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PHONON DISPERSION IN SYSTEMS WITH A PLANAR FERMI SURFACE

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The effect of a planar Fermi surface on the phonon spectrum near $q = 2p_F$ is investigated. Two branches of excitations are found in this region. The reliability of the calculation is examined by means of a sum rule for the spectral weight function. The average and the spread of the spectral distribution are computed.

THIS work is motivated by the theoretical indication,[1] supported by experimental evidence,[2] that the Fermi surface of several intermetallic compounds of the *A*-15 (β-tungsten) crystal structure contains planar sections. We investigate the effect of such planar portions of the Fermi surface on the phonon spectrum in the neighbourhood of $q = 2p_F$. To this end we adopt an idealized picture of an electron gas with a Fermi surface consisting of two parallel planes separated by $2p_F$ and limited by the Brillouin-zone boundaries. Such a system was studied by Alfanas'ev and Kagan,[3] who predict that the phonon spectrum near $2p_F$ differs considerably from the case of a spherical Fermi surface. This shows up in a much stronger Kohn singularity. The origin of this effect is the sharp increase in the phase-space volume available for low energy electron excitations accompanied by the absorption of phonons with $q = 2p_F$. This leads to a strong coupling with such phonons and, thus, to a significant renormalization of the phonon spectrum in this region. One implication of this strong coupling is the breakdown of Migdal's theorem, which asserts that the electron–phonon vertex is described correctly up to the order of $\sqrt{(m/M)}$ (m – electron mass, M – ion mass) by the bare coupling constant. The authors of reference 3 did not calculate the phonon spectrum explicitly.

Note that a planar Fermi surface means that the system is one-dimensional at least in momentum space. The coupled one-dimensional electron–phonon system was studied by Engelsberg and Varga[4] in the framework of the Tomonaga model. This model cannot be applied in our case since it excludes electron excitations across the Fermi surface and is valid only for longwave phonons.

We start from an effective Fröhlich Hamiltonian

$$H = \sum_p \epsilon_p c_p^+ c_p + \sum_q \omega_q^0 a_q^+ a_q + \sum_{p,q} g_q (a_q + a_{-q}^+) c_{p+q}^+ c_p, \tag{1}$$

where a_q, c_p are the phonon and electron destruction operators and g_q is the electron–phonon coupling constant. It is assumed that the long-range effects of the electron–electron interaction are already included in ϵ_p, ω_q^0 and g_q. We characterize the strength of the electron–phonon coupling by a dimensionless parameter λ_q defined by

$$g_q^2 = \frac{\lambda_q \pi^3}{\beta m p_F} \omega_q^0 \tag{2}$$

where $\beta = (\int dp_x dp_y / p_F^2)$. The parameter β is related to the electron density by $n = \beta(p_F/2\pi)^3$. We shall assume that ω_q^0 and λ_q do not vary strongly in the neighbourhood of $q = 2p_F$ and we shall replace them by constants ω_0 and λ. To estimate λ we

write g^2 in the form

$$g^2 = \frac{J^2}{2Mn\omega_0} \tag{3}$$

where J is the matrix element $<k|\nabla U|\, k + 2p_F>$. Semiempirical values of Fermi surface averages of J^2 for various materials were given McMillan.[5] The value of p_F may be estimated from positron annihilation experiments[2] and ω_0 from the Debye temperature. On the grounds of such estimates one gets for V_3Si, $\lambda \approx 0.1$–0.5.

All the information about the phonon spectrum is contained in the phonon Green's function

$$D(q,\omega) = \frac{2\omega_q^0}{\omega^2 - \omega_q^{0\,2} - 2\omega_q^0\Pi(q,\omega) + i\delta}, \quad (\delta = +0), \tag{4}$$

where the phonon self-energy $\Pi(q,\omega)$ is given by

$$\Pi(q,\omega) = \frac{2i}{(2\pi)^4}\int g_q\Gamma(p,\epsilon;\, q,\omega)\, G_0(p+q,\epsilon+\omega)\, G_0(p,\epsilon)\mathrm{d}^3p\mathrm{d}\epsilon \tag{5}$$

where Γ is the electron–phonon vertex function. We have replaced the electron Green's function G by the free Green's function G_0, the argument being that they differ only in a very small region of integration around the Fermi surface. In view of the planar Fermi surface, G_0 depends only on p_z. As a first step we replace Γ by g_q and solve for the poles of $D(q,\omega)$. We thus have on account of equation (2)

$$\Pi_0(q,\omega) = -\lambda_q\omega_q^0\left(\frac{p_F}{m}\right)\frac{i}{8\pi}\int G_0(p+q,\epsilon+\omega)\, G_0(p,\epsilon)\mathrm{d}p\mathrm{d}\epsilon \tag{6}$$

where the Cartesian index z has been suppressed. The real and imaginary parts of $\Pi_0(q,\omega)$ are

$$\mathrm{Re}\,\Pi_0(q,\omega) = -\lambda_q\omega_q^0\frac{p_F}{4q}\ln\left|\frac{(q/2+p_F)^2 - (m\omega/q)^2}{(q/2-p_F)^2 - (m\omega/q)^2}\right|, \tag{7}$$

$$\mathrm{Im}\,\Pi_0(q,\omega) = -\lambda_q\omega_q^0\frac{\pi p_F}{4q}\left[\theta(\epsilon_{q/2+m\omega/q} - \epsilon_F) - \theta(\epsilon_{q/2-m\omega/q} - \epsilon_F)\right]\mathrm{sgn}\,\omega, \tag{8}$$

where $\theta(x) = 1$ for $x > 0$, and $\theta(x) = 0$ for $x < 0$. We are looking for solutions of the equation

$$\omega^2 = \omega_q^{0\,2} + 2\omega_q^0\Pi_0(q,\omega), \tag{9}$$

near $q = 2p_F$. Let us denote $q' = q/2 - p_F$ and consider $|q'| \ll p_F$. We continue analytically the function $\Pi_0(q,\omega)$ to the complex ω-plane, separate the real and imaginary parts of equation (9) and obtain two coupled equations for the real (ω) and imaginary (γ) parts of the phonon frequency:

$$\omega^2 - \gamma^2 = \omega_0^2\left(1 + \frac{\lambda}{8}\ln\left|\frac{[(\omega+2v_Fq')^2+\gamma^2][(\omega-2v_Fq')^2-\gamma^2]}{(8\epsilon_F)^4}\right|\right), \tag{10}$$

$$\omega\gamma = -\frac{\lambda\omega_0^2}{4}\left[\pi\theta(\omega - 2v_F|q'|) + \mathrm{arctg}\,\frac{2\omega\gamma}{(2v_Fq')^2 + \gamma^2 - \omega^2}\right]. \tag{11}$$

In view of the θ-function we consider separately the two possibilities: $\omega < 2v_F|q'|$ and $\omega > 2v_F|q'|$. In the first case the only solution of equation (11) is $\omega\gamma = 0$, namely, either $\omega = 0$ or $\gamma = 0$. There exists formally a solution of equations (10) and (11) with $\omega = 0$, $\gamma \neq 0$, however, we shall see later that the weight of this solution in $D(q,\omega)$ is zero. We therefore are left with $\gamma = 0$, $\omega \neq 0$. Such a solution exists outside an interval of width $2q_0'$ around $q = 2p_F$. This width depends on λ and is approximately given by

$$\frac{\lambda}{2}\ln\left|\frac{4\epsilon_F}{v_Fq_0'}\right| \simeq 1 \tag{12}$$

This interval increases and becomes more asymmetric with respect to $2p_F$ as λ increases. The frequency ω vanishes as q' approaches the end points of this interval from the outside. In the second case, $\omega > 2v_F|q'|$, one finds a solution with $\omega \neq 0$, $\gamma \neq 0$, which exists as long as ω exceeds $v_Fq|(q/2p_F) - 1| \simeq 2v_F|q'|$. A typical phonon spectrum with the two branches is shown in Fig. 1 for $\lambda = 0.25$ and $\omega_0/2\epsilon_F = 0.01$.

So far we have replaced the electron–phonon vertex in equation (5) by the bare coupling constant. This is justified when Migdal's theorem holds. It can be shown in our case[3] that the first order correction to the electron–phonon vertex diverges and a proper renormalization is needed. The simplest renormalization is that which results from summing all ladder diagrams. We have recalculated the phonon spectrum with the self-energy

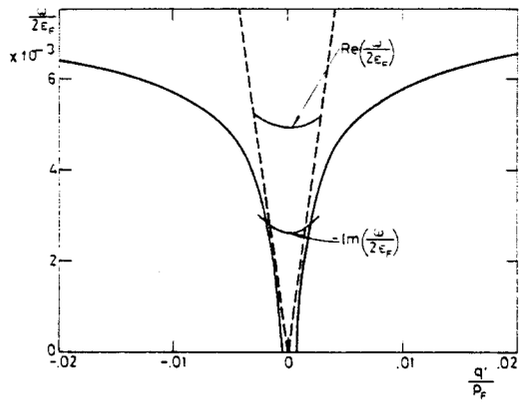

FIG. 1. A typical phonon dispersion curve near $q = 2p_F$ for $\lambda = 0.25$ and $\omega_0/2\epsilon_F = 0.01$. The real and imaginary parts of the damped branch are indicated. The broken lines correspond to $\omega = \pm 2v_F q'$.

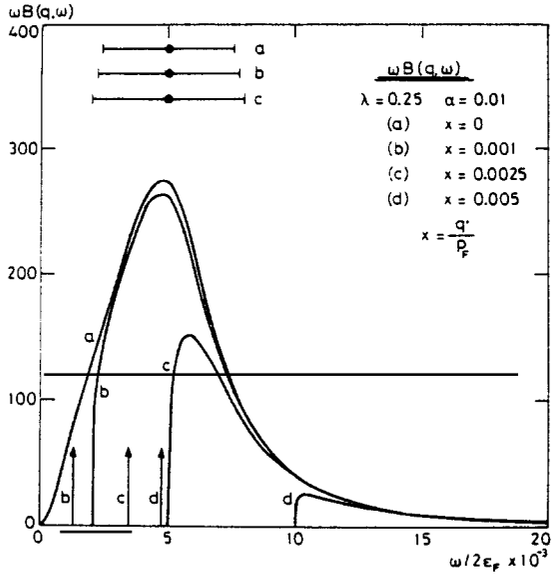

FIG. 2. The function $\omega B(q,\omega)$ for four cases specified by the parameters in the figure. See text for further details.

obtained in this way and found that the previous results are effected only by about 2 per cent. The reason for that is that the vertex diagrams of the ladder-type are very small except for a weak divergence in a very narrow region around the lines $\omega = \pm 2v_F q'$. Since our solutions do not come that close to this region they are not effected appreciably. The details of this calculation will be described elsewhere.

Let us now analyze our results with the help of the spectral weight function $B(q,\omega)$, which is related to $D(q,\omega)$ by

$$B(q,\omega)\,\mathrm{sgn}\omega = -\frac{1}{\pi}\,\mathrm{Im}D(q,\omega). \qquad (13)$$

It is clear from equation (4) with Π_0 replacing Π, that whenever $\mathrm{Im}\,\Pi_0(q,\omega) = 0$, the spectral weight $B(q,\omega)$ is proportional to $\delta(\omega - \omega_q)$, where ω_q is a root of equation (9) on the real ω-axis. It follows from equation (8) that $\mathrm{Im}\,\Pi_0(q,\omega) = 0$ for $\omega < 2v_F|q'|$ and therefore the undamped branch of the phonon spectrum is represented in the spectral distribution by a δ-function. We mentioned before that equations (10) and (11) also have a formal solution with $\omega = 0$, $\gamma \neq 0$, however, $\omega = 0$ is not a root of equation (9) on the real ω-axis and this solution does not carry any spectral weight. The other branch of the phonon spectrum occurs in a region where $\mathrm{Im}\,\Pi_0 \neq 0$. There $B(q,\omega)$ is a continuous function of ω. The function $\omega B(q,\omega)$ is plotted in Fig. 2 for $\lambda = 0.25$, $\omega_0/2\epsilon_F = 0.01$ and several values of q'. The vertical arrows indicate the δ-function contribution of the undamped lower branch. In case (a) the undamped solution does not exist. The centers of the horizontal lines in the upper part of the figure and their lengths show the values of $\omega(q')$ and $\gamma(q')$ for the damped solution. This solution does not exist for case (d).

The spectral weight $B(q,\omega)$ satisfies the sum rule

$$\int_0^\infty \omega B(q,\omega)\,d\omega = \omega_q^0. \qquad (14)$$

We have checked to what extent this sum rule is exhausted by our approximation for $B(q,\omega)$. We find that outside the interval where the undamped solution does not exist, the sum rule is satisfied very well. In this interval, however, the sum rule is not satisfied and for $\lambda = 0.25$ we find that 20 per cent are missing near $q = 2p_F$ which increases to about 80 per cent for $\lambda = 0.5$. This means that in the immediate neighborhood of $q = 2p_F$ our approximation is not good enough and it becomes worse as λ increases. As we saw, this cannot be improved by the inclusion of ladder diagrams. If the physical situation corresponds to $\lambda < 0.25$ then our approximation is quite reliable for all q'.

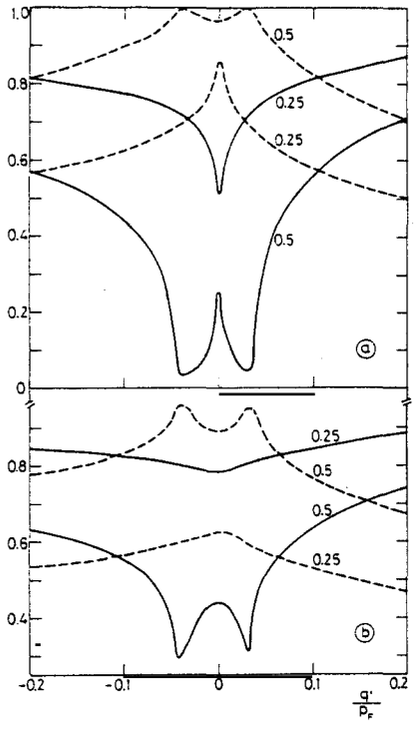

FIG. 3. The function $\bar{\omega}$ (full line) and $<(\omega - \bar{\omega})^2>^{1/2}$ in units of ω_0. (a) $\omega_0/2\epsilon_F = 0.01$, (b) $\omega_0/2\epsilon_F = 0.1$. The numbers on the curves indicate values of λ.

An ideal neutron scattering experiment would resolve the two contributions to $B(q,\omega)$ where the two branches exist. However the experimental resolution may not be sufficient for that. It is therefore instructive, for comparison with experiment, to characterize the spectral distribution by its average $\bar{\omega}$ and by the spread around this average $<(\omega - \bar{\omega})>$. We compute these averages with the weight function $(\omega/\omega_0)\, B(q,\omega)$, rather than with $B(q,\omega)$, because the latter cannot be normalized between 0 and ∞. The functions $\bar{\omega}$ and $<(\omega - \bar{\omega})^2>^{1/2}$ in units of ω_0 are plotted in Fig. 3 for $\lambda = 0.25$, 0.5 and $\omega_0/2\epsilon_F = 0.01$, 0.1. It is hard to say which of the curves represents a physical case because of the uncertainty in the values of the two parameters involved. However, the results indicate that near $q = 2p_F$ one should expect a depression in the center of mass of the spectral distribution accompanied by an increase in the phonon line widths. If these effects are sharp enough to be detected experimentally, it may be possible to locate planar portions of the Fermi surface in β-tungstens by neutron scattering experiments.

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On étudie le spectre de phonons d'un métal dont la surface de Fermi est plane. Deux branches d'excitations sont trouvées dans la région de vecteur d'onde $q \sim 2p_F$. Le calcul est testé au moyen d'une règle de somme sur la densité spectrale: la fréquence moyenne et l'écart quadratique moyen de cette distribution sont calculés.