ELECTRON-PHONON STATES IN HOMOPOLAR CRYSTALS CAUSED BY A STRONG MAGNETIC FIELD

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Submitted February 20, 1969

Zh. Eksp. Teor. Fiz. 57, 1224–1230 (October, 1969)

It is shown that in strong magnetic fields the interaction of the conduction electrons with a homopolar lattice leads to a number of special features. In particular, under certain conditions the formation of electron-phonon states—magnetic "condensons"—possessing a very distinctive spectral structure becomes possible. In this article the longitudinal effective mass of the magnetic "condensons" is calculated in the limiting cases of strong and weak coupling, and also certain effects in semiconductors and semimetals which these states may lead to are indicated.

I. INTRODUCTION. CLASSICAL CONSIDERATION OF A LATTICE

IN[1] it was shown that in strong magnetic fields the interaction of a conduction electron with a classical homopolar lattice leads to the appearance of self-consistent states in which the electron deforms the lattice and is localized in the region created by its deformation; these states are energetically more favorable states of a "bare" electron in an undeformed lattice.

An attempt to find self-consistent states of a similar kind in the absence of a magnetic field was first undertaken in the work by Deĭgen and Pekar,[2] where it was shown that such states (called "condensons" by the authors) do not exist with dimensions significantly exceeding the lattice constant.

The result of article[2] is associated with the fact that without a magnetic field the appearance of a local electron state in a homopolar crystal requires a considerable deformation; in this connection for deformations of large radius the energy losses because of the increase in the free energy of the lattice turn out to be larger than the gain due to localization of the electron. In a strong magnetic field an arbitrarily weak potential well leads to the appearance of localized electronic levels;[3] therefore the self-consistent states obtained in[1] (in what follows we shall call them magnetic "condensons") are energetically favored. For the isotropic case the energy and wave function of a magnetic "condenson" have the form

$$E_0 = -\hbar^2 / 2m^* r_{z0}^2, \tag{1}$$

$$\psi_0(\mathbf{r}) = \frac{1}{\sqrt{4\pi r_{z0}\rho_0}} \frac{\exp\{-\bar{\rho}^2/4\rho_0^2\}}{\operatorname{ch}(z/r_{z0})}, \tag{2}$$

where r_{z0} denotes the radius of the state

$$r_{z0} = \frac{\hbar^2}{2m^*} \frac{16\pi\rho_0^2\rho s^2}{\varepsilon_1^2}, \tag{3}$$

m^* is the effective mass of an electron, $\rho_0 = \sqrt{c\hbar/eH}$ is the characteristic length in the magnetic field H, ϵ_1 is the deformation potential constant, ρ is the density, s is the velocity of sound, $\bar{\rho}$ and z are cylindrical coordinates with the z axis directed along the magnetic field; the energy is measured from μH. Under actual conditions r_{z0} and ρ_0 are much larger than the lattice constant, which justifies the replacement of the lattice by an elastic continuum and the application of the effective mass method. The free energy of a lattice containing a magnetic "condenson" amounts to $(\frac{2}{3})|E_0|$, i.e., the self-energy of a magnetic "condenson" is equal to $(\frac{1}{3})|E_0|$. Formulas (1) and (2) are obtained under the assumption that the electron wave function may be expanded over the states of the first Landau band (with n = 0). Taking the following bands into account lowers the energy of a magnetic "condenson"; the corrections to E_0 and ψ_0 arising in this connection are small provided

$$\frac{|E_0|}{\mu H} = \left(\frac{\rho_0}{r_{z0}}\right)^2 \ll 1. \tag{4}$$

Condition (4) is well satisfied up to actually attainable magnetic fields.

By the method of article[1] it is not difficult to obtain the energies and wave functions of the excited localized self-consistent states, if it is taken into account that as a consequence of the axial symmetry of the problem these states must be numbered by the quantum number m, the projection of the electron orbital momentum in the direction of the magnetic field. In the approximation (4) we have

$$E_m = -\hbar^2 / 2m^* r_{zm}^2, \tag{5}$$

$$\psi_m(\mathbf{r}) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \frac{\exp\{-\bar{\rho}^2/4\rho_0^2\}\,(\bar{\rho}^2/2\rho_0^2)^{m/2}}{\rho_0\sqrt{m!}} \frac{\operatorname{ch}^{-1}(z/r_{zm})}{\sqrt{2r_{zm}}}, \tag{6}$$

$$r_{zm} = (m!)^2 2^{2m}[(2m)!]^{-1} r_{z0}. \tag{7}$$

However, in view of the complexity of the problem in the general case there is no firm assurance that Eq. (6) exhausts all excited localized states of a magnetic "condenson."

We note that the well-known theorem 1 : 2 : 3 : 4 from the theory of polarons[4] is satisfied for the characteristic energies of the obtained magnetic "condenson." In general the picture of the behavior of a conduction electron in a homopolar crystal in the presence of a strong magnetic field in many respects coincides with the polaron picture; in this connection the coupling strength essentially depends on the magnitude of the magnetic field.

The transition from a classical consideration of the lattice to a quantum consideration leads to delocalization of the magnetic "condensons" and to the formation of electron-phonon states with a distinctive spectral structure (these states will also be called magnetic "condensons").

For the isotropic case and in the effective mass approximation the Hamiltonian of the system under consideration has the form

$$H=\frac{1}{2m^*}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2+\sum\hbar\omega_{\mathbf{k}}\left(a_{\mathbf{k}}^*a_{\mathbf{k}}+\frac{1}{2}\right)\times\sum\left(V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{kr}}+V_{\mathbf{k}}^*a_{\mathbf{k}}^*e^{-i\mathbf{kr}}\right), \tag{8}$$

where $a_{\mathbf{k}}^*$ and $a_{\mathbf{k}}$ are phonon creation and annihilation operators, $\omega_{\mathbf{k}} = sk$, and the interaction of an electron with the phonons is written in the deformation potential approximation, i.e., $V_{\mathbf{k}} = i\epsilon_1\sqrt{\hbar k/2V\rho s}$ (V is the volume of the crystal).

The longitudinal effective mass is determined by the dependence of the energy on the value of the projection of the total momentum in the direction of the magnetic field; the operator for this projection

$$P_z=p_z+\sum\hbar k_z a_{\mathbf{k}}^*a_{\mathbf{k}} \tag{9}$$

commutes with H.

In the following sections we calculate the longitudinal effective mass of a magnetic "condenson" in the limiting cases of strong and weak coupling, and also an attempt is made to ascertain the structure of the spectrum of these states.

2. THE CASE OF STRONG COUPLING

We shall use a variational method to construct the wave function of the ground state and of the states nearest to it (with small values of P_Z) in the case of strong coupling. In this connection it is convenient to write the Hamiltonian in the coordinate representation, introducing dimensionless real normal coordinates $q_{\mathbf{k}}$ corresponding to traveling waves (see, for example,[5]) and the quantities $p_{\mathbf{k}} = -i\partial/\partial q_{\mathbf{k}}$ which are canonically conjugate to them:

$$H=\frac{1}{2m^*}\left(\mathbf{p}+\frac{e}{2}\mathbf{A}\right)^2+\frac{1}{2}\sum\hbar\omega_{\mathbf{k}}(q_{\mathbf{k}}^2+p_{\mathbf{k}}^2)-\sqrt{2}\sum|V_{\mathbf{k}}|(q_{\mathbf{k}}\sin\mathbf{kr}+p_{\mathbf{k}}\cos\mathbf{kr}). \tag{10}$$

Although the quantities $\{q_{\mathbf{k}}\}$ do not determine the geometrical configuration of the lattice, it is convenient to write the general form of a state possessing a definite value of P_Z in terms of these coordinates:

$$\Psi_{P_z}(\mathbf{r},\{q_{\mathbf{k}}\})=e^{iP_zz/\hbar}\sum_{\{n_{\mathbf{k}}\}}a_{\{n_{\mathbf{k}}\}}^{P_z}\exp\left\{-iz\sum n_{\mathbf{k}}k_z\right\}\prod_{\mathbf{k}}\Phi_{n_{\mathbf{k}}}(q_{\mathbf{k}}); \tag{11}$$

the summation in (11) runs over all possible sets of the phonon occupation numbers $\{n_{\mathbf{k}}\}$; $a_{\{n_{\mathbf{k}}\}}^{P_z}$ are arbitrary functions of $\overline{\rho}$ and φ. First let us find a function Ψ having the form

$$\Psi(\mathbf{r},\{q_{\mathbf{k}}\})=\varphi(\mathbf{r})\prod_{\mathbf{k}}F_{\mathbf{k}}(q_{\mathbf{k}}) \tag{12}$$

and giving a minimum of the functional

$$\bar{E}(\varphi,\{F_{\mathbf{k}}\})=\int\Psi^*H\Psi\,d\tau\,\Pi\,dq_{\mathbf{k}} \tag{13}$$

under the condition

$$\int\Psi^*\Psi\,d\tau\,\Pi\,dq_{\mathbf{k}}=1.$$

Minimizing $\bar{E}$ with respect to $F_{\mathbf{k}}$ for fixed φ ($\int|\varphi|^2d\tau=1$) leads to the result

$$\Psi_{\mathbf{r}_0}=A\varphi(\mathbf{r}-\mathbf{r}_0)\prod_{\mathbf{k}}\exp\left\{-\frac{(q_{\mathbf{k}}-q_{\mathbf{k}0}(\mathbf{r}_0))^2}{2}\right\}, \tag{14}$$

where A is a normalizing factor;

$$q_{\mathbf{k}0}(\mathbf{r}_0)=\frac{\varepsilon_1}{\sqrt{V\rho s^2\hbar\omega_{\mathbf{k}}}}\int|\varphi(\mathbf{r}-\mathbf{r}_0)|^2e^{-i(\mathbf{kr}-\pi/2)}d\tau. \tag{15}$$

T The electronic part $\Psi_{\mathbf{r}_0}$ in this connection should be a normalized extremum of the functional

$$I(\varphi)=\int\varphi^*\frac{(\mathbf{p}+eA/c)^2}{2m^*}\varphi\,d\tau-\frac{\varepsilon_1^2}{2\rho s^2}\int|\varphi|^4d\tau, \tag{16}$$

which appeared in[1] in connection with a classical consideration of the lattice. Thus, if in the expansion of φ one can confine oneself to only states of the first Landau band (the possibility of such an expansion as usual is determined by condition (4)), then φ coincides with ψ_0 in formula (2). The reason for this consists in the fact that one can regard (12) as an adiabatic approximation, where φ is determined for equilibrium values of the displacements in the ground state.

Now let us construct a superposition of states $\Psi_{\mathbf{r}_0}$ with different $\mathbf{r}_0$. Since all $\mathbf{r}_0$ are equivalent, then in order to calculate the longitudinal effective mass it is necessary to select functions of the form

$$\Psi_{P_z}(\mathbf{r},\{q_{\mathbf{k}}\})=A_{P_z}\int_{-\infty}^{\infty}e^{iP_zz_0/\hbar}\Psi_{\mathbf{r}_0}\,dz_0, \tag{17}$$

where A_{P_Z} is a normalization factor, but $\mathbf{r}_0$ has a unique nonvanishing component z_0. It is easy to show that Ψ_{P_Z} is an eigenfunction of (9) corresponding to the eigenvalue P_Z. Without citing the extremely cumbersome intermediate calculations of the quantity

$$E(P_z)=\int\Psi_{P_z}^*H\Psi_{P_z}\,d\tau\,\Pi\,dq_{\mathbf{k}}, \tag{18}$$

let us write down the first two terms of its expansion in powers of P_Z, which determine the energy of the ground state and the longitudinal effective mass:

$$E(P_z)=E_0\left(1-2\frac{d}{d\beta}\ln I_2\right)+\frac{1}{2}\sum\hbar\omega_{\mathbf{k}}+\frac{P_z^2}{2m^*}\frac{W(I_1,I_2)}{I_2^2}, \tag{19}$$

where E_0 is defined by formula (1);

$$I_1(\beta)=\int_0^{\infty}\frac{y^3}{\operatorname{sh}y}\exp\left\{\beta\frac{y\operatorname{cth}y-1}{\operatorname{sh}^2y}\right\}dy, \tag{20}$$

$$I_2(\beta)=\int_0^{\infty}\frac{y}{\operatorname{sh}y}\exp\left\{\beta\frac{y\operatorname{cth}y-1}{\operatorname{sh}^2y}\right\}dy, \tag{21}$$

and

$$W(I_1,I_2)=I_1\frac{d}{d\beta}I_2-I_2\frac{d}{d\beta}I_1 \tag{22}$$

is the Wronskian of the linearly independent functions $I_1(\beta)$ and $I_2(\beta)$, i.e., for all β we have $W(I_1, I_2) \neq 0$. The dimensionless quantity β determines the strength of the coupling:

$$\beta=2\sqrt{\pi}\frac{E_0\rho_0}{\hbar s}\sim H^{3/2}. \tag{23}$$

The physical meaning of β is especially clear if it is taken into consideration that $\hbar s/\rho_0$ represents the average energy of the acoustic phonons, which most actively interact with an electron in a strong magnetic field. Since

$$\lim_{\beta\to\infty}\frac{d}{d\beta}\ln I_2=\frac{1}{3}, \tag{24}$$

then the self-energy of a magnetic "condenson" tends to $(1/3)|E_0|$ as $\beta \to \infty$, i.e., to its value for a classical lattice. As one would expect, the energy of the ground state $E(0)$ is lower than the minimum of the functional (13) for functions of the form (12).

The longitudinal effective mass $M_{\parallel}^*$ of a "condenson" is given by

$$\frac{M_{\parallel}^*}{m^*} = \frac{I_2^2}{W(I_1, I_2)} \tag{25}$$

For the validity of the method used in this section, it is necessary that the inequality

$$M_{\parallel}^* \gg m^*. \tag{26}$$

be satisfied, which at the present time apparently falls outside the framework of experimental feasibilities.

A machine calculation of $M_{\parallel}^*$ according to formula (25) gives the following result for $\beta = 5$; $M_{\parallel}^* = 2.6\ m^*$, and for $\beta = 10$ we have $M_{\parallel}^* = 6.2\ m^*$:

It is not difficult to carry out a calculation of the longitudinal effective mass for a classical consideration of the lattice. The expression obtained in this connection agrees with the asymptotic form of (25) as as $\beta \to \infty$:

$$\frac{M_{\parallel}^*}{m^*} \approx \frac{4}{15}\beta^2 + O(\beta). \tag{27}$$

We note that the values of β at which the asymptotic form (27) appears are considerably larger than those at which inequality (26) begins to be satisfied.

3. THE CASE OF WEAK COUPLING

In this case it is more convenient to use the Hamiltonian written in the form (8). Let us calculate the longitudinal effective mass to second order in perturbation theory. As a basis for the electron part we choose the functions

$$\varphi_{m,\,p_z}(\mathbf{r}) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \frac{e^{iP_z z/\hbar}}{\sqrt{L}} \left(\frac{\bar{\rho}^2}{2\rho_0^2}\right)^{m/2} \frac{\exp\{-\bar{\rho}^2/4\rho_0^2\}}{\rho_0\sqrt{m!}} \tag{28}$$

with $m \geq 0$, i.e., we again confine our attention to states of the first Landau band; for this purpose in the case of weak coupling the quantity μH must be larger than the characteristic energy of the phonons which are actively interacting with the electron:

$$\hbar s / \rho_0 \mu H \equiv \delta < 1. \tag{29}$$

For $m^* = m_0$ inequality (29) is well satisfied for $H > 10^5$ Oe. Writing the basis in cylindrical coordinates is dictated by the axial symmetry of the problem; one can show that as a consequence of the isotropy of the crystal, functions (28) with different values of m are not coupled by the interaction Hamiltonian in second-order perturbation theory, i.e.,

$$\sum_{\lambda'} \frac{(H_{int})_{\lambda\lambda'}(H_{int})_{\lambda'\lambda''}}{E_\lambda - E_{\lambda'}} = C_{\lambda\lambda''}\delta_{mm''}, \tag{30}$$

where $\lambda = (\{n_k\}; m, p_z)$ denotes the set of quantum numbers which characterize the stationary states of H_0 ($H = H_0 + H_{int}$).

As the initial state we choose $\lambda = (\{0\}; m, p_z)$. A simple calculation leads to the following expression for the second-order correction to the electron's energy:

$$E^{(2)}_{p_z\, m} = \sum_{\mathbf{k}} \left(\frac{p_z^2}{2m^*} - \frac{(\hbar k_z - p_z)^2}{2m^*} - \hbar s k\right)^{-1} \exp\{-k_\rho^2\rho_0^2/2\}\,|V_{\mathbf{k}}|^2, \tag{31}$$

where k_z and k_ρ denote the components of $\mathbf{k}$, respectively, along and transverse to the magnetic field. Thus, in second-order perturbation theory the degeneracy in m is not removed.

With the aid of Eq. (31) one can write the relative change of the longitudinal effective mass as follows:

$$\frac{M_{\parallel}^*}{m^*} = 1 + \frac{4}{\pi(2\pi)^{1/4}}\sqrt{\beta}\,\delta^{3/2}\int_0^\infty e^{-\delta^2 y}\,dy \int_0^\infty \frac{\sqrt{x}\sqrt{x+y}\,dx}{(x+\sqrt{x+y})^3} \tag{32}$$

A numerical calculation indicates that the inner integral in (32) for $y > 0.1$ coincides with its asymptotic expression $(1/8)\pi y^{-1/4}$ correct to within 1 to 2%: Therefore, for $\delta < 1$ when the contribution of the outer integral over the interval $(0, 1/10)$ is small, one can represent expression (32) with an error of the order of 1% in the form

$$\frac{M_{\parallel}^* - m^*}{m^*} = \frac{\Delta m^*}{m^*} = \frac{1}{2}\Gamma\left(\frac{3}{4}\right)\frac{1}{(2\pi)^{1/4}}\sqrt{\beta} \approx 0.4\sqrt{\beta}. \tag{33}$$

Thus, it turns out that in the weak coupling limit the longitudinal effective mass is determined by the same parameter β as for strong coupling although the energy E_0, with the aid of which the quantity β was introduced, loses its clear physical meaning in the case of weak coupling.

Formula (33) is valid under the condition $\Delta m^* \ll m^*$, which corresponds to $\beta \ll 1$. However, for typical semiconductors and magnetic fields of 10^5 to 10^6 Oe, the quantity $\beta = 0(1)$. In the case of intermediate coupling an attempt to evaluate the effective mass of a magnetic "condenson" with the aid of the methods which are applicable in the theory of polarons[6,7] encountered a number of fundamental difficulties. If one "matches" expressions (25) and (33), extrapolating them to the region $\beta = 0(1)$, then as a result a very smooth curve is obtained which gives $\Delta m^* \approx 0.5\ m^*$ for $\beta = 1$. Although the thus obtained values of the effective mass can only be justified emotionally, it is difficult to conceive of anything which would allow a large error in this connection.

4. MAGNETIC "CONDENSONS" IN SEMICONDUCTORS AND SEMIMETALS

In conclusion let us make a few remarks about possible manifestations of magnetic "condensons." Any important effects associated with them can appear only in an "ultraquantum" case, when the characteristic energy of the "bare" electrons, measured from μH, is considerably smaller than μH and at temperatures less than the self-energy of a magnetic "condenson." These conditions apparently are realized for certain semiconductors and semimetals in magnetic fields of 10^5 to 10^6 Oe for temperatures of the order of a few degrees.

The role of the anisotropy of the bare effective mass of the electrons may turn out to be extremely important. If the equal-energy surfaces near the bottom of the band are ellipsoids of revolution, as they are in Ge and Si, then all of the formulas obtained for the case of a scalar effective mass remain in force if the magnetic field is directed along the axis of revolution. In this connection the longitudinal mass $m_{\parallel}^*$ ($\beta \sim m_{\parallel}^*$) of the electron appears in the expressions for the self-energy and for the longitudinal mass of the magnetic

"condenson," but the criteria (4) and (29) are better satisfied the smaller the electron's transverse mass $m_\perp^*$. Therefore, for example, in Ge where $m_\parallel^* \approx 20\, m_\perp^*$, magnetic "condensons" should appear most clearly of all for magnetic field directions which are close to the directions of the largest axes of the effective mass ellipsoids.

We note that a calculation of the spectrum of a magnetic "condenson" without using perturbation theory leads to the removal of the degeneracy in m; for a classical consideration of the lattice this splitting is determined by formula (5). The removal of the degeneracy in m may lead to the appearance of a number of peaks in the density of states of the magnetic "condensons," i.e., the corresponding region of the absorption spectrum must bear a clearly expressed nonmonotonic character.

The effects of magnetic "condensons" as charge carriers will be considered in a separate article. We only note that in a transverse electric field the nature of the motion of a magnetic "condenson" may differ from diffusive motion, to which the existing theories of galvanomagnetic phenomena in semiconductors and semimetals in the presence of strong magnetic fields[8,9] lead.

I wish to take this opportunity to express my gratitude to I. M. Lifshitz, É. I. Rashba, V. L. Vinetskiĭ, and V. P. Galaĭko for a discussion of this work and for valuable comments.

[1] L. S. Kukushkin, ZhETF Pis. Red. 7, 251 (1968) [JETP Lett. 7, 194 (1968)].

[2] M. F. Deĭgen and S. I. Pekar, Zh. Eksp. Teor. Fiz. 21, 803 (1951).

[3] L. S. Kukushkin, Zh. Eksp. Teor. Fiz. 54, 1213 (1968) [Sov. Phys.-JETP 27, 648 (1968)].

[4] S. I. Pekar, Issledovaniya po élektronnoĭ teorii kristallov (Investigations in the Electron Theory of Crystals), Gostekhizdat, 1951.

[5] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford, 1954 (Russ. Transl., IIL, M. 1961).

[6] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. 90, 297 (1953).

[7] R. P. Feynman, Phys. Rev. 97, 660 (1955).

[8] E. Adams and T. Holstein, J. Phys. Chem. Solids 10, 254 (1959).

[9] R. Kubo, S. J. Miyake, and N. Hashitsume, in Solid State Physics (F. Seitz and D. Turnbull, eds.), Vol. 17, pp. 269–364, Academic Press, New York, 1965.

Translated by H. H. Nickle
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