parameters, such as the mean free path, the electron-phonon coupling constant, etc.

1) The diffusion equation was solved for the first time for laser breakdown of solids in[3], but no account was taken there of the energy lost in electron-phonon collisions, which can not be neglected, as shown in[1], for the considered range of pulse durations (10^{-11}–10^{-7} sec).

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Weakly bound excitation states in a crystal

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It is shown that the formation in crystals of bound states by two elementary excitations (two phonons, a phonon and an electron) is possible for an arbitrarily weak interaction between them. This occurs near points in the quasi-momentum space of the excitations at which the two effective masses for the relative motion of the excitations become infinite. The mathematical situation here is similar to the situation that obtains in superconductors during the formation of Cooper pairs. The binding energy turns out to be exponentially small in the coupling constant.

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1. INTRODUCTION

It will be shown in this paper that the formation in crystals of bound states by two elementary excitations (two phonons, a phonon and an electron) interacting arbitrarily weakly with each other is possible. This occurs near certain special points in the quasi-momentum space of the excitations.

The question of the formation of bound states by excitations has attracted considerable attention in recent years. In Wortis's paper[1] two-magnon bound states were investigated. Cohen and Ruvalds,[2] Ruvalds and Zawadowsky,[3] and Agranovich[4] have studied the bound states of phonons. In the cases considered by these authors, however, in order for the formation of bound states to be possible, it is necessary that the phonon interaction energy exceed some threshold value. Another situation obtains, as is well known, in liquid He^4. There, two rotons with an arbitrarily weak attraction between them can form a bound state.[5–7] This is explained by the fact that the energy of the roton as a function of its momentum has a minimum on a whole sphere in momentum space. Thus, this phenomenon is closely connected with the isotropy of the liquid. Kozhushner[8] has discovered that two excitons form a bound state when they interact arbitrarily weakly with each other in a special model in which only the interaction with the nearest neighbors is taken into account.

Some examples of bound-state formation in crystals under conditions when the interaction is weak have been considered by Rashba and Levinson.[9,10] These authors were, however, concerned either with phenomena that occur when the optical-phonon dispersion is neglected or with electrons in a magnetic field, when the situation becomes one-dimensional. Meanwhile, as we shall see, the formation of weakly-bound excitation states is possible in crystals with the most general properties and, thus, should be the rule, rather than the exception.

To see this, let us consider the simpler case when two identical excitations form a bound state. (Phonons belonging to one and the same branch.) Let the dispersion law for the excitations forming the bound state have the form $\omega(\mathbf{k})$, where ω is the excitation energy and $\mathbf{k}$ is the quasi momentum. Henceforth, instead of quasi momentum, we shall always speak of momentum. In this case the question determining the bound-state energy has, as will be shown in the following section of the paper, the form

$$\lambda\int\frac{d^3q/(2\pi)^3}{\varepsilon-\omega(\mathbf{p}/2-\mathbf{q})-\omega(\mathbf{p}/2+\mathbf{q})+i0}=1. \qquad (1)$$

Here λ has the meaning of an effective coupling constant, ε is the bound-state energy, and $\mathbf{p}$ is the bound-state momentum. The function $\varepsilon(\mathbf{p})$ determined by this equation is the dispersion law for this bound state.

It is immediately clear from the form of Eq. (1) that this equation can have a solution for an arbitrarily small small value of the constant λ only if the integral on the left-hand side diverges at some values of ε and $\mathbf{p}$. Indeed, otherwise the left-hand side would, in any case, be smaller than the right-hand side; the divergence of the integral can compensate for the smallness of λ. Let us now indicate the case when such a divergence certainly occurs. For this purpose, let us note that the expression $\omega(\mathbf{p}/2+\mathbf{q})+\omega(\mathbf{p}/2-\mathbf{q})$ is an even function of $\mathbf{q}$ and, therefore, expands in even powers of the components of this vector. Let us now assume that the crystal has a symmetry axis of order higher than two, and let us direct $\mathbf{p}$ along this axis. Then for small $\mathbf{q}$

$$\omega(\mathbf{p}/2+\mathbf{q})+\omega(\mathbf{p}/2-\mathbf{q})\approx 2\omega(\mathbf{p}/2)+a_{\|}(p)q_{\|}^2+a_{\perp}(p)q_{\perp}^2+\sim q^4, \tag{2}$$

where $q_{\|}$ is the component of the vector $\mathbf{q}$ along the symmetry axis, while $q_{\perp}$ is the component of $\mathbf{q}$ in the plane perpendicular to this axis. The coefficients $a_{\|}$ and $a_{\perp}$ are functions of p, and at some value of $p=p_0$ the function $a_{\perp}$ can vanish. It is easy to understand that in this case the integral for $\mathbf{p}=\mathbf{p}_0$ and $\varepsilon=2\omega(\mathbf{p}_0/2)$ ($\mathbf{p}_0$ is a vector equal in magnitude to p_0 and directed along the symmetry axis) diverges at small $\mathbf{q}$. For $a_{\perp}=0$, it is necessary to take terms of order $q_{\perp}^4$ into account on the right-hand side of (2).[1]

To simplify the subsequent computations, we shall assume that the symmetry axis is a 6-fold axis. This assumption does not change the fundamental aspect of the work. Then the terms of fourth order in $\mathbf{q}_{\perp}$ have the same form as in the isotropic case, so that

$$\omega(\mathbf{p}_0/2+\mathbf{q})+\omega(\mathbf{p}_0/2-\mathbf{q})\approx 2\omega(\mathbf{p}_0/2)+a_{\|}(p_0)q_{\|}^2+bq_{\perp}^4. \tag{3}$$

This expression has the meaning of kinetic energy for the relative motion of the excitations (at a given value, $\mathbf{p}=\mathbf{p}_0$, of the resultant momentum). The bound state at small $\mathbf{q}$ can be formed only if this energy has at $\mathbf{q}=0$ a minimum or a maximum (and not a saddle point); in other words, if the constants $a_{\|}$ and b are of the same sign. If $a_{\|}>0$ and $b>0$, i.e., if there is a minimum, then the bound-state energy must lie below the minimum value, $2\omega(\mathbf{p}_0/2)$, of the energy of the two excitations. In the opposite case, when $a_{\|}<0$ and $b<0$, the bound-state energy lies above the maximum. Below we shall, for definiteness, consider the case of a bound state near the minimum (i.e., we shall assume that $a_{\|}>0$ and $b>0$).

It is now easy to verify that the integral in (1) diverges at small $\mathbf{q}$ when $\mathbf{p}=\mathbf{p}_0$ and $\varepsilon=2\omega(\mathbf{p}_0/2)$. Let us substitute (3) into (1), represent d^3q in the form $q_{\perp}dq_{\perp}dq_{\|}d\varphi$, and integrate over the angle φ. Then the integral assumes the form

$$\Pi=-\frac{1}{(2\pi)^2}\int\frac{dq_{\|}q_{\perp}dq_{\perp}}{\delta_0+a_{\|}q_{\|}^2+bq_{\perp}^4},$$

where we have introduced the notation $\delta_0=2\omega(\mathbf{p}_0/2)-\varepsilon$. Integrating over $r_{\|}$, we obtain

$$\Pi=-\frac{1}{4\pi a_{\|}^{1/2}}\int\frac{q_{\perp}dq_{\perp}}{(\delta_0+bq_{\perp}^4)^{1/2}}.$$

At $\delta_0=0$ this integral diverges logarithmically at small $q_{\perp}$. On the other hand, the divergence at large $q_{\perp}$ is connected with the inapplicability of the expansion (2) at such $\mathbf{q}$. In evaluating the integral, it is necessary to truncate it at some $q_{\perp}=\Lambda$ of the order of the reciprocal-lattice constant. Evaluating with allowance for this the integral for $\delta_0\ll b\Lambda^4$, and substituting into (1), we obtain

$$-\left\{\frac{\lambda}{16\pi(a_{\|}b)^{1/2}}\right\}\ln\frac{4b\Lambda^4}{\delta_0}=1,$$

whence the bound-state energy for $p=p_0$ is equal to

$$\varepsilon=2\omega(\mathbf{p}_0/2)-4b\Lambda^4\exp(-2/g),\quad g=-\lambda/8\pi(a_{\|}b)^{1/2}.$$

The quantity

$$\delta_0=4b\Lambda^4\exp(-2/g) \tag{4}$$

has the meaning of excitation binding energy for $\mathbf{p}=\mathbf{p}_0$. We see that a bound state is formed near the point $\mathbf{p}=\mathbf{p}_0$ for an arbitrarily weak interaction between the excitations. It is only necessary for the constant g to be positive, which corresponds to attraction between the excitations.[2] The binding energy, however, turns out to be exponentially small in the coupling constant. The phenomenon under consideration manifests in this an obvious similarity with the Cooper effect in superconductors. The dispersion law for the bound state, i.e., the dependence $\varepsilon(\mathbf{p})$ for $\mathbf{p}=\mathbf{p}_0$, will be determined in Sec. 3.

Let us now discuss in greater detail the question of the existence on the symmetry axis of the point $\mathbf{p}_0$ at which the coefficient $a_{\perp}$ vanishes. For this purpose, let us consider the dispersion curve $\omega(\mathbf{k})$ for the excitations forming the bound state in the case when the vectors $\mathbf{k}$ are directed along the axis. Let $\omega(k_{\|})$ have the shape shown in Fig. 1. (The excitations under consideration may, for example, be optical phonons.) If now we consider $\mathbf{k}$ not only on the axis, then the function $\omega(\mathbf{k})$ can clearly have at the point A a minimum or a saddle point and at B a maximum or a saddle point. Let the point A be a minimum. Then at $p=2k_A$, $a_{\|}>0$ and $a_{\perp}>0$. If now the point B is a maximum, then $a_{\|}(2k_B)<0$, $a_{\perp}(2k_B)<0$, and the coefficient $a_{\perp}$ should vanish somewhere in the interval $2k_A<p<2k_B$. (The vanishing, however, of $a_{\|}$, which for us is unimportant, occurs at some other point.) The same situation obtains if the points A and B are both saddle points. It is clear from the foregoing that the vanishing of $a_{\perp}$ and, consequently, the formation, when the constants have

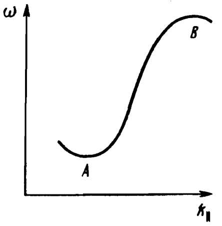
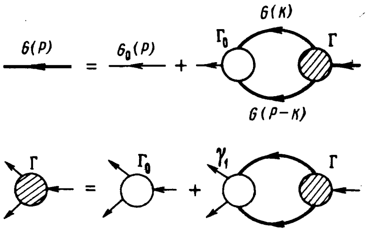


FIG. 1.

the requisite signs, of a bound state should occur in many crystals having a symmetry axis of order higher than two. Other possible cases of bound-state formation by identical excitations will be briefly discussed at the end of Sec. 3.

2. THE BASIC EQUATIONS

The investigation of the question of the bound states of excitations amounts, as a rule, to the investigation of equations of the type (1). This is not surprising, since (1) is the analog of the Schrödinger equation, written in the momentum representation, for a pair of interacting excitations. In our case, in which we are concerned with weakly-bound excitations, it is possible to obtain a closed equation in the general form without any model ideas. The point is that for a small binding energy the process in which the bound state breaks up into its constituent excitations is "almost possible." We shall describe the bound state as a spectral branch determined by a pole of the corresponding Green function.[3] Accordingly, in the equation for this function it is necessary to separate out the diagrams describing the above-indicated disintegration. Such a set of equations was derived by the present author.[11] Diagrammatically, it is of the form



(5)

The vertex parts Γ_0 and γ_1, represented by the unhatched circles, are sums of diagrams that cannot be divided between the ingoing and outgoing ends into parts connected by only one or two lines. The hatched total vertex part Γ, on the other hand, contains all the diagrams, except those connected with each other by only one line.

We shall not write out Eqs. (5) in analytic form. (See[11], formulas (3) and (27); in formula (3) the sign of the right-hand side is wrong and should be changed.) The bound-state energy is determined by the pole of the Green function $G(P)$. The equation for finding this energy is therefore obtained from (5) by neglecting the free term G_0. Let us write down this system, omitting the arguments of the vertex parts:

$$\begin{aligned} G_0^{-1}(P) &= i\int \Gamma_0 G(K)G(P-K)\Gamma\, d^4K/(2\pi)^4, \\ \Gamma &= \Gamma_0 + i\int \gamma_1 G(K)G(P-K)\Gamma\, d^4K/(2\pi)^4. \end{aligned} \tag{6}$$

Equations (6) are exact. They can be simplified, using the assumed smallness of the binding energy. Because of this smallness, the uncertainty in the energy and momenta of the excitations forming the bound state is small; it can be said that the excitations form the bound state with definite momentum values. Mathematically, this manifests itself in the fact that only the small integration domain in which the product of the Green functions is anomalously large is important. Therefore, the vertex parts can be taken out from under the sign of integration. After that, the vertex part Γ can be eliminated from the equations. Finally, the bound-state energy is determined by the equation

$$\frac{i\lambda}{(2\pi)^4}\int G(K)G(P-K)\,d^4K = 1, \tag{7}$$

where

$$\lambda = \gamma_1 + \Gamma_0^2 G_0(P). \tag{8}$$

In (7) the vertex-part arguments K and $P-K$ corresponding to the internal lines in the diagram (5) should be set equal to the energies and momenta of the excitations forming the bound state. Allowance, however, for the dependence on the bound-state momentum P, although permissible, does not also play an important role, since we are interested in only momenta near the singular point $\mathbf{p}_0$. (See the Introduction and Sec. 3.) Therefore, the coefficient λ can be assumed to be a constant. Notice also the growth of the interaction λ as we approach the pole of the Green function G_0, i.e., in the case when the bound-state spectrum is close to some branch of the ordinary excitations. We shall, however, not discuss this question in greater detail.

The Green functions G of the excitations forming the bound state can be taken in the usual form

$$G(K) = [k_4 - \omega(\mathbf{k}) + i0]^{-1}.$$

Carrying out after this the integration over the energy component of the 4-momentum $K\{k_4, \mathbf{k}\}$, we finally obtain:

$$\lambda\Pi(P) \equiv \lambda\int \frac{d^3k/(2\pi)^3}{\varepsilon - \omega(\mathbf{k}) - \omega(\mathbf{p}-\mathbf{k}) + i0} = 1 \tag{9}$$

($P = P\{\varepsilon, \mathbf{p}\}$). This equation determines the dependence $\varepsilon(\mathbf{p})$, i.e., the dispersion law for the bound state.

3. THE DISPERSION LAW FOR A BOUND STATE OF IDENTICAL EXCITATIONS

The quantity δ_0 computed in the Introduction is the binding energy of excitations with a resultant momentum $\mathbf{p} = \mathbf{p}_0$. If $\mathbf{p}$ is changed, the binding energy will change. The dispersion curve for the bound state can also be obtained from Eq. (9). In this section we shall again consider the case of the bound state of identical excitations with one and the same momentum value. In this case it is convenient to make the change of variables

$$\mathbf{k} = \mathbf{p}/2 + \mathbf{q},$$

after which (9) reduces to the Eq. (1) written out above. Let us investigate this equation in greater detail, assuming, as in the Introduction, that the crystal has a 6-fold axis, the coefficient $a_\perp$ vanishing on this axis at a point $\mathbf{p}_0$. As a preliminary, let us write down the expansion in powers of $\mathbf{q}$ of the expression $\omega(\mathbf{p}_0/2 + \mathbf{q})$:

$$\omega(\mathbf{p}_0/2+\mathbf{q})=\omega(p_0/2)+v_0q_\parallel+{}^1/_2a_\parallel q_\parallel^2+\alpha q_\parallel q_\perp^2+{}^1/_2bq_\perp^4. \tag{10}$$

The notation for the coefficients in (10) has been chosen in accordance with (3). The absence of a term with merely $p_\perp^2$ ensures the vanishing of $a_\perp(p)$.

Using (10), we find with the necessary accuracy after simple transformations that

$$\begin{aligned}\omega(\mathbf{p}/2+\mathbf{q})+\omega(\mathbf{p}/2-\mathbf{q})=2\omega(\mathbf{p}/2)+\alpha\Delta p_\parallel q_\perp^2+a_\parallel q_\parallel^2\\ +bq_\perp^4+b(\mathbf{p}_\perp\mathbf{q}_\perp)^2+{}^1/_2bp_\perp^2q_\perp^2,\end{aligned} \tag{11}$$

where $\Delta\mathbf{p}=\mathbf{p}-\mathbf{p}_0$ and $\mathbf{p}_\perp$ is the component of $\Delta\mathbf{p}$ in the plane perpendicular to the symmetry axis.

Let us determine, to begin with, $\varepsilon(\mathbf{p})$ on the symmetry axis, i.e., for $\mathbf{p}_\perp=0$. The computations in this case are again very simple:

$$\begin{aligned}\Pi=\int\frac{d^3q/(2\pi)^3}{\varepsilon-\omega(\mathbf{p}/2+\mathbf{q})-\omega(\mathbf{p}/2-\mathbf{q})}=-\frac{1}{4\pi}\int\frac{q_\perp dq_\perp}{[a_\parallel(\varepsilon'+\alpha\Delta p_\parallel q_\perp^2+bq_\perp^4)]^{1/2}}\\ =-\frac{1}{8\pi(a_\parallel b)^{1/2}}\ln\frac{4b\Lambda}{2(b\varepsilon')^{1/2}+\alpha\Delta p_\parallel}.\end{aligned} \tag{12}$$

Here we have introduced the notation $\varepsilon'=2\omega(\mathbf{p}/2)-\varepsilon$. Let us recall that, by assumption, $a_\parallel>0$ and $b>0$. Substituting (12) into (1), and solving the resulting equation for ε, we obtain

$$\varepsilon(\mathbf{p})=2\omega(\mathbf{p}/2)-[2(b\delta_0)^{1/2}-\alpha\Delta p_\parallel]^2/4b, \tag{13}$$

where δ_0 has the same meaning as in (4). Notice that Eq. (1) has, as is easy to see, a solution only if $2(b\delta_0)^{1/2}>\alpha\Delta p_\parallel$, so that the formula (13) makes sense only in this region.

The formula (13) gives the absolute value of the bound-state energy. A more interesting quantity, however, is the "binding energy," i.e., the distance of the bound-state level from the boundary of the continuous spectrum. For the excitations produced near the minimum of the expression (12), this binding energy is equal to

$$\delta(\mathbf{p})=\varepsilon_m(\mathbf{p})-\varepsilon(\mathbf{p}),$$

where $\varepsilon_m(\mathbf{p})$ is the minimum value of the expression (11) for a given $\mathbf{p}$. It is easy to verify that for p lying on the axis $\varepsilon_m=2\omega(\mathbf{p}/2)$ for $\alpha\Delta p_\parallel>0$ and $\varepsilon_m=2\omega(\mathbf{p}/2)-(\alpha\Delta p_\parallel)^2/4b$ for $\alpha\Delta p_\parallel<0$. With allowance for this, we can rewrite (13) in the final form:

$$\delta=\delta_0\begin{cases}(1-\Delta p_\parallel/r_\parallel)^2, & \Delta p_\parallel>0\\ 1-2\Delta p_\parallel/r_\parallel, & \Delta p_\parallel<0\end{cases} \tag{14}$$

where we have introduced the notation

$$r_\parallel=2(b\delta_0)^{1/2}/\alpha. \tag{15}$$

(For definiteness, we assume that $\alpha>0$.)

For $\Delta p_\parallel=r_\parallel$ the binding energy vanishes, and the bound-state level for $\Delta p_\parallel>r_\parallel$ goes off into the continuous spectrum. The point $\Delta p_\parallel=r_\parallel$ is the end point of the bound-state spectrum in the sense of the paper.[11] According to the classification of that paper, it corresponds to the second mode of termination of the spectrum. For negative values of $\alpha\Delta p_\parallel$ the binding energy increases. It should, however, be borne in mind that $|\Delta p_\parallel|$ should in any case be much less than the reciprocal-lattice constant. This means, as can easily be verified, that the binding energy in any case is much less than $(\delta_0\omega_0)^{1/2}$, where $\omega_0\sim\omega(\mathbf{p}_0/2)$ is a characteristic optical-phonon frequency.

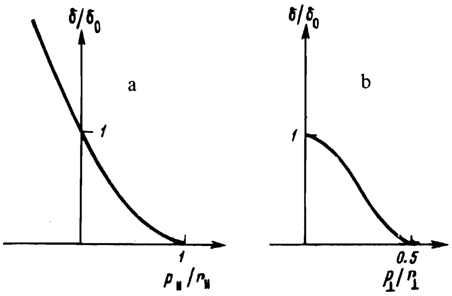


FIG. 2.

The plot of the binding energy $\delta(p_\parallel)$ is shown in Fig. 2a.

Now let the resultant momentum $\mathbf{p}$ be directed not exactly along the symmetry axis, so that $\mathbf{p}-\mathbf{p}_0$ has a component $\mathbf{p}_\perp$ perpendicular to the axis. Let us substitute (11) into the expression for Π and evaluate the $dq_\parallel$ and $dq_\perp$ integrals. Then

$$\Pi=-\frac{1}{16\pi^2(a_\parallel b)^{1/2}}\int_0^{2\pi}\ln\frac{4b\Lambda^2}{2(b\varepsilon')^{1/2}+\alpha\Delta p_\parallel+bp_\perp^2/2+bp_\perp^2\cos^2\varphi}\,d\varphi,$$

where φ is the angle between $\mathbf{q}_\perp$ and $\mathbf{p}_\perp$. The $d\varphi$ integral can be evaluated with the aid of the formula

$$\int_0^{2\pi}\ln(1+a\cos^2\varphi)\,d\varphi=2\pi\ln\frac{1+(1+a)^{1/2}}{2}. \tag{16}$$

We finally have

$$\begin{aligned}\Pi=-\frac{1}{8\pi(a_\parallel b)^{1/2}}\ln\Big\{8b\Lambda^2\Big[\Big(2(b\varepsilon')^{1/2}+\alpha\Delta p_\parallel+\frac{b}{2}p_\perp^2\Big)^{1/2}\\ +\Big(2(b\varepsilon')^{1/2}+\alpha\Delta p_\parallel+\frac{3b}{2}p_\perp^2\Big)^{1/2}\Big]^{-2}\Big\}.\end{aligned} \tag{17}$$

Substituting (17) into (9), and solving the equation, we can find $\varepsilon(\mathbf{p})$. We write out at once the expression for the binding energy $\delta(\mathbf{p})$ with allowance for the fact that the lower boundary of the continuous spectrum, $\varepsilon_m(\mathbf{p})$, now has the form

$$\begin{aligned}\varepsilon_m(\mathbf{p})=2\omega(\mathbf{p}/2)\quad\text{for}\quad\alpha\Delta p_\parallel+{}^1/_2bp_\perp^2>0,\\ \varepsilon_m(\mathbf{p})=2\omega(\mathbf{p}/2)-(\alpha\Delta p_\parallel+{}^1/_2bp_\perp^2)^2/4b\quad\text{for}\quad\alpha\Delta p_\parallel+{}^1/_2bp_\perp^2<0.\end{aligned}$$

The binding energy is equal to

$$\delta(\mathbf{p})=\delta_0\Big\{1-4\Big(\frac{p_\perp}{r_\perp}\Big)^2\Big[1-\frac{1}{4}\Big(\frac{p_\perp}{r_\perp}\Big)^2\Big]-\frac{\Delta p_\parallel}{r_\parallel}\Big\}^2 \tag{18}$$

for $\alpha\Delta p_\parallel+\frac{1}{2}bp_\perp^2>0$ and

$$\delta(\mathbf{p})=\delta_0\Big[1-\Big(\frac{p_\perp}{r_\perp}\Big)^2\Big]\Big\{1-\frac{3p_\perp^2}{r_\perp^2}+\frac{p_\perp^4}{r_\perp^4}-\frac{2\Delta p_\parallel}{r_\parallel}\Big\}$$

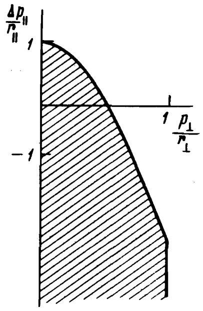


FIG. 3.

for $\alpha\Delta p_\parallel + \frac{1}{2} bp_\perp^2 < 0$; here $r_\parallel = 2^{3/2}\delta_0^{1/4}/b^{1/4}$. The dependence of δ on $p_\perp$ for $\Delta p_\parallel = 0$ is shown in Fig. 2b.

Notice that the binding energy decreases with increasing $p_\perp$, i.e., as we move away from the symmetry axis. The existence domain for the bound state, i.e., the region where $\delta(\mathbf{p}) > 0$, is hatched in Fig. 3. At the boundary, $\delta = 0$. Notice that the characteristic dimension of the existence domain in the direction perpendicular to the axis turns out to be of order $r_\perp \sim \delta_0^{1/4}$, i.e., to be much larger than $r_\parallel \sim \delta_0^{1/2}$.

We have thus far been concerned with states that form near the symmetry axis of the crystal. Let us now consider the question whether the formation of such states not on the axis, but near some "nonsymmetric" point in momentum space is possible. In this case the quadratic terms in the expression for $\omega(\mathbf{p}/2 + \mathbf{q}) + \omega(\mathbf{p}/2 - \mathbf{q})$ have the form $a_{ik} q_i q_k$. Directing the axes along the principal axes of the quadratic form $a_{ik}(\mathbf{p})$, we obtain

$$\omega(\mathbf{p}/2+\mathbf{q}) + \omega(\mathbf{p}/2-\mathbf{q}) \approx 2\omega(\mathbf{p}/2) + a_1 q_1^2 + a_2 q_2^2 + a_3 q_3^2.$$

It is clear that in order for the integral (9) to diverge, it is necessary that two of the coefficients a_i vanish at some point $\mathbf{p}_0$. Let us ascertain how many conditions should be fulfilled for that.

The vanishing of two eigenvalues means that at the point $\mathbf{p}$ the matrix a_{ik} can be represented in the form

$$a_{ik} = l_i l_k,$$

where $\mathbf{l}$ is the eigenvector (of the matrix) corresponding to that eigenvalue that does not vanish. Eliminating three of the components l_i from these six equalities, we find:

$$a_{12}^2 = a_{11}a_{22}, \quad a_{13}^2 = a_{11}a_{33}, \quad a_{23}^2 = a_{22}a_{33}. \tag{19}$$

The conditions (19) should be regarded as three equations for the determination of the three components of the vector $\mathbf{p}_0$ near which the bound state is formed. The fact that the number of equations is equal to the number of unknowns implies that such a point does, generally speaking, exist, so that the formation of such a state is possible also at points not on the axis of the crystal. Let us emphasize in this connection that the above-considered case of the formation of the state on the symmetry axis is an independent case, and not simply a particular case of a general case. Indeed, it is quite improbable that the point $\mathbf{p}_0$ will accidentally fall on the axis. Meanwhile, the arguments given in the Introduction precisely show that the location of $\mathbf{p}_0$ exactly on the axis is as probable as its location at a nonsymmetric point. On the other hand, from the experimental point of view, the search for the states lying near the axis is probably simpler because of the smaller degree of arbitrariness. Taking into account this circumstance and also the great complexity of the formulas in the nonsymmetric case, we shall not investigate this case.

Notice also that the formation of a weakly-bound state near a symmetry plane of the crystal is also possible. Indeed, for $\mathbf{p}$ lying in the symmetry plane, the terms quadratic in $\mathbf{q}$ are of the form

$$a_z q_z^2 + a_{\alpha\beta} q_\alpha q_\beta,$$

where the z axis is directed perpendicular to the plane and the indices α, β number the components of vectors in the plane. The coefficients a_z, $a_{\alpha\beta}$ depend now on the two components of the vector $\mathbf{p}$ in the plane. These two components can, generally speaking, be chosen such that a_z and one of the eigenvalues of the matrix $a_{\alpha\beta}$ vanish simultaneously. In this case the point $\mathbf{p}_0$ will lie exactly in the plane.

4. THE BOUND STATES OF DIFFERENT EXCITATIONS

Now let the excitations forming the bound states be different. Of special interest here are electron-phonon bound states in a semiconductor, i.e., weakly-bound polarons. The excitations may also be two phonons of different branches or two phonons belonging to one and the same branch, but going into the bound state with different quasi-momentum values.

The equation for the determination of the bound-state energy in the case of two different excitations also has the form (9), with the only difference that $\omega(\mathbf{k}) + \omega(\mathbf{p} - \mathbf{k})$ is replaced by

$$\omega_1(\mathbf{k}) + \omega_2(\mathbf{p}-\mathbf{k}), \tag{20}$$

where ω_1 and ω_2 are the energies of the excitations forming the bound state. In the preceding case, owing to symmetry, there could be no terms linear in $\mathbf{q}$ in the denominator of (1). Now they should first of all be eliminated. For this purpose, let us find the minimum of the expression (20) as a function of $\mathbf{k}$ for a given $\mathbf{p}$.[4] Let this minimum occur at $\mathbf{k} = \mathbf{k}_0$. (Naturally, $\mathbf{k}_0$ is a function of $\mathbf{p}$: $\mathbf{k}_0 = \mathbf{k}_0(\mathbf{p})$.) Let us set $\mathbf{k} = \mathbf{k}_0(\mathbf{p}) + \mathbf{q}$. Since the expression (20) has a minimum at $\mathbf{k} = \mathbf{k}_0$, its expansion in powers of $\mathbf{q}$ will no longer contain linear terms.[5] Let us again assume that the crystal has a symmetry axis of order greater than two. Let us direct $\mathbf{p}$ along the symmetry axis. Then

$$\begin{aligned}\omega_1(\mathbf{p}-\mathbf{k}) + \omega_2(\mathbf{k}) &= \omega_1(\mathbf{p}-\mathbf{k}_0-\mathbf{q}) + \omega_2(\mathbf{k}_0+\mathbf{q}) \\ &\approx \omega_1(\mathbf{p}-\mathbf{k}_0) + \omega_2(\mathbf{k}_0) + a_\perp q_\perp^2 + a_\parallel q_\parallel^2\end{aligned} \tag{21}$$

and the coefficient $a_\perp$ can vanish on the axis at some point $\mathbf{p} = \mathbf{p}_0$.

Notice that the earlier-considered case of identical excitations fits into this general scheme, but there, on account of the symmetry of the problem, we always had $\mathbf{k}_0 = \mathbf{p}/2$. There is, however, one important difference. It consists in the fact that now the left-hand side of (21) is no longer an even function of $\mathbf{q}$. Meanwhile, in order for a bound state to exist, it is necessary that this expression for $\mathbf{p} = \mathbf{p}_0$ contain no terms of third order in $\mathbf{q}$. This condition will be fulfilled automatically if the symmetry axis is at least a fourfold axis. The presence of such an axis is in this case a necessary condition for the existence of the effects under consideration. The formation of weakly-bound states by two different excitations at a nonsymmetric point and in a symmetry plane is impossible.

Let us again carry out specific computations for a sixfold axis. It turns out here that it is more convenient to carry out the expansion not about the point $\mathbf{k}_0(\mathbf{p})$, but about the point $\mathbf{k}_0(\mathbf{p}_\parallel)$, where $\mathbf{p}_\parallel$ is the component of $\mathbf{p}$ along the axis. In other words, we set $\mathbf{k} = \mathbf{k}_0(\mathbf{p}_\parallel) + \mathbf{q}$. Let us at once write down the expansion of (20) in powers of $\mathbf{q}$ from general considerations, leaving out the formulas connecting the expansion coefficients with the derivatives of the functions ω_1 and ω_2. It is important that when $\mathbf{p}$ is not directed exactly along the axis the point $\mathbf{k}_0(\mathbf{p}_\parallel)$ be not a minimum point and the expansion contain terms linear in $\mathbf{q}_\perp$ (but not in $\mathbf{q}_\parallel$). With allowance for this we have:

$$\omega_1(\mathbf{p}-\mathbf{k})+\omega_2(\mathbf{k})\approx\varepsilon_0(\mathbf{p})+\alpha\Delta p_\parallel q_\perp{}^2-2\beta\mathbf{p}_\perp\mathbf{q}_\perp+a_\parallel q_\parallel{}^2+bq_\perp{}^4. \tag{22}$$

We have introduced the notation

$$\varepsilon_0=\omega_1[\mathbf{p}-\mathbf{k}_0(\mathbf{p}_\parallel)]+\omega_2[\mathbf{k}_0(\mathbf{p}_\parallel)].$$

In view of the presence in (22) of a term linear in $\mathbf{p}_\perp$, it is not necessary to consider terms of higher order in this quantity.

Notice first of all that on the axis, i.e., for $\mathbf{p}_\perp = 0$, the expansions (22) and (11) coincide. This means that for a momentum directed along the axis the binding energy for different excitations is also given by the formula (14). The situation naturally changes when there is deviation from the axis. After performing the $dq_\parallel$ integration, we obtain for the integral Π the expression

$$\Pi=\frac{1}{8\pi^2 a_\parallel{}^{1/2}}\int\frac{q_\perp dq_\perp d\varphi}{(\varepsilon'+\alpha\Delta p_\parallel q_\perp{}^2-2\beta p_\perp q_\perp\cos\varphi+bq_\perp{}^4)^{1/2}} \tag{23}$$

where $\varepsilon' = \varepsilon_0 - \varepsilon$.

The integral (23) cannot be evaluated in its general form. We can obtain only asymptotic formulas for small and large $p_\perp$. We shall restrict ourselves to the determination for small and large $p_\perp$ of the boundary of the existence domain for the bound state, i.e., of the surface equation $\delta(\mathbf{p}) = 0$ in momentum space.

Let us begin with small values of $p_\perp$. Let us first of all determine the lower boundary of the continuous spectrum, i.e., the minimum value of the expression (22) for a given $\mathbf{p}$. To the minimum corresponds the value $\cos\vartheta = 1$. (For definiteness, let us assume that $\alpha > 0$, $\beta > 0$.) For $\Delta p_\parallel > 0$ and for small $p_\perp$, the term $bq_\perp^4$ is negligible near the minimum. The minimum is then attained at $q_\perp = \beta p_\perp/\alpha\Delta p_\parallel$ and the minimum value of the energy is equal to

$$\varepsilon_m=\varepsilon_0-\beta^2 p_\perp{}^2/\alpha\Delta p_\parallel \quad\text{or}\quad \varepsilon_m{}'=\beta^2 p_\perp{}^2/\alpha\Delta p_\parallel.$$

Let us denote the value of Π for $\varepsilon' = \varepsilon_m$ by Π_m, differentiate Π_m twice with respect to $f = \beta p_\perp$, and make the change of variables $q_\perp = xf/a_\perp$, where $a_\perp = \alpha\Delta p_\parallel$. (In view of the good convergence of the integral, we can replace the upper integration limit by infinity.) As a result, we have

$$\frac{\partial^2\Pi_m}{\partial f^2}=-\frac{3bf}{8\pi^2(a_\parallel^{1/2}a_\perp^{9/2})}\int_0^\infty\int_0^{2\pi}\frac{(1-x\cos\varphi)x\,dx\,d\varphi}{[1+x^2-2x\cos\varphi+(f^2b/a_\perp{}^3)x^4]^{5/2}}.$$

For small f, only large values of x are important in the integral, so that we can neglect the unit term in the denominator and restrict ourselves to the first term in the expansion of this denominator in powers of $2x\cos\varphi$. After the computations, we obtain

$$\frac{\partial^2\Pi_m}{\partial f^2}=\frac{b^{1/2}}{2\pi a_\parallel^{1/2}a_\perp{}^3} \tag{24}$$

On the other hand, for $f = 0$, as can easily be obtained directly from (23), we have

$$\Pi_m(0)=-\frac{1}{8\pi(a_\parallel b)^{1/2}}\ln\frac{4b\Lambda^2}{a_\perp},\qquad \frac{\partial\Pi_m(0)}{\partial f}=0.$$

Integrating (24) with these boundary conditions, we obtain

$$\Pi_m=-\frac{1}{8\pi(a_\parallel b)^{1/2}}\left[\ln\frac{4b\Lambda^2}{\alpha\Delta p_\parallel}-\frac{2b\beta^2 p_\perp{}^2}{\alpha^3(\Delta p_\parallel)^3}\right].$$

If we substitute this expression into Eq. (9), we directly obtain a relation between $\Delta p_\parallel$ and $p_\perp$ on the surface $\delta(\mathbf{p}) = 0$, i.e., at the boundary of the existence domain for the bound state. After simple transformations, we obtain the equation for this boundary in the form

$$1-\Delta p_\parallel/r_\parallel=(p_\perp/s_\perp)^2, \tag{25}$$

where $r_\parallel$ has the same meaning as in (15), while

$$s_\perp=2b^{1/4}\delta_0^{3/4}/\beta, \tag{26}$$

the formula (25) being valid provided $p_\perp/s_\perp \ll 1$. The quantity $s_\perp$ characterizes the transverse dimension of the existence domain for the bound state of different excitations. Notice that $s_\perp \sim \delta_0^{3/4}$, while for identical excitations the corresponding quantity is $r_\perp \sim \delta_0^{1/4}$, so that if the δ_0 in the two cases are of the same order of magnitude, then

$$s_\perp \ll r_\perp.$$

Let us now determine the boundary in the limit of large $p_\perp \gg s_\perp$. It is easy to verify that to large $p_\perp$ on the boundary correspond large negative values of $\alpha\Delta p_\parallel$.

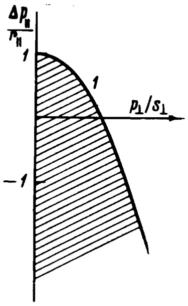


FIG. 4.

More precisely, $|\Delta p_\parallel| \gg r_\parallel$, $\Delta p_\parallel < 0$. (We assume that $\alpha > 0$ and $\beta > 0$.) In this case the term with f in the integral for Π_m is small compared to the remaining terms, and is important only near the minimum of the denominator. Therefore, we can replace in it q by its value, q_m, at the minimum. After this, the integral over $q_\perp$ can be computed as in the derivation of (12). Taking into account the fact that

$$\varepsilon_m' = -a_\perp q_m^2 + 2 f q_m - b q_m^4$$

and noting that we can, with the necessary accuracy, set

$$q_m = |a_\perp|^{1/2} / (2b)^{1/2}, \quad a_\perp = \alpha \Delta p_\parallel,$$

we find after expanding in powers of f:

$$\Pi_m = \frac{1}{16\pi^2 (a_\parallel b)^{1/2}} \int_0^{2\pi} \ln \frac{2\Lambda^2 |b\alpha\Delta p_\parallel|^{1/2}}{2^{1/2} \beta p_\perp (1 - \cos\varphi)} d\varphi = \frac{1}{8\pi (a_\parallel b)^{1/2}} \ln \frac{2\Lambda^2 |2b\alpha\Delta p_\parallel|^{1/2}}{\beta p_\perp}.$$

The $d\varphi$ integral can be evaluated according to the formula

$$\frac{1}{\pi} \int_0^\pi \ln(1 - \cos\varphi) d\varphi = -\ln 2.$$

Substituting Π_m into (9), and solving the equation, we find the equation for the boundary for large $p_\perp$:

$$-\Delta p_\parallel / r_\parallel = (p_\perp / s_\perp)^2. \tag{27}$$

Formally, this is the asymptotic form of the same parabola whose asymptotic form for small $p_\perp$ was found above. The existence domain for the bound state of different excitations is the hatched region in Fig. 4. The quantity $p_\perp / s_\perp$ is plotted along the abscissa axis, while the quantity $\Delta p_\parallel$ is plotted along the ordinate axis.

Thus, we see that bound states of the type under consideration should probably quite often exist in crystals. They should be searched for, first and foremost, near high-order symmetry axes in momentum space. The most direct method of detection is the observation of the inelastic scattering of neutrons. The exponential smallness of the binding energy is hardly a serious obstacle to their detection, since in reality the interaction is not too weak. On the other hand, the picture may be smeared because of the damping of the excitations. It is clear from the form of the basic equation (9) that, if ω_1 and ω_2 have imaginary parts γ_1 and γ_2, then they can be neglected only when the quite rigid condition $\gamma_1 + \gamma_2 \ll \delta_0$ is satisfied. The level width for the excitations forming the bound state should be less than the binding energy. Therefore, it is necessary to work at low temperatures and choose the excitation branch for which decay is forbidden.

Notice also that even if the sign of the interaction is such that the bound state is not formed, the density of two-particle states will all the same have some singularity near the point $\mathbf{p}_0$. This density remains finite at the boundary of the two-particle spectrum, which can also be revealed experimentally.

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[1)] In the model considered in[8] the right-hand side of (2) does not, at some value of $\mathbf{p}$, depend on $\mathbf{q}$ at all. In the general case such a situation is, of course, impossible.

[2)] This pertains to the case $a_\parallel > 0$, $b > 0$. In the opposite case, when $a_\parallel < 0$, $b < 0$, it is necessary for g to be negative too, so that the bound state near the maximum is formed when there is repulsion between the excitations.

[3)] It may seem that the bound state should be sought as a pole of the vertex part and not of the Green function. It can easily be seen, however, that the poles of the two functions coincide in a system in which the conversion of the excitation into two is possible.

[4)] We are again considering the case of a bound state with energy below the boundary of the continuous spectrum.

[5)] Compare similar arguments in Kazarinov and Konstantinov's paper.[12]

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