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Dynamics of Bloch Electrons in a Magnetic Field

Prasanta K. Misra
Department of Physics, Utkal University, Bhubaneswar-4, Orissa, India
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A class of representations for Bloch electrons in a magnetic field is obtained by using only the translational properties of the Hamiltonian. The condition that these basis functions reduce to Bloch functions for zero magnetic field is included to obtain a set of magnetic Bloch functions. Since no approximation is made at any stage, these results may be carried over to a many-particle formulation. This representation is used to derive the well-known theorems for describing the motion of Bloch electrons in a magnetic field. In all cases the previous results are shown to be modified in the same manner, i.e., the wave vector $\vec{k}$ is to be replaced by the operator $\underline{\vec{K}}$ symmetrically. Thus the appropriate space for describing the motion of Bloch electrons in a magnetic field is an operator space and not the wave-vector space.

I. INTRODUCTION

The motion of Bloch electrons in a magnetic field has been studied by many authors.[1-13] Some authors have used the effective-Hamiltonian formalism,[1,3-7] while others have considered the translational properties[2,8-10] in the presence of a magnetic field. Different authors have used different basis functions to formulate the effective Hamiltonian. But, as noted by Kohn,[4] the form of the effective Hamiltonian is not unique. It depends sensitively on the choice of the basis functions. Also, the way the solution is obtained is influenced by the choice of the basis functions. It has been realized that the complex problem of Bloch electrons in a magnetic field can be enormously simplified by the right choice of the basis functions.

It is well known that in the case of Bloch electrons in a magnetic field, the Bloch functions do not form a useful representation, as there are singular interband matrix elements. The Bloch functions are a consequence of invariance under a lattice translation, and in a magnetic field the difficulty is that the expression for the interaction energy contains the electron coordinates, so that the periodicity of the Hamiltonian is lost. Therefore, Harper[2] introduced Bloch-type eigenfunctions which reduce to Bloch functions in the limit of zero magnetic field. The Luttinger-Kohn functions[3] can be considered as a localized form of these functions. Subsequently, different basis functions were used by Wannier,[5] Blount,[6] and Roth,[7] all of which reduce to the Bloch functions in the limit of zero magnetic field. We can regard these as different types of magnetic Bloch functions. However, it was not possible to show that the magnetic Bloch functions formed a complete set. Thus, when these functions were used to obtain an effective Hamiltonian in the form of a power series in B, the question of convergence of the series was not answered. The use of an effective Hamiltonian could only be justified asymptotically as B approaches zero.[6]

Brown[8,11] has applied the theory of group representations to the Bloch electrons in a magnetic field. He has shown that the set of operators which commute with the Hamiltonian, which he called the magnetic translation operators, form a ray group. These operators form a subgroup of the operators for a free electron in a magnetic field.[9] However, there is a difficulty in the generalization of the Born–von Kármán boundary conditions, and Brown has shown that the periodic boundary conditions can be invoked only if the magnetic field is in the direction of some lattice vector. In this case the energy eigenfuctions, which are N-fold degenerate, serve as basis functions and a set of generalized Wannier functions can be constructed. These representations are characterized by a wave vector $\vec{q}$ whose domain is smaller than the Brillouin zone by a factor N in each of the directions normal to the field. However, this method is not useful for the more general case where the magnetic field is in an arbitrary direction, since suitable basis functions have to be found without invoking any periodic boundary conditions.

Zak[9,12,13] has introduced a kq representation in which the states are specified by eigenvalues of finite translations in the direct and reciprocal spaces. Here $\vec{q}$ 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. However, when he considers the dynamics of Bloch electrons in external fields, he winds up in the magnetic Bloch-function representation before deriving the "standard results." Thus, it is not clear as to how this representation simplifies the problem of Bloch electrons in a magnetic field.

It is clear from the foregoing remarks that, while it has been realized that the problem of Bloch electrons in a magnetic field can be enormously simplified by the right choice of the basis functions, no attempt has been made to obtain a complete set of functions based on the symmetry of the problem except in the special case where the magnetic field is along a lattice vector.[8,11] It was assumed that it would not be possible to use symmetry properties for the general case when the magnetic field is in an arbitrary direction, since the periodic boundary conditions can not be used.

In Sec. II, we show that it is possible to obtain a class of representations for Bloch electrons in a magnetic field in an arbitrary direction from considerations of translational symmetry properties alone. If we put in the condition that these functions reduce to Bloch functions for zero magnetic field, then they become the Roth functions.[7] Therefore, these functions should be the right choice for the basis functions for simplification of this complex problem. Further, no approximation is made at any stage, and therefore the results may be carried over to a many-particle formulation.

In Sec. III, we show that the well-known theorems for describing the motion of Bloch electrons in a magnetic field can be derived in a very simple manner by using this representation. It is shown that in all cases the previous results are to be modified. Our results reduce to these well-known results only in the limit of zero magnetic field. It is also shown that our results indicate that in a magnetic field the motion of Bloch electrons should be described in an operator space and not in the wave-vector space, as has been done till now. This operator space reduces to the wave-vector space in the limit of zero magnetic field. Some of these results have already been derived by Zak[12,13] by essentially using the same representation, though he starts out in a different representation, but we rederive them in a simple and straightforward way for the sake of completeness.

II. BASIS FUNCTIONS

The Hamiltonian for an electron in a periodic potential and a uniform magnetic field is

$$H=\frac{1}{2m}\left[\underline{\vec{p}}+\frac{e}{c}\vec{A}(\vec{r})\right]^2+V(r), \tag{1}$$

where $\vec{A}(\vec{r})$ is the vector potential and e is the magnitude of the electronic charge. In the linear gauge, for a uniform magnetic field, we have

$$\vec{A}(\vec{r})=\vec{r}\cdot\nabla\vec{A}\ , \tag{2}$$

where $\nabla\vec{A}$ is a constant dyadic. There is no loss of generality in selecting this gauge, since the results can be proved for an arbitrary gauge by performing a gauge transformation.

There is a translation operation under which the Hamiltonian is invariant, even though it is not invariant under pure spatial translation. There is a simple physical reason for this. If a charged particle is transported from one point of a periodic lattice to an equivalent one, it would be necessary to exert a force to cancel the effect of the magnetic field so that the charge is in an equivalent state of motion at the new site. This gives rise to an impulse which corresponds to the shift in kinetic momentum. So the operators which commute with the Hamiltonian should incorporate this momentum shift. The set of operators which commute with the Hamiltonian are called magnetic translation operators.[8] We now want to obtain the magnetic translation operator in the linear gauge.

Let

$$\underline{\vec{P}}=\underline{\vec{p}}+(e/c)\,\vec{r}\cdot\nabla\vec{A}\ . \tag{3}$$

It can be easily shown that the components of $\underline{\vec{P}}$ do not commute with one another. From (1) and (3), we have

$$H=\underline{P}^2/2m+V(r)\,. \tag{4}$$

Let

$$\underline{\vec{P}}_0=\underline{\vec{p}}+(e/c)\nabla\vec{A}\cdot\vec{r}. \tag{5}$$

The components of $\underline{\vec{P}}_0$ do not commute:

$$[\underline{P}_{0x},\underline{P}_{0y}]=(ie\hbar/c)B\,, \tag{6}$$

where B is the magnetic field which is taken in the z direction. It can be shown that

$$[\underline{\vec{P}},\underline{\vec{P}}_0]=0\ . \tag{7}$$

From (4) and (7) we have

$$[H,e^{i\vec{R}\cdot\underline{\vec{P}}_0}]=0\ , \tag{8}$$

where $\vec{R}$ is a lattice vector. So in the linear gauge, the magnetic translation operator is

$$T(\vec{R})=e^{i\vec{R}\cdot\underline{\vec{P}}_0}\ . \tag{9}$$

It can be easily shown that these operators form a ray group. Further, if $\psi(\vec{r},t)$ is an eigenfuction of H, $T(\vec{R})\psi(\vec{r},t)$ must also be an eigenfunction of H.

Let $\phi_{n\vec{k}}(\vec{r},\vec{B})$ be a complete set of orthonormal basis functions, where $\vec{k}$ is the reduced wave vector and n is a band index. The existence of magnetic translation operators shows that some types of bands exist. We know that for completely free electrons the eigenfunctions of the Hamiltonian are the plane waves which are therefore natural choices for the basis functions:

$$\phi^0_{n\vec{k}}(\vec{r},\vec{B}=0)=e^{i\vec{G}_n\cdot\vec{r}}e^{i\vec{k}\cdot\vec{r}}, \tag{10}$$

where $\vec{G}_n$ is any reciprocal-lattice vector. We also know that for electrons in a periodic potential ($B=0$), the eigenfunctions of the Hamiltonian are the Bloch functions, which are therefore natural choices for basis functions:

$$\phi_{n\vec{k}}(\vec{r},\vec{B}=0)=U_{n\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}\ , \tag{11}$$

where $U_{n\vec{k}}(\vec{r})$ is periodic in $\vec{r}$. So for electrons in a periodic potential and in a uniform magnetic field, we write

$$\phi_{n\vec{k}}(\vec{r},\vec{B})=\underline{\vec{C}}_n e^{i\vec{k}\cdot\vec{r}} ,\tag{12}$$

where $\underline{\vec{C}}_n$ is an operator which will be some function of $\vec{k}$, $\vec{B}$, and $\vec{r}$. We note that this does not involve any approximation. We can always find an operator to obtain a function from another function. We now expand the wave function $\psi(\vec{r},t)$ in terms of these basis functions:

$$\psi(\vec{r},t)=\sum_{n\vec{k}}\phi_{n\vec{k}}(\vec{r})\psi_n(\vec{k},t),\tag{13}$$

where $\psi_n(\vec{k},t)$ are the time-dependent functions. It is understood that we shall go to the limit of continuous $\vec{k}$, but we keep the summation for convenience. From (12) and (13), we have

$$\psi(\vec{r},t)=\sum_{n\vec{k}}\{\underline{\vec{C}}_n e^{i\vec{k}\cdot\vec{r}}\}\psi_n(\vec{k},t).\tag{14}$$

We can write this as

$$\psi(\vec{r},t)=\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}\underline{\vec{D}}_n\psi_n(\vec{k},t),\tag{15}$$

where

$$\underline{\vec{D}}_n=(\underline{\vec{C}}_n^*)^\dagger ,\tag{16}$$

and $(\underline{\vec{C}}_n^*)^\dagger$ is the Hermitian conjugate of the complex conjugate of $\underline{\vec{C}}_n$. In deriving (15) from (14), it appears as if an approximation is involved, that $\underline{\vec{C}}_n$ does not depend on the gradient with respect to $\vec{r}$. But this is not true. We could easily start with (15), which is as good a starting point, and which does not involve any approximation. Here $\underline{\vec{D}}_n$ does not contain ∇_r since $\psi_n(\vec{k},t)$ is independent of $\vec{r}$ and $\psi(\vec{r},t)$ is not an operator. Then (14) can be obtained from (15), and $\underline{\vec{D}}_n$ and $\underline{\vec{C}}_n$ are related as in (16). From (9) and (15) we obtain

$$T(\vec{R})\psi(\vec{r},t)=\exp\left[i\vec{R}\cdot\left(\underline{\vec{p}}+\frac{e}{c}\nabla\vec{A}\cdot\vec{r}\right)\right]\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}\underline{\vec{D}}_n\psi_n(\vec{k},t).\tag{17}$$

Also

$$\vec{r}\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}\vec{D}_n\psi_n(\vec{k},t)=\sum_{n\vec{k}}\{-i\nabla_k e^{i\vec{k}\cdot\vec{r}}\}\vec{D}_n\psi_n(\vec{k},t) .\tag{18}$$

Since $i\nabla_k$ is Hermitian, we have

$$\vec{r}\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}\underline{\vec{D}}_n\psi_n(\vec{k},t)=\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}i\nabla_k\underline{\vec{D}}_n\psi_n(\vec{k},t).\tag{19}$$

From (17) and (19), we obtain

$$T(\vec{R})\psi(\vec{r},t)=\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}e^{i\vec{R}\cdot(\underline{\vec{p}}+\hbar\vec{K}_0)}\underline{\vec{D}}_n\psi_n(\vec{k},t),\tag{20}$$

where

$$\vec{K}_0=\vec{k}+(e/\hbar c)\nabla\vec{A}\cdot i\nabla_k .\tag{21}$$

Since $T(\vec{R})\psi(\vec{r},t)$ is also an eigenfunction of H, we can write in analogy with (15)

$$T(\vec{R})\psi(\vec{r},t)=\psi'(\vec{r},t)=\sum_{n\vec{k}}e^{i\vec{k}\cdot\vec{r}}\underline{\vec{D}}_n\psi_n'(\vec{k},t).\tag{22}$$

From the translational property, (20) and (22) should have the same form. So it follows that $e^{i\vec{R}\cdot(\underline{\vec{p}}+\hbar\underline{\vec{K}}_0)}$ must commute with $\underline{\vec{D}}_n$. This is necessary in the case of $e^{i\vec{R}\cdot\underline{\vec{p}}}$, but with $e^{i\hbar\vec{R}\cdot\underline{\vec{K}}_0}$ there could be a phase factor involved. But commuting is sufficient. [It is important to note that $\underline{\vec{K}}_0$ commutes with the effective Hamiltonian in Eq. (40).] Therefore, $\underline{\vec{D}}_n$ must be periodic in $\vec{r}$. However, we note that the components of $\underline{\vec{K}}_0$ do not commute. It can be shown that

$$[\underline{K}_{0x},\underline{K}_{0y}]=ieB/\hbar c .\tag{23}$$

We define

$$\underline{\vec{K}}=\vec{k}+(e/\hbar c)\ \vec{A}(i\nabla_k) .\tag{24}$$

In the linear gauge

$$\underline{\vec{K}}=\vec{k}+(e/\hbar c)i\nabla_k\cdot\nabla\vec{A} .\tag{25}$$

It can be shown that

$$[\underline{K}_x,\underline{K}_y]=-ieB/\hbar c\tag{26}$$

and

$$[\underline{\vec{K}},\underline{\vec{K}}_0]=0 .\tag{27}$$

Therefore, $\underline{\vec{D}}_n$ must be a function of $\underline{\vec{K}}$. Also, since the different components of $\underline{\vec{K}}$ do not commute, $\underline{\vec{D}}_n$ can always be defined as a symmetric function of $\underline{\vec{K}}$. Therefore, from the translational properties we require $\underline{\vec{D}}_n$ to be periodic in $\vec{r}$ as well as to depend on $\underline{\vec{K}}$. This defines a class of representation for Bloch electrons in a magnetic field. Included in this class are the magnetic Bloch functions, the orthogonalized-plane-wave representation,[14] and the $\vec{k}\cdot\vec{p}$ representation.[15] It also includes the representation of Blount,[6] which omits small matrix elements of the potential and which is a better representation near a magnetic breakdown region.

From the translational properties of Bloch electrons, in the absence of any external field, we require that our basis functions must reduce to Bloch functions for $B=0$. We shall now show that, if we put in this condition, that the Roth functions[7] are obtained as the natural choice for the basis functions. From (11), (12), and (16), we note that for $B=0$, $D_{n\underline{\vec{K}}}(\vec{r})$ must reduce to $U_{n\vec{k}}(\vec{r})$. We also note that both $D_{n\underline{\vec{K}}}(\vec{r})$ and $U_{n\vec{k}}(\vec{r})$ are periodic in $\vec{r}$. Further, $D_{n\underline{\vec{K}}}(\vec{r})$ is a symmetric function of $\underline{\vec{K}}$, and $\underline{\vec{K}}$ reduces to $\vec{k}$ for $B=0$. Therefore, the simplest choice for $D_{n\underline{\vec{K}}}(\vec{r})$ is that it is the operator obtained from $U_{n\vec{k}}(\vec{r})$ by replacing $\vec{k}$ by $\underline{\vec{K}}$ in a symmetric manner. Therefore,

$$D_{n\underline{\vec{K}}}(\vec{r})=U_{n\underline{\vec{K}}}(\vec{r}) .\tag{28}$$

We know that any symmetric function $f(\underline{\vec{K}})$ can be expanded as

$$f(\underline{\vec{K}})=\int d\vec{\rho}\,e^{-i\underline{\vec{K}}\cdot\vec{\rho}}f(\vec{\rho}) .\tag{29}$$

Therefore, we have, since $\underline{\vec{K}}$ is Hermitian,

$$f^\dagger(\underline{\vec{K}})=\int d\vec{\rho}\,e^{i\underline{\vec{K}}\cdot\vec{\rho}}f^*(\vec{\rho}) ,\tag{30}$$

from which we have

$$f^{\dagger}(\underline{\vec{K}})=[f(\underline{\vec{K}})^{*}]^{*} . \quad (31)$$

Therefore, we have

$$[f^{\dagger}(\underline{\vec{K}})]^{*}=f(\underline{\vec{K}}^{*}). \quad (32)$$

From (16), (28), and (32), we obtain

$$C_{n\underline{\vec{K}}}=U_{n\underline{\vec{K}}^{*}}. \quad (33)$$

From (12) and (33), the basis functions are

$$\phi_{n\vec{k}}(\vec{r})=U_{n\underline{\vec{K}}^{*}}(\vec{r})\,e^{i\vec{k}\cdot\vec{r}} . \quad (34)$$

These functions were first used by Roth[7] as basis functions for Bloch electrons in a magnetic field. Roth had used these functions intuitively, "with less motivation" (Appendix of Ref. 7), and the justification of their use was that they yielded the correct results. However, we have made use of the invariance properties of the Hamiltonian to obtain these functions.

We note that $\phi_{n\vec{k}}(\vec{r})$ are not normalized. The normalization is determined by the matrix

$$N_{nn'}(\underline{\vec{K}})=\int d\vec{r}\;U^{\dagger}_{n\underline{\vec{K}}}\,U_{n'\underline{\vec{K}}} . \quad (35)$$

A set of functions $V_{n\underline{\vec{K}}}$ can be built from $U_{n\underline{\vec{K}}}$ by using the multiplication theorem[7] for symmetric operators. It has been shown by Roth[16] that

$$V_{n\underline{\vec{K}}}=U_{n\underline{\vec{K}}}+\left[\frac{i}{2}\sum_{n'}U_{n'\vec{k}}\,\vec{h}\cdot\int d\vec{r}\,\nabla_k U^{*}_{n'\vec{k}}\times\nabla_k U_{n\vec{k}}+\cdots\right], \quad (36)$$

where

$$\vec{h}=e\vec{B}/2\hbar c . \quad (37)$$

Here we have followed the notation of Zak[12] that the rectangular brackets mean that, in the expression inside them, $\vec{k}$ is replaced by $\underline{\vec{K}}$ symmetrically; i.e., $[f(\vec{k})]$ is the value obtained after $\vec{k}$ is replaced by $\underline{\vec{K}}$ symmetrically in $f(\vec{k})$. We shall use this notation in what follows. So the orthonormal basis functions are

$$\phi_{n\vec{k}}(\vec{r})=V_{n\underline{\vec{K}}^{*}}(\vec{r})\,e^{i\vec{k}\cdot\vec{r}} . \quad (38)$$

We also note that the Roth functions[7] are obtained from the condition that the basis functions should reduce to Bloch functions for $B=0$, but the other functions mentioned above have the same translational properties.

III. DYNAMICS OF BLOCH ELECTRONS

We shall now show that the well-known theorems for describing the motion of Bloch electrons in a magnetic field can be derived in a very simple manner by using the above representation. We shall also show that in all cases the previous results are to be modified. Our results reduce to the previous results only in the limit of zero magnetic field. Some of these results have been already derived by Zak[12] by using essentially the magnetic Bloch function representation, though he starts out in the kq representation, but we rederive them in a more simple and straightforward way for the sake of completeness.

Using the above representation, we obtain

$$\langle\underline{\vec{K}}\rangle=\sum_{n\vec{k}}\psi^{*}_{n}(\vec{k},t)\underline{\vec{K}}\,\psi_{n}(\vec{k},t). \quad (39)$$

By using the same representation, it has been shown by Roth[16] that the effective Hamiltonian is

$$H_{nn'}(\underline{\vec{K}})=\mathcal{E}_{n}(\underline{\vec{K}})\,\delta_{nn'}+hH'_{nn'}(\underline{\vec{K}})+\cdots . \quad (40)$$

From (39) and (40), we have

$$\frac{d\langle\underline{\vec{K}}\rangle}{dt}=\frac{1}{i\hbar}\langle[\underline{\vec{K}},\mathcal{E}(\underline{\vec{K}})]\rangle. \quad (41)$$

Using the multiplication theorem,[7] we obtain

$$[\underline{\vec{K}},\mathcal{E}(\underline{\vec{K}})]=-\frac{ie}{\hbar c}[\nabla_k\mathcal{E}]\times\vec{B}, \quad (42)$$

where, in our notation, $[\nabla_k\mathcal{E}]$ is the result obtained after $\vec{k}$ is replaced by $\underline{\vec{K}}$ symmetrically in $\nabla_k\mathcal{E}$. From (41) and (42), we obtain

$$\frac{d\langle\underline{\vec{K}}\rangle}{dt}=-\frac{e}{\hbar c}\langle[(1/\hbar)\nabla_k\mathcal{E}]\times\vec{B}\rangle . \quad (43)$$

Comparing this with the classical result

$$m\dot{\vec{V}}=-(e/c)\vec{V}\times\vec{B} , \quad (44)$$

we find that in a magnetic field, the kinetic momentum is $\hbar\underline{\vec{K}}$ and the velocity is $[(1/\hbar)\nabla_k\mathcal{E}]$. Here the brackets mean that $\vec{k}$ is replaced by $\underline{\vec{K}}$ symmetrically in $(1/\hbar)\nabla_k\mathcal{E}$. We have already shown that $\vec{k}$ is replaced by $\underline{\vec{K}}$ in the periodic part of the Bloch function. Thus in a magnetic field the wave vector $\vec{k}$ is replaced by the operator $\underline{\vec{K}}$, and the appropriate space is the $\underline{\vec{K}}$ space and not the $\vec{k}$ space. This is confirmed by the fact that in a magnetic field, the variables k_x, k_y, and k_z are no longer good quantum numbers. However, since the magnetic field is taken in the z direction, $\underline{K}_z=k_z$, and from (43) it follows that $\underline{K}_z$ is a constant of motion. From (26), we have

$$[\underline{K}_x,(c\hbar^2/eB)\underline{K}_y]=\hbar/i . \quad (45)$$

We draw an analogy between this equation and the ordinary commutation rule between coordinates and momenta

$$[p_x,q_x]=\hbar/i \quad (46)$$

by making the identification

$$p_x=\underline{K}_x,\quad q_x=(c\hbar^2/eB)\underline{K}_y . \quad (47)$$

We apply the Bohr-Sommerfeld quantization condition

$$\oint p_x\,dq_x=2\pi(n+\gamma)\hbar, \quad (48)$$

where n is a positive integer and γ is some "phase factor." We substitute (47) in (48) to find

$$\oint \underline{K}_x d\underline{K}_y = \frac{2\pi(n+[\gamma(\vec{k})])eB}{c\hbar} = [A(\vec{k})], \tag{49}$$

where the integral runs along the curve bounding a cross section of a surface of constant energy perpendicular to the field and has a value equal to the area $[A(\vec{k})]$ of this cross section. Therefore, the area in $\vec{\underline{K}}$ space $[A(\vec{k})]$, the operator corresponding to the area of the orbit, is quantized for constant energy and constant k_z. This is a generalization of the Onsager relation.[17] We note that $[\gamma(\vec{k})]$ is an operator obtained from $\gamma(\vec{k})$ by replacing $\vec{k}$ with $\vec{\underline{K}}$. The operator nature of γ has been clearly established by Roth,[18] who has derived a similar relation for the cross-sectional area of the orbit. This result has also been derived by Zak,[12] but he missed the point that $[\gamma(\vec{k})]$ is an operator.

We shall now derive an expression for the effective mass. From (40), we have

$$\frac{d}{dt}\left[\frac{1}{\hbar}\nabla_k \mathcal{E}\right] = \frac{1}{i\hbar^2}[[\nabla_k \mathcal{E}], [\mathcal{E}(\vec{k})]], \tag{50}$$

where on the right-hand side the outside bracket means the commutation relation. Using the multiplication rule,[7] we obtain

$$\frac{d}{dt}\left[\frac{1}{\hbar}\nabla_k \mathcal{E}\right] = -\frac{e}{\hbar^3 c}\left[\frac{\partial^2 \mathcal{E}}{\partial\vec{k}\,\partial\vec{k}}(\nabla_k \mathcal{E} \times \vec{B})\right]. \tag{51}$$

From (42) and (43), we have

$$\frac{d}{dt}\vec{\underline{K}} = -\frac{e}{\hbar^2 c}[\nabla_k \mathcal{E} \times \vec{B}]\ . \tag{52}$$

From (51) and (52), we obtain

$$\frac{d}{dt}\left[\frac{1}{\hbar}\nabla_k \mathcal{E}\right] = \hbar\left[\frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}}{\partial\vec{k}\,\partial\vec{k}}\,\dot{\vec{k}}\right]\ . \tag{53}$$

We have already shown that in a magnetic field, the kinetic momentum is $\hbar\vec{\underline{K}}$ and the velocity $\vec{\underline{V}}$ is $[(1/\hbar)\nabla_k \mathcal{E}]$. Therefore, we can write (53) as

$$m^* \dot{\vec{\underline{V}}} = \hbar\dot{\vec{\underline{K}}}, \tag{54}$$

where $1/m^*$ is the inverse effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}}{\partial\vec{k}\,\partial\vec{k}}. \tag{55}$$

Equation (54) is the familiar expression, except that $\vec{k}$ is to be replaced by $\vec{\underline{K}}$ symmetrically.

We have seen that the area of cross section depends on the energy of the state whose quantum number is n. From the definition of the cyclotron frequency, we have

$$d\mathcal{E}/dn = \hbar\omega_c. \tag{56}$$

From (49) and (56), we obtain the expression for cyclotron frequency

$$\omega_c = \frac{2\pi eB}{c\hbar^2}\left(\frac{dA}{d\mathcal{E}}\right)^{-1}\ . \tag{57}$$

The cyclotron mass is defined as

$$m_c = eB/c\omega_c. \tag{58}$$

From (57) and (58), we obtain the familiar expression for the cyclotron mass

$$m_c = \frac{\hbar^2}{2\pi}\frac{dA}{d\mathcal{E}}\ . \tag{59}$$

The operator corresponding to the orbit radius is given by the relation

$$m_c \vec{\underline{\rho}}\,\omega_c^2 = e\hbar\, m_c^{-1}\vec{\underline{K}} \times \vec{B}. \tag{60}$$

From (58) and (60), we have

$$\vec{\underline{\rho}} = (c\hbar/eB^2)\vec{\underline{K}} \times \vec{B}. \tag{61}$$

It can be easily shown that

$$\hbar(\vec{\underline{K}} - \vec{\underline{K}}_0) \times \vec{B} = (e/c)\,B^2\,(i\nabla_k)_\perp, \tag{62}$$

where $(i\nabla_k)_\perp$ is the component of $i\nabla_k$ perpendicular to the magnetic field. From (61) and (62) we have

$$(i\nabla_k)_\perp = \vec{\underline{\rho}} + \vec{\underline{\rho}}_0, \tag{63}$$

where

$$\vec{\underline{\rho}}_0 = -(\hbar c/eB^2)\vec{\underline{K}}_0 \times \vec{B}. \tag{64}$$

Since $\vec{\underline{K}}_0$ commutes with the effective Hamiltonian, $\vec{\rho}_0$ is a constant of motion. From (23) and (64), we have

$$[\rho_{0x}, \rho_{0y}] = i\hbar c/eB. \tag{65}$$

Thus ρ_{0x} and ρ_{0y} can be considered as equivalent to a canonical coordinate and momentum pair. The area is $2\pi n\hbar c/eB$, and so the number of states per unit area is

$$eB/2\pi\hbar c. \tag{66}$$

This gives the degeneracy of the Landau levels.

Thus the well-known results are obtained in a very simple way by considering the motion of Bloch electrons in $\vec{\underline{K}}$ space. The conjugate operators $\underline{K}_x$ and $\underline{K}_y$ describe one degree of freedom, the conjugate operators $\underline{K}_{0x}$ and $\underline{K}_{0y}$ describe another degree of freedom, and $\underline{K}_z = k_z$ describes the third degree of freedom.

IV. CONCLUSIONS

In this paper it has been shown that it is possible to obtain a class of representations for Bloch electrons in a magnetic field by using only the translational properties of the Hamiltonian. If we put in the condition that the basis functions reduce to Bloch functions for zero magnetic field, then these become the magnetic Bloch functions first used by Roth.[7] Since no approximation has been made at any stage, these results may be carried over to a many-particle formulation.

Note that the completeness of the set of the Roth functions has not been proved. However, there are sets of this class of representation which are complete, i.e., the $\vec{k}\cdot\vec{p}$ representation[15] and the plane-wave representation.

This representation has been used to derive some well-known results. First, expressions for the kinetic momentum and the velocity of the electron in the magnetic field have been derived. Then a generalized Onsager relation[17] for the area in $\vec{K}$ space was derived. In all cases it was shown that the previous results are to be modified in the same manner, i.e., the wave vector $\vec{k}$ is to be replaced by the operator $\vec{K}$ symmetrically. Expressions for the effective mass, the cyclotron mass, and the cyclotron frequency were also derived in a simple way. Thus the appropriate space for describing the motion of Bloch electrons in the magnetic field is an operator space and not the wave-vector space. The same principle can be applied to the pseudopotential theory of metals in a magnetic field. It has been shown[19] that the vector $\vec{k}$ in the zero-field pseudopotential is to be replaced by the operator $\vec{K}$ in the magnetic pseudopotential. Some of the results in the section on dynamics have been derived by Zak[12,13] by using essentially the same representation, though he started out in a different representation, but here they have been rederived in a simple and straightforward way for the sake of completeness.

[1]J. M. Luttinger, Phys. Rev. 84, 814 (1951).
[2]P. G. Harper, Proc. Phys. Soc. (London) A68, 874 (1955).
[3]J. M. Luttinger and W. Kohn, Phys. Rev. 97, 869 (1955).
[4]W. Kohn, Phys. Rev. 115, 1460 (1959).
[5]G. H. Wannier and D. R. Fredkin, Phys. Rev. 125, 1910 (1962).
[6]E. I. Blount, Phys. Rev. 126, 1636 (1962).
[7]L. M. Roth, J. Phys. Chem. Solids 23, 433 (1962).
[8]E. Brown, Phys. Rev. 133, A1038 (1964).
[9]J. Zak, Phys. Rev. 136, A776 (1964).
[10]P. G. Harper, J. Phys. Chem. Solids 28, 495 (1967).
[11]E. Brown, Phys. Rev. 166, 626 (1968).
[12]J. Zak, Phys. Rev. 168, 686 (1968).
[13]J. Zak, Phys. Rev. 177, 1151 (1969).
[14]P. K. Misra and L. M. Roth, Phys. Rev. 177, 1089 (1969).
[15]L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. 50, 58 (1936); E. O. Kane, J. Phys. Chem. Solids 8, 38 (1959).
[16]L. M. Roth, Phys. Rev. 133, A542 (1964).
[17]L. Onsager, Phil. Mag. 43, 1006 (1952).
[18]L. M. Roth, Phys. Rev. 145, 434 (1966).
[19]P. K. Misra, J. Phys. Chem. Solids (to be published).

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New First-Order Phase Transition in High-Purity Ytterbium Metal

E. Bucher, P. H. Schmidt, A. Jayaraman, K. Andres,
J. P. Maita, K. Nassau, and P. D. Dernier
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 17 February 1970)

A first-order magnetic phase transition has been observed in high-purity Yb metal. It is characterized by a paramagnetic-to-diamagnetic transition with a large degree of hysteresis between 100 and 360 °K, and appears to be associated with an fcc-hcp martensitic transformation. The occurrence of this transition is characteristic of high-purity metal and has not been previously reported. Several other properties such as the specific heat at 0 and 106 kOe, the volume and resistance changes the low-temperature resistivity, x-ray data, and the pressure and strain dependence of the transition are discussed. The diamagnetic phase is not superconducting above 0.015 °K. The fcc phase was obtained from the hcp phase by applying strain at room temperature and was also investigated. It shows a strongly temperature-dependent paramagnetic susceptibility down to 1.4 °K, but no magnetic ordering could be detected down to 1.0 °K.

I. INTRODUCTION

Ytterbium metal is known to exist in three different crystallographic modifications, namely, fcc, bcc, and hcp.[1,2] Of these, the bcc phase is the high-temperature phase while the fcc phase is stable at atmospheric pressure and up to about 660 °C. It was believed that the hcp phase was impurity stabilized and had a narrow range of stability between about 300 and 700 °C, at atmospheric pressure.[1] High-pressure studies on Yb have shown that the fcc-bcc phase boundary has a negative slope and that a fcc-bcc transition could be induced by pres-