Dynamics of Electrons in Solids in External Fields. II

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Further applications of the *kq* representation to the dynamics of electrons in solids are carried out. The Bloch theory of conduction electrons is reformulated in the new representation. The symmetry of the problem is discussed in light of the *kq* representation. In particular, the motion of an electron in both a periodic potential and a constant magnetic field is developed on a firm quantum-mechanical basis. A complete and orthonormal set of magnetic Bloch functions is defined. These functions are shown to obey the magnetic translation symmetry, and it is for this reason that they are very useful in describing the motion of a Bloch electron in a magnetic field.

I. INTRODUCTION

IN a recent publication[1] (to be referred to as I) the *kq* representation was used for describing the motion of electrons in solids in external fields. It was shown that well-known results of the dynamics can be reproduced by using this representation in a very simple and natural way. The reason for this is that **k** and **q** are the most natural coordinates for problems connected with periodic potentials. Indeed, the quasimomentum **k** gives the momentum of an electron in the crystal within **K**, a vector of the reciprocal lattice. **k** is a conserved quantity and is of very great importance in the Bloch theory of conduction electrons. The coordinate **q** has the meaning of a quasicoordinate and gives the location of the electron inside a unit cell of the Bravais lattice without specifying in which of the unit cells the electron is. Such a specification of the position is very closely connected with the motion in a periodic potential because the latter is a function of the quasicoordinate **q** only. The *kq* representation uses therefore the natural coordinates **k** and **q** of a crystal and the very important concepts of unit cells in the direct and reciprocal lattice. One is to expect that the dynamics of electrons in solids will assume the simplest form when described in terms of the quasimomentum **k** and the quasicoordinate **q**.

In this paper further applications of the *kq* representation to the Bloch theory of conduction electrons are given. In Sec. II the motion of an electron in a periodic potential is described in the new representation. This section serves also as an introduction to the later material and gives a general view on conservation laws in the motion of electrons in solids. Section III deals with the problem of a Bloch electron in a magnetic field.[1–4] The use of the *kq* representation leads to a definition of a complete and orthonormal set of functions. These functions are used in developing an effective-Hamiltonian theory to any order in the magnetic field. In Sec. IV it is shown that the set of functions defined in this paper obey the magnetic translation symmetry. This is pointed out as a very important reason for the usefulness of these functions. By using them, the effective-Hamiltonian theory becomes very transparent and straightforward.

II. MOTION OF AN ELECTRON IN A PERIODIC POTENTIAL

Let us start this section by reviewing the main features of the *kq* representation. As was shown in I, translations in direct and reciprocal spaces

$$T(\mathbf{R}_n)=\exp(i\mathbf{p}\cdot\mathbf{R}_n)\,, \qquad (1)$$

$$T(\mathbf{K}_m)=\exp(i\mathbf{r}\cdot\mathbf{K}_m)\,, \qquad (2)$$

form a complete set of commuting operators and can therefore be used for specifying a complete set of states in quantum mechanics. The eigenstates $\psi_{kq}(\mathbf{r})$ of operators (1) and (2) for a special choice of phase are [I(30)]

$$\psi_{kq}(\mathbf{r})=[\tau/(2\pi)^3]^{1/2}\sum_{\mathbf{R}_n}\exp(i\mathbf{k}\cdot\mathbf{R}_n)\delta(\mathbf{r}-\mathbf{q}-\mathbf{R}_n)\,. \qquad (3)$$

The basic operators **p** and **r** then become [I(31), (32)]

$$\mathbf{p}=-i(\partial/\partial\mathbf{q})\,, \qquad (4)$$

$$\mathbf{r}=i(\partial/\partial\mathbf{k})+\mathbf{q}\,. \qquad (5)$$

k and **q**, the quasimomentum and quasicoordinate in (3), assume values in the first Brillouin zone and the unit cell of a Bravias lattice correspondingly. Any function $\psi(\mathbf{r})$ in the r representation is connected to its *kq* transform $C(\mathbf{kq})$ as follows:

$$\psi(\mathbf{r})=\int d\mathbf{k}\,d\mathbf{q}\,C(\mathbf{kq})\psi_{kq}(\mathbf{r})\,. \qquad (6)$$

The inverse transformation is

$$C(\mathbf{kq})=\int \psi(\mathbf{r})\psi_{kq}^*(\mathbf{r})d\mathbf{r}\,. \qquad (6')$$

Because of the structure of $\psi_{kq}(\mathbf{r})$, Eq. (3), the bound-

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ary conditions on $C(\mathbf{kq})$ are [I(40), (41)]

$$C(\mathbf{k}+\mathbf{K}_m,\mathbf{q})=C(\mathbf{kq}), \tag{7}$$

$$C(\mathbf{k},\mathbf{q}+\mathbf{R}_n)=\exp(i\mathbf{k}\cdot\mathbf{R}_n)C(\mathbf{kq}). \tag{8}$$

Schrödinger's equation for a Bloch electron in magnetic and electric fields $\mathbf{H}$ and $\mathbf{E}$ in the kq representation is [I(36)]

$$\left\{\left[-i\frac{\partial}{\partial\mathbf{q}}+\frac{e}{2c}\mathbf{H}\times\left(i\frac{\partial}{\partial\mathbf{k}}+\mathbf{q}\right)\right]^2\Big/2m+V(\mathbf{q})+e\mathbf{E}\cdot\left(i\frac{\partial}{\partial\mathbf{k}}+\mathbf{q}\right)\right\}C(\mathbf{kq})=\epsilon C(\mathbf{kq}). \tag{9}$$

It is important to point out that no matter what physical problem one considers, the boundary conditions on $C(\mathbf{kq})$ are the same [conditions (7) and (8)].

In this section we limit ourselves to the discussion of the motion of a Bloch electron in the absence of external fields. Equation (9) then will become

$$\left[\frac{1}{2m}\left(-i\frac{\partial}{\partial\mathbf{q}}\right)^2+V(\mathbf{q})\right]C(\mathbf{kq})=\epsilon C(\mathbf{kq}). \tag{10}$$

This equation is the same as in the r representation

$$\left[\frac{1}{2m}\left(-i\frac{\partial}{\partial\mathbf{r}}\right)^2+V(\mathbf{r})\right]\psi(\mathbf{r})=\epsilon\psi(\mathbf{r}). \tag{11}$$

The latter has as its solutions Bloch functions

$$\psi_{nk_B}(\mathbf{r})=\exp(ik_B\cdot\mathbf{r})u_{nk_B}(\mathbf{r}), \tag{12}$$

where $\mathbf{k}_B$ is the quasimomentum of the state and n is the band index (the reason for using a notation $\mathbf{k}_B$ is explained below). By using formula (6′) one finds

$$\begin{aligned}C_{nk_B}(\mathbf{kq})&=\int d\mathbf{r}\,\psi_{nk_B}(\mathbf{r})\psi_{kq}^*(r)\\&=\psi_{nk_B}(\mathbf{q})\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m)\\&=\psi_{nk}(\mathbf{q})\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m).\end{aligned} \tag{13}$$

Relation (13) gives the Bloch functions in the kq representation. It is easy to check that if $\psi_{nk_B}(\mathbf{r})$ is a solution of Eq. (11) corresponding to the energy $\epsilon_n(\mathbf{k}_B)$, so will $C_{nk_B}(\mathbf{kq})$ be a solution of Eq. (10) for the same energy. The physical meaning of solution (13) is very simple: $C_{nk_B}(\mathbf{kq})$ does not vanish only when $\mathbf{k}$ (which is an independent coordinate) equals $\mathbf{k}_B$ (which is a constant of the motion and is used for specifying a Bloch state) within a vector of the reciprocal lattice $\mathbf{K}_m$. Both $\mathbf{k}$ and $\mathbf{k}_B$ specify eigenvalues of the translation operators in direct space, (1), and as such there is no difference between them. In the description of $C_{nk_B}(\mathbf{kq})$, however, $\mathbf{k}$ and $\mathbf{k}_B$ have different roles, this being the reason for their different notation. It is also easy to check that $C_{nk_B}(\mathbf{kq})$ in (13) is an eigenfunction of the translation operator $T(\mathbf{R}_n)$:

$$T(\mathbf{R}_n)C_{nk_B}(\mathbf{kq})=\exp(i\mathbf{k}_B\cdot\mathbf{R}_n)C_{nk_B}(\mathbf{kq}). \tag{14}$$

This is the Bloch theorem written in the kq representation. It is interesting to discuss this theorem in more detail in the light of the $\mathbf{k}$ and $\mathbf{q}$ variables.

In quantum mechanics one can measure precisely either the coordinate $\mathbf{r}$ of a particle or its momentum $\mathbf{p}$. Both of them cannot be measured simultaneously because they do not commute. The same is true, in general, about a function of $\mathbf{r}$ and a function of $\mathbf{p}$. If, however, one is interested in partial information about, say, the coordinate, then one could at the same time also measure to some extent the momentum. An example of such a partial information about the coordinate $\mathbf{r}$ and the momentum $\mathbf{p}$ are the quasicoordinate $\mathbf{q}$ and the quasimomentum $\mathbf{k}$. The latter carry the most information one can get simultaneously about $\mathbf{r}$ and $\mathbf{p}$. In the Bloch theorem one specifies states by both the eigenvalues of the energy operator (11), which is a function of $\mathbf{r}$, and the eigenvalue of translation operators (1), that depend on $\mathbf{p}$. The dependence of the Hamiltonian (11) on $\mathbf{r}$ can be expressed by means of the translation operators $T(\mathbf{K}_n)$ in reciprocal space (2). This is achieved by expanding the periodic potential $V(\mathbf{r})$ in a Fourier series

$$\begin{aligned}H&=\mathbf{p}^2/2m+\sum_{\mathbf{K}_m}V(\mathbf{K}_m)\exp(i\mathbf{K}_m\cdot\mathbf{r})\\&=\mathbf{p}^2/2m+\sum_{\mathbf{K}_m}V(\mathbf{K}_m)T(\mathbf{K}_m),\end{aligned} \tag{15}$$

where $V(\mathbf{K}_m)$ are the Fourier coefficients of the periodic potential $V(\mathbf{r})$. As was mentioned before, in general, a function of $\mathbf{r}$ (the Hamiltonian) and a function of $\mathbf{p}[T(\mathbf{R}_n)]$ do not commute and they do not have common eigenstates. In the special case considered here, it is because of the commutativity of $T(\mathbf{R}_n)$ and $T(\mathbf{K}_m)$ [relations (1) and (2)] that the translations $T(\mathbf{R}_n)$ commute with the Hamiltonian and that the Bloch theorem holds. We see therefore that the fundamental operators $T(\mathbf{R}_n)$ and $T(\mathbf{K}_m)$ are of very great significance in the Bloch theorem.

Because of the Bloch theorem, $\mathbf{k}_B$ is a conserved quantity in the quantum-mechanical description of the motion of an electron in a periodic potential. Is there any classical anlog for this conservation law? It is known in classical mechanics[5] that any function of $\mathbf{r}$ and $\mathbf{p}$ that gives vanishing Poisson brackets with the Hamiltonian is a constant of motion. The spatial symmetry of a classical system can be expressed in terms of infinitesimal transformations: Generating functions G of infinitesimal transformations that leave the Hamil-

[5] Herbert Goldstein, *Classical Mechanics* (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1950).

tonian invariant are constants of motion. For example, an infinitesimal translation in the x direction is generated by $G=p_x$. There is, however, no such theorem in classical mechanics with respect to finite transformations. The invariance of the classical Hamiltonian for a periodic potential $V(\mathbf{r})$ with respect to a finite translation, $\mathbf{r}\rightarrow\mathbf{r}+\mathbf{R}_n$, does not lead to any conservation law. In order to see better the fundamental difference between the quantum-mechanical and classical description of the problem let us consider the operators $T(\mathbf{R}_n)$ and $T(\mathbf{K}_m)$. As was mentioned before, it is because of the commutativity of these operators that the Bloch theorem holds and therefore that $\mathbf{k}_B$ can be defined in quantum mechanics. Classically, there are no functions of the form (1) and (2) that give vanishing Poisson brackets.[6] It is for this reason that $\mathbf{k}_B$ cannot be introduced classically. The conclusion is that the quasimomentum $\mathbf{k}_B$ is a purely quantum-mechanical concept that has no classical analog.

In some cases it can be more convenient to work with the function $U(\mathbf{kq})$ that is connected to $C(\mathbf{kq})$ by the relation [I(42)]

$$C(\mathbf{kq})=\exp(i\mathbf{k}\cdot\mathbf{q})U(\mathbf{kq}). \tag{16}$$

For an electron in a periodic potential, $U(\mathbf{kq})$ satisfies the equation

$$\left[\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}\right)^2\Big/2m+V(\mathbf{q})\right]U(\mathbf{kq})=\epsilon U(\mathbf{kq}). \tag{17}$$

According to (13) and (16), the Bloch solutions of Eq. (17) are

$$U_{nk_B}(\mathbf{kq})=u_{nk}(\mathbf{q})\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m), \tag{18}$$

where $u_{nk}(\mathbf{q})$ is the periodic part of the Bloch function. The phase transformation (16) will also change the expressions for the basic operators $\mathbf{p}$ and $\mathbf{r}$ [(4) and (5)]. They will become

$$\mathbf{p}=-i(\partial/\partial\mathbf{q})+\mathbf{k}, \tag{19}$$

$$\mathbf{r}=i(\partial/\partial\mathbf{k}). \tag{20}$$

Accordingly, the translation operators $T(\mathbf{R}_n)$ and $T(\mathbf{K}_m)$ will be

$$T(\mathbf{R}_n)=\exp\left[i\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}\right)\cdot\mathbf{R}_n\right], \tag{21}$$

$$T(\mathbf{K}_m)=\exp\left[i\left(i\frac{\partial}{\partial\mathbf{k}}\right)\cdot\mathbf{K}_m\right]. \tag{22}$$

One can easily check that $U_{nk_B}(\mathbf{kq})$ in (18) is an eigenfunction of $T(\mathbf{R}_n)$ with the eigenvalue $\exp(i\mathbf{k}_B\cdot\mathbf{R}_n)$, which is to be expected according to the Bloch theorem.

[6] A general discussion of this problem is given in a paper by Yakir Aharonov and Aage Petersen (private communication).

It is interesting to compare Eq. (17) with the usual equation for the periodic part $u_{nk_B}(\mathbf{r})$ of the Bloch function (12). From (11) and (12) one has

$$\left[\left(-i\frac{\partial}{\partial\mathbf{r}}+\mathbf{k}_B\right)^2\Big/2m+V(\mathbf{r})\right]u_{nk_B}(\mathbf{r}) =\epsilon_n(\mathbf{k}_B)u_{nk_B}(\mathbf{r}). \tag{23}$$

The energy in Eq. (23) is periodic in $\mathbf{k}_B$ with the period of the reciprocal lattice vectors $\mathbf{K}_m$. However, neither the Hamiltonian in (23) nor the functions $u_{nk_B}(\mathbf{r})$ have such periodicity. This difficulty is avoided in Eq. (17) and solution (18) which are periodic in $\mathbf{k}_B$.

To complete this section let us consider the Bloch representation in addition to the r representation and the kq representation that were already considered here. The wave function $B_n(\mathbf{k}_B)$ in the Bloch representation (nk_B representation) can be obtained by expanding $U(\mathbf{kq})$[$C(\mathbf{kq})$ or $\psi(\mathbf{r})$] in Bloch functions $U_{nk_B}(\mathbf{kq})$

$$U(\mathbf{kq})=\sum_{nk_B}B_n(\mathbf{k}_B)U_{nk_B}(\mathbf{kq}) =\sum_n B_n(\mathbf{k})u_{nk}(\mathbf{q}), \tag{24}$$

where the last equality was obtained by using the explicit form (18) for $U_{nk_B}(\mathbf{kq})$. The simple relation (24) (with no integral over $\mathbf{k}$!) was already used before [I(47)] in the derivation of an effective Hamiltonian for a Bloch electron in a magnetic field. For comparison let us write the expansion of $\psi(\mathbf{r})$ in Bloch functions

$$\psi(\mathbf{r})=\sum_{nk_B}B_n(\mathbf{k}_B)\psi_{nk_B}(\mathbf{r}). \tag{25}$$

In the latter expansion there is also the integration over $\mathbf{k}_B$ which may complicate the calculations considerably [It is clear that if expansion (24) would be performed for $C(\mathbf{kq})$, the result on the right-hand side would contain $\psi_{nk}(\mathbf{q})$, again without integration over $\mathbf{k}$.] It follows from relation (24) that the transformation between the kq representation and the nk_B representation is given by $U_{nk_B}(\mathbf{kq})$ in (18). In the Bloch representation Eq. (17) becomes

$$\epsilon_n(\mathbf{k}_B)B_n(\mathbf{k}_B)=\epsilon B_n(\mathbf{k}_B). \tag{26}$$

The solution of Eq. (26) for the energy $\epsilon=\epsilon_l(\mathbf{k}_B')$ is

$$B_n^{lk_B'}(\mathbf{k}_B)=\delta_{nl}\sum_{K_m}\delta(\mathbf{k}_B-k_B'-\mathbf{K}_m). \tag{27}$$

The function (27) will clearly give for $U(kq)$ in Eq. (24) the function $U_{lk_B'}(\mathbf{kq})$ which one should expect to get.

In summary, the connections between functions $\psi(\mathbf{r})$, $C(\mathbf{kq})$, and $B_n(\mathbf{k})$ (in the r representation, kq representation, and nk representation correspondingly) are given by the following relations: The function $\psi(\mathbf{r})$ is connected to the function $C(\mathbf{kq})$ by relation (6), the function

$\psi(\mathbf{r})$ is connected to $B_n(\mathbf{k})$ by relation (25), and $C(\mathbf{kq})$ is connected to $B_n(\mathbf{k})$ by (24) with $u_{nk}(\mathbf{q})$ replaced by $\psi_{nk}(\mathbf{q})$.

III. EFFECTIVE HAMILTONIAN FOR A BLOCH ELECTRON IN A MAGNETIC FIELD

In paper I it was shown that the kq representation is very convenient for deriving an effective Hamiltonian for a Bloch electron in a magnetic field. The well-known result was obtained for the zero order in magnetic field effective Hamiltonian,[2–4] and the higher-order terms were shown to coincide with the corresponning terms in Roth's paper.[3] Because of its clear nature and simplicity, the kq representation makes it possible to develop a very simple and straightforward effective Hamiltonian theory to any order in magnetic field.

The Schrödinger equation in the kq representation for a Bloch electron in a magnetic field is [I(43)]:

$$\left\{\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m+V(\mathbf{q})\right\}U(\mathbf{kq})=\epsilon U(\mathbf{kq}).\quad(28)$$

The idea of an effective Hamiltonian[2–4] is to write Eq. (28) in a Bloch-type $n k_B$ representation and to keep to some approximation only one-band terms. Assume that a general transformation is performed from the wave function $U(\mathbf{kq})$ in the kq-representation to the wave function $B_n(\mathbf{k}_B)$ in the $n k_B$ representation

$$U(\mathbf{kq})=\sum_{nk_B}(\mathbf{kq}|n\mathbf{k}_B)B_n(\mathbf{k}_B),\quad(29)$$

where $(kq|n\mathbf{k}_B)$ is the transformation matrix. It was already shown [relation (24)] that if the proper Bloch functions were used in transformation (29), $(\mathbf{kq}|n\mathbf{k}_B)$ would be replaced by $U_{nk_B}(\mathbf{kq})$ and (29) would go over to (24). Imagine, however, that some modified Bloch functions are used in (29), like the Kohn-Luttinger functions,[2,4] or the Roth functions.[3] Then $(\mathbf{kq}|n\mathbf{k}_B)$ is different from $U_{nk_B}(\mathbf{kq})$. Let us assume that $(\mathbf{kq}|n\mathbf{k}_B)$ form an orthonormal set of functions. One also has to make sure that $(\mathbf{kq}|n\mathbf{k}_B)$ form a complete set of functions because otherwise expansion (29) would not be valid. We therefore require that

$$\int d\mathbf{k}\,d\mathbf{q}\,(n\mathbf{k}_B|\mathbf{kq})(\mathbf{kq}|n'\mathbf{k}_B')=\delta_{nn'}\delta(\mathbf{k}_B-\mathbf{k}_B'),\quad(30)$$

$$\sum_{nk_B}(\mathbf{kq}|n\mathbf{k}_B)(n\mathbf{k}_B|\mathbf{k}'\mathbf{q}')=\delta(\mathbf{k}-\mathbf{k}')\delta(\mathbf{q}-\mathbf{q}').\quad(31)$$

Relation (30) expresses orthonormality, while (31) gives completeness. By using relations (29) and (30), Schrödinger's equation (28) in the modified Bloch representation, nk_B, will become

$$\sum_{n'k_B'}H_{nn'}(\mathbf{k}_B\mathbf{k}_B')B_{n'}(\mathbf{k}_B')=\epsilon B_n(\mathbf{k}_B).\quad(32)$$

The following notation was used in (32):

$$H_{nn'}(\mathbf{k}_B\mathbf{k}_B')=\int d\mathbf{k}\,d\mathbf{q}\,(n\mathbf{k}_B|\mathbf{kq})\times\left[\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m+V(\mathbf{q})\right]\times(\mathbf{kq}|n'\mathbf{k}_B').\quad(33)$$

Let us also introduce a notation that was used in I. Given a function $S(\mathbf{k}_B)$ [or $S(\mathbf{k})$] one can define [I(59)]

$$[S(\mathbf{k}_B)],\quad(34)$$

where the rectangular brackets mean that $S(\mathbf{k}_B)$ was first symmetrized as a function of $\mathbf{k}_B$ and then $\mathbf{k}_B$ replaced by $\mathbf{k}_B+(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k}_B)$. In notation (34) the existence of an effective Hamiltonian for Eq. (32) is expressed by the requirement that

$$H_{nn'}(\mathbf{k}_B\mathbf{k}'_B)=\delta_{nn'}[H_n(\mathbf{k}_B)]\sum_{\mathbf{K}_m}\delta(\mathbf{k}_B-\mathbf{k}_B'-\mathbf{K}_m),\quad(35)$$

where $[H_n(\mathbf{k}_B)]$ operates on the δ function. If relation (35) is satisfied, Eq. (32) becomes an effective-Hamiltonian equation

$$[H_n(\mathbf{k}_B)]B_n(\mathbf{k}_B)=\epsilon B_n(\mathbf{k}_B).\quad(36)$$

The main idea of an effective Hamiltonian is that Eq. (36) is a one-band equation and that $[H_n(\mathbf{k}_B)]$ is a function of $\mathbf{k}_B+(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k}_B)$. This is a very attractive result and it is known[2–4] that $[H_n(\mathbf{k}_B)]$ in (36) can be constructed to any order in the magnetic field $\mathbf{H}$. It is interesting to compare the exact equation (28) with the effective Hamiltonian equation (36). In the first of them there are derivatives with respect to $\mathbf{k}$ only to second order, while the latter equation is a difference equation and contains therefore derivatives with respect to $\mathbf{k}_B$ to any order. To see this difference better let us write down the Hamiltonian of Eq. (36) in a more explicit form. By definition

$$[H_n(\mathbf{k}_B)]=\sum_l H_n(\mathbf{R}_l)\times\exp\left[i\left(\mathbf{k}_B+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}_B}\right)\cdot\mathbf{R}_l\right],\quad(37)$$

where $H_n(\mathbf{R}_l)$ are the Fourier coefficients of the expansion of $H_n(\mathbf{k}_B)$ and the reason that there is a sum over Bravais lattice vectors $\mathbf{R}_l$ is because $H_n(\mathbf{k}_B)$ turns out to be periodic with respect to vectors $\mathbf{K}_m$ of the reciprocal lattice[2] (see also the proof at the end of Sec. III). It is clear that an operator (37) leads to a difference equation in (36). Being a difference equation, Eq. (36) connects $B_n(\mathbf{k}_B)$ with different $\mathbf{k}_B$ in the Brillouin zone. On the contrary, Eq. (28) [or any exact equation (32)] is diagonal in $\mathbf{k}$ because it is known that the Hamiltonian of a Bloch electron in a magnetic field is diagonal in $\mathbf{k}$ with respect to any Bloch-type states.[2,4,7] There is therefore a qualitative difference between the effective Hamiltonian equation (36) and the exact equation (28).

To lowest order in magnetic field $H^{(0)}$, it is easy to check that Eq. (35) is satisfied by [see definition (33)]

$$(\mathbf{kq}|n\mathbf{k}_B)=[u_{nk}(\mathbf{q})]\sum_{K_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m), \quad (38)$$

$$H_n(\mathbf{k}_B)=\epsilon_n(\mathbf{k}_B). \quad (39)$$

In Eq. (38), $u_{nk}(\mathbf{q})$ is the periodic part of the Bloch function (18), and $[u_{nk}(\mathbf{q})]$ operates on the δ function. $\epsilon_n(\mathbf{k}_B)$ in (39) is the one-band energy of the solid under consideration in the absence of a magnetic field. In order to verify that (38) and (39) satisfy relation (35), we use the multiplication rule for functions in rectangular brackets, I(61) [see also Appendix I, (A1)–(A4)]. The left-hand side of Eq. (35) will become, to zero order in $\mathbf{H}$,

$$\int d\mathbf{q}\,[u_{nk_B}^*(\mathbf{q})][H(\mathbf{k}_B\mathbf{q})][u_{n'k_B}(\mathbf{q})]\sum_{\mathbf{K}_m}\delta(\mathbf{k}_B-\mathbf{k}_B'-\mathbf{K}_m)$$
$$=\delta_{nn'}[\epsilon_n(\mathbf{k}_B)]\sum_{\mathbf{K}_m}\delta(\mathbf{k}_B-\mathbf{k}_B'-\mathbf{K}_m), \quad (40)$$

which coincides with the right-hand side of Eq. (35). It is also easy to check that the transformation function (38) satisfies the completeness (31) and the orthonormality (30) conditions to zero order in the magnetic field. Take, for example, the completeness condition (31): To zero order in $\mathbf{H}$ we have [see formulas (A1), (A3), (A4) in Appendix I]:

$$\sum_{nk_B}(\mathbf{kq}|n\mathbf{k}_B)(n\mathbf{k}_B|\mathbf{k}'\mathbf{q}')$$
$$=\sum_n[u_{nk}(\mathbf{q})][u_{nk}^*(\mathbf{q})]\sum_{K_m}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{K}_m)$$
$$=\delta(\mathbf{k}-\mathbf{k}')\delta(\mathbf{q}-\mathbf{q}'). \quad (41)$$

For arriving at result (41) the completeness of the $u_{nk}(\mathbf{q})$ was used. The orthonormality of (38) to zero order in magnetic field can also be easily checked. Since the transformation function (38) satisfies Eq. (35) and the conditions (30) and (31) to zero order in magnetic field, it will lead, when used in expansion (29), from Eq. (28) to the effective Hamiltonian Eq. (36):

$$[\epsilon_n(\mathbf{k}_B)]B_n(\mathbf{k}_B)=\epsilon B_n(\mathbf{k}_B). \quad (42)$$

Result (42) gives the well-known effective Hamiltonian equation to zero order in magnetic field.[1–4] Let us point out that if our only task would be to arrive at Eq. (42), we could do it in a very simple way without developing all the arguments that follow expansion (29). Compare Eq. (28) for a Bloch electron in a magnetic field with Eq. (17) for a Bloch electron. The only difference between these two equations is that in the former $\mathbf{k}+(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k})$ appears instead of $\mathbf{k}$ in Eq. (17). We know, however, that if $U_{nk_B}(\mathbf{kq})$ in (18) is used as a transformation function in (29) [or (24)], Bloch's equation (17) assumes the form (26). One should therefore expect that the transformation function (38), where $\mathbf{k}$ in $u_{nk}(\mathbf{q})$ is replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k})$, will lead from Eq. (28) to the effective Hamiltonian Eq. (42). This is straightforwardly checked by expanding $U(\mathbf{kq})$ in (28) according to relation (29) with the transformation function (38), multiplying both sides of Eq. (28) by $(n\mathbf{k}_B|\mathbf{kq})$, integrating over $\mathbf{k}$ and $\mathbf{q}$, and using the multiplication rule (A1). Of course, one would have to check orthonormality and completeness of (38) to zero order in the magnetic field. The discussion that followed expansion (29) will, however, be needed for deriving an effective-Hamiltonian equation to higher order in the magnetic field.

Before going to higher-order terms let us show that the transformation functions (38) coincide with the Roth functions,[3] $\Phi_{nk_B}(\mathbf{r})$, that were used in the derivation of an effective Hamiltonian. For showing this, let us find the kq transform [see relations (6′) and (16)] of $\Phi_{nk_B}(\mathbf{r})$

$$U_{nk_B}{}^R(\mathbf{kq})=\exp(-i\mathbf{k}\cdot\mathbf{q})C_{nk_B}{}^R(\mathbf{kq})$$
$$=\exp(-i\mathbf{k}\cdot\mathbf{q})\int\Phi_{nk_B}(\mathbf{r})\psi_{kq}^*(\mathbf{r})dr$$
$$=[u_{nk}(\mathbf{q})]\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m). \quad (43)$$

The superscript R in (43) stands for Roth's function and in the derivation of result (43), the definition of $\Phi_{nk_B}(\mathbf{r})$ [Ref. 3, Eq. (10)] and expression (3) for $\psi_{kq}(\mathbf{r})$ were used. We see therefore that $(\mathbf{kq}|n\mathbf{k}_B)$ in (38) is just the kq transform of Roth's function $\Phi_{nk_B}(\mathbf{r})$. In Ref. 3 it was assumed that $\Phi_{nk_B}(\mathbf{r})$ form a complete system of functions. In I and in relation (41) this was shown to be correct to zero order in the magnetic field. It is clear, that for developing an effective Hamiltonian theory to higher-order terms, one has to make sure that the functions $(\mathbf{kq}|n\mathbf{k}_B)$ used in expansion (29) form a complete system of functions to the desired order in the magnetic field.

As was already checked, the transformation functions (38) form a complete and orthonormal set of functions to zero order in magnetic field. Let us now show that for sufficiently small magnetic fields it is possible to construct a set of functions $\Phi_{nk_B}(\mathbf{kq})$ which are orthonormal and complete to any order in magnetic field. Define a matrix[3]

$$[N_{mn}(\mathbf{k})]=\int d\mathbf{q}\,[u_{mk}^*(\mathbf{q})][u_{nk}(\mathbf{q})]. \quad (44)$$

The matrix $[N(\mathbf{k})]$ can be given another form by using

[7] E. I. Blount, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1961), Vol. 13.

the matrix $[S(\mathbf{k})]$ that was defined in paper I [I(55), (59)] (See formula (A1) in Appendix I)

$$[N(\mathbf{k})]=[S(\mathbf{k})]^\dagger[S(\mathbf{k})]=I+[N^{(1)}(\mathbf{k})]+[N^{(2)}(\mathbf{k})]+\cdots, \quad (45)$$

where

$$N^{(1)}(\mathbf{k})=-ih_{\alpha\beta}\frac{\partial S(\mathbf{k})^\dagger}{\partial k_\alpha}\frac{\partial S(\mathbf{k})}{\partial k_\beta},$$
$$N^{(2)}(\mathbf{k})=-\tfrac{1}{2}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}\frac{\partial^2 S(\mathbf{k})^\dagger}{\partial k_{\alpha_1}\partial k_{\alpha_2}}\frac{\partial^2 S(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}}, \quad (45')$$

and

$$[S_{mn}(\mathbf{k})]=\int d\mathbf{q}\, u_{m0}^*(\mathbf{q})[u_{nk}(\mathbf{q})]. \quad (46)$$

The superscripts in (45) and (45′) denote the order of the magnetic field. The existence of an inverse matrix for $[N(\mathbf{k})]$ is of very great importance to what follows. In order to be able to define $[N(\mathbf{k})]^{-1}$ we assume that the magnetic field is sufficiently small so that the commutator expansion in (45) holds. The assumption of a commutator expansion is very crucial in the entire theory of effective Hamiltonians.[2–4] By making this assumption, the matrix $[N(\mathbf{k})]$ can be inverted

$$[N(\mathbf{k})]^{-1}=\{I+[N^{(1)}(\mathbf{k})]+[N^{(2)}(\mathbf{k})]+\cdots\}^{-1}=I-[N^{(1)}(\mathbf{k})]-[N^{(2)}(\mathbf{k})]+[N^{(1)}(\mathbf{k})]^2+\cdots.$$

Let us use this inverse matrix for defining functions

$$\Phi_{nk_B}(\mathbf{kq})=(\mathbf{kq}|n\mathbf{k}_B)=\sum_l [u_{lk}(\mathbf{q})][N_{ln}(\mathbf{k})]^{-1/2}\times\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m), \quad (47)$$

where

$$[N(\mathbf{k})]^{-1/2}=\{I+[N^{(1)}(\mathbf{k})]+[N^{(2)}(\mathbf{k})]+\cdots\}^{-1/2}=I-\tfrac{1}{2}[N^{(1)}(\mathbf{k})]-\tfrac{1}{2}[N^{(2)}(\mathbf{k})]+\tfrac{3}{8}[N^{(1)}(\mathbf{k})]^2+\cdots. \quad (47')$$

As will be seen below the matrix $[N(\mathbf{k})]^{-1/2}$ in (47) serves as an "orthonormalization factor," and it can be checked that the functions $\Phi_{nk_B}(\mathbf{kq})$ form an orthonormal (30) and complete (31) set of functions. Orthonormality of (47) follows at once:

$$\int d\mathbf{k}\, d\mathbf{q}\,(n\mathbf{k}_B|\mathbf{kq})(\mathbf{kq}|n'\mathbf{k}_B')=\{[N(\mathbf{k}_B)]^{-1/2}[S(\mathbf{k}_B)]^\dagger[S(\mathbf{k}_B)][N(\mathbf{k}_B)]^{-1/2}\}_{nn'}\times\sum_{\mathbf{K}_m}\delta(\mathbf{k}_B-\mathbf{k}_B'-\mathbf{K}_m)=\delta_{nn'}\delta(\mathbf{k}_B-\mathbf{k}_B'), \quad (48)$$

where formulas (A3), (A4), (45), and (46) were used. The left-hand side of the completeness condition (31) is given by

$$\sum_{ll'} u_{l0}(\mathbf{q})u_{l'0}^*(\mathbf{q}')\{[S(\mathbf{k})][N(\mathbf{k})]^{-1}[S(\mathbf{k})]^\dagger\}_{ll'}\times\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{K}_m). \quad (49)$$

This means that in order to prove completeness, one has to prove the relation

$$[S(\mathbf{k})][N(\mathbf{k})]^{-1}[S(\mathbf{k})]^\dagger=I, \quad (50)$$

where I is a unit matrix. It is easily seen that any power of the matrix on the left-hand side of (50) equals the matrix iteslf. Such a matrix can be either zero or I. Zero is excluded because relation (50) was proven before [see proof (41)] to zero order in magnetic field. It follows therefore that relation (50) holds to any order in magnetic field. This proves that the functions (47) form a complete set of functions to any order in magnetic field.[8]

The complete and orthonormal set of functions (47) will now be used in constructing effective Hamiltonians to higher order in magnetic field. It was already shown that expansion (29) leads to Eq. (32) [with notation (33)] when the transformation functions $(\mathbf{kq}|n\mathbf{k}_B)$ form an orthonormal set. It was also shown that in order to arrive at an effective Hamiltonian, Eq. (36), to some order in the magnetic field one has to prove that the Hamiltonian (33) can be given the form (35) to the same order in magnetic field. By using expression (47) for the transformation function, the Hamiltonian (33) in its matrix form becomes ($\mathbf{k}$ is used instead of $\mathbf{k}_B$)

$$H(\mathbf{kk}')=[U(\mathbf{k})]^\dagger[H(\mathbf{k})][U(\mathbf{k})]\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{K}_m), \quad (51)$$

where the following notation was assumed:

$$[U(\mathbf{k})]=[S(\mathbf{k})][N(\mathbf{k})]^{-1/2}, \quad (52)$$

$$H_{mn}(\mathbf{k})=\int d\mathbf{q}\, u_{m0}^*(\mathbf{q})\left\{\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}\right)^2\Big/ 2m+V(\mathbf{q})\right\}u_{n0}(\mathbf{q}). \quad (53)$$

Having the Hamiltonian (51) in the nk representation ($\mathbf{k}$ is used instead of $\mathbf{k}_B$), one can write the equation for $B_n(\mathbf{k})$ in (29)

$$\sum_{n'}\{[U(\mathbf{k})]^\dagger[H(\mathbf{k})][U(\mathbf{k})]\}_{nn'}B_{n'}(\mathbf{k})=\epsilon B_n(\mathbf{k}). \quad (54)$$

This equation is a multiband effective-Hamiltonian equation for a Bloch electron in a magnetic field. It has a significant advantage over this type of equation in

[8] In previous work (Refs. 3 and 4) completeness was assumed to any order in magnetic field. This is not at all obvious. A discussion of this problem with Professor Laura M. Roth and Dr. E. I. Blount and their comments were very much appreciated. The author is in particular grateful to Professor Roth for pointing out in a private communication the possibility of defining the inverse matrix $[N(\mathbf{k})]^{-1}$.

Ref. (1) [I(65)] and in other publicatons[2–4] in that on the right-hand side of (54) there is only a diagonal term. This fact makes the diagonalization procedure of Eq. (54) very simple because any unitary transformation of (54) will keep the right-hand side diagonal.

Let us describe the diagonalization procedure of Eq. (54). By using the commutator expansion (A1), the Hamiltonian of Eq. (54) can be written as a power series in the magnetic field

$$[U(\mathbf{k})]^\dagger[H(\mathbf{k})][U(\mathbf{k})]=[H_0(\mathbf{k})]=[H^{(0)}(\mathbf{k})]+[H^{(1)}(\mathbf{k})]+[H^{(2)}(\mathbf{k})]+\cdots, \quad (55a)$$

where (see Appendix II)

$$H^{(0)}(\mathbf{k})=\epsilon^{(0)}(\mathbf{k}), \quad (55b)$$

$$H^{(1)}(\mathbf{k})=(S^\dagger HS)^{(1)}-\{N^{(1)}(\mathbf{k}),\epsilon^{(0)}(\mathbf{k})\}, \quad (55c)$$

$$H^{(2)}(\mathbf{k})=(S^\dagger HS)^{(2)}-\{N^{(1)}(\mathbf{k}),(S^\dagger HS)^{(1)}\}-\{N^{(2)}(\mathbf{k})-\tfrac{3}{4}(N^{(1)}(\mathbf{k}))^2,\,\epsilon^{(0)}(\mathbf{k})\}+ih_{\alpha\beta}\left\{\frac{\partial N^{(1)}(\mathbf{k})}{\partial k_\alpha},\frac{\partial\epsilon^{(0)}(\mathbf{k})}{\partial k_\beta}\right\}. \quad (55d)$$

Here, the curly brackets of any two functions $A(\mathbf{k})$ and $B(\mathbf{k})$ denote a symmetrical product

$$\{A(\mathbf{k}),B(\mathbf{k})\}=\tfrac{1}{2}[A(\mathbf{k})B(\mathbf{k})+B(\mathbf{k})A(\mathbf{k})].$$

In (55b), $\epsilon^{(0)}(\mathbf{k})$ is the energy spectrum in the absence of the magnetic field [in (39) and (42) it is denoted by $\epsilon(\mathbf{k})$]. The notation $[H_0(\mathbf{k})]$ of the Hamiltonian (55a) expresses the fact that the latter is diagonal to zero order in magnetic field, and to the lowest order one obtains again the effective Hamiltonian equation (42). The higher-order terms in (55a) contain nondiagonal elements and, as is shown below, their removal to any order in the magnetic field can be achieved by a unitary transformation. Let us start with removing nondiagonal terms in (55a) to first order in magnetic field. Define a unitary transformation

$$\exp\{i[T^{(1)}(\mathbf{k})]\}=I+i[T^{(1)}(\mathbf{k})]+\cdots, \quad (56)$$

where $[T^{(1)}(\mathbf{k})]$ is a Hermitian matrix and is of first order in magnetic field. By applying transformation (56) to the Hamiltonian (55a), the latter will assume the form (to first order in magnetic field)

$$H_1(\mathbf{k})=H^{(0)}(\mathbf{k})+i(H^{(0)}(\mathbf{k})T^{(1)}(\mathbf{k})-T^{(1)}(\mathbf{k})H^{(0)}(\mathbf{k}))+H^{(1)}(\mathbf{k})+\cdots. \quad (57)$$

One can now choose $T^{(1)}(\mathbf{k})$ in such a way that the nondiagonal terms in (57) vanish to first order in magnetic field

$$T_{nn'}^{(1)}(\mathbf{k})=i\frac{H_{nn'}^{(1)}(\mathbf{k})}{\epsilon_n^{(0)}(\mathbf{k})-\epsilon_{n'}^{(0)}(\mathbf{k})},\quad n'\neq n \quad (58)$$

$$T_{nn}^{(1)}(\mathbf{k})=0. \quad (59)$$

It is easy to check that the matrix defined by (58) and (59) is Hermitian and (56) is therefore a unitary transformation. The notation $H_1(\mathbf{k})$ with the subscript 1 in (57) means that the transformed Hamiltonian is diagonal to first order in magnetic field

$$H_1(\mathbf{k})=\epsilon^{(0)}(\mathbf{k})+\epsilon^{(1)}(\mathbf{k})+\cdots, \quad (60)$$

where $\epsilon^{(0)}(\mathbf{k})=\epsilon(\mathbf{k})$ is the energy spectrum of the solid in the absence of the magnetic field and $\epsilon^{(1)}(\mathbf{k})$ is the diagonal part of $H^{(1)}(\mathbf{k})$ in (57) [or (55a)]. The diagonality of the Hamiltonian [Eq. (60)] to first order in the magnetic field was achieved by starting with a Hamiltonian (55a) which was diagonal to zero order in magnetic field and by using a unitary transformation (56). It is clear that the same process can now be used for diagonalizing the Hamiltonian (60) to second and higher order in magnetic field. Assume, for example, that the Hamiltonian is already diagonal to pth order in magnetic field

$$H_p(\mathbf{k})=\epsilon^D(\mathbf{k})+H^{(p+1)\prime}(\mathbf{k})+\cdots, \quad (61)$$

where $\epsilon^D(\mathbf{k})$ is the diagonal Hamiltonian containing terms up to pth order in magnetic field

$$\epsilon^{(D)}(\mathbf{k})=\epsilon^{(0)}(\mathbf{k})+\cdots+\epsilon^{(p)}(\mathbf{k}), \quad (62)$$

and $H^{(p+1)\prime}(\mathbf{k})$ has nondiagonal terms of the order $(p+1)$ in magnetic field. Let us show that a unitary matrix can be defined

$$\exp\{i[T^{(p+1)}(\mathbf{k})]\}=I+i[T^{(p+1)}(k)]+\cdots \quad (63)$$

that will make the Hamiltonian (61) diagonal to the order $(p+1)$ in magnetic field. Under transformation (63) the Hamiltonian (61) will become [to order $(p+1)$]

$$H_{p+1}(\mathbf{k})=\epsilon^D(\mathbf{k})+i(\epsilon^{(0)}(\mathbf{k})T^{(p+1)}(\mathbf{k})-T^{(p+1)}(\mathbf{k})\epsilon^{(0)}(\mathbf{k}))+H^{(p+1)\prime}(\mathbf{k})+\cdots. \quad (64)$$

Again, $T^{(p+1)}(\mathbf{k})$ can be chosen in such a way that the nondiagonal elements of $H_{p+1}(\mathbf{k})$ vanish to the order $p+1$ in magnetic field

$$T_{nn'}^{(p+1)}(\mathbf{k})=i\frac{H_{nn'}^{(p+1)\prime}(\mathbf{k})}{\epsilon_n^{(0)}(\mathbf{k})-\epsilon_{n'}^{(0)}(\mathbf{k})},\quad n'\neq n \quad (65)$$

$$T_{nn}^{(p+1)}(\mathbf{k})=0. \quad (66)$$

The matrix $T^{(p+1)}(\mathbf{k})$ defined by (65) and (66) is Hermitian and (63) is therefore a unitary matrix. This completes the proof that a unitary matrix exists [relation (63)] that transforms the Hamiltonian (61), which is diagonal to pth order in magnetic field, into a Hamiltonian

$$H_{p+1}(\mathbf{k})=\epsilon^D(\mathbf{k})+\epsilon^{(p+1)}(\mathbf{k})+\cdots, \quad (67)$$

which is diagonal to the order $p+1$ in magnetic field. The term $\epsilon^{(p+1)}(\mathbf{k})$ in (67) is the diagonal part of $H^{(p+1)\prime}(\mathbf{k})$ in (61). Since p is completely arbitrary, the above procedure can be used for diagonalizing the

Hamiltonian (55a) step by step to any power in the magnetic field. It is to be pointed out that the unitarity of transformation (63) is of very great importance. It is because of this fact that one does not have to worry about the right-hand side of Eq. (54), which stays diagonal automatically during the entire diagonalization procedure. This leads to a significant simplification of the previous methods[3,4] where the diagonalization procedure has to be carried out on both sides of the multiband equation.

In conclusion of this section let us show that the method developed here enables one to prove in a straightforward way that the effective Hamiltonian is a periodic function in $\mathbf{k}$ with the periodicity of the reciprocal-lattice vectors.[2] A very simple formula was given in Appendix II [A(15)] for the product $[S^\dagger(\mathbf{k})]\times[H(\mathbf{k})][S(\mathbf{k})]$. It was shown there that each term in the rectangular brackets of formula (A15) is periodic in $\mathbf{k}$. The same argument can be used to show that each term in the rectangular brackets of the expansion (47′) of $[N(\mathbf{k})]^{-1/2}$ is periodic in $\mathbf{k}$ [see definition (45′)]. It follows therefore that all the expressions (55b)–(55d) for the effective Hamiltonian are periodic in $\mathbf{k}$. This will be also true for the effective Hamiltonian on each stage of diagonalization because the matrix $T(\mathbf{k})$ that is used in this diagonalization process [formulas (58), (59) or, in general, (65), (66)] is itself periodic in $\mathbf{k}$. This completes the proof that both the diagonal and nondiagonal terms in the effective Hamiltonian $H_{\text{eff}}(\mathbf{k})$, to any order in magnetic field and at any stage of diagonalization, are periodic in $\mathbf{k}$ with the periodicity of the reciprocal-lattice vectors.

IV. DISCUSSION

The effective-Hamiltonian theory in this paper was developed by using an orthonormal and complete set of functions $\Phi_{nk_B}(\mathbf{kq})$ [Eq. (47)]. In order to define these functions the assumption was made that the magnetic field is sufficiently small so that the inverse matrix $[N(\mathbf{k})]^{-1}$ can be defined. After making this assumption, one gets a multiband effective-Hamiltonian equation [Eq. (59)] which is correct to any order in magnetic field. The diagonalization procedure becomes then straightforward and very simple. It is interesting to ask the question what is so special about the functions $\Phi_{nk_B}(\mathbf{kq})$ that makes the entire theory look so elegant and straightforward. The answer lies in their symmetry. As was pointed out before,[9] the Bloch functions or Kohn-Luttinger functions[2] with the proper symmetry of Schrödinger's equation in the absence of external fields cannot serve as a suitable basis for expanding solutions of Eq. (28) for a Bloch electron in a magnetic field. The reason for this is that the symmetry of Schrödinger's equation in the absence of a magnetic field [Eq. (10)] is completely different from the symmetry of Eq. (28). The latter equation has the symmetry of the magnetic translation group[10] while Eq. (10) is invariant under the regular translations [Eq. (1)]. As is known,[9] the regular translation group and the magnetic translation group have a completely different structure. The behavior of Bloch functions [Eq. (13)] under regular translations $T(\mathbf{R}_n)$ [Eq. (21)] is given by relation (14). Let us check how the functions $\Phi_{nk_B}(\mathbf{kq})$ in (47) behave under magnetic translations[10]:

$$\tau(\mathbf{R}_n)=\exp\left[i\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}-\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)\cdot\mathbf{R}_n\right]. \quad (68)$$

One finds

$$\tau(\mathbf{R}_n)\Phi_{nk_B}(\mathbf{kq})=\exp(i\mathbf{k}_B\cdot\mathbf{R}_n)\Phi_{nk_B+(e/2c)\mathbf{H}\times\mathbf{R}_n}(\mathbf{kq}). \quad (69)$$

The last relation is obtained by using the fact that any function of $\mathbf{k}+(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k})$ commutes with $\mathbf{k}-(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k})$. As seen from relation (69), the functions $\Phi_{nk_B}(\mathbf{kq})$ transform into one another according to the symmetry required by the magnetic translation group.[11] It is for this reason that the functions $\Phi_{nk_B}(\mathbf{kq})$ form the proper set for expanding the solution of Schrödinger's equation for a Bloch electron on a magnetic field.[9] The $\mathbf{k}_B$ in $\Phi_{nk_B}(\mathbf{kq})$ specifies the magnetic translations and plays a similar role to the $\mathbf{k}_B$ vector in the Bloch functions [relation (14)], where it specifies the regular translations. One can therefore call $\Phi_{nk_B}(\mathbf{kq})$ the magnetic Bloch functions.

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APPENDIX I: COMMUTATOR EXPANSIONS

As was shown by Roth[3] the following formula holds for any two functions $A(\mathbf{k})$ and $B(\mathbf{k})$:

$$[A(\mathbf{k})][B(\mathbf{k})]$$

$$=[\exp\{-i(e/2c)\mathbf{H}\cdot\nabla_k\times\nabla_{k'}\}A(\mathbf{k})B(\mathbf{k}')|_{\mathbf{k}'=\mathbf{k}}]$$

$$=[A(\mathbf{k})B(\mathbf{k})]-ih_{\alpha\beta}\left[\frac{\partial A(\mathbf{k})}{\partial k_\alpha}\frac{\partial B(\mathbf{k})}{\partial k_\beta}\right]$$

$$-\tfrac{1}{2}h_{\alpha\beta}h_{\alpha'\beta'}\left[\frac{\partial^2 A(\mathbf{k})}{\partial k_\alpha\partial k_{\alpha'}}\frac{\partial^2 B(\mathbf{k})}{\partial k_\beta\partial k_{\beta'}}\right]+\cdots, \quad (A1)$$

where the rectangular brackets mean that the function inside is first symmetrized with respect to the components of $\mathbf{k}$ and then $\mathbf{k}$ is replaced by $\mathbf{k}+(e/2c)\mathbf{H}$

[9] J. Zak, Phys. Rev. **136**, A776 (1964).

[10] J. Zak, Phys. Rev. **134**, A1602 (1964).

[11] J. Zak, Phys. Rev. **134**, A1607 (1964).

$\times i(\partial/\partial\mathbf{k})$ [see formula (34)], and

$$h_{\alpha\beta}=\epsilon_{\alpha\beta\gamma}eH^{\gamma}/2c,$$

with $\epsilon_{\alpha\beta\gamma}$ being the antisymmetric unit tensor. [In I a factor $\frac{1}{2}$ is missing in the third term of formulas I(61) and (63).] In a way similar to the proof of formula (A1), one can prove that

$$[A(\mathbf{k})]^{-}[B(\mathbf{k})]^{-}=[\exp\{i(e/2c)\mathbf{H}\cdot\nabla_k\times\nabla_k\}\times A(\mathbf{k})B(\mathbf{k}')|_{\mathbf{k}'=\mathbf{k}}]^{-},\quad \text{(A2)}$$

where $[\ \ ]^{-}$ mean that the function inside is first symmetrized with respect to the components of $\mathbf{k}$ and then $\mathbf{k}$ is replaced by $\mathbf{k}-(e/2c)\mathbf{H}\times i(\partial/\partial\mathbf{k})$.

It can be checked that

$$[A(\mathbf{k}_B)]^{-}\delta(\mathbf{k}-\mathbf{k}_B)=[A(\mathbf{k})]\delta(\mathbf{k}-\mathbf{k}_B).\qquad \text{(A3)}$$

In order to prove (A3) let us write its left-hand side explicitly

$$\begin{aligned}[A(\mathbf{k}_B)]^{-}\delta(\mathbf{k}-\mathbf{k}_B)&=\int d\lambda\,A(\lambda)\exp\left\{i\left(\mathbf{k}_B-i\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial k_B}\right)\cdot\lambda\right\}\delta(\mathbf{k}-\mathbf{k}_B)\\&=\int d\lambda\,A(\lambda)\exp\left\{i\left(\mathbf{k}+i\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)\cdot\lambda\right\}\delta(\mathbf{k}-\mathbf{k}_B)\\&=[A(\mathbf{k})]\delta(\mathbf{k}-\mathbf{k}_B),\end{aligned}$$

which is equal to the right-hand side of (A3). In the last proof $A(\lambda)$ is the Fourier transform of $A(\mathbf{k}_B)$.

Another formula that was used in the text [see derivation of (40), (41), (48), and (49)] is that if

$$\begin{aligned}(\mathbf{kq}|n\mathbf{k}_B)&=[u_{nk}(\mathbf{q})]\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m)\\&=\sum_l u_{l0}(\mathbf{q})[S_{ln}(\mathbf{k})]\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m),\end{aligned}$$

then its complex conjugate $(n\mathbf{k}_B|\mathbf{kq})$ is given by

$$\begin{aligned}(n\mathbf{k}_B|\mathbf{kq})&=[u^*_{nk}(\mathbf{q})]^{-}\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m)\\&=\sum_l u^*_{l0}(\mathbf{q})[S^*_{ln}(\mathbf{k}_B)]\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m).\qquad \text{(A4)}\end{aligned}$$

The proof of (A4) is as follows:

$$\begin{aligned}(n\mathbf{k}_B|\mathbf{kq})&=(\mathbf{kq}|n\mathbf{k}_B)^*\\&=[u_{nk}(\mathbf{q})]^*\sum_{K_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m)\\&=\int u^*_{n\lambda}(\mathbf{q})\exp\left[-i\left(\mathbf{k}-i\frac{e}{2c}H\times i\frac{\partial}{\partial\mathbf{k}}\right)\right]d\lambda\times\sum_{K_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m)\\&=[u^*_{nk}(q)]^{-}\sum_{\mathbf{K}_m}\delta(\mathbf{k}-\mathbf{k}_B-\mathbf{K}_m).\end{aligned}$$

$u_{n\lambda}(\mathbf{q})$ here is the Fourier transform of $u_{nk}(\mathbf{q})$. The last equality of (A4) follows from the definition of $S(\mathbf{k})$ [relation (46)] and from (A3).

APPENDIX II: GENERAL EXPRESSION FOR THE HAMILTONIAN

Let us now give a commutator expansion of the Hamiltonian (55a). By using definition (52) for $[U(\mathbf{k})]$, one has

$$[H_0(\mathbf{k})]=[N(\mathbf{k})]^{-1/2}[S(\mathbf{k})]^{\dagger}[H(\mathbf{k})]\times[S(\mathbf{k})][N(\mathbf{k})]^{-1/2}.\quad \text{(A5)}$$

An expansion for $[S(\mathbf{k})]^{\dagger}[H(\mathbf{k})][S(\mathbf{k})]$ to second order in magnetic field was already given in I [I(66)]. It is possible to derive a general formula for this triple product to any order in magnetic field. Since $[H(\mathbf{k})]$ in (A5) is a quadratic function of $[\mathbf{k}]$ [relation (53)] one has

$$[H(\mathbf{k})][S(\mathbf{k})]=[H(\mathbf{k})S(\mathbf{k})]-ih_{\alpha\beta}\left[\frac{\partial H(\mathbf{k})}{\partial k_\alpha}\frac{\partial S(\mathbf{k})}{\partial k_\beta}\right]-\tfrac{1}{2}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}\left[\frac{\partial^2 H(\mathbf{k})}{\partial k_{\alpha_1}\partial k_{\alpha_2}}\frac{\partial^2 S(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}}\right].\quad \text{(A6)}$$

There are no higher-order terms in (A6). The matrix $S(\mathbf{k})$ is unitary [I(54)] and any term in (A6) can be multiplied inside the brackets by the products $S(\mathbf{k})S^{\dagger}(\mathbf{k})=S^{\dagger}(\mathbf{k})S(\mathbf{k})=I$. The first term will become $S(\mathbf{k})\epsilon^{(0)}(\mathbf{k})$, because, as was pointed out before [I(51*a*)], $S(\mathbf{k})$ diagonalizes $H(\mathbf{k})$. $\epsilon^{(0)}(\mathbf{k})$ here is the energy spectrum of the solid in the absence of the magnetic field. For the second and third terms in (A6) define the following quantities[3]:

$$\begin{aligned}x_\alpha(\mathbf{k})_{nn'}&=i\left(S^{\dagger}(\mathbf{k})\frac{\partial S(\mathbf{k})}{\partial k_\alpha}\right)_{nn'}\\&=i\int u^*_{nk}(\mathbf{q})\frac{\partial u_{n'k}(\mathbf{q})}{\partial k_\alpha}d\mathbf{q},\end{aligned}\qquad \text{(A7)}$$

$$\begin{aligned}v_\alpha(\mathbf{k})_{nn'}&=\left(S^{\dagger}(\mathbf{k})\frac{\partial H(\mathbf{k})}{\partial k_\alpha}S(\mathbf{k})\right)_{nn'}\\&=\frac{1}{m}\int u^*_{nk}(\mathbf{q})\left(-i\frac{\partial}{\partial q_\alpha}+k_\alpha\right)u_{n'k}(\mathbf{q})d\mathbf{q}.\end{aligned}\qquad \text{(A8)}$$

Expression (A6) can now be written in the following form:

$$[H(\mathbf{k})][S(\mathbf{k})]=[S(\mathbf{k})\epsilon^{(0)}(\mathbf{k})]+[S(\mathbf{k})E^{(1)}(\mathbf{k})]+[S(\mathbf{k})E^{(2)}(\mathbf{k})],\quad \text{(A9)}$$

where

$$E^{(1)}=-h_{\alpha\beta}v_\alpha(\mathbf{k})x_\beta(\mathbf{k}),\qquad \text{(A10)}$$

$$E^{(2)}=\frac{1}{2m}h_{\alpha\beta}h_{\alpha\beta'}\left(i\frac{\partial x_\beta(\mathbf{k})}{\partial k_{\beta'}}+x_{\beta'}(\mathbf{k})x_\beta(\mathbf{k})\right).\quad \text{(A11)}$$

The terms in (A9) are of zero, first, and second order in magnetic field, correspondingly. For obtaining expression (A11), the relation was used

$$S^{\dagger}(\mathbf{k})\frac{\partial^2 S(\mathbf{k})}{\partial k_\alpha \partial k_\beta}=-i\frac{\partial x_\alpha(\mathbf{k})}{\partial k_\beta}-x_\beta(\mathbf{k})x_\alpha(\mathbf{k}). \quad (A12)$$

The last equality is straightforwardly obtained from definition (A7). By using expression (A9) one has

$$[S^{\dagger}(\mathbf{k})][H(\mathbf{k})][S(\mathbf{k})]$$
$$=\Big[\epsilon^{(0)}(\mathbf{k})-ih_{\alpha\beta}\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_\alpha}\frac{\partial}{\partial k_\beta}(S(\mathbf{k})\epsilon^{(0)}(\mathbf{k}))-\tfrac{1}{2}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}$$
$$\times\frac{\partial^2 S^{\dagger}(\mathbf{k})}{\partial k_{\alpha_1}\partial k_{\alpha_2}}\frac{\partial^2}{\partial k_{\beta_1}\partial k_{\beta_2}}(S(\mathbf{k})\epsilon^{(0)}(\mathbf{k}))+E\cdots+{}^{(1)}(\mathbf{k})$$
$$-ih_{\alpha\beta}\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_\alpha}\frac{\partial}{\partial k_\beta}(S(\mathbf{k})E^{(1)}(\mathbf{k}))-\tfrac{1}{2}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}$$
$$\times\frac{\partial^2 S^{\dagger}(\mathbf{k})}{\partial k_{\alpha_1}\partial k_{\alpha_2}}\frac{\partial^2}{\partial k_{\beta_1}\partial k_{\beta_2}}(S(\mathbf{k})E^{(1)}(\mathbf{k}))+\cdots+E^{(2)}(\mathbf{k})$$
$$-ih_{\alpha\beta}\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_\alpha}\frac{\partial}{\partial k_\beta}(S(\mathbf{k})E^{(2)}(\mathbf{k}))-\tfrac{1}{2}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}$$
$$\times\frac{\partial^2 S^{\dagger}(\mathbf{k})}{\partial k_{\alpha_1}\partial k_{\alpha_2}}\frac{\partial^2}{\partial k_{\beta_1}\partial k_{\beta_2}}(S(k)E^{(2)}(k))+\cdots\Big]. \quad (A13)$$

In order to write expression (A13) in a compact form let us define a matrix

$$N_{\beta_1\beta_2\cdots\beta_m}{}^{(n)}(\mathbf{k})=\frac{(-i)^n}{n!}h_{\alpha_1\beta_1}h_{\alpha_2\beta_2}\ldots h_{\alpha_n\beta_n}$$
$$\times\frac{\partial^{(n)}S^{\dagger}(\mathbf{k})}{\partial k_{\alpha_1}\cdots\partial k_{\alpha_n}}\frac{\partial^{(n-m)}S(\mathbf{k})}{\partial_{\beta_{m+1}}\cdots\partial_{\beta_n}}, \quad (A14)$$

where summation is understood on repeated indeces. The matrix (A14) is of the nth order in magnetic field and is a generalization of the definition (45′) in the text. By using definition (A14), the expression (A13) can be given the following simple form:

$$[S^{\dagger}(k)][H(k)][S(k)]$$
$$=\sum_{m=0}^{n}\sum_{n=0}^{\infty}C_n{}^m\Big[N_{\beta_1\beta_2\cdots\beta_m}{}^{(n)}(\mathbf{k})\frac{\partial^{(m)}E(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}\cdots\partial k_{\beta_m}}\Big], \quad (A15)$$

where $C_n{}^m$ is the binomial coefficient of the $(m+1)$ term and

$$E(\mathbf{k})=\epsilon^{(0)}(\mathbf{k})+E^{(1)}(\mathbf{k})+E^{(2)}(\mathbf{k}). \quad (A16)$$

The form (A15) is very useful and enables one to write a general expression for the nth-order term in $[S^{\dagger}(\mathbf{k})][H(\mathbf{k})][S(\mathbf{k})]$:

$$\sum_{m=0}^{n}C_n{}^mN_{\beta_1\beta_2\cdots\beta_m}{}^{(n)}(\mathbf{k})\frac{\partial^{(m)}\epsilon^{(0)}(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}\cdots\partial k_{\beta_m}}$$
$$+\sum_{m=0}^{n-1}C_{n-1}{}^mN_{\beta_1\beta_2\cdots\beta_m}{}^{(n-1)}(\mathbf{k})\frac{\partial^{(m)}E^{(1)}(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}\cdots\partial k_{\beta_m}}$$
$$+\sum_{m=0}^{n-2}C_{n-2}{}^mN_{\beta_1\beta_2\cdots\beta_m}{}^{(n-2)}(\mathbf{k})\frac{\partial^{(m)}E^{(2)}(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}\cdots\partial k_{\beta_m}}. \quad (A17)$$

For example, to second order in magnetic field, expression (A15) becomes

$$(S^{\dagger}HS)^{(0)}=\epsilon^{(0)}(\mathbf{k}), \quad (A18)$$

$$(S^{\dagger}HS)^{(1)}=N^{(1)}\epsilon^{(0)}(\mathbf{k})+N_{\beta_1}{}^{(1)}\frac{\partial\epsilon^{(0)}(\mathbf{k})}{\partial k_{\beta_1}}+E^{(1)}(\mathbf{k}), \quad (A19)$$

$$(S^{\dagger}HS)^{(2)}=N^{(2)}(\mathbf{k})\epsilon^{(0)}(\mathbf{k})+2N_{\beta_1}{}^{(2)}(\mathbf{k})\frac{\partial\epsilon^{0}(\mathbf{k})}{\partial k_{\beta_1}}$$
$$+N_{\beta_1\beta_2}{}^{(2)}(\mathbf{k})\frac{\partial^2\epsilon^{(0)}(\mathbf{k})}{\partial k_{\beta_1}\partial k_{\beta_2}}+N^{(1)}(\mathbf{k})E^{(1)}(\mathbf{k})$$
$$+N_{\beta_1}{}^{(1)}(\mathbf{k})\frac{\partial E^{(1)}}{\partial k_{\beta_1}}+E^{(2)}(\mathbf{k}). \quad (A20)$$

Having the general formula (A15) and by using the expansion (47′) for $[N(\mathbf{k})]^{-1/2}$ one can get an expression for the Hamiltonian (A5) to any order in magnetic field. To second order in magnetic field this is given in text [formulas (55a)-(55d)].

In conclusion of this Appendix let us show that $N_{\beta_1\beta_2\cdots\beta_m}{}^{(n)}(\mathbf{k})$ in (A14) and $E(\mathbf{k})$ in (A16) are periodic in $\mathbf{k}$ with the periodicity of the reciprocal lattice vectors. By using the definition of $S(\mathbf{k})$ [formula (46)] one has

$$\left(\frac{\partial^{(n)}S^{\dagger}(\mathbf{k})}{\partial k_{\alpha_1}\partial k_{\alpha_2}\cdots\partial k_{\alpha_n}}\frac{\partial^{(n-m)}S(\mathbf{k})}{\partial k_{\beta_{m+1}}\cdots\partial k_{\beta_n}}\right)_{ll'}$$
$$=\int\frac{\partial^{(n)}u_{lk}{}^*(\mathbf{q})}{\partial k_{\alpha_1}\partial k_{\alpha_2}\cdots\partial k_{\alpha_n}}\frac{\partial^{(n-m)}u_{l'k}(\mathbf{q})}{\partial k_{\beta_{m+1}}\cdots\partial k_{\beta_n}}dq. \quad (A21)$$

From the behavior of the periodic part of the Bloch function, $u_{lk}(\mathbf{q})$, as a function of $\mathbf{k}$, it follows that the expression (A21) is periodic in $\mathbf{k}$. In a similar way one shows that $E(\mathbf{k})$ [A(16), (A10), A(11)] is periodic in $\mathbf{k}$ [see definition (A7) and (A8)].