CONCLUSIONS

In this study, we have attempted to determine the extent to which the independent-particle model describes the angular correlation of the photons emitted when positrons and electrons annihilate in metals and, hence, to evaluate the experiment as a technique for studying the electronic structure of metals. We have concluded that the independent-particle model provides a good first approximation to the angular distribution, even in very anisotropic metals, but that some of the detailed structure which the model predicts is probably reduced by the Coulomb correlations in the system.

The electronic structures of the heavy rare-earth metals have been shown to be rather similar, and the angular distributions which we have observed are qualitatively in agreement with the relativistic augmented-plane-wave calculations of Keeton and Loucks. The structure in the c-axis distributions has been shown to be related to those aspects of the Fermi surface which are believed to be important in determining the magnetic structures. In particular, the difference between Gd and the other magnetic hcp rare-earth metals can be qualitatively understood. The modification of the Fermi surface in the helically ordered magnetic phase of Ho has the expected effect of reducing the structure in the c-axis angular distribution. The electronic structure of the equiatomic Ho-Er alloy has been shown to be similar to those of the constituent metals although a rigid-band model is not apparently strictly applicable.

ACKNOWLEDGMENTS

We have been greatly assisted in this work by the interest and encouragement of Professor T. L. Loucks, whose calculations have allowed a much more detailed interpretation of our results than would otherwise have been possible. O. Dietrich kindly performed the convolution of the theoretical distribution with the resolution function. Valuable discussions with Dr. D. R. Gustafson, who constructed much of the apparatus used in this experiment, and the advice and encouragement of Professor D. J. Zaffarano are gratefully acknowledged. The rare-earth metals and alloys used in this work were kindly supplied by B. J. Beaudry and Professor F. H. Spedding, and invaluable help in growing the single crystals was given by Professor S. Legvold and his group.

PHYSICAL REVIEW VOLUME 168, NUMBER 3 15 APRIL 1968

Dynamics of Electrons in Solids in External Fields

J. ZAK*

Department of Physics and Francis Bitter National Magnet Laboratory,† Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received 11 December 1967)

A quantum-mechanical representation is defined by means of finite translations in direct and reciprocal space. The eigenfunctions of the finite translations are found and their connection with Bloch functions and Wannier functions is established. The new representation is used for describing the motion of a Bloch electron in a magnetic and in an electric field. For the first problem, well-known results are reproduced in an extremely simple and natural way. It is also shown that the representation introduced in this paper gives a straightforward way to compare classical and quantum dynamics for a Bloch electron in external magnetic and electric fields.

I. INTRODUCTION

THE motion of electrons in solids (Bloch electrons) in external magnetic and electric fields has attracted great attention both experimentally and theoretically during all periods in the development of solid-state physics. The reason for this is that very many properties of solids, and in particular their energy spectrum, can be measured by performing experiments in external fields. For example, all the vast field of magneto- and electro-optics and Fermi-surface measurements by the de Haas–van Alphen technique is based on this kind of experiment. It is therefore natural that many papers have been published on the motion of Bloch electrons in external fields.[1–4] The final results derived in the mentioned papers have a very simple physical interpretation and are closely related to the dynamics of unperturbed Bloch electrons. This is a common feature of all theories for the given problem, and physically one should expect that the perturbed motion will in one way or another be connected to the unperturbed one. The mentioned papers[1–4] differ, however, by their approach to the problem, namely, different

* Permanent address: Department of Physics, Technion—Israel Institute of Technology, Haifa, Israel.

† Supported by the U. S. Air Force of Scientific Research.

[1] W. Kohn, Phys. Rev. **115**, 1460 (1959); see this paper for other references.

[2] Laura M. Roth, J. Phys. Chem. Solids **23**, 433 (1962).

[3] Gregory H. Wannier, Rev. Mod. Phys. **34**, 645 (1962); see this paper for other references.

[4] E. I. Blount, Phys. Rev. **126**, 1636 (1962).

basis functions are used in them for expanding the solution of the perturbed motion. It is a very interesting demonstration of the well-known fact that the way the solution is obtained is influenced by the choice of the quantum-mechanical representation. Roth's[2] and Blount's[4] papers treat the problem of a Bloch electron in a magnetic field and were written in order to simplify Kohn's[1] method. Although their task was achieved, there still was a feeling that there must be a much simpler method to obtain results with such a simple physical structure.

In this paper it is shown that the clue for the solution of the problem does indeed lie in the right choice of the basis functions. For this purpose a quantum-mechanical representation recently introduced by the author[5] is used. In this representation the states are specified by eigenvalues of finite translations in the direct and reciprocal spaces. It turns out that in this representation Schrödinger's equation for a Bloch electron in external fields (magnetic and electric) becomes an equation in six independent variables and contains side by side the Bloch motion, the motion in the external fields, and a term that couples them. Such an equation was predicted before[3] and more recently obtained[6,7] on the basis of some assumptions but never rigorously proven because of the lack of a suitable representation. Since we now have a proof of this equation, its connection with the original Schrödinger's equation becomes completely clear, and it can be used, as we will show in this paper, as a very powerful tool for describing the motion of a Bloch electron in external magnetic and electric fields.

In Sec. II the new representation is described and its connection with other representations is given. In Sec. III we discuss the equation for a Bloch electron in external magnetic and electric fields in the new representation. Section IV deals with a Bloch electron in a magnetic field. It is shown how the well-known results can be obtained in an extremely simple and natural way. In Sec. V a general description of the problem is given in terms of the Ehrenfest theorem in quantum mechanics.

II. kq REPRESENTATION

In a previous paper[5] it was proven that finite translations in the direct and reciprocal space form a complete set of commuting operators[8] that can be used to obtain a representation in quantum mechanics. Since the mentioned paper[5] was only a brief letter, in this section we are going to reconstruct what we call the kq representation.

Let us start with a one-dimensional case and let x and p be the coordinate and the momentum that satisfy the commutation relation

$$[p,x]=-i, \tag{1}$$

where we have assumed $h=1$. It is known that for a spinless particle (spin will not be taken into account in this paper) either the operator x or the operator p forms a complete set of commuting operators.[8] This means, for example, that x can be chosen to specify a complete set of functions $\delta(x-x_0)$, which are eigenfunctions of x,

$$x\delta(x-x_0)=x_0\delta(x-x_0), \tag{2}$$

where $\delta(x-x_0)$ is the Dirac δ function and x_0 is the eigenvalue of x in the state $\delta(x-x_0)$. Any function of x, say $\psi(x)$, can be expanded in the set $\delta(x-x_0)$

$$\psi(x)=\int C(x_0)\delta(x-x_0)dx_0, \tag{3}$$

where the integration is over the whole x axis. Let us now define an operator

$$T(a)=\exp(ipa), \tag{4}$$

where a is a constant. This operator represents a finite translation in x space,[9]

$$T(a)\psi(x)=\psi(x+a). \tag{5}$$

It is well known that the operators (4) for a and any multiple of a are of very great importance in solid-state physics, where a has the meaning of a lattice constant. Their importance comes from the fact that they commute with the Hamiltonian for a periodic potential, the period being given by the lattice constant. For example, the Bloch theorem for an electron in a periodic lattice[10] is obtained by requiring that the solution of Schrödinger's equation is also an eigenfunction of $T(a)$:

$$T(a)\psi_k(x)=\exp(ika)\psi_k(x). \tag{6}$$

Here k specifies the eigenvalue of the translation operator $T(a)$ and k assumes values from 0 to $2\pi/a$ or from $-\pi/a$ to π/a. It is clear that Eq. (6) itself does not define the function $\psi_k(x)$ completely and it only requires that $\psi_k(x)$ has the form of a Bloch function

$$\psi_k(x)=\exp(ikx)u_k(x), \tag{7}$$

where $u_k(x)$ is periodic in x with the period a. One way of defining the function $\psi_k(x)$ completely is to require that it satisfies Schrödinger's equation. The function $\psi_k(x)$ will now have a band index n that specifies the energy eigenvalues,

$$\psi_{nk}(x)=\exp(ikx)u_{nk}(x). \tag{8}$$

This is the way Bloch functions are specified by means

[5] J. Zak, Phys. Rev. Letters **19**, 1385 (1967).
[6] H. C. Praddaude, Phys. Rev. **140**, A1292 (1965).
[7] P. G. Harper, J. Phys. Chem. Solids **82**, 495 (1967).
[8] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, New York, 1958).
[9] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, Ltd., London, 1958).
[10] C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, New York, 1963).

of a continuous variable k which comes from the translation symmetry and a discrete energy band index[11] n.

Another way of defining $\psi_k(x)$ in (7) completely is to find operators that commute with $T(a)$ and that form together with $T(a)$ a complete set. Let us define another operator

$$T(b)=\exp(ixb), \tag{9}$$

where b is a constant satisfying

$$ab=2\pi. \tag{10}$$

One can easily check that the commutation relation of $T(a)$ and $T(b)$ vanishes:

$$[T(a),T(b)]=0. \tag{11}$$

This just means that $T(a)$ and $T(b)$ commute. We state that $T(a)$ and $T(b)$ form a complete set of commuting operators. It is clear that any function of $T(a)$ and $T(b)$ will commute with both $T(a)$ and $T(b)$. The question is, however, whether one can find additional operators that are not functions of $T(a)$ and $T(b)$ and that commute with the set $T(a)$, $T(b)$. The answer to this question is negative. Any function of x and p that commutes with both $T(a)$ and $T(b)$ is a function of the latter operators only. To prove this we use a known theorem[12] that any function f of the operators x and p can be written

$$f(xp)=\frac{1}{2\pi}\int \exp(i\alpha p+i\beta x) \times \mathrm{Tr}[f(xp)\exp(-i\alpha p-i\beta x)]d\alpha d\beta, \tag{12}$$

where Tr means trace. Assume now that $f(xp)$ commutes with $T(a)$ and $T(b)$. The only exponentials in (12) will then be with $\alpha=na$ and $\beta=mb$ because only they commute with both $T(a)$ and $T(b)$. Therefore, the requirement that $f(xp)$ commutes with $T(a)$ and $T(b)$ will lead relation (12) to a sum over exponentials

$$\exp(inap+imbx), \tag{13}$$

and $f(xp)$ becomes a function of $T(a)$ and $T(b)$ only. This is the proof that $T(a)$ and $T(b)$ form a complete set of commuting operators. The constants a and b were chosen arbitrarily with the only limitation that they satisfy relation (10). As we mentioned already, in solids a usually has the meaning of a lattice constant and then b according to (10) will have the meaning of a constant in the reciprocal lattice.

The operator $T(a)$ gives a translation by a in the direct space (x space). It can be seen that the operator $T(b)$ gives a translation by $-b$ in the reciprocal space (p space)

$$T(b)\psi(p)=\psi(p-b), \tag{14}$$

because the operator x in the p representation is given by $i(\partial/\partial p)$. The operators $T(a)$ and $T(b)$ are therefore finite translations in the direct and reciprocal spaces, respectively. In solids these operators can be given a very simple meaning of being translations by Bravais-lattice and reciprocal-lattice vectors.

Having proven that $T(a)$ and $T(b)$ form a complete set of commuting operators, let us now find their eigenfunctions. It was mentioned already that the eigenfunctions of $T(a)$ are Bloch functions ψ_k given by relation (7). We now require that they also be eigenfunctions of $T(b)$:

$$T(b)\psi_{kq}(x)=\exp(iqb)\psi_{kq}(x). \tag{15}$$

Here q specifies the eigenvalues of $T(b)$ in the same way as k does it for $T(a)$ in (6). The reason for having such similar relations is because $T(a)$ and $T(b)$ are unitary operators with eigenvalues given by $\exp(ika)$ and $\exp(iqb)$, respectively. In relation (15) q assumes values from 0 to $2\pi/b$ or from $-\pi/b$ to π/b in complete analogy with the values k assumes. In solid-state physics one would say that k varies in the first Brillouin zone while q varies in the first symmetric unit cell.[10] From requirement (15) we get that $\psi_{kq}(x)$ has to be of the form

$$\psi_{kq}(x)=f(kq)\sum_n \delta(x-q-na)\exp(ikna), \tag{16}$$

where the function $f(kq)$ is still to be defined from the normalization of $\psi_{kq}(x)$. That $\psi_{kq}(x)$ is an eigenfunction of both $T(a)$ and $T(b)$ is very easy to check just by verifying relations

$$T(a)\psi_{kq}(x)=\exp(ika)\psi_{kq}(x), \tag{17}$$

$$T(b)\psi_{kq}(x)=\exp(iqb)\psi_{kq}(x). \tag{18}$$

Let us now check the orthogonality of $\psi_{kq}(x)$ for different eigenvalues kq:

$$\int \psi_{kq}^*(x)\psi_{k'q'}(x)dx=b|f(kq)|^2\delta(k-k')\delta(q-q'). \tag{19}$$

For ψ_{kq} to be normalized $|f(kq)|=1/\sqrt{b}$. The function ψ_{kq} then becomes

$$\psi_{kq}(x)=\frac{1}{\sqrt{b}}\sum_n \delta(x-q-na)\exp(ikna). \tag{20}$$

Being eigenfunctions of a complete set of commuting operators $T(a)$ and $T(b)$, the functions ψ_{kq} form a complete set of functions. Any function of x can be expanded in them. One of the checks of the completeness of $\psi_{kq}(x)$ is that

$$\int \psi_{kq}^*(x)\psi_{kq}(x')dkdq=\delta(x-x'), \tag{21}$$

where the integration is over unit cells in the direct and reciprocal lattices.

While constructing the eigenfunctions of $T(a)$ and $T(b)$ we used functions of x and this is why the final result (2) is given in the x representation. It is easy, for

[11] G. F. Koster, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1957), Vol. 5.
[12] H. J. Groenewold, Physica **12**, 405 (1946).

example, to get ψ_{kq} in the p representation by taking a Fourier transform of relation (20):

$$\psi_{kq}(p)=\frac{1}{\sqrt{a}}\exp(-ikq)\sum_n \delta(p-k-nb) \times\exp(-iqnb). \quad (22)$$

Finally, the eigenfunctions of $T(a)$ and $T(b)$ can be written in their own representation (in the kq representation):

$$\psi_{k'q'}(kq)=\delta(k-k')\delta(q-q'). \quad (23)$$

To complete the construction of the kq representation let us find expressions for the operators x and p in it. We start with the operator p:

$$\langle k'q'|p|kq\rangle=\int dpdp'\langle kq|p\rangle\langle p|p|p'\rangle\langle p'|k'q'\rangle$$

$$=\int dpp\langle kq|p\rangle\langle p|k'q'\rangle$$

$$=-i\frac{\partial}{\partial q'}\delta(q'-q)\delta(k'-k). \quad (24)$$

In deriving the result (24) we used expression (22) and the relation $\langle p|kq\rangle=\psi_{kq}(p)$. Similarly one finds an expression for the operator x:

$$\langle k'q'|x|kq\rangle=i\frac{\partial}{\partial k'}\delta(k'-k)\delta(q'-q) +q'\delta(k'-k)\delta(q'-q). \quad (25)$$

There is no doubt that the expression we obtained for the operators x and p depends on the choice of the phase we made in the function $\psi_{kq}(x)$. As we will see later, this choice makes the functions in the kq representation be Bloch-type functions. Alternatively, expressions (24) and (25) can be written as follows:

$$p=-i\partial/\partial q, \quad (26)$$

$$x=i(\partial/\partial k)+q. \quad (27)$$

This completes the construction of the kq representation: We have a complete set of commuting operators (4) and (9), their eigenfunctions (20), which form a complete set of eigenfunctions, and expressions for the basic operators x and p.

Until now we wrote the results for a one-dimensional case but the generalization to three dimensions is straightforward. The translations will be

$$T(\mathbf{R}_n)=\exp(i\mathbf{p}\cdot\mathbf{R}_n), \quad (28)$$

$$T(\mathbf{K}_m)=\exp(i\mathbf{r}\cdot\mathbf{K}_m), \quad (29)$$

where $\mathbf{R}_n=n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$, $\mathbf{K}_m=m_1\mathbf{b}_1+m_2\mathbf{b}_2+m_3\mathbf{b}_3$ with integer $n_1, n_2, n_3, m_1, m_2, m_3$ and $\mathbf{a}_i\cdot\mathbf{b}_j=2\pi\delta_{ij}$. The complete set of the operators is defined on the basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ while all the other operators in (28) and (29) are functions of them. The eigenfunctions in three dimensions will be

$$\psi_{kq}(\mathbf{r})=\left[\frac{\tau}{(2\pi)^3}\right]^{1/2}\sum_{\mathbf{R}_n}\delta(\mathbf{r}-\mathbf{q}-\mathbf{R}_n)\exp(i\mathbf{k}\cdot\mathbf{R}_n), \quad (30)$$

where τ is the volume of a unit cell in the direct space and the vectors $\mathbf{k}$ and $\mathbf{q}$ vary in the cells built on the vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ and $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, respectively. Again, the connection with the concepts of a Bravais lattice and a reciprocal lattice is obvious. Finally, the operators $\mathbf{p}$ and $\mathbf{r}$ in the three-dimensional case are

$$\mathbf{p}=-i\partial/\partial\mathbf{q}, \quad (31)$$

$$\mathbf{r}=i(\partial/\partial\mathbf{k})+\mathbf{q}. \quad (32)$$

The kq representation has a number of very interesting features. First of all, it is a representation in which the operators $\mathbf{r}$ and $\mathbf{p}$ are partly defined together. By giving $\mathbf{k}$ and $\mathbf{q}$ one can tell where in unit cells of $\mathbf{k}$ space and $\mathbf{q}$ space the values of the operators $\mathbf{p}$ and $\mathbf{r}$ are, but one cannot tell in which of the cells they are. This follows from the fact that $\mathbf{k}$ and $\mathbf{k}+\mathbf{K}_m$ define the same eigenvalue of $\exp(i\mathbf{p}\cdot\mathbf{R}_n)$ and similarly, $\mathbf{q}$ and $\mathbf{q}+\mathbf{R}_n$ define the same eigenvalue of $\exp(i\mathbf{r}\cdot\mathbf{K}_m)$. Of course, the possibility of defining partly $\mathbf{r}$ and $\mathbf{p}$ together does not violate the uncertainty principle. However, working with $\mathbf{k}$ and $\mathbf{q}$ together, which means with $\mathbf{p}$ and $\mathbf{r}$ partly together, makes the quantum-mechanical description very close to the Hamiltonian classical description. This will be shown in Sec. V. Another interesting feature of the kq representation is its connection to the Bohr-Sommerfeld quantization rules. Let us consider a one-dimensional case. It is known[9] that for finding energy levels one can use the condition

$$\oint pdx=2\pi\hbar(n+\gamma), \quad (33)$$

where the integration is on a closed path in phase space, n is an integer which gives the quantum state number n, and γ is a phase factor which we assume here to be zero. One can write relation (33) in a different way:

$$\oint pdx/2\pi\hbar=n, \quad (34)$$

and interpret the left-hand side of it[9] as the number of quantum states contained in the area of phase space $\oint pdx$. This is just the well-known rule that the number of quantum states in an area of phase space is given by this area divided by $2\pi\hbar$. In the kq representation the area of the elementary region where k and q vary is $2\pi/a\times 2\pi/b=2\pi$ or $2\pi\hbar$ if $\hbar$ is not assumed to be 1. Every point in this elementary cell gives a different quantum state. Allow now the kq values to cover the whole plane and we get the phase space. The number of times that a definite quantum state appears in an area

$\oint p dx$ is given by this area divided by $2\pi\hbar$ because every quantum state appears once in the area $2\pi\hbar$. We therefore can associate a more precise meaning to formula (34), namely, n gives the number of times a given quantum state appears in the area $\oint p dx$ or the weight of every quantum state. It is in this meaning that formula (34) is used in integration over phase space in statistical mechanics.[13] One usually replaces the classical elementary area $dpdx$ by $dpdx/2\pi\hbar$.

It is also interesting to compare the functions $\psi_{kq}(\mathbf{r})$ in (30) with functions one uses in the Bloch theory of solids. First of all, $\psi_{kq}(\mathbf{r})$ is a Bloch-type function because it satisfies relation (17). However, while Bloch functions ψ_{nk} have a discrete band index and a continuous wave vector $\mathbf{k}$, the functions ψ_{kq} are specified by two continuous vectors $\mathbf{k}$ and $\mathbf{q}$. As we will see in the next section, this will lead us to a six-dimensional equation from which one can obtain a very good insight of the motion in external fields. A function very often used is the Wannier function.[3] The expression (30) is of the same type as the one that connects Bloch functions with Wannier functions. The only difference is that the Wannier function appears instead of the δ functions in (30).[10] One can therefore say that the Wannier functions that are defined through the ψ_{kq} Bloch-type functions are infinitely localized, and instead of having a discrete band index, they are defined by a continuous vector $\mathbf{q}$. This infinite localization of the Wannier-type functions $\delta(\mathbf{r}-\mathbf{q}-\mathbf{R}_n)$ is just the feature that is needed in describing the dynamics of Bloch electrons in external fields.[2,3]

Other features of the kq representation will become apparent in the following sections.

III. SCHRÖDINGER'S EQUATION IN THE kq REPRESENTATION

In this section we obtain the equation for an electron in a periodic potential and constant magnetic and electric fields in the kq representation. In doing so we start with Schrödinger's equation for this problem in the r representation

$$\left[\left(\mathbf{p}+\frac{e}{2c}\mathbf{H}\times\mathbf{r}\right)^2\Big/2m+V(\mathbf{r})+e\mathbf{E}\cdot\mathbf{r}\right]\psi(\mathbf{r})=\epsilon\psi(\mathbf{r}), \quad (35)$$

where $V(\mathbf{r})$ is the periodic potential, $\mathbf{H}$ and $\mathbf{E}$ are the magnetic and electric fields, respectively, and e is the charge of the electron with a minus sign ($e>0$). By using expressions (31) and (32), this equation can be written in the kq representation:

$$\left\{\left[-i\frac{\partial}{\partial\mathbf{q}}+\frac{e}{2c}\mathbf{H}\times\left(i\frac{\partial}{\partial\mathbf{k}}+\mathbf{q}\right)\right]^2\Big/2m+V(\mathbf{q})+e\mathbf{E}\cdot\left(i\frac{\partial}{\partial\mathbf{k}}+\mathbf{q}\right)\right\}C(\mathbf{kq})=\epsilon C(\mathbf{kq}), \quad (36)$$

[13] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, Ltd., London, 1958).

where $C(\mathbf{kq})$ is the wave function in the kq representation. That the periodic potential is just a function of $\mathbf{q}$ follows from its periodicity which enables the expansion

$$V(\mathbf{r})=\sum_{\mathbf{K}_m}V(\mathbf{K}_m)\exp(i\mathbf{K}_m\cdot\mathbf{r}), \quad (37)$$

where $\mathbf{K}_m$ are vectors of the reciprocal lattice defined earlier. Expression (37) contains the operators $T(\mathbf{K}_m)$ and since $C(\mathbf{kq})$ satisfies relation (40) below, the exponential in (37) can be replaced by $\exp(i\mathbf{K}_m\cdot\mathbf{q})$ which leads to $V(\mathbf{q})$. This makes the kq representation particularly useful for treating problems with a periodic potential. The wave function $C(\mathbf{kq})$ is connected to $\psi(\mathbf{r})$ in Eq. (35) by the relation

$$\psi(\mathbf{r})=\int d\mathbf{k}d\mathbf{q}\,C(\mathbf{kq})\psi_{kq}(\mathbf{r}), \quad (38)$$

where $\psi_{kq}(\mathbf{r})$ are the eigenfunctions (30) of the operators (28) and (29), and the integration is over the unit cells in $\mathbf{k}$ and $\mathbf{q}$ space. The inverted formula is

$$C(\mathbf{kq})=\int d\mathbf{r}\psi(\mathbf{r})\psi_{kq}{}^*(\mathbf{r}). \quad (39)$$

From the expression (30) for ψ_{kq} it follows that $C(\mathbf{kq})$ satisfies the following conditions:

$$C(\mathbf{k}+\mathbf{K}_m,\mathbf{q})=C(\mathbf{k},\mathbf{q}), \quad (40)$$

$$C(\mathbf{k},\mathbf{q}+\mathbf{R}_m)=\exp(i\mathbf{k}\cdot\mathbf{R}_m)C(\mathbf{k},\mathbf{q}). \quad (41)$$

These are the boundary conditions on $C(\mathbf{kq})$ and we see that the latter are Bloch-type functions, they are periodic with respect to $\mathbf{k}$, and produce a phase factor $\exp(i\mathbf{k}\cdot\mathbf{R}_n)$ when $\mathbf{q}$ is replaced by $\mathbf{q}+\mathbf{R}_n$.

Equation (36) contains six independent variables $\mathbf{k}$ and $\mathbf{q}$. This does not mean that the number of degrees of freedom of the problem has changed. The only thing that happened is that instead of having three variables $\mathbf{r}$ in an infinite region we have now six variables $\mathbf{k}$, $\mathbf{q}$ that are restricted to unit cells in $\mathbf{k}$ and $\mathbf{q}$ spaces. This change leads to a very important consequence. While in Eq. (35) there are infinite terms caused by the magnetic and electric fields when $\mathbf{r}\to\infty$, none such terms appear in Eq. (36) because $\mathbf{k}$ and $\mathbf{q}$ are limited to unit cells only. In order to appreciate more fully the significance of Eq. (36), let us perform a phase transformation by looking for $C(\mathbf{kq})$ in a form

$$C(\mathbf{kq})=\exp(i\mathbf{k}\cdot\mathbf{q})U(\mathbf{kq}). \quad (42)$$

The equation for $U(\mathbf{kq})$ will be

$$\left[\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m+V(\mathbf{q})+e\mathbf{E}\cdot i\frac{\partial}{\partial\mathbf{k}}\right]U(\mathbf{kq})=\epsilon U(\mathbf{kq}). \quad (43)$$

The boundary conditions on $U(\mathbf{kq})$ are accordingly

$$U(\mathbf{k}+\mathbf{K}_m,\mathbf{q})=\exp(-i\mathbf{r}\cdot\mathbf{K}_m)U(\mathbf{k},\mathbf{q}), \quad (44)$$

$$U(\mathbf{k},\mathbf{q}+\mathbf{R}_m)=U(\mathbf{k},\mathbf{q}). \quad (45)$$

These conditions are the same that the periodic part of the Bloch function u_{nk} in (8) satisfies. In fact, if one assumes in Eq. (43) $H=E=0$, one has

$$\left[\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}\right)^2\Big/2m+V(\mathbf{q})\right]U(\mathbf{kq})=\epsilon U(\mathbf{kq}), \quad (46)$$

which is the same equation that $u_{nk}(\mathbf{r})$ satisfies.[10] In (46) the vector $\mathbf{k}$ can be used for specifying the function U and the energy ϵ and for a given $\epsilon_n(\mathbf{k})$ the solution of (46) is just $u_{nk}(\mathbf{q})$.

In the general equation (43) both $\mathbf{k}$ and $\mathbf{q}$ are variables, and solutions have to be found for ϵ that are independent of $\mathbf{k}$ and $\mathbf{q}$. An equation of the type of (43) for $\mathbf{H}=0$ was given already in Ref. 3 and applied in describing the dynamics of Bloch electrons in an external electric field. However, instead of the real energy ϵ, a variable W appears which is $\mathbf{k}$-dependent and which is in some limiting way connected to the energy of the system. Equation (43) was also obtained in Refs. 6 and 7 and shown to be very useful in the effective-mass approximation. In Ref. 6, Eq. (43) was obtained by using a set of functions that was assumed to be complete. Although not stated explicitly, the boundary conditions on the wave function in Ref. 6 are the same as are given by relations (44) and (45). In Ref. 7, Eq. (43) was obtained for the magnetic field only by using symmetry properties of Schrödinger's equations for a Bloch electron in a magnetic field. It was pointed out before[14] that it is doubtful whether the functions used by Harper can be solutions of Schrödinger's equation. In fact, by using his functions Harper obtains Eq. (43) for $E=0$; however, with boundary conditions on U which are in error.[5] It is only now when Eq. (43) is derived on a firm quantum-mechanical basis that the variables in it and the wave function become well defined.

As was mentioned before, Eq. (43) contains six variables $\mathbf{k}$, $\mathbf{q}$. It can be seen that the terms in Eq. (43) that depend on $\mathbf{q}$ give simply a Bloch Hamiltonian, while the terms that contain only $\mathbf{k}$ represent a Fourier transform of the Hamiltonian (35) for $V(\mathbf{r})=0$. It follows therefore that in Eq. (43) the Bloch motion and the motion in external fields appear side by side. The term that contains both variables $\mathbf{k}$ and $\mathbf{q}$ couples these two motions.[6,7] This feature of Eq. (43) corresponds to the general picture for the motion of Bloch electrons in perturbed crystals.[10]

In conclusion of this section we expand $U(\mathbf{kq})$ in solutions of the unperturbed equation (46), $u_{nk}(\mathbf{q})$. Both $U(\mathbf{kq})$ and $u_{nk}(\mathbf{q})$ satisfy the same boundary conditions (44) and (45), and therefore

$$U(\mathbf{kq})=\sum_n B_n(\mathbf{k})u_{nk}(\mathbf{q}), \quad (47)$$

with coefficients $B_n(\mathbf{k})$ that are periodic in $\mathbf{k}$, the period being the vectors $\mathbf{K}_m$ of the reciprocal lattice. Let us note that the summation in (47) is only on the band index. This differs from the usual expressions[1,2] where summation on $\mathbf{k}$ is also performed. It turns out[1,15] that for constructing effective one-band Hamiltonians it is more convenient to use the functions $u_{n0}(\mathbf{q})$ in the expansion (47). We then have

$$U(\mathbf{kq})=\sum_n A_n(\mathbf{k})u_{n0}(\mathbf{q}), \quad (48)$$

where

$$u_{nk}(\mathbf{q})=\sum_m S_{mn}(\mathbf{k})u_{m0}(\mathbf{q}) \quad (49)$$

and

$$A_n(\mathbf{k})=\sum_l S_{nl}(\mathbf{k})B_l(\mathbf{k}). \quad (50)$$

Formula (48) is obtained just by expanding $u_{nk}(\mathbf{q})$ in (47) according to (49), which is always possible because $u_{n0}(\mathbf{q})$ form a complete system with respect to any periodic function,[15] and by using the definition (50). The convenience of expansion (48) is given by the fact that in it the variables $\mathbf{k}$ and $\mathbf{q}$ are completely separated.

The following observation will be of very great importance in the next sections where we describe the motion of a Bloch electron in external fields. Let us substitute in Eq. (46) for $E=H=0$ the expansion (47), then multiply Eq. (46) from the left by $u_{mk}^*(\mathbf{q})$ and integrate over $\mathbf{q}$. We obtain the following equation for $B_n(\mathbf{k})$:

$$\epsilon_m(\mathbf{k})B_m(\mathbf{k})=\epsilon B_m(\mathbf{k}), \quad (51)$$

which is just the equation for a Bloch electron without external fields. If we do the same with the expansion (48), an equation for $A_m(\mathbf{k})$ is obtained.

$$\left(\epsilon_m(0)+\frac{k^2}{2m}\right)A_m(\mathbf{k})+\sum_n\frac{\mathbf{k}\cdot\mathbf{p}_{mn}}{m}A_n(\mathbf{k})=\epsilon A_m(\mathbf{k}), \quad (52)$$

where

$$\mathbf{p}_{mn}=-i\int u^*_{m0}(\mathbf{q})\frac{\partial}{\partial\mathbf{q}}u_{n0}(\mathbf{q})d\mathbf{q}. \quad (53)$$

It is therefore seen that while Eq. (51) has no interband terms, Eq. (52) is a coupled system of equations. We know, however, what kind of transformation one has to perform on $A_n(\mathbf{k})$ [formula (50)] in order to get rid of all the interband terms and to pass from Eq. (52) to Eq. (51):

$$\sum_n\{S^\dagger(\mathbf{k})H(\mathbf{k})S(\mathbf{k})\}_{mn}B_n(\mathbf{k})=\sum_n\epsilon_m(\mathbf{k})\delta_{mn}B_n(\mathbf{k})=\epsilon B_m(\mathbf{k}). \quad (51')$$

The matrix $S(\mathbf{k})$, by means of which this transformation is carried out, is unitary, as can be seen either by comparing the right-hand sides of Eqs. (51) and (52) or by

[14] J. Zak, Phys. Rev. **136**, A1647 (1964).

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

a straightforward calculation:

$$\{S^\dagger(\mathbf{k})S(\mathbf{k})\}_{nm}$$
$$=\sum_\alpha S^*(\mathbf{k})_{\alpha n}S_{\alpha m}(\mathbf{k})$$
$$=\sum_\alpha \int u_{\alpha 0}(\mathbf{q})u_{nk}{}^*(\mathbf{q})d\mathbf{q}\int u_{\alpha 0}{}^*(\mathbf{q}')u_{mk}(\mathbf{q}')d\mathbf{q}'$$
$$=\delta_{nm}, \tag{54}$$

where we have used completeness of the functions u and the definition of $S(\mathbf{k})$ from (49):

$$S_{mn}(\mathbf{k})=\int u_{m0}{}^*(\mathbf{q})u_{nk}(\mathbf{q})d\mathbf{q}. \tag{55}$$

Since one-band effective Hamiltonians are obtained by transforming away interband terms, the transformation (55) will be used extensively in the next sections.

IV. BLOCH ELECTRON IN A MAGNETIC FIELD

In this section we reproduce the well-known one-band effective Hamiltonian for a Bloch electron in a magnetic field.[1,2,4] The reason for doing it again is to show that the kq representation, introduced in this paper, makes the problem trivial. We want to solve Eq. (43) for $E=0$:

$$\left[\left(-i\frac{\partial}{\partial\mathbf{q}}+\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m+V(\mathbf{q})\right]$$
$$\times U(\mathbf{kq})=\epsilon U(\mathbf{kq}). \tag{56}$$

Let us use expansion (48) for $U(\mathbf{kq})$, then multiply Eq. (56) by $u_{m0}{}^*(\mathbf{q})$ from the left and integrate over $\mathbf{q}$. The result is

$$\left[\epsilon_{m0}(0)+\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m\right]A_m(\mathbf{k})$$
$$+\sum_n\left[\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)\cdot\mathbf{p}_{mn}\Big/m\right]A_n(\mathbf{k})$$
$$=\epsilon A_m(\mathbf{k}). \tag{57}$$

Equation (57) for a Bloch electron in a magnetic field is the same as Eq. (52) for $\mathbf{H}=0$ with $\mathbf{k}$ replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. The usual problem of constructing an effective one-band Hamiltonian is to get rid of the interband terms in (57). We know, however, how to do it for Eq. (52) and to pass to Eq. (51) which has no interband elements. This was achieved by the transformation (50), where the unitary matrix $S(\mathbf{k})$ is given in (55). Since Eq. (57) can be obtained from Eq. (52) by replacing in the latter $\mathbf{k}$ by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$, we can expect that the matrix $S(\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k})$, where $\mathbf{k}$ is replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$, will transform away the interband elements in Eq. (57). As we will see, this is almost the case. The problem is that the matrix $S(\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k})$ is not well defined because the components of the vector $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ do not commute with each other:

$$\left[\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)_\alpha,\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)_\beta\right]$$
$$=-\frac{e}{c}\epsilon_{\alpha\beta\gamma}H^\gamma, \tag{58}$$

where $\epsilon_{\alpha\beta\gamma}$ is the unit antisymmetric tensor in all the three indices and a summation on repeated indices is understood. Let us mention at this point that Blount in his paper[4] arrived at the same equation (57) and was faced with the same problem. He works, however, with a semiclassical mixed representation where the commutation relation (58) is replaced by quite complicated multiplication rules on functions. It is for this reason that his diagonalization procedure becomes rather complicated.

One possible way of defining the matrix $S\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ from $S(\mathbf{k})$ is to symmetrize in the latter all the products of the components of the vector $\mathbf{k}$ [for example, to write $\frac{1}{2}(k_xk_y+k_yk_x)$ instead of k_xk_y] and then to replace $\mathbf{k}$ by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. The function that is obtained in such a procedure will be denoted by

$$[S(\mathbf{k})], \tag{59}$$

where the rectangular brackets mean that $S(\mathbf{k})$ was first symmetrized as a function of $\mathbf{k}$ and then $\mathbf{k}$ replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. Notation (59) will be used in what follows.

Let us now show that the operator $[S(\mathbf{k})]$ diagonalizes the Hamiltonian in Eq. (57) to the lowest order in magnetic field. The meaning of diagonalizing Eq. (57) to different powers in the magnetic field[1,2,4] will become clear below. It is first to be noted that $[S(\mathbf{k})]$ is not unitary. For checking it we want to find

$$[S^\dagger(\mathbf{k})][S(\mathbf{k})], \tag{60}$$

where we have used the fact that rectangular brackets and conjugation are commuting operations. In order to be able to use formula (54) we have to write the product (60) as a symmetric function of the variable $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. Although each term in (60) is symmetric, their product will in general no longer be so. In the paper by Roth[2] a rule is given how to expand a product of any two functions $[A(\mathbf{k})][B(\mathbf{k})]$ in a power series of the magnetic field where the coefficients are symmetric functions in the components of $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. The rule is as follows (to second order in the magnetic field):

$$[A(\mathbf{k})][B(\mathbf{k})]$$
$$=[A(\mathbf{k})B(\mathbf{k})]-ih_{\alpha\beta}\left[\frac{\partial A(\mathbf{k})}{\partial k_\alpha}\times\frac{\partial B(\mathbf{k})}{\partial k_\beta}\right]$$
$$-h_{\alpha\beta}h_{\alpha'\beta'}\left[\frac{\partial^2A(\mathbf{k})}{\partial k_\alpha\partial k_{\alpha'}}\times\frac{\partial^2B(\mathbf{k})}{\partial k_\beta\partial k_{\beta'}}\right]+\cdots, \tag{61}$$

where the summation on repeated indices is understood. The definition of a function in rectangular brackets is given in (59) and

$$h_{\alpha\beta}=\epsilon_{\alpha\beta\gamma}eH^{\gamma}/2c. \tag{62}$$

In (62), $\epsilon_{\alpha\beta\gamma}$ is the antisymmetric unit tensor and H^{γ} is the γ component of the magnetic field. By applying formula (61) to the product in (60) we find

$$[S^{\dagger}(\mathbf{k})][S(\mathbf{k})]=I-ih_{\alpha\beta}\left[\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_{\alpha}}\times\frac{\partial S(\mathbf{k})}{\partial k_{\beta}}\right]$$
$$-h_{\alpha\beta}h_{\alpha'\beta'}\left[\frac{\partial^2 S^{\dagger}(\mathbf{k})}{\partial k_{\alpha}\partial k_{\alpha'}}\times\frac{\partial^2 S(\mathbf{k})}{\partial k_{\beta}\partial k_{\beta'}}\right], \tag{63}$$

where I is a unit matrix and was obtained by using formula (53) for the unitarity of $S(\mathbf{k})$. We see therefore that to the lowest order in the magnetic field the matrix $[S(\mathbf{k})]$ is unitary.

It is now very easy to show that $[S(\mathbf{k})]$ diagonalizes Eq. (57) to the lowest order in magnetic field. Indeed, by using $[S(\mathbf{k})]$ for transforming $A_n(\mathbf{k})$ to new functions $B_n(\mathbf{k})$,

$$A(\mathbf{k})=[S(\mathbf{k})]B(\mathbf{k}), \tag{64}$$

Eq. (57) becomes

$$[S^{\dagger}(\mathbf{k})][H(\mathbf{k})][S(\mathbf{k})]B(\mathbf{k})=\epsilon[S^{\dagger}(\mathbf{k})][S(\mathbf{k})]B(\mathbf{k}), \tag{65}$$

where $[H(\mathbf{k})]$ is the Hamiltonian of (57) which is originally written in such a symmetrized way. The right-hand side of Eq. (65) was already written as a power series in the magnetic field. Let us use formula (61) and do the same with the left-hand side of (65). We have

$$[S^{\dagger}(\mathbf{k})][H(\mathbf{k})][S(\mathbf{k})]=[S^{\dagger}(\mathbf{k})H(\mathbf{k})S(\mathbf{k})]-ih_{\alpha\beta}\left\{\left[S^{\dagger}(\mathbf{k})\frac{1}{m}(p_{\alpha}+k_{\alpha})\frac{\partial S(\mathbf{k})}{\partial k_{\beta}}\right]+\left[\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_{\alpha}}\times\frac{\partial}{\partial k_{\beta}}(H(\mathbf{k})S(\mathbf{k}))\right]\right\}$$
$$-h_{\alpha\beta}h_{\alpha'\beta'}\left\{\frac{1}{2m}\left[S^{\dagger}(\mathbf{k})\frac{\partial^2 S(\mathbf{k})}{\partial k_{\beta}\partial k_{\beta'}}\right]\delta_{\alpha\alpha'}+\left[\frac{\partial S^{\dagger}(\mathbf{k})}{\partial k_{\alpha}}\times\frac{\partial}{\partial k_{\beta}}\left(\frac{1}{m}(p_{\alpha'}+k_{\alpha'})\frac{\partial S(\mathbf{k})}{\partial k_{\beta'}}\right)\right]\right.$$
$$\left.+\frac{1}{2}\left[\frac{\partial^2 S^{\dagger}(\mathbf{k})}{\partial k_{\alpha}\partial k_{\alpha'}}\times\frac{\partial^2}{\partial k_{\beta}\partial k_{\beta'}}(H(\mathbf{k})S(\mathbf{k}))\right]\right\}, \tag{66}$$

where again as before the rectangular brackets mean that the function inside is symmetrized with respect to the components of $\mathbf{k}$, and $\mathbf{k}$ is replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. The quantity p_{α} in formula (66) is a matrix with elements given by formula (53) while k_{α} is clearly a scalar matrix. In the lowest order of the magnetic field Eq. (65) for any band n becomes

$$[\epsilon(\mathbf{k})]B_n(\mathbf{k})=\epsilon B_n(\mathbf{k}). \tag{67}$$

This equation follows at once from (66), (63), and (51′). The result (67) is the same as was obtained before.[1,2,4] One-band effective Hamiltonians in higher powers of the magnetic field can be obtained by diagonalizing Eq. (65) and making use of the expressions (63) and (66). We will not do it here because Eq. (65) together with the expressions (63) and (66) is exactly the result of Roth's paper[2] [Eq. (24) together with formulas (45), (46), (50), (51), (52), and (56)]. It is to be mentioned, however, that the derivation in Ref. 2 was based on an assumption of completeness of some set of functions while in this paper the kq representation was used which was proven to produce a complete set of functions. In some sense one can say that the reproduction of the results of Ref. 2 by means of the kq representation is a proof of the completeness of the functions used in Ref. 2.

V. FUNDAMENTAL DYNAMICS IN THE BLOCH THEORY OF SOLIDS

Two theorems have been very widely used for describing the motion of a Bloch electron in external electric and magnetic fields. These theorems are[10,16]

$$\dot{\mathbf{k}}=-e\mathbf{E}, \tag{68}$$

$$\dot{\mathbf{k}}=-(e/c)\mathbf{v}\times\mathbf{H}, \tag{69}$$

where $\dot{\mathbf{k}}$ is the time derivative of the $\mathbf{k}$ vector and $\mathbf{v}$ is assumed to be the velocity of a Bloch electron in the state specified by the vector $\mathbf{k}$. Because of their importance many proofs of theorems (68) and (69) have been presented in the literature. Having the kq representation it is interesting to rederive these theorems.

Let us start with the electric-field case. The motion is described by Eq. (43) with $\mathbf{H}=0$. The coordinates in this equation $\mathbf{k}$ and $\mathbf{q}$ give the eigenvalues of translations $\exp(i\mathbf{p}\cdot\mathbf{a})$ and $\exp(i\mathbf{r}\cdot\mathbf{b})$, respectively. The rate of change in time of $\mathbf{k}$ is defined by the Hamiltonian H of (43) with $\mathbf{H}=0$ and is as follows:

$$\dot{\mathbf{k}}=i[H,\mathbf{k}]=-e\mathbf{E}.$$

We see therefore that Eq. (68) follows straightforwardly

[16] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, New York, 1965).

in the kq representation. It is worthwhile to mention the meaning of Eq. (68). When there is only a periodic potential, the eigenvalues $\exp(i\mathbf{k}\cdot\mathbf{a})$ of translations $\exp(i\mathbf{p}\cdot\mathbf{a})$ are constants of motion. If in addition to a periodic potential there is also an electric field present, the eigenvalues $\exp(i\mathbf{k}\cdot\mathbf{a})$ are no longer constant in time and are given as follows:

$$\exp(i[\mathbf{k}-e\mathbf{E}t]\cdot\mathbf{a}). \tag{70}$$

It is to be noted that expression (68) or (70) is exact and has nothing to do with a one-band approximation.

The equation for the magnetic case is given in (56). If we would try to calculate $\dot{\mathbf{k}}$ from (56) by using the relation $\dot{\mathbf{k}}=i[H,\mathbf{k}]$, this would lead us to a gauge-dependent result.[16] This is not surprising because only the combination $\mathbf{k}+(e/2c)H\times i\partial/\partial\mathbf{k}$ is gauge-independent. In fact, the classical analog of (69) is

$$m\dot{\mathbf{v}}=(e/c)\mathbf{v}\times\mathbf{H}, \tag{71}$$

with the velocity $\mathbf{v}$ on the left-hand side and not the $\mathbf{k}$ vector as in (69).

In order to find an equation for a Bloch electron in a magnetic field that corresponds to (71) for a free electron, we use the result of the preceding section. It was shown there (and is well known[1,2,4]) that in the lowest order of the magnetic field, the one-band Hamiltonian is given by $[\epsilon_n(\mathbf{k})]$, where the rectangular brackets mean here that $\epsilon_n(\mathbf{k})$ is first symmetrized with respect to different components of the vector $\mathbf{k}$ and then $\mathbf{k}$ is replaced by $\mathbf{k}+(e/2c)H\times i\partial/\partial\mathbf{k}$. The derivative with respect to time of the vector $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ (which is the velocity operator for an electron in a magnetic field) is as follows:

$$(d/dt)[\mathbf{k}]=i[[\epsilon_n(\mathbf{k})],[\mathbf{k}]], \tag{72}$$

where on the right-hand side the outside brackets mean just the commutation relation. By using formula (61) one finds that to first order in the magnetic field, relation (72) will be

$$\frac{d}{dt}[\mathbf{k}]=-\frac{e}{c}\left[\frac{\partial\epsilon_n(\mathbf{k})}{\partial\mathbf{k}}\right]\times\mathbf{H}. \tag{73}$$

In deriving Eq. (73), which is correct to first order in the magnetic field, we took only the zero-order term in the effective one-band Hamiltonian, because higher-order terms in the effective Hamiltonian would lead to higher-order terms in (73).

It follows therefore that the correct equation for describing the motion of a Bloch electron in a magnetic field[3] is (73) and not (69). The reason that Eq. (69) leads to correct results when used in a semiclassical theory of transport[10] is easily seen by comparing (69) with (73). The only difference between these two equations is that in the latter $\mathbf{k}$ is replaced by $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ which is just a relabeling of the variable. It is clear that one has to have in mind the velocity components $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ and not $\mathbf{k}$ when using the equation of motion for a Bloch electron in a magnetic field.

The next question to ask is what kind of an equation does one get for a Bloch electron in both a magnetic and electric field. We saw that for the electric case the vector $\mathbf{k}$ appears in the equation of motion, while in the magnetic case the vector $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ appears. To find the equation of motion when both fields are present we need an effective one-band Hamiltonian. Let us show that the matrix $[S(\mathbf{k})]$ given by (55) and (59) diagonalizes the equation for a Bloch electron in both an electric and magnetic field to zero order of the magnetic field (as before) and to first order in the electric field. By using expansion (48) one gets from (43) the following equation for $A_n(\mathbf{k})$:

$$\left[\epsilon_m(0)+\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)^2\Big/2m\right]A_m(\mathbf{k})+e\mathbf{E}\cdot i\frac{\partial}{\partial\mathbf{k}}A_m(\mathbf{k})$$
$$+\sum_n\left\{\left[\left(\mathbf{k}+\frac{e}{2c}\mathbf{H}\times i\frac{\partial}{\partial\mathbf{k}}\right)\cdot\mathbf{p}_{mn}\right]\Big/m\right\}$$
$$\times A_n(\mathbf{k})=\epsilon A_m(\mathbf{k}). \tag{74}$$

This equation differs from the one for a magnetic field only by the presence of the diagonal term containing the electric field. By applying the transformation $[S(\mathbf{k})]$ to the part of the Hamiltonian in (79) that does not depend on the electric field, we get the same result as before to the zero order in magnetic field, namely, $[\epsilon_n(\mathbf{k})]$ as in Eq. (67). The part of the Hamiltonian that depends on $\mathbf{E}$ will become

$$[S^\dagger(\mathbf{k})]e\mathbf{E}\cdot i\frac{\partial}{\partial\mathbf{k}}[S(\mathbf{k})]$$
$$=eE\cdot i\frac{\partial}{\partial\mathbf{k}}+[S^\dagger(\mathbf{k})]e\mathbf{E}\cdot\left(i\frac{\partial}{\partial\mathbf{k}}[S(\mathbf{k})]\right). \tag{75}$$

In the second term the derivative with respect to $\mathbf{k}$ can be replaced by the derivative with respect to $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ and we can therefore apply formula (61) to this term. In zero order of the magnetic field and first order in the electric field the effective one-band Hamiltonian of (74) will be

$$[\epsilon_n(\mathbf{k})]+e\mathbf{E}\cdot\left(i\frac{\partial}{\partial\mathbf{k}}+[\mathbf{x}_{nn}(\mathbf{k})]\right), \tag{76}$$

where

$$\mathbf{x}_{nn}(\mathbf{k})=\int u_{nk}{}^*i\frac{\partial}{\partial\mathbf{k}}u_{nk}d\mathbf{q}. \tag{77}$$

When $\mathbf{H}=0$, expression (76) goes over into the known one-band effective Hamiltonian for a Bloch electron in an electric field only.[17] We can now find the time deriva-

[17] E. N. Adams, Phys. Rev. **107**, 698 (1957).

tive of $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$. By using (76) and (61) one gets in the lowest order of magnetic and electric fields

$$\frac{d}{dt}[\mathbf{k}]=-e\left(\mathbf{E}+\frac{1}{c}\left[\frac{\partial\epsilon_n(\mathbf{k})}{\partial\mathbf{k}}\right]\times\mathbf{H}\right). \tag{78}$$

It is again to be noted that formula (78) differs from the one commonly used in transport theory. In the latter no rectangular brackets appear. As was already mentioned, this difference is not essential in the semiclassical transport theory because it means just using a different notation for the vector $\mathbf{k}$. There is no doubt, however, that quantum mechanically Eqs. (73) and (78) without the rectangular brackets are completely meaningless because then the noncommutativity of the components of $\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}$ becomes essential. This is best demonstrated in the derivation of Onsager's relation ($\mathbf{E}=0$). Let us assume that $\mathbf{H}$ is in the z direction and denote

$$\chi^+=\mathbf{k}+(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}. \tag{79}$$

$\chi_z^+=k_z$, and according to (73) is a constant of motion. The other two components χ_x^+ and χ_y^+ satisfy relation (58), and the Bohr-Sommerfeld quantization rule (33) for them is ($\hbar$ is not assumed to be 1)

$$\oint\chi_x^+d\chi_y^+=\frac{2\pi eH}{\hbar c}(n+\gamma). \tag{80}$$

On the left-hand side we have an area in the χ space $S(\epsilon,\chi_z)$ for a given energy ϵ and χ_z^+. Relation (80) can therefore be written

$$S(\epsilon,\chi_z^+)=(2\pi eH/\hbar c)(n+\gamma), \tag{81}$$

which is Onsager's relation.[18] By using the coordinates χ^+ we did not take into account all the degrees of freedom of the three-dimensional problem. The couple of conjugate coordinates χ_x^+, χ_y^+ describes one degree of freedom, while $\chi_z^+=k_z$ describes another one. The third degree of freedom can be described by the x and y components of the vector[19]:

$$\chi^-=\mathbf{k}-(e/2c)\mathbf{H}\times i\partial/\partial\mathbf{k}. \tag{82}$$

Their commutation relation is

$$[\chi_x^-,\chi_y^-]=ieH/c. \tag{83}$$

Both χ_x^- and χ_y^- commute with the Hamiltonian $[\epsilon_n(\mathbf{k})]$ and the commuting set of operators [see expressions (4), (9), and (10)]

$$\exp(i\chi_x^-A),\quad \exp(i\chi_y^-B), \tag{84}$$

with

$$AB=2\pi c/eH, \tag{85}$$

can be used for specifying eigenstates[20] of $[\epsilon_n(\mathbf{k})]$. The complete specification of the eigenstates of $[\epsilon_n(\mathbf{k})]$ will therefore be given by the number n in (81) by k_z and by the eigenvalues of the operators (84). Since the Hamiltonian $[\epsilon_n(\mathbf{k})]$ does not depend on the latter, this leads to the known degeneracy of Landau levels which in our description will be given by the number of states contained in area of variation of χ_x^-, χ_y^-. This area equals $2\pi/AB$ and the number of states is therefore[18]

$$eH/2\pi\hbar c. \tag{86}$$

In conclusion we would like to remark that this paper shows how well-known results can be reproduced in a simple and very natural way by using the kq representation.

ACKNOWLEDGMENTS

The author would like to thank Professor Y. Aharonov for making available prior to publication his results on the use of modular operators in describing the significance of potentials in quantum mechanics. It is also a pleasure to the author to express his gratitude to the Physics Department and the Francis Bitter National Magnet Laboratory, M.I.T., for their kind hospitality.

[18] L. Onsager, Phil. Mag. **43**, 1006 (1952).

[19] R. Kubo, H. Hasegawa, and N. Hashitsume, J. Phys. Soc. Japan **14**, 56 (1959).

[20] J. Zak, Phys. Rev. **134**, A1602 (1964); **134**, A1607 (1964).