THE ZONE ENERGY SPECTRUM IN THE PRESENCE OF A MAGNETIC FIELD

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Eigenfunctions (in the **k**-representation) are derived which describe the motion of an electron with an arbitrary dispersion law in a magnetic field, account being taken of two zones (and in particular of overlapping ones). A criterion for the applicability of the one-zone approximation is obtained.

THE state of an electron moving in the periodic field of a crystal is described, as is well known, by the wave vector **k** and by the number of the allowed energy zone s. If the crystal is placed in an external field, electric or magnetic, the eigenfunction of the electron is generall described in the form of an expansion

$$\psi = \sum_s \int g_s(\mathbf{k})\,\psi_{\mathbf{k}s}\,d\mathbf{k}, \qquad (1)$$

covering all zones. However, if the external field satisfies the conditions for quasi-classical behavior (in the case of a magnetic field, this means that the minimum radius of rotation of the electron $\alpha_0 = \sqrt{\hbar c/eH}$ must be significantly larger than the lattice constant a), then a single zone can play the principal role in the expansion (1), as before. The aim of the present note is the clarification of the condition of admissibility of such a single zone approximation and the discovery of the eigenfunction (1) for this case. For simplicity of description, we shall consider only two zones, s and r.

We give the name "jump at a given point" to the energy difference $E_s(\mathbf{k}) - E_r(\mathbf{k})$ at a given point of **k**-space. Such a discontinuity can exist even in the presence of zones overlapping in energy. Inasmuch as $E_s(\mathbf{k})$ and $E_r(\mathbf{k})$ are different functions of **k**, the discontinuity at the point as a rule exists although the case of coincidence of E_s and E_r for some **k** can occur (degenerate zones). It will be shown below that the condition for admissibility of the single zone approximation in the magnetic field is the existence of a sufficiently large discontinuity at points lying on a given isoenergetic surface.

The problem of taking neighboring zones into account was considered previously by the author,[1] and also, in a much less general form, by Adams,[2] and Luttinger and Kohn.[3] In the presence of a magnetic field directed along the z axis and described by the vector potential $A_x = -Hy$, $A_y = A_z = 0$, it is expedient to write the expansion (1) in Bloch eigenfunctions, as was shown by the author:[4,1]

$$\psi_{\mathbf{k}s} = \sum_{\mathbf{h}} b_{\mathbf{h}s}(k_1, k_2, k_3)\, e^{i(\mathbf{k}+2\pi\mathbf{h})\mathbf{r}}, \qquad (2)$$

in which k_1 is replaced by $k_1 + y/\alpha_0^2$. We use Eq. (I) of reference 1 for $g_s(\mathbf{k})$, setting the potential of the electric field in it equal to zero, keeping the non-diagonal (interzone) "magnetic terms" of order α_0^{-2}, and leaving out two zones. Equation (I) can be described in the case under consideration in the form of a set of equations

$$\hat{E}_s g_s - \alpha_0^{-2}\hat{H}_{sr} g_r = E g_s, \qquad \hat{E}_r g_r - \alpha_0^{-2}\hat{H}_{rs} g_s = E g_r. \qquad (3)$$

Here (see, for example, references 4 and 1) $\hat{E}_s$ is the operator obtained from $E_s(k_1, k_2, k_3)$ by the substitution $k_1 \to k_1 - (1/i\alpha_0^2)\,\partial/\partial k_2$ and $\hat{H}_{sr}$ is an operator of the same type as $\hat{E}_s$, $\hat{E}_r$, depending, however, not only on the dispersion law of the electron in the crystal, but also on the wave functions in the zones s and r.

Those states are of interest to us in which g_r is small in comparison with g_s. We satisfy the system (3) by setting

$$g_r = \alpha_0^{-2}\Phi(\mathbf{k})\, g_s. \qquad (4)$$

Discarding terms of order α_0^{-4}, we obtain for g_s the "single zone" equation $\hat{E}_s g_s = E g_s$, the solution of which, as shown in reference 4, has the form

$$g_s = \left(\frac{\partial E_s}{\partial \varkappa_{1s}}\right)^{-1/2} \exp\left\{ + i\alpha_0^2 k_1 k_2 - i\alpha_0^2 \int_0^{k_2} \varkappa_{1s}\, dk_2 \right\},$$

$\varkappa_{1s}$ is the solution of the equation $E_s(\varkappa_{1s}, k_2, k_3) = E$.

Substituting (4) in the second equation of (3), we find $\Phi(\mathbf{k})$ (we can remove this quantity from

under the operator $\hat{E}_r$ since it is slowly changing). The action of the operator $\hat{H}_{rs}$ on g_s reduces after transformation to multiplication of g_s by the function $F_{rs}(\mathbf{k})$, which depends on the dispersion law and the wave functions in both zones [see (2)]:

$$F_{rs}(\mathbf{k}) = \sum_{\mathbf{h}} b_{\mathbf{h}r}(\mathbf{k}) \left\{ \frac{\hbar^2}{m}(k_2 + 2\pi h_2) \frac{\partial b_{\mathbf{h}s}}{\partial k_1} - \frac{\partial b_{\mathbf{h}s}}{\partial k_2} \frac{\partial E_s}{\partial k_1} \right\}. \quad (5)$$

The final form of g_r will be

$$g_r(\mathbf{k}) = \frac{i\alpha_0^{-2} F_{rs}(k)}{E_r(\varkappa_{1s}, k_2, k_3) - E_s(\varkappa_{1s}, k_2, k_3)} g_s(\mathbf{k}). \quad (6)$$

Consequently, the criterion for the admissibility of the single zone approximation has the form

$$|E_r(\mathbf{k}) - E_s(\mathbf{k})| \gg \alpha_0^{-2} F_{rs}. \quad (7)$$

The quantity F_{rs} is of order $\hbar^2/m^*$, where m^* is the effective mass in the basic zone (s); therefore, the inequality (7) can be written in the form

$$|E_r(\mathbf{k}) - E_s(\mathbf{k})| \gg \mu^* H. \quad (8)$$

It must be kept in mind that the inequalities (8) and (7), in accord with (8), must hold at points in $\mathbf{k}$-space lying on a surface of constant energy $E_s(\mathbf{k}) = E$.

Without calculation, we write down the corresponding criterion for an electron placed in crossed homogeneous magnetic H and electric F fields [it is assumed that the principal reason for the appearance of interzone terms is the electric field; in other words, we have the criterion (8)]:

$$|E_r(\mathbf{k}) - E_s(\mathbf{k})| \gg eFam/m^*, \quad (9)$$

(a is the lattice constant). In the absence of a magnetic field, as was shown in reference 1, the inequality (9) holds again; however, in the presence of a magnetic field, only those points of $\mathbf{k}$-space enter into (9) which lie on a surface of constant energy.

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[1] G. E. Zilberman, JETP **36**, 1465 (1959), Soviet Phys. JETP **9**, 1040 (1959).

[2] E. Adams, Phys. Rev. **89**, 63 (1953).

[3] J. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

[4] G. E. Zil'berman, JETP **32**, 296 (1957); **33**, 387 (1957); Soviet Phys. JETP **5**, 208 (1957); **6**, 299 (1958).

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