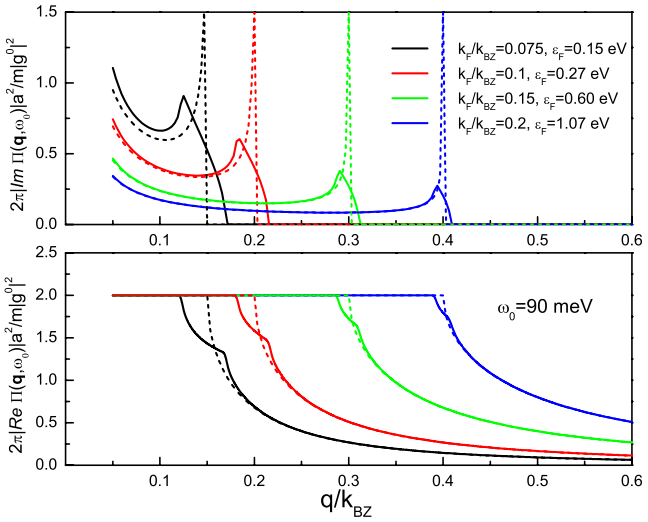

FIG. 1. (Color online) The imaginary and real parts of the normalized polarization operator $2\pi|\Pi(\mathbf{q},\omega=\omega_0)|a^2/m|g^0|^2$ as a function of the reduced wave vector q/k_{BZ}, for different fillings k_F/k_{BZ}. Solid lines represent the exact results, and the dashed lines the approximate solution [Eq. (17)]. The four different sets correspond, from left to right, to four increasing values of k_F/k_{BZ}.

$$\mathrm{Re}\,\Pi(\mathbf{q},0)\simeq -\frac{m|g^0|^2}{\pi a^2}\left[1-\theta(q-2k_F)\sqrt{1-\left(\frac{2k_F}{q}\right)^2}\right]=-\frac{m|g^0|^2}{\pi a^2}[1-\theta(Q-1)\sqrt{1-Q^{-2}}]. \quad (19)$$

In the opposite limit,

$$\mathrm{Re}\,\Pi(\mathbf{q}\to 0,\omega)\approx -\frac{m|g^0|^2}{2\pi a^2}\left(\frac{qk_F}{m\omega}\right)^2.$$

The momentum dependence of the absolute values of the imaginary (the upper panel) and real parts (the lower panel) of Eqs. (16) (solid lines) and (17) (short-dash lines) at $\omega=\omega_0=90$ meV as the functions of the reduced wave vector q/k_{BZ} [$k_{BZ}=\pi/a$ is the Brillouin zone (BZ) vector, or the radius of the Wigner-Seitz cylinder] is shown in Fig. 1. Fermi vectors $k_F/k_{BZ}=0.075, k_F/k_{BZ}=0.1, k_F/k_{BZ}=0.15$, and $k_F/k_{BZ}=0.2$ correspond to $\varepsilon_F=0.15$, 0.27, 0.60, and 1.07 eV, respectively.

Along the imaginary (Matsubara) axis, the polarization operator has the following form:

$$\Pi_M(\mathbf{q},i\omega_n)=-\frac{m|g^0|^2}{\pi a^2}\left[1+\frac{\sqrt{Q^4-Q^2-(\omega_n/4Q\varepsilon_F)+\sqrt{[Q^4-Q^2-(\omega_n/4Q\varepsilon_F)]^2+(Q\omega_n/4\varepsilon_F)^2}}}{\sqrt{2}Q^2}\right], \quad (20)$$

where $\omega_n=2\pi nT$. T is temperature and $n=0,\pm1,\pm2,\ldots,\pm\infty$. $\Pi_M(\mathbf{q},i\omega_n\to0)$ coincides with Eq. (19).

II. PHONON RENORMALIZATION IN TWO-DIMENSIONAL SYSTEMS

First, let us consider the *approximate* polarization operator from Eq. (17). Then

$$\omega_{\mathbf{q}}^{app}=\omega_0\sqrt{1-2\zeta[1-\theta(q-2k_F)\sqrt{1-(2k_F/q)^2}]} \quad (21)$$

and, according to Eqs. (12) and (17),

$$\Gamma_{\mathbf{q}}^{app}=\frac{m|g^0|^2}{2\pi a^2MV_Fq}\frac{\theta(2k_F-q)}{\sqrt{1-(q/2k_F)^2}}=\frac{\zeta\omega_0^2}{4\varepsilon_F}\frac{\theta(1-Q)}{Q\sqrt{1-Q^2}}, \quad (22)$$

where we have introduced, following Ref. 17, an *auxiliary* coupling constant $\zeta=N(0)|g^0|^2/M\omega_0^2$ (some authors use another dimensionless constant $\lambda_0=2\zeta$). $\Omega_{\mathbf{q}}=\omega_{\mathbf{q}}^{app}+i\Gamma_{\mathbf{q}}^{app}$ gives the renormalized frequency and the damping [see Eqs. (11) and (12)]. For $q\leqslant2k_F$,

$$\frac{\Gamma_{\mathbf{q}}^{app}}{\omega_{\mathbf{q}}^{app}}=\frac{\varsigma\omega_0}{4\varepsilon_F\sqrt{1-2\zeta}}\frac{1}{Q\sqrt{1-Q^2}}. \quad (23)$$

This expression diverges in the limits $Q\to0$ and $Q\to1$.

Turning now to the exact Eq. (15), we observe that in the lowest order in ω/ε_F

$$\Pi(q\to2k_F,\omega)=-\frac{m|g^0|^2}{\pi a^2}\left[1-(1+i)\sqrt{\frac{\omega}{8\varepsilon_F}}\right].$$

This leads to

$$\omega_{2k_F}\simeq\omega_0\sqrt{1-2\zeta},$$

$$\Gamma_{2k_F}=\frac{\zeta\omega_0^2}{\omega_{2k_F}}\sqrt{\frac{\omega_{2k_F}}{8\varepsilon_F}},$$

and

$$\frac{\Gamma_{2k_F}}{\omega_{2k_F}}=\frac{\zeta}{1-2\zeta}\sqrt{\frac{\omega_0\sqrt{1-2\zeta}}{8\varepsilon_F}}. \quad (24)$$

This ratio remains finite in the limit $Q\to1$, although the approximate expression of Eq. (23) diverges for any system with a cylindrical Fermi surface. Of course, the singularity at $Q\to0$ is also unphysical and, in principle, can be treated in a similar way. The common point is that, in both cases, the well-known popular formula

$$\frac{\Gamma_{\mathbf{q}}}{\omega_{\mathbf{q}}}=\frac{|g_0^2|}{M}\sum_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})=\frac{|g_0^2|}{M(2\pi a)^2}\int\frac{dk}{|\mathbf{v}(\mathbf{k})\times\mathbf{v}(\mathbf{k}+\mathbf{q})|} \quad (25)$$

is not valid near the singularity. We do not consider the $Q\to0$ case in this paper, but it is worth noting that there are other issues relevant in that limit, but not near the Kohn singularity, such as the Landau threshold and applicability of the Migdal theorem.

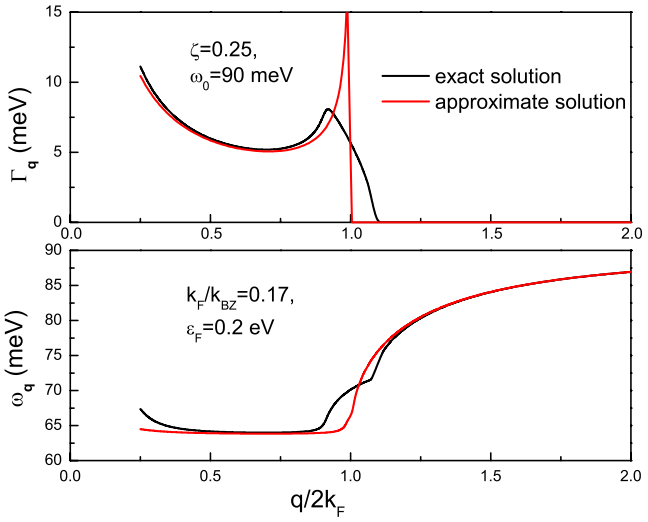

FIG. 2. (Color online) The linewidth $\Gamma_{\mathbf{q}}$ and the renormalized phonon frequency $\omega_{\mathbf{q}}$ obtained by using the approximation of Eq. (17) and the exact expression Eq. (15), for the following parameters: the bare phonon frequency $\omega_0=90$ meV and the bare constant of EPI $\zeta=1/4$. The filling corresponds to $k_F/k_{BZ}=0.17$ and $\varepsilon_F=0.2$ eV.

The results for the linewidth $\Gamma_{\mathbf{q}}$ and the renormalized phonon frequency $\omega_{\mathbf{q}}$ obtained by using the approximate polarization operator as functions of the reduced wave vector $Q=q/2k_F$ are shown in Fig. 2 by red lines. Parameters are the following: the bare phonon frequency $\omega_0=90$ meV and the bare constant of EPI $\zeta=1/4$. The ratio k_F/k_{BZ} is equal to 0.17. It corresponds to $\varepsilon_F=0.2$ eV.

The approximate result agrees with that of Ref. 4 (their Fig. 4). The exact result (black lines) has been obtained by a numerical solution of Eqs. (8) and (9) using the polarization operator from Eq. (15). The latter, in contrast to the approximate expression, shows two shoulders in the wave vector dependence of the renormalized frequency $\omega_{\mathbf{q}}$ (see also $|\mathrm{Re}\,\Pi(\mathbf{q},\omega_0)|$ in the bottom panel of Fig. 2). The first one corresponds to the maximum of $|\mathrm{Im}\,\Pi(\mathbf{q},\omega)|$ (or $\Gamma_{\mathbf{q}}$) and the second one to the vanishing of these values.

III. ELECTRON SELF-ENERGY

The electron self-energy is expressed via the electron and phonon Green functions:

$$\Sigma(p)=ig^0\int G(p-k)D(k)\Gamma(p,p-k,k)\frac{d^{D+1}k}{(2\pi)^{D+1}},$$

where $p=\{\mathbf{p},\varepsilon\}$. It was shown by Migdal[8] that one can neglect the vertex corrections $\Gamma(p,p-k,k)\simeq g^0(1+\sqrt{m/M})$ and that the function $G(\varepsilon,\mathbf{k})$ differs from the bare electron Green function [Eq. (7)] only in the narrow interval of momenta $|k-k_F|\lesssim\omega_{ph}/V_F$ and frequencies $|\omega|\lesssim\omega_{ph}$. Thus, the full electron Green function $G(p)$ can be substituted by the corresponding function for noninteracting electrons [Eq. (7)]. Using Eq. (3), the electron self-energy for $T=0$ becomes (see, e.g., Refs. 18 and 19)

$$\Sigma(\mathbf{k},\omega)=\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\frac{|g^0|^2}{2M\omega_{\mathbf{q}}}\int d\xi\left[\frac{\theta(\xi)}{\omega-\xi-\omega_{\mathbf{q}}+i\Gamma_{\mathbf{q}}}+\frac{\theta(-\xi)}{\omega-\xi+\omega_{\mathbf{q}}-i\Gamma_{\mathbf{q}}}\right].$$

This is a trivial generalization of the standard expressions on the finite phonon linewidth case. Let us average the self-energy over the Fermi surface

$$\Sigma(\omega)=\frac{1}{N(0)}\sum_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}})\Sigma(\mathbf{k},\omega)$$
$$=-\frac{1}{N(0)M}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\frac{|g^0|^2}{4\omega_{\mathbf{q}}}\left\{\ln\frac{\Gamma_{\mathbf{q}}^2+(\omega_{\mathbf{q}}-\omega)^2}{\Gamma_{\mathbf{q}}^2+(\omega_{\mathbf{q}}+\omega)^2}+2i\left[\tan^{-1}\left(\frac{\omega_{\mathbf{q}}-\omega}{\Gamma_{\mathbf{q}}}\right)-\tan^{-1}\left(\frac{\omega_{\mathbf{q}}+\omega}{\Gamma_{\mathbf{q}}}\right)\right]\right\}.$$

The limit $\lambda=-\lim_{\omega\to 0}\mathrm{Re}\,\Sigma(\omega)/\omega$ is nothing but the standard electron-phonon coupling constant

$$\lambda_{\Gamma}=\frac{1}{MN(0)}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\frac{1}{\Gamma_{\mathbf{q}}^2+\omega_{\mathbf{q}}^2}$$
$$=\sum_{\mathbf{q}}\tilde{N}_{\mathbf{q}}(0)\frac{|g^0|^2}{M}\frac{1}{\Gamma_{\mathbf{q}}^2+\omega_{\mathbf{q}}^2},\qquad(26)$$

where we introduced the phase space function (sometimes called "nesting function")

$$\tilde{N}_{\mathbf{q}}(0)=\frac{1}{N(0)}\sum_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k}+\mathbf{q}}).\qquad(27)$$

For a 2D cylindrical Fermi surface, we have

$$\tilde{N}_{\mathbf{q}}(0)=\frac{\theta(1-Q)}{4\pi\varepsilon_F Q\sqrt{1-Q^2}},\qquad(28)$$

which diverges at $Q\to 0$ and $Q\to 1$. Following Ref. 9, we can introduce the "mode λ" via the expression $\lambda=\Sigma_{\mathbf{q}}\lambda_{\mathbf{q}}$. Then

$$\lambda_{\mathbf{q}}=\tilde{N}_{\mathbf{q}}(0)\frac{|g^0|^2}{M}\frac{1}{\Gamma_{\mathbf{q}}^2+\omega_{\mathbf{q}}^2}.$$

In the weak-damping approximation, we recover the standard formula

$$\lambda_{\mathbf{q}}^{app}=\tilde{N}_{\mathbf{q}}(0)\frac{|g^0|^2}{M}\Big/\omega_{\mathbf{q}}^2,\qquad(29)$$

but for $\Gamma_{\mathbf{q}}\gg\omega_{\mathbf{q}}$, the contribution of strongly damped phonons to total $\lambda_{\mathbf{q}}$ is suppressed.

The result (26) we can get also if we introduce, according to Eq. (3), a generalized Eliashberg function

$$\alpha_{\Gamma}^2(\omega)F(\omega)=\frac{1}{2\pi MN(0)}\sum_{\mathbf{k},\mathbf{q}}\frac{\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})}{2\omega_{\mathbf{q}}}\frac{1}{2}\left[\frac{\Gamma_{\mathbf{q}}}{(\omega-\omega_{\mathbf{q}})^2+\Gamma_{\mathbf{q}}^2}-\frac{\Gamma_{\mathbf{q}}}{(\omega+\omega_{\mathbf{q}})^2+\Gamma_{\mathbf{q}}^2}\right]$$
$$=\frac{1}{2\pi M}\sum_{\mathbf{q}}\frac{\tilde{N}_{\mathbf{q}}(0)|g^0|^2}{2\omega_{\mathbf{q}}}\frac{1}{2}\left[\frac{\Gamma_{\mathbf{q}}}{(\omega-\omega_{\mathbf{q}})^2+\Gamma_{\mathbf{q}}^2}-\frac{\Gamma_{\mathbf{q}}}{(\omega+\omega_{\mathbf{q}})^2+\Gamma_{\mathbf{q}}^2}\right].\qquad(30)$$

The second term in this expression cancels out the nonphysical behavior at low and high frequencies. Otherwise, λ_{Γ} would have been divergent. Equations (26) and (30) are general and valid not only for the 2D systems, where phase space factor [Eq. (27)] is divergent.

For $\Gamma_{\mathbf{q}}\ll\omega_{\mathbf{q}}$, we have

$$\alpha_{app}^2(\omega)F(\omega)=\frac{1}{N(0)M}\sum_{\mathbf{k},\mathbf{q}}\frac{\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})}{2\omega_{\mathbf{q}}}\delta(\omega-\omega_{\mathbf{q}})$$
$$=\frac{1}{2\pi N(0)}\sum_{\mathbf{q}}\frac{\Gamma_{\mathbf{q}}^{app}}{\omega_{\mathbf{q}}}\delta(\omega-\omega_{\mathbf{q}}),\qquad(31)$$

where in the last equality we have used the approximate Eq. (12). Note that Eq. (31) is a consequence of the fact that the damping $\Gamma_{\mathbf{q}}^{app}$, according to Eq. (12), can be expressed via the nesting function [Eq. (27)] and both are determined by the same function $\mathrm{Im}\,\Pi'(q,0)\equiv d\,\mathrm{Im}\,\Pi(q,\omega)/d\omega|_{\omega=0}$. In a general case, these functions can be different. This result, without using the pole approximation for the phonon Green function, can be trivially obtained in the Matsubara formalism. In this case, one does not need to solve the Dyson equation. In the lowest order in coupling for $T=0$, the self-energy has a form

$$\Sigma(i\varepsilon,\mathbf{k})=-i\int\frac{d(i\omega)}{2\pi}\sum_{\mathbf{k}',\nu}|g^0|^2D_{M\nu}(i\omega+i\varepsilon,\mathbf{k},\mathbf{k}')\times\frac{1}{i\omega-\varepsilon_{\mathbf{k}'}-\Sigma(i\omega,\mathbf{k}')},$$

where

$$D_{M\nu}(i\omega,\mathbf{k},\mathbf{k}') = (1/\pi)\int_0^\infty d\Omega\ \mathrm{Im}\, D(\Omega + i\delta,\mathbf{k},\mathbf{k}')[(i\omega-\Omega)^{-1} - (i\omega+\Omega)^{-1}]. \quad (32)$$

We can also average the self-energy over the Fermi surface $\Sigma(i\varepsilon)=\Sigma_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}})\Sigma(i\varepsilon,\mathbf{k})/N(0)$:

$$\Sigma(i\varepsilon) = \frac{1}{N(0)}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}}) \times|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}D_M(\mathbf{q},i\omega)\int_{-\infty}^{\infty}\frac{d\xi}{i(\varepsilon-\omega)-\xi}.$$

The integral $\int_{-\infty}^{\infty}\frac{d\xi}{i(\varepsilon-\omega)-\xi}=-i2\pi\,\mathrm{sign}(\varepsilon-\omega)$ allows us to calculate the *physical* coupling constant λ

$$\lambda = -\left.\frac{\partial\Sigma_{el}(i\varepsilon)}{\partial i\varepsilon}\right|_{\varepsilon\to 0} = -\lim_{\varepsilon\to 0}\frac{1}{N(0)}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}}) \times|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\int\frac{d\omega}{2\pi}D(\mathbf{q},i\omega)2\pi\delta(\varepsilon-\omega)$$

$$= -\frac{1}{N(0)}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})D_M(\mathbf{q},i0)$$

$$= -\frac{1}{N(0)}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\frac{1}{D_{M0}^{-1}(i0)-\Pi_M(\mathbf{q},i0)}.$$

On the Matsubara axes, for a 2D system, according to Eq. (20), the phase space factor vanishes for $q>2k_F$ and $\Pi_M(q\leqslant 2k_F,i0)=-2\zeta\omega_0^2$ is a constant [see Eqs. (20) and (19)]. Using Eqs. (2) and (32), we get $D_{M0}^{-1}(i0)=-M\omega_0^2$ and

$$\lambda = \zeta/(1-2\zeta). \quad (33)$$

In a 3D case, $\Pi_M(\mathbf{q},i0)$ is a rather complicated function of q and Eq. (33) is only an approximation (as was probably first mentioned by Fröhlich[17]). The physical meanings of the coupling constants λ and ζ are that they are measures of the renormalization of the phonon frequency from ω_0 to $\omega_{\mathbf{q}}$ (cf. a discussion for 3D systems in Ref. 20).

Turning back to the 2D case, according to Eq. (26), we can neglect all divergent contributions near $Q=0$ and $Q=1$. Elsewhere, we can use Eq. (29).

One should keep in mind that the *conventional coupling constant* is $\lambda=\zeta/(1-2\zeta)$. This parameter determines electronic properties (Fermi velocities, T_c, etc.). The other parameter, $\zeta=\lambda/(1+2\lambda)<1/2$, defines the observable phonon frequency, $\omega_{\mathbf{q}}=\omega_0\sqrt{1-2\zeta}$.

CONCLUSIONS

First of all, the standard well-known expression

$$\alpha^2(\omega)F(\omega) = \frac{1}{2\pi N(0)}\sum_{\mathbf{q}}\frac{\Gamma_{\mathbf{q}}}{\omega_{\mathbf{q}}}\delta(\omega-\omega_{\mathbf{q}}) \equiv \frac{1}{N(0)M}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\frac{\delta(\varepsilon_{\mathbf{k}})|g^0|^2\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})}{2\omega_{\mathbf{q}}}\delta(\omega-\omega_{\mathbf{q}})$$

is valid only in the lowest order in the bare phonon linewidth, $\Gamma_{\mathbf{q}}$, which is not an acceptable approximation in the case of strong Kohn singularities, and particularly for a cylindrical Fermi surface. $\Gamma_{\mathbf{q}}$ in this approximation is not the actual phonon linewidth; as opposed to $\Gamma_{\mathbf{q}}$, determined by the oversimplified Eq. (12), the real phonon linewidth does not diverge even for an ideally cylindrical Fermi surface. Second, following Eq. (33) derived above, the more accurate treatment presented here still respects the old sum rules that the total λ for a cylindrical Fermi surface and parabolic bands do not depend on filling.

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