Experimental investigation of nonpair ion–ion interaction via conduction electrons in aluminum

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The method of inelastic neutron scattering and a triaxial spectrometer were used to investigate an isolated singularity of the transverse phonon branch along the [100] direction of an Al single crystal in the vicinity of the wave vector $q/q_{max} \approx 0.2$. The aim was to identify this singularity as due to a three-particle process, i.e., due to the manifestation of a nonpair ion–ion interaction, in contrast to the already observed Kohn anomaly of the same branch ($q/q_{max} \approx 0.76$). This was done by determining the group velocities $\partial\omega/\partial\mathbf{q}$ of phonons along the [100] and [10ξ] directions (here, $\xi = 0.176$, which corresponds to 10° inclination relative to the [100] direction). The measurements of the velocity $\partial\omega/\partial\mathbf{q}$ along the latter (asymmetric) direction were made for different phonon polarizations. It was established that "splitting" of the singularities occurred along the [10ξ] direction, the nature of this splitting and the polarization dependence indicating that the singularity at $q/q_{max} \approx 0.42$ was of the three-particle type. An analysis was made of the influence of the Fermi surface nonsphericity on the fine structure of the dispersion curves of nontransition metals.

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1. INTRODUCTION

Beginning from Kohn's paper,[1] who was the first to demonstrate the existence of singularities of the electron gas polarizability associated with the properties of the Fermi surface of a metal and manifested in the phonon dispersion curves, these singularities or anomalies have been continuously attracting attention from the experimental and theoretical points of view. The singularities are due to an abrupt boundary in the distribution of conduction electrons in the phase space, which gives rise to a logarithmic divergence of the group phonon velocity $\partial\omega/\partial\mathbf{q}$ when the wave vector $\mathbf{q}$ corresponds to a transition of an electron from one point on the Fermi surface to another with the opposite velocity. Similar singularities have been also predicted for spin waves.[2]

The Kohn anomalies were first observed by Brockhouse *et al.* in lead[3] by the method of inelastic scattering of thermal neutrons. Subsequently, these anomalies were investigated for nontransition [Zn (Ref. 4), Al (Ref. 5)] and transition [Nb (Ref. 6), Cu (Ref. 7)] metals. Weymouth and Stedman[5] determined the group velocity of phonons in Al and they achieved a high momentum and energy resolution; this enabled them to record not only the existence of the Kohn anomalies but also to estimate their relative magnitudes. As shown in several theoretical papers,[8-10] these amplitudes largely depend on such important characteristics of a metal as the curvature of the Fermi surface, size of the energy gaps in the band structure, and the nature of the electron–ion interaction.

Brovman and Kagan[11] developed a self-consistent many-electron theory of perturbations in nontransition metals and used it to predict the existence of new anomalies of the phonon dispersion curves: these are the "three-particle" singularities,[12] reflecting the nonpair nature of the ion–ion interaction. Brovman and Kagan[11] showed that the dynamic matrix of the vibrations can be represented as a series in powers of the electron–ion interaction potential ($V_\mathbf{G}/\varepsilon_F$):

$$D_{\alpha\beta}(\mathbf{q}) = D^{(1)}_{\alpha\beta}(\mathbf{q}) + D^{(2)}_{\alpha\beta}(\mathbf{q}) + D^{(3)}_{\alpha\beta}(\mathbf{q}) + \dots \tag{1}$$

Here and later, we shall consider a monatomic lattice; $D^{(1)}_{\alpha\beta}$ is the dynamic matrix of vibrations of the ion lattice in the field of a homogeneous noninteracting electron gas; $D^{(n)}_{\alpha\beta}$ are the corrections due to the n-th order of the perturbation theory.

The contributions to the square of the phonon frequency made by $D^{(2)}_{\alpha\beta}$ and $D^{(3)}_{\alpha\beta}$ are

$$[\omega_j^{(2)}(\mathbf{q})]^2 = \frac{\Omega_0}{M} 2 \Big\{ \sum_{\mathbf{G}} [\zeta_j^2(\mathbf{q},\mathbf{G}) V^2_{\mathbf{q}+\mathbf{G}} \Gamma^{(2)}(\mathbf{q}+\mathbf{G}, -\mathbf{q}-\mathbf{G})] - \sum_{\mathbf{G}\neq 0} [\dots]_{\mathbf{q}=0} \Big\}, \tag{2}$$

$$[\omega_j^{(3)}(\mathbf{q})]^2 = \frac{\Omega_0}{M} 6 \Big\{ \sum_{\mathbf{G}_1\mathbf{G}_2} [\zeta_j(\mathbf{q},\mathbf{G}_1)\zeta_j(\mathbf{q},\mathbf{G}_2) V_{\mathbf{q}+\mathbf{G}_1} V_{-\mathbf{q}-\mathbf{G}_2} V_{\mathbf{G}_2-\mathbf{G}_1} \times \Gamma^{(3)}(\mathbf{q}+\mathbf{G}_1, -\mathbf{q}-\mathbf{G}_2, \mathbf{G}_2-\mathbf{G}_1)] - \sum_{\mathbf{G}_1\neq\mathbf{G}_2\neq 0} [\dots]_{\mathbf{q}=0} \Big\}, \tag{3}$$

where

$$\zeta_j(\mathbf{q},\mathbf{G}) = (\mathbf{q}+\mathbf{G})\mathbf{e}_j(\mathbf{q}), \tag{4}$$

$\mathbf{q}$ is the phonon wave vector, $\mathbf{G}$ is the reciprocal lattice vector, $\mathbf{e}_j(\mathbf{q})$ is the vector of the polarization of the j-th vibration mode, $V_\mathbf{G}$ is the Fourier component of the pseudopotential of the electron–ion interaction, and ε_F is the Fermi energy.

The multipoles $\Gamma^{(2)}$ and $\Gamma^{(3)}$ (see Brovman and Kagan[11]) describe the properties of a homogeneous electron gas of a given density and largely determine the nature of the phonon spectra of metals. In particular, for certain values of the wave vector these multipoles become singular and this gives rise to anomalies in the phonon spectra, which can be observed experimentally. For example, the Kohn anomalies are usually associated with the singularity $\Gamma^{(2)}$.

The presence in Eq. (1) of the term $D^{(3)}_{\alpha\beta}$ effectively

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implies allowance for the nonpair interaction between ions via conduction electrons. In this case the electrons can be scattered additionally by the third ion and thus provide an indirect interaction between a pair of ions, which now becomes of the three-particle type and whose inclusion makes it possible to predict qualitatively new singularities in the phonon spectra of metals. The existence of this nonpair interaction is responsible for the asymmetry of the frequency splitting at the point K of the Brillouin zone of hexagonal metals, as found experimentally for Be, Mg, Zn, and Cd (Refs. 13-16).

Another example of the three-particle interaction is provided by the appearance of singularities of the group phonon velocity $\partial\omega/\partial\mathbf{q}$, which—in contrast to the local manifestation of the nonpair nature of the ion–ion forces at the point K—may, like the Kohn anomalies, determine largely the fine structure of the phonon spectrum as a whole. This is because in spite of the presence in Eq. (3) for $[\omega_j^{(3)}(\mathbf{q})]^2$ of an additional—compared with $[\omega_j^{(2)}(\mathbf{q})]^2$—small parameter (V_G/ε_F), the root singularity of $\Gamma^{(3)}$ (Ref. 11) [which is stronger than the logarithmic Kohn singularity of $\Gamma^{(2)}$] can be detected directly by experiments in which the group phonon velocity is measured. In particular, the calculations of $\partial\omega/\partial\mathbf{q}$ for Al reported by Brovman and Kagan[11] demonstrate that the anomalies associated with the three-particle and Kohn singularities are of the same order of magnitude. This makes it realistic to consider experimental detection and investigation of three-particle singularities of the group phonon velocity.

Weymouth and Stedman[5] investigated the Kohn singularities in the case of Al and observed at least two anomalies which could not be identified as being of the Kohn type. Although Brovman and Kagan showed[11] that the positions of these anomalies can be deduced easily from the geometric conditions for three-particle singularities, there have been no direct experimental studies of the nature of these anomalies of $\partial\omega/\partial\mathbf{q}$.

We investigated a singularity of the transverse phonon branch along the [100] direction of an Al single crystal in the vicinity of the wave vector $q/q_{max} \approx 0.43$ with the aim of identifying it as a three-particle singularity, distinct from the Kohn anomaly observed for the same branch ($q/q_{max} \approx 0.76$). Here, q_{max} denotes the maximum value of the phonon wave vector within the Brillouin zone for a given direction of $\mathbf{q}$.

2. POSITIONS OF SINGULARITIES ON DISPERSION CURVES

The positions of diametral Kohn singularities in the spherical Fermi surface model are governed by the condition

$$|\mathbf{q}+\mathbf{G}|=2k_F, \tag{5}$$

where k_F is the radius of the Fermi sphere. In the case of the transverse phonon branch of Al along the [100] direction, the position of the singularity at $q/q_{max} \approx 0.76$ is easily deduced from the condition (5) for $\mathbf{G}=(1, \pm 1, \pm 1)$.[1)] Moreover, in a fairly wide region near $q/q_{max} \approx 0.43$ we find that for any value of G there are no diametral transitions giving rise to a Kohn singularity.

The positions of three-particle singularities on dispersion curves are found from the condition (see Brovman and Kagan[11]) that the radius of a circle passing through the vertices of an acute-angled triangle of sides $(\mathbf{q}+\mathbf{G}_1)$, $(-\mathbf{q}-\mathbf{G}_2)$, and $(\mathbf{G}_2-\mathbf{G}_1)$ is k_F. In the subsequent analysis it will be convenient to use a vector $\mathbf{G}_3=\mathbf{G}_2-\mathbf{G}_1$. Table I gives all the reciprocal lattice vectors forming triangles equivalent from the point of view of the symmetry of the fcc structure for a given direction of the wave vector $\mathbf{q}\|[100]$ and governing the position of a three-particle singularity at $q/q_{max}=0.46$ [if $2k_F=2.255(2\pi/a)$]. Table I gives also the values of the polarization factor [see Eqs. (2)-(4)]:

$$\zeta_{3T}=\zeta_T(\mathbf{q}, \mathbf{G}_1)\zeta_T(\mathbf{q}, \mathbf{G}_2), \tag{6}$$

which governs the conditions of existence of three-particle singularities of the group velocity of phonons belonging to branches with different transverse polarizations ($\mathbf{e}_T\|z$ and $\mathbf{e}_T\|y$). It follows from Table I that a three-particle singularity should be observed for both polarizations but in the $\mathbf{e}_T\|z$ case the contribution to the singularity is made by the first and fourth groups of the vectors $\mathbf{G}_i$, whereas in the $\mathbf{e}_T\|y$ case, the second and third groups are important. Thus, if $\mathbf{q}\|[100]$, the transverse branch (which is then doubly degenerate) should exhibit a three-particle singularity at $q/q_{max}=0.46$ (Ref. 11).

However, if the wave vector $\mathbf{q}$ is inclined away from the high-symmetry direction [100], for example, if it is inclined by an angle φ in the XZ plane [$\mathbf{q}^*=q^*(\cos\varphi, 0, \sin\varphi)$], then the first group of the reciprocal lattice vectors $\mathbf{G}_j$ in Table I is no longer equivalent to the fourth group in the $\mathbf{e}_T\|z$ case. We then have split singularities which can be explained as follows. Figure 1 shows the reciprocal lattice planes of Al, shown by thick lines in a reciprocal lattice cell in Fig. 2; the triangles based on the arguments of $\Gamma^{(3)}$, $\mathbf{G}_2$, and $\mathbf{G}_3$ belong to the first group of vectors in Table I and $\mathbf{G}_2'$ and $\mathbf{G}_3'$ to the fourth group. It is clear from Fig. 1 that in the case of phonons with $\mathbf{q}\|[100]$, the triangles

TABLE I.

Groups	$\mathbf{G}_1$			$\mathbf{G}_2$			$\mathbf{G}_3=\mathbf{G}_2-\mathbf{G}_1$			ξ_{3z}	ξ_{3y}
	x	y	z	x	y	z	x	y	z		
1	1	1	1	0	0	2	−1	−1	1	2	0
	1	−1	1	0	0	2	−1	1	1	2	0
	0	0	2	1	1	1	1	1	−1	2	0
	0	0	2	1	−1	1	1	−1	−1	2	0
2	1	1	1	0	2	0	−1	1	−1	0	2
	1	−1	1	0	−2	0	−1	−1	−1	0	2
	0	2	0	1	1	1	1	−1	1	0	2
	0	−2	0	1	−1	1	1	1	1	0	2
3	1	1	−1	0	2	0	−1	1	1	0	2
	1	−1	−1	0	−2	0	−1	−1	1	0	2
	0	2	0	1	1	−1	1	−1	−1	0	2
	0	−2	0	1	−1	−1	1	1	−1	0	2
4	1	1	−1	0	0	−2	−1	−1	−1	2	0
	1	−1	−1	0	0	−2	−1	1	−1	2	0
	0	0	−2	1	1	−1	1	1	1	2	0
	0	0	−2	1	−1	−1	1	−1	1	2	0

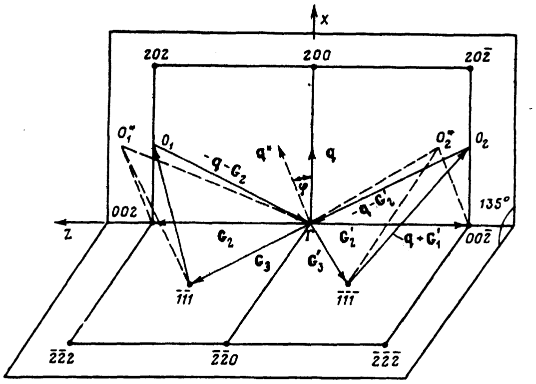

FIG. 1. Splitting of a three-particle singularity when the phonon wave vector **q** is inclined at an angle φ relative to the [100] direction.

with sides ($\mathbf{q}+G_1$), ($-\mathbf{q}-G_2$), G_3 and ($\mathbf{q}+G_1'$), ($-\mathbf{q}-G_2'$), G_3' are equal and make equivalent contributions to a given singularity. When **q** is inclined at an angle φ in the XZ plane (it is denoted by $\mathbf{q}^*$ in Fig. 1), the sides of the triangles change in different ways and the condition for these triangles to be inscribed in circles of radius k_F gives rise to different values of q_1^* and q_2^* at which there are singularities. Similar reasoning applies also to the second and third group of vectors in Table I. The positions of three-particle singularities calculated in the spherical Fermi surface approximation are given in Table II for an inclination of **q** in the XZ plane by an angle $\varphi=10°$ relative to the [100] direction. Moreover, Table II gives the polarization factors ζ_{3T} of Eq. (6) from which we can deduce that the singularities associated with the first and fourth groups of vectors should be observed for $\mathbf{e}_T \| z$ and those associated with the second and third groups should be found in the $\mathbf{e}_T \| y$ case. The relative amplitudes of the singularities are proportional to the product ζ_{3T} and at the number of triangles N contributing equivalently to a given singularity (the values of these products are given in the last two columns of Table II). In the calculations of ζ_{3T} allowance is made for the fact that in the case when **q** is inclined relative to the [100] direction the polarization vectors should not be parallel to y and z.

We shall now discuss the behavior of a diametral Kohn singularity with $q/q_{\max}\approx 0.76$ when **q** is inclined to [100]. This singularity should split into two components and the components should be associated with transverse branches of different polarizations. Figure 3 demonstrates the splitting of a Kohn singularity in the spherical Fermi surface case. Here, G and G′ are the reciprocal lattice sites of the (1, ±1, ±1) type. For $\varphi=0$, we find that $q_1^*=q_2^*=q$ and that G and G′ make equivalent contributions to the same singularity. If $\varphi\neq 0$, it is clear that $q_1^*\neq q_2^*$ and then G and G′ correspond to different Kohn singularities. The calculated positions of these singularities, polarization factors, and total intensities are given in Table III for $\varphi=10°$.

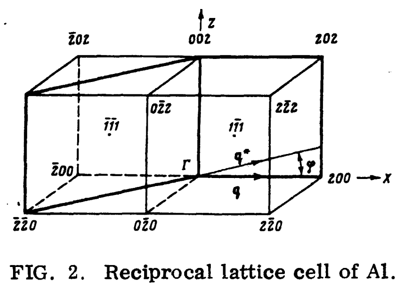

FIG. 2. Reciprocal lattice cell of Al. The thick lines identify the planes in Fig. 1.

TABLE II.

Groups	q^*/q_{max}	ζ_{3z}	ζ_{3y}	$N\zeta_{3z}$	$N\zeta_{3y}$
1	0.35	1.59	0.0	6.35	0.0
2	0.42	−0.003	2.0	−0.01	8.0
3	0.50	0.005	2.0	0.02	8.0
4	0.60	2.31	0.0	9.23	0.0

3. EXPERIMENTS

The different polarization dependences of the singularities discussed above provide an opportunity for an experimental confirmation of the three-particle nature of the anomaly in the vicinity of $q/q_{\max}\approx 0.43$ of the transverse branch directed along [100] in Al. We determined the velocities $\partial\omega/\partial\mathbf{q}$ of phonons along the [100] and [10ξ] directions ($\xi=0.176$, which corresponds to an inclination at an angle of $\varphi=10°$ relative to the [100] axis). Lifting of the degeneracy of the transverse vibration branches along the [10ξ] direction enabled us to investigate phonons with $\mathbf{e}_T\|z$ and $\mathbf{e}_T\|y$, which was ensured by orienting a sample in different ways.[2)]

Our measurements were carried out at room temperature using a triaxial crystal spectrometer and neutrons generated in the IRT-M reactor at the I. V. Kurchatov Institute of Atomic Energy.[17] Our sample was a single-crystal Al cylinder (the cylinder axis was parallel to the [010] crystallographic direction) with a mosaic angle of ~20′. Natural collimation ensured that the divergence of the neutron beam incident on the sample was ~25′. Multislit collimators placed in front of an analyzer crystal and detector produced scattered beams of 30′ and 20′ divergence, respectively. The monochromator and analyzer functions in the spectrometer were performed by copper single crystals with the (111) reflection planes and a mosaic angle of ~20′. The

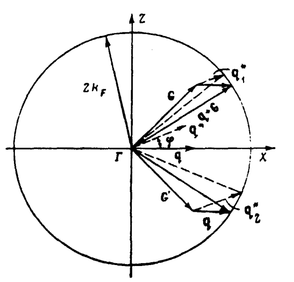

FIG. 3. Splitting of a Kohn singularity when the phonon wave vector **q** is inclined at an angle φ relative to the [100] direction.

TABLE III.

q^*/q^*_{max}	ζ_z^2	ζ_y^2	$N\zeta_z^2$	$N\zeta_y^2$
0.69	0.76	1.0	1.52	2.0
0.84	1.10	1.0	2.20	2.0

calculated momentum resolution was then 0.015 (in units of q/q_{max}) and the increase in the phonon wave vector in the measurements of $\partial\omega/\partial\mathbf{q}$ was selected to be 0.02. In the measurements carried out on phonons along the [100] and [10ξ] directions in the $\mathbf{e}_T \| z$ case the crystallographic direction [010] of the sample was orthogonal to the scattering plane. For $\mathbf{q}\|[10\xi]$ and $\mathbf{e}_T \| y$ the normal to the scattering plane was in the XZ coordinate plane and it was inclined at 10° relative to the [001] axis. All the measurements were carried out by the method of constant momentum transfer (constant Q) of Ref. 18 for two fixed values of the wavelengths of the incident neutrons: 1.2 and 1.35 Å. The selection of this method was justified because investigations of low-energy transverse branches revealed extensive intervals of scanning of the phase space in which there was little change in the focusing conditions and the corrections associated with a change in the analyzer reflectivity within one maximum were fairly small. Moreover, we compared the group phonon velocities differing in respect of the polarization vector but equivalent from the point of view of the measurement geometry, which ensured the necessary relative precision.

The phonon frequency ω was found by approximating the experimental maxima with a Gaussian. The error in the frequency $\delta\omega$, governed by the statistical precision of the measurements, was calculated by analogy with Ref. 19:

$$\delta\omega=\delta\omega_{1/2}\frac{N_m^{1/2}}{N_m-N_b}\frac{1}{n^{1/2}},\qquad(7)$$

where $\delta\omega_{1/2}$ is the width of the measured maximum at midamplitude, N_m is the number of counts at the maximum, N_b is the background, and n is the number of experimental points across the full width of the measured maximum.

4. RESULTS OF MEASUREMENTS AND DISCUSSION

Two singularities, at $q/q_{max}=0.42$ and $q/q_{max}=0.77$, can be seen (Fig. 4) in the dependence of the phonon group velocity on q/q_{max} along the [100] direction; the positions of these singularities are in good agreement with the results of Weymouth and Stedman.[5] As pointed out in Sec. 2, an analysis carried out in the spherical Fermi surface model gives similar positions of the singularities: at $q/q_{max}=0.46$ there should be a three-particle anomaly associated with the set of the reciprocal lattice vectors given in Table I and at $q/q_{max}=0.76$ there should be a diametral Kohn anomaly with vectors of the G=(1, ±1, ±1) type.

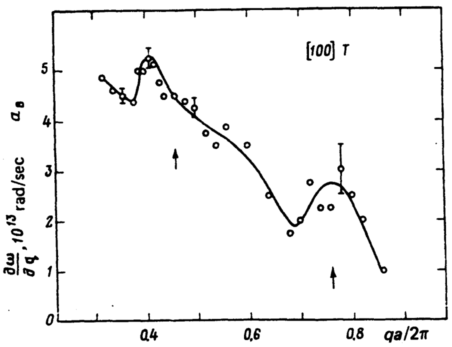

FIG. 4. Group velocity of transverse phonons along the [100] direction. The arrows identify the positions of the three-particle and Kohn singularities calculated in the spherical Fermi surface approximation (a in units of a_B).

Figure 5 gives the results of measurements of the velocity $\partial\omega/\partial\mathbf{q}$ along the [10ξ] direction for the phonon polarization vectors $\mathbf{e}_T \| y$ and $\mathbf{e}_T \| z$. We can see that the singularities are split and the nature of the splitting of the second singularity is qualitatively the same for $\mathbf{e}_T \| z$ and $\mathbf{e}_T \| y$. On the other hand, the splitting of the first singularity depends strongly on the phonon polarization vector. For $\mathbf{e}_T \| z$, the splitting is much greater than for $\mathbf{e}_T \| y$, in which case the momentum resolution is insufficient for exact localization of the singularities. The arrows in Fig. 5 identify the three-particle singularities calculated in the approximation of the spherical Fermi surface.

A comparison of the results obtained for $\partial\omega/\partial\mathbf{q}$ along the [10ξ] direction with the calculations shows that the nature of splitting and polarization dependence of the first singularity are in qualitative agreement with the properties predicted for a three-particle singularity, whereas the behavior of the second singularity is in agreement with that expected of a Kohn anomaly. However, there are quantitative differences between the experimental and calculated results which include a considerable (10-15%) disagreement between the calculated positions of the three-particle singularities along the [100] and [10ξ] directions and a somewhat smaller discrepancy (~5%) for the Kohn singularity along the

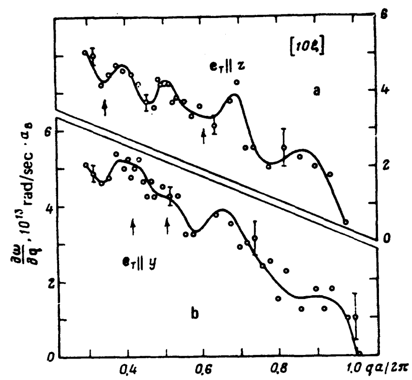

FIG. 5. Group velocity of transverse phonons along the [10ξ] direction. The arrows identify the positions of the three-particle and Kohn singularities calculated in the spherical Fermi surface approximation (a in units of a_B).

[10ξ] direction in the $\mathbf{e}_T \| y$ case (Fig. 5). These discrepancies can be due, on the one hand, to some possible systematic errors and, on the other, to incorrect theoretical estimates based on the spherical Fermi surface approximation. When the latter is allowed for, the shifts of the singularity positions δq may reach values proportional to the energy gap characterized by the dimensionless parameter $\Delta = (V_G/\varepsilon_F)$, which is observed experimentally for the singularities with $q/q_{max} = 0.42$.

However, allowance for the real Fermi surface shape affects not only the positions of the singularities but also gives rise to additional anomalies of the phonon spectrum, known as the nondiametral Kohn singularities. Electron transitions corresponding to these singularities are represented by dashed lines in Fig. 6, which shows the simplest Fermi surface in the model of two gaps in the reduced zone scheme. The continuous lines in Fig. 6 represent a triangle, which is based on the arguments $\Gamma^{(3)}$ (see Sec. 2) and which governs the position of the three-particle singularity with the phonon wave vector $q_0^{(3)}$. The values of $q_G^{(2)}$ (Fig. 7) at which there are nondiametral Kohn singularities may differ from $q_0^{(3)}$ by $\sim\delta q$. However, it can be shown that the amplitude of the singularities associated with nondiametral transitions is governed by the region of the strongest coherent modification of the electron spectrum. Since the dimensions of this region are small and of the order of the parameter Δ for simple metals, it follows that the amplitudes of nondiametral Kohn singularities are also small. In fact, these amplitudes are related to a correction to $\pi_0(\mathbf{q})$ (π_0 is the polarization operator of a noninteracting homogeneous electron gas), allowing for the nonsphericity of the Fermi surface:

$$\pi(\mathbf{q}) = \pi_0(\mathbf{q}) + \delta\pi(\mathbf{q}). \tag{8}$$

If $|\mathbf{q}|$ is close to the position of a nondiametral singularity, we find that

$$\delta\pi \propto \Delta^{1/2}, \tag{9}$$

and in all the other cases[3)] we obtain $\delta\pi \propto \Delta^2$.

Bearing in mind that

$$\Gamma^{(2)}(\mathbf{q}, -\mathbf{q}) = -\frac{1}{2}\frac{\pi(\mathbf{q})}{\varepsilon(\mathbf{q})}, \tag{10}$$

where $\varepsilon(\mathbf{q})$ is the static dielectric function, we can easily show that the correction to the square of the phonon frequency [see Eq. (2)] is associated with allowance for the real Fermi surface:

$$\delta[\omega_j^{(2)}(\mathbf{q})]^2 \propto \Delta^{1/2}\omega_p^2(V_{\mathbf{q}+G}/\varepsilon_F)^2, \tag{11}$$

the whole contribution of the third order of the perturbation theory being

$$[\omega_j^{(3)}(\mathbf{q})]^2 \propto \Delta\,\omega_p^2(V_{\mathbf{q}+G}/\varepsilon_F)^2, \tag{12}$$

where ω_p^2 is the square of the plasma frequency.

To within terms of the third order in the perturbation theory, we have

$$\omega_j^2(\mathbf{q}) = [\omega_j^{(1)}(\mathbf{q})]^2 + [\omega_{0j}^{(2)}(\mathbf{q})]^2 + \delta[\omega_j^{(2)}(\mathbf{q})]^2 + [\omega_j^{(3)}(\mathbf{q})]^2, \tag{13}$$

and the phonon frequency is

$$\omega_j(\mathbf{q}) \approx \omega_{0j}(\mathbf{q}) + \frac{1}{2\omega_{0j}(\mathbf{q})}(\delta[\omega_j^{(2)}(\mathbf{q})]^2 + [\omega_j^{(3)}(\mathbf{q})]^2), \tag{14}$$

where

$$\omega_{0j}(\mathbf{q}) = ([\omega_j^{(1)}(\mathbf{q})]^2 + [\omega_{0j}^{(2)}(\mathbf{q})]^2)^{1/2}.$$

Substituting Eqs. (11) and (12) into Eq. (14), we obtain

$$\omega_j(\mathbf{q}) \sim \omega_{0j}(\mathbf{q}) + \frac{\Delta\omega_p^2}{2\omega_{0j}(\mathbf{q})}\left(\frac{V_{\mathbf{q}+G}}{\varepsilon_F}\right)^2(\Delta^{1/2}+1). \tag{15}$$

Since the characteristic size of the interval of the wave vector variation, where $\delta[\omega^{(2)}]^2$ and $[\omega^{(3)}]^2$ are important, is of the order of δq and the changes in the corrections to $\omega_{0j}(\mathbf{q})$ are of the order of their own magnitude $\delta\omega \sim (\delta[\omega^{(2)}]^2 + [\omega^{(3)}]^2)/\omega_0$, then allowing for the smoothness of the function $\omega_{0j}(\mathbf{q})$ in the vicinity of $\mathbf{q}$ described above, we obtain $\partial\omega/\partial\mathbf{q} \propto \delta\omega/\delta q$ and, since $\delta q \propto \Delta q_{max}$, we find that

$$\frac{\partial\omega}{\partial\mathbf{q}} \propto \frac{\omega_p^2(V_{\mathbf{q}+G}/\varepsilon_F)^2}{2\omega_{0j}(\mathbf{q})q_{max}}(\Delta^{1/2}+1). \tag{16}$$

It follows from the above expression that the ratio of the contributions made to the group velocity by a nondiametral Kohn singularity and a three-particle singularity is proportional to $\Delta^{1/2}$. In the case of Al this ratio is of the order of 0.1–0.15 and the influence of a diametral singularity on the behavior of $\partial\omega/\partial\mathbf{q}$ in the vicinity of a three-particle anomaly is slight.

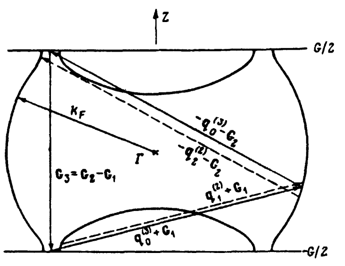

FIG. 6. Simplified Fermi surface in the model of two gaps The dashed lines are nondiametral Kohn transitions and the continuous lines represent the condition for the existence of a three-particle singularity.

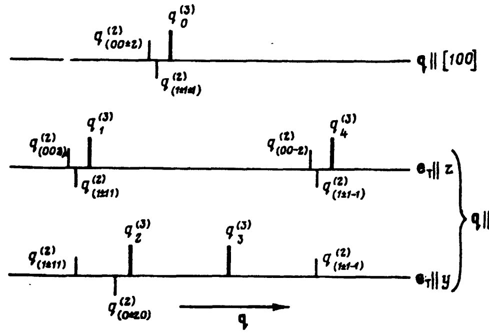

FIG. 7. Diagram showing positions of all types of singularities in the vicinity of $q/q_{max} = 0.46$ subject to allowance for the real shape of the Fermi surface ($q_G^{(2)}$ is the position of a nondiametral Kohn singularity governed by the site $\mathbf{G}$ and $q_i^{(3)}$ is the position of a three-particle singularity).

It follows from the above analysis that the experimental values of the group velocity of transverse phonons along the [100] and [10ξ] directions in the aluminum lattice demonstrate that the singularity of the dispersion branch at $q/q_{max} = 0.42$ is of the three-particle type, i.e., it is associated with a nonpair ion-ion interaction via conduction electrons. The fact that the three-particle and diametral Kohn singularities may be comparable in amplitude demonstrates the need to allow for the nonpair interaction if a correct understanding of the fine structure of the dispersion curves is desired. Undoubtedly, further experimental and theoretical studies of the Kohn and particularly three-particle singularities from the point of view of the influence of the real Fermi surface will extend considerably our knowledge of the electron and phonon spectra, and of the special features of the electron-ion interaction in metals.

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[1)]The components of the reciprocal lattice vectors are given in units of $2\pi/a$, where a is the lattice constant measured in terms of a_B.

[2)]Throughout our analysis of the results for the [10ξ] direction we shall understand that the conditions $\mathbf{e}_T \parallel z$ and $\mathbf{e}_T \parallel y$ are not satisfied rigorously.

[3)]This result was first obtained by Yu. Kagan, V. V. Pushkarev, and A. Kholas.

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