Proper Functions for a Bloch Electron in a Magnetic Field*

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Functions are defined as products of a properly symmetrized function for a free electron in a magnetic field and of a Bloch-type function. An equation is derived for the Bloch-type function, and it is shown that in general the energy for a Bloch electron in a magnetic field is obtained by superimposing Landau levels on the energy spectrum of the crystal. The treatment is based on the symmetry of the equation for a Bloch electron in magnetic field.

I. INTRODUCTION

In developing the effective-mass approximation the solution of Schrödinger's equation for a Bloch electron in a magnetic field is expanded in Bloch functions or Kohn-Luttinger–type functions.[1–3] In doing so great difficulties arise because the magnetic field introduces terms into Schrödinger's equation which in the basis of Bloch functions give infinite matrix elements. It was pointed out[4] that from symmetry arguments one should not expect the Bloch functions to be a proper system of functions for expanding the solution of a Bloch electron in a magnetic field. The reason for this is that the magnetic translation group[5] is not a subgroup of the usual translation group, and therefore the Bloch functions which are symmetry-adapted for the usual translation group are not suitable for constructing functions with the proper symmetry of the magnetic translation group.

In this paper symmetry adapted functions are constructed for a Bloch electron in a magnetic field in the same form as Bloch functions are constructed. The latter consist of a product of two functions:

$$\psi_k(\mathbf{r})=\exp\{i\mathbf{k}\cdot\mathbf{r}\}u_k(\mathbf{r}). \tag{1}$$

The first factor is a free-electron function, while the second is a periodic function with the periodicity of the potential energy. Function (1) is an eigenfunction of the translation operators

$$T(\mathbf{R}_n)=\exp\{(i/\hbar)\mathbf{p}\cdot\mathbf{R}_n\}, \tag{2}$$

with $\mathbf{p}$ the momentum operator and $\mathbf{R}_n$ a Bravais lattice vector. In fact, the free-electron function itself is an eigenfunction of the translation operators (2), and the periodic function $u_k(\mathbf{r})$ is introduced in order that $\psi_k(\mathbf{r})$ be a solution of Schrödinger's equation.

The same idea will be used in the second section of this paper for constructing functions for a Bloch electron in a magnetic field. We will look for functions that are symmetry adapted with respect to the magnetic translation group,[6] and that are written as a product of two functions: a function that is a solution for an electron in a magnetic field properly symmetrized to be an eigenfunction of the magnetic translation operators[4,7] for a Bloch electron in a magnetic field, and a function that is analogous to a Bloch function. In the last section we derive an effective Schrödinger's equation for a Bloch electron in a magnetic field, and find a general picture for the energy spectrum.

II. CONSTRUCTION OF THE FUNCTIONS

First, symmetry-adapted functions are constructed for the magnetic translation group from the eigenfunctions for an electron in a magnetic field. To do this we assume that we know the solutions of the equation

$$\frac{(\mathbf{p}+(e/c)\mathbf{A})^2}{2m}\psi(\mathbf{r})=E\psi(\mathbf{r}), \tag{3}$$

where $e>0$ and $\mathbf{A}$ is the vector potential in the gauge

$$\mathbf{A}=\tfrac{1}{2}[\mathbf{H}\times\mathbf{r}]. \tag{4}$$

$\mathbf{H}$ is the magnetic field. We also assume that the third axis is chosen in the direction of the magnetic field, and that otherwise the coordinate system is arbitrary.[8] The operators that commute with the Hamiltonian in (3) are[4]

$$\tau(\mathbf{R})=\exp\{(i/\hbar)(\mathbf{p}-(e/c)\mathbf{A})\cdot\mathbf{R}\}, \tag{5}$$

where $\mathbf{R}$ is an arbitrary vector. For our choice of the coordinate system the operators $\tau(\mathbf{a})$ and $\tau(\mathbf{c})$ commute ($\mathbf{a}$ is a vector in the direction of the first axis, $\mathbf{c}$ in the direction of the third axis), and we can always choose the solutions of Eq. (3) to be also eigenfunctions of $\tau(\mathbf{a})$ and $\tau(\mathbf{c})$:

$$\left.\begin{aligned}\tau(\mathbf{a})\psi_q&=\exp\{i\mathbf{q}\cdot\mathbf{a}\}\psi_q\\ \tau(\mathbf{c})\psi_q&=\exp\{i\mathbf{q}\cdot\mathbf{c}\}\psi_q\end{aligned}\right\}. \tag{6}$$

The functions ψ_q are therefore specified by the two-dimensional vector $\mathbf{q}$ in plane 1–3. This specification

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[6] J. Zak, Phys. Rev. **134**, A1607 (1964).
[7] E. Brown, Phys. Rev. **133**, A1038 (1964).
[8] The explicit expression for the function $\psi(\mathbf{r})$ is known in a Cartesian coordinate system and can therefore be obtained in any system by a coordinate transformation.

follows from the symmetry of the problem. There is also a quantum number n that defines the Landau levels. The solutions of Eq. (3) are therefore fully specified by $\mathbf{q}$ and $n:\psi_{nq}$. The eigenvalues of Eq. (3) depend only on n and q_H (the component of $\mathbf{q}$ in the direction $\mathbf{H}$):

$$E_{nq_H}=(n+\tfrac{1}{2})\hbar\omega+(\hbar^2q^2{}_H)/(2m). \tag{7}$$

In a Cartesian coordinate system ψ_{nq} is given[9]

$$\psi_{nq}(\mathbf{r})=A_n\exp\{-ixy/2\lambda^2+i\mathbf{q}\cdot\mathbf{r}\}\phi_n((y-q_x\lambda^2)/\lambda), \tag{8}$$

where A_n is a normalization constant and $\lambda=(\hbar c/eH)^{1/2}$ is the radius of the first cyclotron orbit.

The equation for a Bloch electron in a magnetic field is

$$\left[\frac{(\mathbf{p}+(e/c)\mathbf{A})^2}{2m}+V(\mathbf{r})\right]\psi=E\psi, \tag{9}$$

and the operators that commute with the Hamiltonian in (9) are the magnetic translation operators[5,7]:

$$\tau(\mathbf{R}_n)=\exp\{(i/\hbar)(\mathbf{p}-(e/c)\mathbf{A})\cdot\mathbf{R}_n\}. \tag{10}$$

As was shown before,[5,6] it is possible to construct a group of the operators (10), called the magnetic translation group, and to find symmetry adapted functions for this group. However, for arbitrary magnetic fields no wave-type solutions of the equation (9) exist, and since in this paper we are interested in constructing Bloch-type functions, we will therefore deal with "rational" magnetic fields[4,7,10]:

$$\frac{\mathbf{H}\cdot\mathbf{a}_1\times\mathbf{a}_2}{hc/e}=\frac{2n}{N}, \tag{11}$$

where $\mathbf{a}_1$, $\mathbf{a}_2$ are unit cell vectors, $\mathbf{H}$ is the magnetic field chosen in the direction of the third unit cell vector $\mathbf{a}_3$, and n, N are integers with no common factor. When condition (11) is fulfilled, the magnetic translation group possesses a commutative subgroup[4] which can be constructed on the vectors:

$$\mathbf{R}_N=n_1\mathbf{a}_1+n_2N\mathbf{a}_2+n_3\mathbf{a}_3, \tag{12}$$

where n_1, n_2, n_3 are integers. It thus follows that for "rational" magnetic fields solutions of Eq. (9) can be constructed which are also eigenfunctions of the magnetic translation operators $\tau(\mathbf{R}_N)$. We will construct such functions in the following way. Let us note that without requiring that the functions satisfy Eq. (9), we can easily find functions that are eigenfunctions of all the operators $\tau(\mathbf{R}_N)$ by properly symmetrizing the solutions ψ_{nq} of Eq. (3) for an electron in a magnetic field. Such a symmetrization was already carried out before[7,4] for functions in a Cartesian coordinate system, and a similar result is obtained for functions ψ_{nq} in a general coordinate system:

$$\phi_{nk}(\mathbf{r})=\sum_{m=-\infty}^{\infty}\exp\{-2\pi imm_2\}\tau(mN\mathbf{a}_2)\psi_{nq}(\mathbf{r}), \tag{13}$$

where

$$\mathbf{k}=\mathbf{q}+m_2(\mathbf{K}_2/N)=m_1\mathbf{K}_1+m_2(\mathbf{K}_2/N)+\mathbf{m}_3\mathbf{K}_3. \tag{14}$$

Here $\mathbf{K}_1$, $\mathbf{K}_2$, and $\mathbf{K}_3$ are the unit cell vectors of the reciprocal lattice (the vector $\mathbf{q}$ is limited to vary in the two-dimensional Brillouin Zone). The coordinate system in which the functions ψ_{nq} were found is now chosen to coincide with the directions $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ of the unit cell vectors. It is clear that the functions ϕ_{nk} are eigenfunctions of the commuting operators $\tau(\mathbf{R}_N)$:

$$\tau(\mathbf{R}_N)\phi_{nk}(\mathbf{r})=\exp\{i\mathbf{k}\mathbf{R}_N\}\phi_{nk}(\mathbf{r}). \tag{15}$$

For the operators $\tau(\mathbf{a}_1)$ and $\tau(\mathbf{a}_3)$, relation (15) follows from (6), and for $\tau(N\mathbf{a}_2)$ it follows from the symmetrization procedure (13).

After having functions $\phi_{nk}(\mathbf{r})$ with the transformation properties (15), we can now look for functions which, apart from having the latter transformation properties, will also satisfy Schrödinger's Eq. (9). The most natural way to do this is to look for functions which are products of $\phi_{nk}(\mathbf{r})$ with an unknown function $w_{nk}(\mathbf{r})$:

$$\Phi_{nk}(\mathbf{r})=\phi_{nk}(\mathbf{r})w_{nk}(\mathbf{r}). \tag{16}$$

In order for $\Phi_{nk}(\mathbf{r})$ to be an eigenfunction of all the magnetic translation operators $\tau(\mathbf{R}_N)$, i.e.,

$$\tau(\mathbf{R}_N)\Phi_{nk}(\mathbf{r})=\exp\{i\mathbf{k}\cdot\mathbf{R}_N\}\Phi_{nk}(\mathbf{r}), \tag{17}$$

the functions $w_{nk}(\mathbf{r})$ have to be periodic with the periods $\mathbf{a}_1$ and $N\mathbf{a}_2$:

$$w_{nk}(\mathbf{r}+\mathbf{R}_N)=w_{nk}(\mathbf{r}). \tag{18}$$

The index n is introduced in $w_{nk}(\mathbf{r})$ to show that in general the latter will depend on the Landau level index n; this dependence will arise from the requirement that $\Phi_{nk}(\mathbf{r})$ satisfies Schrödinger's equation.

The functions $\Phi_{nk}(\mathbf{r})$ have a very simple structure, which is in full analogy with the Bloch functions (1): The first factor $\phi_{nk}(\mathbf{r})$ is the function for a "free" electron in a magnetic field (in the Bloch functions, the first factor is a free-electron function), while the second factor $w_{nk}(\mathbf{r})$ is periodic [Eq. (18)] and plays the same role in the functions $\Phi_{nk}(\mathbf{r})$ as the periodic part $u_{nk}(\mathbf{r})$ plays in the Bloch function.

Another interesting point about the functions $\Phi_{nk}(\mathbf{r})$ is that they are of the same form as those obtained in the effective mass approximation.[1] This fact becomes obvious if we define the function $\Phi_{nk}(\mathbf{r})$ in a slightly different way:

$$\bar{\Phi}_{nk}=\phi_{n0}(\mathbf{r})\exp\{i\mathbf{k}\cdot\mathbf{r}\}w_{nk}(\mathbf{r})=\phi_{n0}(\mathbf{r})\bar{\psi}_{nk}(\mathbf{r}). \tag{19}$$

It is clear that $\bar{\Phi}_{nk}(r)$ also satisfies relation (17) because

[9] M. H. Johnson, B. A. Lippmann, Phys. Rev. 76, 828 (1949).

[10] For the purpose of this paper, it is more convenient to have the "rationality" condition with the factor 2 on the right-hand side because then the representation of the operator $\tau(\mathbf{R}_N)$ is $\exp\{i\mathbf{k}\cdot\mathbf{R}_N\}$ [Eq. (10) in Ref. 4].

$\phi_{n0}(\mathbf{r})$ satisfies (15) for $\mathbf{k}=0$. In addition, the functions

$$\bar{\psi}_{nk}(\mathbf{r})=\exp\{i\mathbf{k}\cdot\mathbf{r}\}w_{nk}(\mathbf{r}) \qquad (20)$$

have the same transformation properties under the operations $T(\mathbf{R}_N)$ as the Bloch functions have. Indeed,

$$T(\mathbf{R}_N)\bar{\psi}_{nk}(\mathbf{r})=\exp\{i\mathbf{k}\cdot\mathbf{R}_N\}\bar{\psi}_{nk}(\mathbf{r}), \qquad (21)$$

which is just a transformation that a Bloch function $\psi_k(\mathbf{r})$ undergoes. We have therefore shown that a general solution of the Eq. (9) for a Bloch electron in a magnetic field can be written as a product of a solution $\phi_{n0}(\mathbf{r})$ of a free electron in a magnetic field, and of a function $\bar{\psi}_{nk}(\mathbf{r})$ that has the transformation properties of a Bloch function. In the effective-mass approximation the result is very similar.[1] There the function is given by a product of a solution (unsymmetrized) for a free electron in a magnetic field, and of a Bloch function for a given $\mathbf{k}$. In the functions $\bar{\Phi}_{nk}(\mathbf{r})$ the Bloch function is replaced by the function $\bar{\psi}_{nk}(\mathbf{r})$, which satisfies the same transformation relation (21) as a Bloch function ψ_k. The similarity between the functions $\bar{\Phi}_{nk}$ and the functions obtained in the effective-mass approximation is thus very close.

To conclude this section let us find the expansion of $\bar{\psi}_{nk}(\mathbf{r})$ in Bloch functions. It should be noted that the wave vector $\mathbf{k}$ in $\bar{\Phi}_{nk}$ is defined according to (14) and therefore varies only in a part of the Brillouin zone. This was caused by the fact that the commutative magnetic translation group was defined on the Bravais lattice vectors $\mathbf{R}_N$. Take a Bloch function ψ_{k_j} for any wave vector $\mathbf{k}_j$ which differs from $\mathbf{k}$ by a vector $(2\pi/N)jK_2$, with $j=0, 1, \cdots, N-1$. All such Bloch functions ψ_{k_j} undergo the transformation

$$T(\mathbf{R}_N)\psi_{k_j}=\exp\{i\mathbf{k}\cdot\mathbf{R}_N\}\psi_{\kappa_j}. \qquad (22)$$

It therefore follows that the expansion of $\bar{\psi}_{nk}(\mathbf{r})$ in Bloch functions will be

$$\bar{\psi}_{nk}(r)=\sum_{lj} C_{lj}\psi_{lk_j}, \qquad (23)$$

where l is the band index and

$$\mathbf{k}_j=\mathbf{k}+(2\pi/N)j\mathbf{K}_2,\quad j=0,1,\cdots,N-1. \qquad (24)$$

Using expansion (23) and the expression (19) for $\bar{\Phi}_{n\kappa}$ we can now state that a solution of the equation for a Bloch electron in a magnetic field for a given $\mathbf{k}$ can be written as a product of a properly symmetrized function for a free electron in a magnetic field $\phi_{n0}(\mathbf{r})$, and of a sum over Bloch functions for different bands and for $\mathbf{k}_j$ given by (24) with a fixed $\mathbf{k}$.

III. EQUATION FOR $\bar{\psi}_{nk}$

In this section we derive an equation for $\bar{\psi}_{nk}$. Let us put $\bar{\Phi}_{nk}$ from relation (19) into Schrödinger's equation (9):

$$\left[\frac{(p+(e/c)\mathbf{A})^2}{2m}+V(\mathbf{r})\right]\phi_{n0}\bar{\psi}_{nk}=E\phi_{n0}\bar{\psi}_{nk}. \qquad (25)$$

According to the construction of ϕ_{n0} [relation (13) for $\mathbf{k}=0$], it satisfies the following equation:

$$\frac{(\mathbf{p}+(e/c)\mathbf{A})^2}{2m}\phi_{n0}(\mathbf{r})=\hbar\omega(n+\tfrac{1}{2})\phi_{n0}(\mathbf{r}). \qquad (26)$$

Thus, by differentiating the product $\phi_{n0}\bar{\psi}_{nk}$ in Eq. (25) and by dividing both sides of (25) by $\phi_{n0}(\mathbf{r})$, the following equation is obtained for $\bar{\psi}_{nk}$:

$$\left[\frac{p^2}{2m}+V(r)+\hbar\omega(n+\tfrac{1}{2}) + \frac{(1/m)(\mathbf{p}+(e/c)\mathbf{A})\phi_{n0}(\mathbf{r})}{\phi_{n0}(\mathbf{r})}\cdot\mathbf{p}\right]\bar{\psi}_{nk}=E\bar{\psi}_{nk}. \qquad (27)$$

Since $\bar{\psi}_{nk}$ has to satisfy relation (21), and since Eq. (27) was derived from general symmetry considerations, we have to expect that the operator on the right-hand side of Eq. (27) will commute with all the translations $T(\mathbf{R}_N)$. Otherwise, it would be impossible to require that the solutions of Eq. (27) satisfy also relation (21). In order to check that the operator on the right-hand side of Eq. (27) commutes with $T(\mathbf{R}_N)$, we have to check that

$$\frac{(\mathbf{p}+(e/c)\mathbf{A})\phi_{n0}(\mathbf{r})}{\phi_{n0}(\mathbf{r})}\cdot\mathbf{p}$$

commutes with $T(\mathbf{R}_N)$, because it is obvious that the other terms of the above operator commute with $T(\mathbf{R}_N)$. According to the definition of $\phi_{nk}(\mathbf{r})$ [relation (13)], we have

$$\begin{aligned}T(\mathbf{R}_N)\phi_{nk}(\mathbf{r}) &= \sum_{m=-\infty}^{\infty}\exp\{-2\pi imm_2\}T(\mathbf{R}_N)\tau(mN\mathbf{a}_2)\psi_{nq}(\mathbf{r})\\ &= \sum_{m=-\infty}^{\infty}\exp\{-2\pi imm_2\}\times\exp\left\{\frac{i}{\hbar}\frac{e}{c}\mathbf{A}\cdot\mathbf{R}_N\right\}\tau(mN\mathbf{a}_2)\tau(\mathbf{R}_N)\psi_{nq}(\mathbf{r})\\ &= \sum_{m=-\infty}^{\infty}\exp\{-2\pi imm_2\}\exp\left\{\frac{i}{\hbar}\frac{e}{c}\mathbf{A}\cdot\mathbf{R}_N\right\}\times\tau((m+n_2)N\mathbf{a}_2)\tau(n_1\mathbf{a}_1+n_3\mathbf{a}_3)\psi_{nq}(\mathbf{r}).\end{aligned}$$

Since $\psi_{nq}(\mathbf{r})$ satisfies Eq. (6), we finally have

$$T(\mathbf{R}_N)\phi_{n0}(\mathbf{r})=\exp\left\{\frac{i}{\hbar}\frac{e}{c}\mathbf{A}\cdot\mathbf{R}_N\right\}\phi_{n0}(\mathbf{r}). \qquad (28)$$

Thus

$$T(\mathbf{R}_N)\frac{(\mathbf{p}+(e/c)\mathbf{A})\phi_{n0}(\mathbf{r})}{\phi_{n0}(\mathbf{r})}\cdot\mathbf{p}=\frac{[\mathbf{p}+(e/c)\mathbf{A}+(e/c)\mathbf{A}(\mathbf{R}_N)]\exp\{(i/\hbar)(e/c)\mathbf{A}(\mathbf{r}+\mathbf{R}_N)\cdot\mathbf{R}_N\}\phi_{n0}(\mathbf{r})}{\exp\{(i/\hbar)(e/c)\mathbf{A}(\mathbf{r}+\mathbf{R}_N)\cdot\mathbf{R}_N\}\phi_{n0}(\mathbf{r})}\cdot\mathbf{p}$$

$$=\frac{(\mathbf{p}+(e/c)\mathbf{A})\phi_{n0}(\mathbf{r})}{\phi_{n0}(\mathbf{r})}\cdot\mathbf{p}. \quad (29)$$

The last equality follows from the relation

$$\mathbf{p}\exp\left\{\frac{i}{\hbar}\frac{e}{c}\mathbf{A}\cdot\mathbf{R}_N\right\}\phi_{n0}(\mathbf{r})$$
$$-\exp\left\{\frac{i}{\hbar}\frac{e}{c}\mathbf{A}\cdot\mathbf{R}_N\right\}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{R}_N)\right]\phi_{n0}(\mathbf{r}). \quad (30)$$

We have therefore proved that the operator on the right-hand side of Eq. (27) is invariant under all the translations $T(\mathbf{R}_N)$. The functions $\bar{\psi}_{nk}(\mathbf{r})$ can thus be chosen in the form (20), and the equation for $w_{nk}(\mathbf{r})$ will be

$$\left[\frac{(\mathbf{p}+\hbar\mathbf{k})^2}{2m}+V(\mathbf{r})+\hbar\omega(n+\tfrac{1}{2})+\frac{(1/m)(\mathbf{p}+(e/c)\mathbf{A})\phi_{n0}(\mathbf{r})}{\phi_{n0}(\mathbf{r})}\right.$$
$$\left.\times(\mathbf{p}+\hbar\mathbf{k})\right]w_{nk}(\mathbf{r})=Ew_{nk}(\mathbf{r}). \quad (31)$$

Equation (31) can be considered as an effective Hamiltonian equation for the problem of a Bloch electron in a magnetic field. As we see, this Hamiltonian depends on the Landau level n and in addition contains the whole Bloch Hamiltonian. It therefore follows that in general the energy levels and the functions of Eq. (31) will depend on both the energy-band index of the crystal l and the Landau level index n: $E=E_{ln}(k)$, $w=w_{lnk}$. This result is a general expression of the effective-mass approximation. In particular, when the last term in Eq. (31) can be neglected (it is not clear at this stage under what conditions this can be done), the energy and the functions will be as follows:

$$E_{ln}(\mathbf{k}_j)=\epsilon_l(\mathbf{k}_j)+\hbar\omega(n+\tfrac{1}{2}), \quad (32)$$

$$w_{ln\mathbf{k}_j}=\psi_{lk_j}(\mathbf{r}). \quad (33)$$

Here $\epsilon_l(\mathbf{k}_j)$ is the energy of a Bloch electron in band l with the wave vector $\mathbf{k}_j$. The function $\bar{\Phi}_{nk}$ will thus be a product of a free-electron function in a magnetic field ϕ_{n0} and a Bloch function $\psi_{lk_j}(\mathbf{r})$:

$$\bar{\Phi}_{lnk}(\mathbf{r})=\phi_{n0}(\mathbf{r})\psi_{lk_j}(\mathbf{r}). \quad (34)$$

It is clear that such a simple form of the spectrum (32), when the energy of a Bloch electron in a magnetic field is given by a sum of a Bloch energy for a fixed $\mathbf{k}_j$ and an energy of a Landau level n is very idealized and, in general, we will have to take into account the perturbation that is introduced by the last term in Eq. (31). The development of a perturbation procedure for Eq. (31) is a subject for a future publication. Here we will note that the functions w_{lnk} satisfy relation (18), and therefore Eq. (31) has to be investigated only in a finite region: $\mathbf{a}_1$, $N\mathbf{a}_2$, $\mathbf{a}_3$. This is a very great advantage, because there is no need to carry out integrations over the whole space, when a perturbation theory is developed. As was mentioned in the introduction such integrations lead to infinite matrix elements and to serious complications.

In conclusion we find that in general a solution of Schrödinger's equation for a Bloch electron in a magnetic field (9) can be written as follows:

$$\bar{\Phi}_{lnk}(\theta)=\phi_{n0}(\mathbf{r})\bar{\psi}_{lnk}(\mathbf{r}), \quad (35)$$

where $\phi_{n0}(\mathbf{r})$ is a solution of the equation for a free electron in a magnetic field (13), and $\bar{\psi}_{lnk}(\mathbf{r})$ is a Bloch-type function that satisfies Eq. (27). The index l specifies an energy band of the crystal, the index n-a Landau level and $\mathbf{k}$ follows from the symmetry of the problem.

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