

netization, thus working against the antiferromagnetic exchange as well as the anisotropy forces.

With regard to the distribution of the ferromagnetic spin density, it is difficult on the basis of these few reflections to assign any unique interpretation to our results. What is clear, however, is that the ferromagnetic component has a significant different spin density distribution from the antiferromagnetic component. In other words, the spin density in this compound must be thought of as a vector rather than a scalar function, that is, varying spatially in direction as well as magnitude. It may very well be that this is a special case of a more general phenomenon that occurs whenever spin-orbit coupling is present. Because of the smallness of

the effect, it is impossible in the present case to get much of a detailed picture of such a spin density, other than to show that it exists and probably resides in directions away from the antiferromagnetic superexchange bonds. It is planned to investigate the phenomenon further in other antiferromagnets where the canting angle is larger, such as the rare-earth orthoferrites.

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One-Dimensional Equation for a Two-Dimensional Bloch Electron in a Magnetic Field

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The properties of the symmetry-adapted functions for the irreducible representations of the magnetic translation group are used to derive a one-dimensional difference-differential equation for a two-dimensional Bloch electron in a constant magnetic field.

THE dynamics of an electron in a two-dimensional periodic potential and a constant magnetic field perpendicular to the plane of motion is discussed. Using symmetry-adapted functions, defined previously, an exact one-dimensional Schrödinger equation for this "two-dimensional Bloch electron in a magnetic field" has been derived. Since no approximations were introduced in this derivation, our one-dimensional equation contains all the information for describing the dynamics of the problem. By contrast, in all other existing methods, such as the effective-mass approximation, the equations are approximate.

It is well known that the energy spectrum of a free electron in a magnetic field consists of two parts: one part is connected with the motion in the direction of the magnetic field and is continuous; the other part comes from the motion in the plane perpendicular to the magnetic field and is discrete. The effective-mass approximation¹⁻³ shows that one may expect this same division of the energy spectrum to hold also in the case of a Bloch electron in a magnetic field. Since quantum

effects in solids are connected with the discrete part of the energy spectrum, it is of great interest to investigate the behavior of a Bloch electron in the plane perpendicular to the external magnetic field.

To derive the one-dimensional equation, symmetry-adapted functions for a Bloch electron in a magnetic field⁴ are used. In the case of "rational" magnetic fields^{5,6} these functions are given by

$$\psi_j^{lk}(\mathbf{r}) = \exp\{i\mathbf{k}\cdot\mathbf{r}\} \exp\left\{-i\left(j + \frac{1}{4\pi}\mathbf{K}_2\cdot\mathbf{r}\right)\frac{n}{N}\mathbf{K}_1\cdot\mathbf{r}\right\} \times w_{lk}(\mathbf{r} + j\mathbf{a}_2) \cdots \quad (1)$$

Here j takes values from 0 to $N-1$, l is the magnetic-band index, \mathbf{K}_1 and \mathbf{K}_2 are unit-cell vectors of the reciprocal lattice,

$$\mathbf{k} = m_1\mathbf{K}_1/N + m_2\mathbf{K}_2/N, \quad 0 \leq m, m_2 < 1 \quad (2)$$

⁴ J. Zak, Phys. Rev. **134**, A1602, A1607 (1964).

⁵ The rationality of the magnetic field is defined here by the relation $\mathbf{H}\cdot\mathbf{a}_1\times\mathbf{a}_2/(hc/|e|) = n/N$, where \mathbf{H} is the magnetic field, $\mathbf{a}_1, \mathbf{a}_2$ are the unit cell vectors, $hc/|e|$ is the elementary fluxon, and n, N are integers. This relation differs by a factor of 2 from the relation (42) in Ref. 4 and is more convenient, because it leads to representations of dimensionality N for both even and odd N . [See also E. Brown, Phys. Rev. **133**, A1038 (1964) and Ref. 6.]

⁶ J. Zak, Phys. Rev. **136**, A776 (1964).

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¹ E. I. Blount, Phys. Rev. **126**, 1636 (1962).

² A. B. Pippard, Proc. Roy. Soc. (London) **A270**, 1 (1962).

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

and the function w_{lk} satisfies the conditions

$$w_{lk}(\mathbf{r} + \mathbf{a}_1) = w_{lk}(\mathbf{r}) \quad (3)$$

$$w_{lk}(\mathbf{r} + N\mathbf{a}_2) = \exp\{im\mathbf{K}_1 \cdot \mathbf{r}\} w_{lk}(\mathbf{r}). \quad (4)$$

The two-dimensional Schrödinger equation for a Bloch electron in a magnetic field is

$$\{[\mathbf{p} + (e/c)\mathbf{A}]^2/2m + V(\mathbf{r})\}\psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (5)$$

Let us find the equation that the function $w_{lk}(\mathbf{r} + j\mathbf{a}_2)$ in Eq. (1) satisfies⁷ (the index l is omitted here because it does not enter the equation). Since the function w_k is periodic in direction \mathbf{a}_1 [relation (3)] it can be expanded in a Fourier series

$$w_{lk}(\mathbf{r} + j\mathbf{a}_2) = \sum_m C_m[\mathbf{K}_2 \cdot (\mathbf{r} + j\mathbf{a}_2)] \exp\{im\mathbf{K}_1 \cdot \mathbf{r}\}. \quad (6)$$

From Eq. (4) we obtain the following relation between the coefficients:

$$C_{m+lN}[\mathbf{K}_2 \cdot (\mathbf{r} + j\mathbf{a}_2 + lN\mathbf{a}_2)] = C_m[\mathbf{K}_2 \cdot (\mathbf{r} + j\mathbf{a}_2)]. \quad (7)$$

This recurrence formula allows one to find all the coefficients when n coefficients, say, C_0, C_1, \dots, C_{n-1} , are known. Expanding the periodic potential $V(\mathbf{r})$ in a Fourier series

$$V(\mathbf{r}) = \sum_m V_m(\mathbf{K}_2 \cdot \mathbf{r}) \exp\{im\mathbf{K}_1 \cdot \mathbf{r}\}, \quad (8)$$

by substituting the symmetry adapted function (1) into the Schrödinger equation (5), and by using relations (6) and (7) we obtain n coupled equations for defining the coefficients C_m [$m=0, 1, \dots, n-1$]. These coupled equations will not be written down here⁸; instead we treat the special case for $n=1$. In this case only one coefficient, say C_0 , has to be defined and its equation is as follows (we put $j=0$ because the energy does not depend on this index):

$$\left[\frac{1}{2m} \left(p_y \hat{K}_2 + \hbar \mathbf{k} - \frac{\hbar K_1 K_2}{2\pi N} y \hat{K}_1 \right)^2 + V \left(p_y \frac{2\pi N}{\hbar K_1 K_2}, y \right) \right] C_0(y) = EC_0(y). \quad (9)$$

Here \hat{K}_1 and \hat{K}_2 are unit vectors in the direction of the unit-cell vectors $\mathbf{K}_1, \mathbf{K}_2$, respectively,

$$y = \hat{K}_2 \cdot \mathbf{r}, \quad p_y = \hat{K}_2 \cdot \mathbf{p}, \quad (10)$$

$$V \left(p_y \frac{2\pi N}{\hbar K_1 K_2}, y \right) = \sum_l V_l(y) \exp \left\{ il p_y \frac{2\pi N}{\hbar K_2} \right\}. \quad (11)$$

For a discussion of Eq. (9), it is more convenient to perform a unitary transformation and to introduce the dependence of \mathbf{k} into the potential energy. This is

⁷ A similar method was used in the paper by P. G. Harper, Proc. Phys. Soc. (London) A68, 879 (1955). However, Harper uses different starting functions which are not specified according to the irreducible representations of the magnetic translation group. It is therefore doubtful whether these functions can be solutions of Schrödinger's equation.

⁸ The case of the coupled equations will be discussed in a future publication.

achieved by the following transformation:

$$\psi(y) = \exp \left\{ im_1 \frac{2\pi}{\hbar K_2} p_y \right\} \exp \left\{ im_2 \frac{K_2}{N} y \right\} C_0(y). \quad (12)$$

The final equation is

$$\left[\frac{1}{2m} \left(p_y \hat{K}_2 - \frac{\hbar K_1 K_2}{2\pi N} y \hat{K}_1 \right)^2 + V \left(p_y \frac{2\pi N}{\hbar K_1 K_2} - m_2 \frac{2\pi}{K_1}, y + m_1 \frac{2\pi}{K_2} \right) \right] \psi(y) = E\psi(y) \quad (13)$$

or, according to definition (11) of the potential energy,

$$\begin{aligned} & \frac{1}{2m} \left(p_y \hat{K}_2 - \frac{\hbar K_1 K_2}{2\pi N} y \hat{K}_1 \right)^2 \psi(y) \\ & + \sum_l V_l \left(y + m_1 \frac{2\pi}{K_2} \right) \exp \{ -2\pi i l m_2 \} \\ & \times \psi \left(y + \frac{2\pi N}{K_2} l \right) = e\psi(y). \quad (13a) \end{aligned}$$

Equation (13), or (13a), is a one-dimensional differential-difference equation which replaces the two-dimensional Schrödinger Eq. (5). For deriving Eq. (13), or (13a), we used the rationality condition on the magnetic field⁵ with $n=1$

$$\mathbf{H} \cdot \mathbf{a}_1 \times \mathbf{a}_2 / (hc/|e|) = 1/N. \quad (14)$$

Apart from condition (14) no other assumptions have been made.

The energy spectrum that follows from Eq. (13), or (13a), is in agreement with the general description given in Refs. 4 and 6, and in the paper cited in Ref. 5. For a fixed \mathbf{k} vector (fixed m_1 and m_2), we get an infinite set of energy levels. If one ignores the dependence of the potential of its first coordinate, i.e., if one assumes from the beginning a one-dimensional equation,² this set of energy levels will be discrete, because for very large y one can neglect V in Eq. (13) and one gets a simple harmonic-oscillator equation. This is no longer true when V depends also on p_y . In this latter case, the energy spectrum for a fixed \mathbf{k} can be either discrete or continuous: for the discrete case the dependence of the energy on \mathbf{k} will lead to a magnetic band structure or what is usually called Landau-level broadening⁶; the continuous case is more complicated and requires special investigation.

The dependence of E on \mathbf{k} is given through the dependence of the potential energy on \mathbf{k} . Thus, the symmetry of the energy as a function of the \mathbf{k} vector is defined by the symmetry of the potential energy.

Equation (13), or (13a), is very convenient for applying a perturbation procedure when the potential energy can be considered as a small perturbation. Equation (13a) shows at once the orbits that will be coupled by the periodic potential, namely, those orbits will be coupled that are shifted by $(2\pi N/K_2)l$, for any integer l .

Equation (13) [and also Eq. (13a)] becomes much simpler for the special case of cubic symmetry

$$\left[\frac{1}{2}\hbar\omega(q^2+p^2)+V(\lambda p-m_2a, \lambda q+m_1a)\right]\psi(q)=E\psi(q) \quad (15)$$

where

$$\omega = |e|H/mc, \quad \lambda q = y, \quad (\hbar/\lambda)p = p_y, \\ \lambda^2 = \hbar c/eH, \quad [p, q] = -i.$$

For a one-dimensional potential the energy spectrum of Eq. (15) will be independent of the particular coordinate upon which the potential energy depends. This is to be expected physically, because for a magnetic field perpendicular to the plane of motion both directions x and y are equivalent.

As an example, let us treat Eq. (15) for the potential

$$V = V_0(\cos 2\pi x/a + \cos 2\pi y/a). \quad (16)$$

We have

$$\left[\frac{1}{2}\hbar\omega(q^2+p^2)+V_0\cos(2\pi\lambda p/a-2\pi m_2)\right. \\ \left.+V_0\cos(2\pi\lambda q/a+2\pi m_1)\right]\psi(q)=E\psi(q). \quad (17)$$

Equation (17) looks very simple and is fully symmetric in q and p . It can be called the Mathieu problem for a two-dimensional Bloch electron in a magnetic field.

Because of the symmetry in q and p the potential energy of the Hamiltonian in Eq. (17) contains a diagonal part with respect to states of a harmonic oscillator. To find this diagonal part let us write the Hamiltonian H of Eq. (17) in terms of annihilation (y) and creation (y^\dagger) operators

$$y = (q+ip)/\sqrt{2}, \\ y^\dagger = (q-ip)/\sqrt{2}. \quad (18)$$

We get

$$H = H_0 + H',$$

$$H_0 = \frac{\hbar\omega}{2}(y^\dagger y + y y^\dagger) \\ + V_0 \exp\left(-\frac{\pi N}{2}\right) [\cos 2\pi m_1 + \cos 2\pi m_2] \\ \times \sum_{s=0}^{\infty} (-1)^s \frac{(\pi N)^s}{(s!)^2} y^{\dagger s} y^s, \quad (19a)$$

$$H' = \frac{V_0}{2} \exp\left(-\frac{\pi N}{2}\right) \sum_{r \neq s=0}^{\infty} M_{rs}(m_1 m_2) \\ \times \frac{[(\sqrt{2}\pi/a)\lambda]^{r+s}}{r!s!} y^{\dagger r} y^s, \quad (19b)$$

where N is given by relation (14), and

$$M_{rs}(m_1 m_2) \\ = i^{r+s} \exp(2\pi i m_1) + (-i)^{r+s} \exp(-2\pi i m_1) \\ + (-1)^s \exp(2\pi i m_2) + (-1)^r \exp(-2\pi i m_2). \quad (20)$$

Equations (19), (19a), and (19b) show the structure of the Hamiltonian: H_0 is diagonal in the harmonic-oscillator states, while H' has only off-diagonal elements. By neglecting H' in the Hamiltonian [Eq. (19)] we get the following energy spectrum:

$$E_n^{(0)} = \hbar\omega(n + \frac{1}{2}) + V_0(\cos 2\pi m_1 + \cos 2\pi m_2) \\ \times L_n(\pi N) \exp(-\frac{1}{2}\pi N), \quad (21)$$

where $L_n(\pi N)$ is a Laguerre polynomial. Expression (21) gives a very simple description of the Landau-level broadening and was also obtained by a perturbation treatment in Ref. 6.

It is interesting to note that by using Pippard's argument² it is very easy to derive the magnetic breakdown criterion^{1,2} from relation (21). To do this, let us evaluate the second term in Eq. (21) for large quantum numbers n (metals). The order of magnitude of this term can be found by using the asymptotic expression for $L_n(\pi N)$. We have

$$V_0(\pi N n)^{-1/4} (\cos 2\pi m_1 + \cos 2\pi m_2). \quad (22)$$

According to Pippard,² magnetic breakdown occurs when the broadening caused by the term [Eq. (22)] is smaller than $\hbar\omega$

$$\hbar\omega > 4V_0(\pi N n)^{-1/4}. \quad (23)$$

Since $V_0 \sim \Delta E$ (the first Fourier coefficient of the potential V_0 is of the order of the energy gap ΔE), and since both n and N are of the order of $E_F/\hbar\omega$ (E_F is the Fermi energy), relation (23) leads to the usual magnetic breakdown criterion

$$\Delta E < (\hbar\omega E_F)^{1/2}.$$

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