Bloch Electrons in a Uniform Magnetic Field*

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The physical periodicity of a space lattice is not destroyed by the presence of a uniform magnetic field. It is shown that a ray group of unitary operators, isomorphic to pure translations, commutes with the Hamiltonian in this case. Such a group has the characteristic property that $AB=\exp[i\phi(A,B)]C$, where A, B, and C are elements of the group and ϕ is a numerical factor. Representation theory applied to this group yields the characteristic degeneracies of levels in magnetic fields, as well as the transformation properties of eigenfunctions. By means of these it is possible to construct an effective Hamiltonian appropriate to finite magnetic fields in crystals.

1. INTRODUCTION

THE theoretical understanding of the behavior of electrons in crystalline potentials is enormously simplified by virtue of the invariance properties of the Hamiltonian under the operations of the space group. The well-known Bloch form of the eigenfunctions is a consequence of invariance under lattice translations. Although these solutions are no longer appropriate when the solid is perturbed, it is often possible to take advantage of the periodic part of the Hamiltonian by use of the effective Hamiltonian formalism.[1] In its simplest form this procedure consists of replacing the effect of the unperturbed Hamiltonian by an operator $E(\mathbf{P})$ obtained from an energy band $E(\hbar\mathbf{k})$. This procedure is not directly applicable to the case of magnetic fields. Onsager[2] had suggested an effective Hamiltonian of the form $H_{\text{eff}}(\mathbf{P}+e\mathbf{A}/c)$, where $\mathbf{A}$ is the vector potential in some arbitrary gauge. Kohn[3] demonstrated the validity of such an expression, if one allows the functional form of the Hamiltonian to depend on the magnetic field $\mathbf{B}$. His paper and similar more recent ones[4,5] make use of an expansion in powers of the magnetic field strength $\mathbf{B}$, so that the results may be valid only in an asymptotic sense.

A different approach has been taken by Wannier and Fredkin.[6,7] Their procedure makes use of the fact that, in a certain sense, periodicity is not destroyed by a uniform magnetic field. Thus, they postulate the existence of Bloch-type eigenfunctions, which reduce to Bloch functions when the magnetic field is reduced to zero. These functions were first introduced by Harper[8] who showed that they have transformation properties appropriate to a periodic lattice in a uniform magnetic field.

The present paper is similar in approach to that of Wannier *et al.*, in that it makes use of the periodicity that exists in the presence of a uniform magnetic field. There is a simple physical way to see why there should be a type of translation operation under which the Hamiltonian is invariant, even though it is not invariant under pure spatial translation. Classically, if one were to transport a particle of charge q from one point of a periodic lattice to an equivalent one, it would be necessary to exert a force along the way, given by

$$\mathbf{F}=-q(\mathbf{v}\times\mathbf{B}/c), \tag{1}$$

in order to cancel the effect of the magnetic field, so that the charge is in an equivalent state of motion at the new site. Integrating Eq. (1) with respect to time yields an expression for the impulse which must be provided in transporting an electron through a lattice displacement $\mathbf{R}_n$,

$$\mathbf{I}=-q(\mathbf{R}_n\times\mathbf{B}/c). \tag{2}$$

This impulse corresponds to the shift in kinetic momentum $\boldsymbol{\pi}=\mathbf{P}-q\mathbf{A}/c$ which must be provided, in addition to the shift in position, to leave the charged particle in an invariant condition. In a quantum mechanical formalism one should therefore expect that the operators which commute with the Hamiltonian are not pure spatial translations, but rather, those which incorporate the corresponding momentum shift. This turns out to be the case. The form of the operator which carries this out is the product of the translation operator and the Peierls' phase term.[9] These operators will be referred to as magnetic translation operators, since they depend on the field and become pure translations as the field approaches zero.

The set of magnetic translation operators does not quite form a group since the product of any two of them is not necessarily one of the set. However, in all cases the product only differs by at most a multiplicative factor of magnitude unity. The operators may be said to form a group up to a factor, or more simply a ray group. It thus turns out to be possible to make use of all the powerful tools of the theory of group representations in the treatment of electrons in uniform

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magnetic fields and periodic potentials. It is the object of this paper to exploit these methods to show: (1) to what extent degeneracy of energy levels is a function of the magnetic field B, (2) the transformation properties of the energy eigenfunctions, (3) the existence of an effective Hamiltonian of the Onsager form. Some of these results have been reported elsewhere.[10] In a recent paper, Fischbeck[11] has made use of magnetic translations to investigate points (1) and (2). The approach used in the present treatment is group theoretical and in a form more convenient for generalization.

One of the obstacles encountered by Wannier and Fredkin,[6] in establishing the existence of an effective Hamiltonian, was the lack of an orthonormal set of basis functions on which to base the formalism. The group theoretical approach used here clearly establishes the existence of such a set of functions, which are the magnetic analog of Wannier functions. This makes the existence proof simple for arbitrary fields. Still a further benefit from formulating the problem on a group theoretical basis stems from the fact that the results are independent of any approximation. Thus, for example, the results may be carried over to a many-particle formulation.

2. THE MAGNETIC TRANSLATION OPERATORS

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

$$H=(1/2m)(\mathbf{P}+e\mathbf{A}/c)^2+V(\mathbf{r}), \tag{3a}$$

$$\mathbf{A}=-\tfrac{1}{2}(\mathbf{r}\times\mathbf{B}), \tag{3b}$$

where $\mathbf{A}$ is the vector potential. This gauge is selected for convenience. There is no loss of generality in this choice, since the results for an arbitrary gauge may be obtained by performing a gauge transformation on the resulting eigenfunctions. We shall use this gauge throughout this paper. The components of $(\mathbf{P}+e\mathbf{A}/c)$ do not commute with one another. This fact is responsible for the peculiar structure which the eigenfunctions have. However, a direct calculation yields[12]

$$[(\mathbf{P}-e\mathbf{A}/c)_i,\ (\mathbf{P}+e\mathbf{A}/c)_j]=0;\quad i,j=1,2,3, \tag{4}$$

from which it follows that an arbitrary function of $\mathbf{P}+e\mathbf{A}/c$ commutes with one of $\mathbf{P}-e\mathbf{A}/c$.

We define a magnetic translation operator,

$$T(\mathbf{R}_n)=\exp[-i\mathbf{R}_n\cdot(\mathbf{P}-e\mathbf{A}/c)/\hbar], \tag{5}$$

which clearly commutes with the first term in the Hamiltonian. In the absence of a magnetic field, $\mathbf{A}$ vanishes and this reduces to a pure translation operator

$$\mathrm{T}(\mathbf{R}_n)=\exp[-i\mathbf{R}_n\cdot\mathbf{P}/\hbar], \tag{6a}$$

$$\mathrm{T}(\mathbf{R}_n)\psi(\mathbf{r})=\psi(\mathbf{r}-\mathbf{R}_n). \tag{6b}$$

[10] E. Brown, Bull. Am. Phys. Soc. 8, 256 (1963).
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[12] This result is valid in the gauge of Eq. (3b).

Using Eqs. (3), (5), and (6) we have, for an arbitrary function $\psi(\mathbf{r})$,

$$\begin{aligned}T(\mathbf{R}_n)\psi(\mathbf{r})&=\exp[-ie\mathbf{R}_n\cdot(\mathbf{r}\times\mathbf{B})/2c\hbar]\psi(\mathbf{r}-\mathbf{R}_n)\\&=\exp[+i(\mathbf{R}_n\times\boldsymbol{\beta})\cdot\mathbf{r}/2]\psi(\mathbf{r}-\mathbf{R}_n),\end{aligned} \tag{7}$$

where $\boldsymbol{\beta}=e\mathbf{B}/\hbar c$. This result follows from the fact that the two terms in the exponent of Eq. (5) commute with one another.[12] It then follows that

$$[T(\mathbf{R}_n),H]=0, \tag{8}$$

where $\mathbf{R}_n$ is an arbitrary lattice vector. This important result allows one to make use of group theory in this problem. The situation differs from the zero-field case in two important ways: (1) the magnetic translations do not commute with one another and (2) the product of an arbitrary two magnetic translations is not necessarily one of them. In order to see this we write

$$\begin{aligned}&T(\mathbf{R}_1)T(\mathbf{R}_2)\\&\quad=\exp[(i/2)(\mathbf{R}_1\times\boldsymbol{\beta})\cdot\mathbf{r}]\mathrm{T}(\mathbf{R}_1)\\&\qquad\qquad\times\exp[(i/2)(\mathbf{R}_2\times\boldsymbol{\beta})\cdot\mathbf{r}]\mathrm{T}(\mathbf{R}_2)\\&\quad=\exp[(i/2)[(\mathbf{R}_1+\mathbf{R}_2)\times\boldsymbol{\beta}]\cdot\mathbf{r}]\mathrm{T}(\mathbf{R}_1)\mathrm{T}(\mathbf{R}_2)\\&\qquad\qquad\times\exp[(-i/2)(\mathbf{R}_2\times\boldsymbol{\beta})\cdot\mathbf{R}_1]\\&\quad=T(\mathbf{R}_1+\mathbf{R}_2)\exp[(-i/2)(\mathbf{R}_1\times\mathbf{R}_2)\cdot\boldsymbol{\beta}].\end{aligned} \tag{9}$$

Using Eq. (9) twice we find

$$T(\mathbf{R}_1)T(\mathbf{R}_2)=T(\mathbf{R}_2)T(\mathbf{R}_1)\exp[-i(\mathbf{R}_1\times\mathbf{R}_2)\cdot\boldsymbol{\beta}]. \tag{10}$$

It follows from Eq. (9) that the product of any sequence of magnetic translations that form a closed path is $e^{i\phi}$, where ϕ is a real number proportional to the magnetic flux through the path; $\phi=$flux $(e/2\hbar c)$.

The ray group of magnetic translations is as basic to the study of magnetic-field problems as the simple translation group is to the perfect crystal. It follows from Eq. (8), if an energy eigenvalue is M-fold degenerate, with eigenfunctions ψ_m, that

$$T(\mathbf{R}_n)\psi_m=\sum_{l=1}^{M}D_{lm}(\mathbf{R}_n)\psi_l. \tag{11}$$

From Eqs. (9) and (11) it follows that the matrices $D(\mathbf{R}_n)$ satisfy

$$\begin{aligned}D(\mathbf{R}_1)D(\mathbf{R}_2)&=D(\mathbf{R}_1+\mathbf{R}_2)\\&\qquad\times\exp[(-i/2)(\mathbf{R}_1\times\mathbf{R}_2)\cdot\boldsymbol{\beta}]\end{aligned} \tag{12}$$

and thus form a ray representation of the translation group.

Up to this point we have been dealing with an infinite crystal and an infinite group. It is convenient to work with finite groups for the purpose of examining irreducible representations. To this end it is worthwhile to explore the possibility of applying appropriate boundary conditions to a finite crystal so as not to destroy the group properties. We, therefore, restrict our attention to a finite lattice of dimensions $N_1\mathbf{a}_1$, $N_2\mathbf{a}_2$, $N_3\mathbf{a}_3$, where $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are primitive translation

vectors. The natural generalization of the Born-von Karman boundary conditions is to restrict the eigenfunctions to go into themselves under magnetic translations corresponding to the full finite lattice.

$$T(N_i\mathbf{a}_i)\psi=\psi;\quad i=1,2,3. \tag{13}$$

In the zero-field case Eq. (13) reduces to the Born-von Karman boundary conditions. There is an essential difference between the magnetic and the zero-field cases, however. In the zero-field case, if one of the eigenfunctions in the infinite lattice goes into itself under some macroscopic translation, then so do all the functions obtained from it by lattice translations. This result does not carry over to the magnetic translations. This can be seen from the following. Assume ψ is an eigenfunction satisfying the boundary conditions of Eq. (13). The functions,

$$\phi_m=T(\mathbf{R}_m)\psi, \tag{14}$$

are then also eigenfunctions. Then from Eq. (10) it follows that

$$T(N_i\mathbf{a}_i)\phi_m=\exp[-iN_i(\mathbf{a}_i\times\mathbf{R}_m)\cdot\boldsymbol{\beta}]\phi_m. \tag{15}$$

From this it follows that Eq. (13) can be satisfied for all functions simultaneously only if

$$N_i(\mathbf{a}_i\times\mathbf{R}_m)\cdot\boldsymbol{\beta}=\text{Multiple of } 2\pi. \tag{16}$$

It follows from Eq. (16) that magnetically periodic boundary conditions[13] can only be invoked if $\boldsymbol{\beta}$ is of the form

$$\boldsymbol{\beta}=\mathbf{R}2\pi\Omega^{-1}l/N, \tag{17}$$

where Ω is the volume of a primitive cell, $\mathbf{R}$ is some primitive lattice vector,[14] and l and N are integers with no common factor. The magnetic field must therefore be in the direction of some lattice vector.

We shall assume Eq. (17) to be fulfilled and examine its consequences in the next section.

The artificial conditions expressed by Eqs. (13) and (17) are imposed for the sake of dealing with a finite group and should be regarded in the same spirit as the imposition of Born-von Karman boundary conditions in the zero-field case. The physical boundary conditions in a finite crystal are quite different from those imposed here. However, if one seeks bulk properties the actual boundary conditions are of little consequence. It is necessary, of course, to recognize for weak magnetic fields, for which the classical orbits of electrons can be large, that the physical size of the specimen should be large in order for the results of such a theory to be applicable even at the absolute zero of temperature. It is shown in Sec. 4 that the boundary conditions yield the correct number of states.

[13] In what follows we refer to the condition of Eq. (13) as magnetically periodic.

[14] Any lattice vector of the form $\Sigma\, n_i a_i$, for which there is no factor common to all n_i, is primitive.

3. IRREDUCIBLE REPRESENTATIONS

The magnetic translations are unitary operators. From this it follows that the matrix representations are unitary, if the basis functions are orthonormal. It is a straightforward matter to show that all the theorems leading to the derivations of the orthogonality relations for unitary representations of groups[15] are also applicable to the ray representations discussed here. These derivations are carried out in the Appendix.

One of the consequences of the orthogonality relations is that the sum of the squares of the dimensionalities of the irreducible representations equals the order of the group. Moreover, if the sum of the squares of the magnitudes of the traces of the matrices of a given representation equals the order of the group, the representation is irreducible. These two statements are sufficient to determine all the irreducible representations of the finite group under discussion.

Assuming Eq. (17) to hold, there is no loss in choosing the primitive vector $\mathbf{a}_3$ to be along the magnetic field,

$$\boldsymbol{\beta}=(2\pi/\Omega)(l/N)\mathbf{a}_3. \tag{18}$$

The commutation relations between the magnetic translations corresponding to the primitive translations are then given by

$$\begin{aligned}&[T(\mathbf{a}_3),T(\mathbf{a}_1)]=[T(\mathbf{a}_3),T(\mathbf{a}_2)]=0,\\ &T(\mathbf{a}_1)T(\mathbf{a}_2)=e^{-i2\pi l/N}T(\mathbf{a}_2)T(\mathbf{a}_1).\end{aligned} \tag{19}$$

The smallest crystal size for which it is possible to impose magnetically periodic boundary conditions is essentially two dimensional, being one unit cell thick in the $\mathbf{a}_3$ direction. It is N by N in the $\mathbf{a}_1$, $\mathbf{a}_2$ plane. The group thus consists of N^2 operations. This domain, being the smallest one for which periodic boundary conditions can be applied, is conveniently called the *magnetic unit cell.*

For this special case consider the N by N matrices

$$\begin{aligned}&D_{jk}(\mathbf{a}_3)=\delta_{j,k}=D_{jk}(0),\\ &D_{jk}(\mathbf{a}_1)=\delta_{j,k}e^{i(j-1)2\pi l/N};\quad j,k=1,2,\cdots N,\\ &D_{jk}(\mathbf{a}_2)=\delta_{j,k-1};\quad (\mathrm{mod}N).\end{aligned} \tag{20}$$

The remaining matrices in the representation can be found by application of Eq. (12). Thus,

$$\begin{aligned}&D_{jk}(n_1\mathbf{a}_1)=\delta_{j,k}e^{i(j-1)2\pi ln_1/N},\\ &D_{jk}(n_2\mathbf{a}_2)=\delta_{j,k-n_2}.\end{aligned} \tag{21}$$

From these we can find the general matrix

$$\begin{aligned}D_{jk}(n_1\mathbf{a}_1+n_2\mathbf{a}_2)&=\exp[in_1n_2\boldsymbol{\beta}\cdot(\mathbf{a}_1\times\mathbf{a}_2)/2]\\ &\quad\times\sum D_{jm}(n_1\mathbf{a}_1)D_{mk}(n_2\mathbf{a}_2),\\ &=\exp\left\{i\pi\frac{ln_1}{N}[n_2+2(j-1)]\right\}\delta_{j,k-n_2};\quad (\mathrm{mod}N).\end{aligned} \tag{22}$$

[15] See, for example, E. P. Wigner, *Gruppentheorie* (Frederick Vieweg und Sohn, Braunschweig, Germany, 1931) [English transl.: J. J. Griffin, *Group Theory* (Academic Press Inc., New York, 1959)].

These matrices form a representation of the given group. Moreover the traces of all the matrices are zero, with the exception of the one corresponding to the identity, which has a trace of N. The sum of the squares of the traces is thus N^2, which is the order of the group. The representation is therefore irreducible. Moreover, the square of its dimensionality is also N^2, which means there can be no other nonequivalent irreducible representation.

In summary, for the group of N^2 elements corresponding to putting magnetically periodic boundary conditions on the magnetic unit cell, we find only one irreducible representation of dimensionality N. For this special case all the eigenvalues are N-fold degenerate. A set of partner functions for this representation may be obtained by use of group projection operators.[15]

The first partner will be of the form

$$f_0(\mathbf{r})=\eta\sum_{\mathbf{R}_n}D_{11}^*(\mathbf{R}_n)T(\mathbf{R}_n)g(\mathbf{r}), \tag{23}$$

where $g(\mathbf{r})$ is an arbitrary function,[16] and η is a normalization coefficient. The labels of the partners are chosen from zero to $N-1$, rather than unity to N, for convenience in what follows. Making use of Eq. (22) we find

$$f_0(\mathbf{r})=\eta\sum_{n=1}^{N}T(n\mathbf{a}_1)g(\mathbf{r}). \tag{24}$$

The other partners of the given representation are simply related to one another by

$$T(-m\mathbf{a}_2)f_n(\mathbf{r})=f_{m+n}(\mathbf{r});\quad (\mathrm{mod}N), \tag{25}$$

$$T(\mathbf{a}_1)f_n(\mathbf{r})=e^{in2\pi l/N}f_n(\mathbf{r}). \tag{26}$$

The choice of basis functions for a degenerate representation is not unique. The fact that Eqs. (25) and (26) place translations along $\mathbf{a}_1$ and $\mathbf{a}_2$ on a different footing is due to the special choice of $D(\mathbf{a}_1)$, $D(\mathbf{a}_2)$. An equivalent representation could be found which interchanges the roles of $\mathbf{a}_1$ and $\mathbf{a}_2$.

The limitation to a single magnetic cell is easily relaxed. Consider a crystal, with magnetically periodic boundary conditions, of dimensions $N_1\mathbf{a}_1$, $N_2\mathbf{a}_2$, $N_3\mathbf{a}_3$, where $N_1=M_1N$, $N_2=M_2N$, and the magnetic field is oriented as before. We can form new representations for the larger group of $N_1N_2N_3$ operations from the one already discussed. For this group there are $M_1M_2N_3$ representations of dimensionality N. The matrices corresponding to the translations $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ differ from those already given only by a phase factor. These representations can be labeled by a vector with reciprocal space components of $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$. Thus

$$D^{\mathbf{q}}(\mathbf{a}_j)\equiv e^{-iq_ja_j}D(\mathbf{a}_j);\quad j=1,2,3, \tag{27}$$

where the possible values of q_i are given by

$$q_i=2\pi C_i/(N_ia_i);\quad i=1,2,3$$
$$C_1=0,1,\cdots,M_1-1;\quad C_2=0,1,\cdots,M_2-1;\quad C_3=0,1,\cdots,N_3-1. \tag{28}$$

It should be noted that the spacing of the $\mathbf{q}$ vectors is the same as the zero-field $\mathbf{k}$ vectors, being governed by the crystal dimensions. However, the domain of $\mathbf{q}$, is reduced in the $\mathbf{a}_1$ and $\mathbf{a}_2$ directions by a factor N. It is seen that this result is consistent with the identification of the domain of dimensions $N\mathbf{a}_1$, $N\mathbf{a}_2$, $\mathbf{a}_3$ as a magnetic unit cell.

Using projection operators once again, it is found that

$$f_0^{\mathbf{q}}(\mathbf{r})=\eta\sum_{n_1,n_2,n_3}\times\exp[+i(q_1n_1a_1+q_3n_3a_3+q_2n_2Na_2)]\times T(n_1\mathbf{a}_1)T(n_3\mathbf{a}_3)T(n_2N\mathbf{a}_2)g(\mathbf{r}), \tag{29}$$

which is a generalization of a Bloch sum. In addition

$$f_m^{\mathbf{q}}(\mathbf{r})=e^{-imq_2a_2}T(-m\mathbf{a}_2)f_0^{\mathbf{q}}(\mathbf{r}). \tag{30}$$

From these relations it follows by a straightforward calculation that

$$T(-\mathbf{R}_n)f_m^{\mathbf{q}}(\mathbf{r})=\exp\{i[\mathbf{q}+(m+n_2/2)(\boldsymbol{\beta}\times\mathbf{a}_2)]\cdot\mathbf{R}_n\}f_{m+n_2}^{\mathbf{q}}(\mathbf{r}), \tag{31}$$

where $\mathbf{R}_n=n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$. This equation completely specifies the transformation properties of the basis functions of the irreducible representations.

There is an alternative way of labeling the functions so as to show their superficial resemblance to Bloch functions. For this purpose we define

$$B(\mathbf{r};\mathbf{q}+m\boldsymbol{\beta}\times\mathbf{a}_2)=f_m^{\mathbf{q}}(\mathbf{r}). \tag{32}$$

In terms of these functions Eq. (31) becomes

$$T(-\mathbf{R}_n)B(\mathbf{r};\mathbf{k})=\exp\{i[\mathbf{k}+\boldsymbol{\beta}\times n_2\mathbf{a}_2/2]\cdot\mathbf{R}_n\}B(\mathbf{r};\mathbf{k}+\boldsymbol{\beta}\times n_2\mathbf{a}_2). \tag{33}$$

The domain of $\mathbf{k}$ and $\mathbf{q}$ are different. The vector $\mathbf{q}$ is restricted to a magnetic zone, which is a Brillouin zone, for a lattice in which the magnetic cell plays the role of unit cell. It is thus smaller than the Brillouin zone by a factor N^2. The domain of $\mathbf{k}$ is extended in the a_1^* direction by a factor N, so that its domain is smaller than the Brillouin zone by a factor N.

It is to be emphasized that the form of Eq. (31) is a result of the special choice of gauge, and the arbitrary choice of basis functions within a degenerate set. The function $B(\mathbf{r};\mathbf{q})$ goes into itself, times a phase factor, under the magnetic translations which are confined to the lattice plane normal to $\mathbf{a}_2^*$. Under magnetic translations to the mth neighboring plane, the vector index $\mathbf{k}$ changes to $\mathbf{k}'=\mathbf{k}+\boldsymbol{\beta}\times n_2\mathbf{a}_2+\boldsymbol{\kappa}$. The last term in the sum corresponds to a translation in reciprocal space necessary to bring $\mathbf{k}'$ into the first zone.

[16] The function $g(\mathbf{r})$ is not completely arbitrary. If it were orthogonal to the first partner by virtue of symmetry, its projection would be zero.

It is instructive to examine what happens in the limit as the size of the crystal becomes infinite. In this case the spectrum of allowed wave vectors $\mathbf{q}$ (or $\mathbf{k}$) becomes quasicontinuous, being a function only of the crystal dimensions. The energy is then a continuous function of $\mathbf{k}$. This can be called a magnetic subband. Thus, a band splits, under the influence of a magnetic field; into N-magnetic subbands.

In general one can expect these subbands to group into clusters. This follows from the fact that N, and the domain of $\mathbf{q}$ can change drastically for infinitesimal changes in $\mathbf{B}$. For example, if $\mathbf{B}$ changes to $\mathbf{B}(M-1)/M$, where M is a large integer such that $l(M-1)$ and NM have no common factor, then the degeneracy changes from N to NM. The number of subbands has thus been changed by a factor M. However, the level density really hasn't changed much since the perturbation is small. This effect has an analog in the zero-field case. Suppose, for example, in a one dimensional lattice every Mth cell had its potential altered infinitesimally. The lattice constant would increase by a factor M and the domain of $\mathbf{k}$ would be reduced by the same factor. Thus, there would be M of the newer bands in place of the original one with only an infinitesimal change in the density of states. In the energy range occupied by a single band there then would be M bands of smaller extent. The resulting energy spectrum would then consist of clusters of M bands. In the magnetic case we may expect a similar phenomenon in the clustering of magnetic bands. The empty lattice results of the next section support this point of view.

4. THE EMPTY LATTICE

The theory discussed above is applicable to the case of a vacuum, for which exact results are available. When the appropriate boundary conditions are applied, it is convenient to refer to the vacuum as the empty lattice, a special case useful for testing a theory. The Schrödinger equation in the gauge of Eq. (3b) for a magnetic field in the z direction is, in atomic units,

$$-\nabla^2\psi+i\beta\left(y\frac{\partial\psi}{\partial x}-x\frac{\partial\psi}{\partial y}\right)+\frac{\beta^2}{4}(x^2+y^2)\psi=E\psi, \quad (34)$$

with solutions,

$$\psi_{k_x,k_z}{}^n=\phi_n(y-k_x/\beta)e^{-i\beta xy/2}e^{i(k_xx+k_zz)}, \quad (35a)$$

where ϕ_n satisfies the harmonic oscillator equation,

$$-\partial^2\phi_n/\partial y^2+\beta^2y^2\phi_n=E_n\phi_n, \quad (35b)$$

and

$$E_n=(2n+1)\beta+k_z{}^2. \quad (35c)$$

These solutions are a complete set of linearly independent functions. The infinite fold degeneracy should be noted by the fact that the energy is independent of k_x.

We pick a Cartesian unit cell of sides a, b, c. The operations $T_x(a)$, $T_y(b)$, $T_z(c)$ designate magnetic translations along x, y, z of amounts a, b, and c respectively,

$$\begin{aligned}T_x(a)f(x,y,z)&=f(x-a,\,y,\,z)e^{-i\beta ay/2},\\ T_y(b)f(x,y,z)&=f(x,\,y-b,\,z)e^{i\beta bx/2},\\ T_y(c)f(x,y,z)&=f(x,\,y,\,z-c).\end{aligned} \quad (36)$$

These operators are applied to the solutions of Eq. (34) with the results

$$T_x(a)\psi_{k_x,k_z}{}^n=e^{-ik_xa}\psi_{k_x,k_z}{}^n, \quad (37a)$$

$$T_y(b)\psi_{k_x,k_z}{}^n=\psi_{k_x+\beta b,k_z}{}^n, \quad (37b)$$

$$T_z(c)\psi_{k_x,k_z}{}^n=e^{-ik_zc}\psi_{k_x,k_z}{}^n. \quad (37c)$$

Since the z dependence is of no interest, being the same as in the zero-field case, we shall neglect it. If we want the eigenfunctions to be invariant to $T_x(N_1a)$, we must restrict k_x to be a multiple of $2\pi/(N_1a)$ as in the zero-field case. In addition, we must require $(k_x+\beta b)$ to be of this form also, so that

$$\beta ab=2\pi l_1/N_1=2\pi l/N, \quad (38)$$

where l/N is the reduced form of l_1/N_1. From Eqs. (37) and (38) it is found that

$$T_y(Nb)\psi_{k_x}{}^n=\psi_{k_x+2\pi l/a}{}^n. \quad (39)$$

This function has the same transformation properties under T_x and T_z as does $\psi_{k_x}{}^n$. The functions $\psi_{k_x}{}^n$ do not yet have the proper periodicity under T_y but the superposition of degenerate functions given by

$$\begin{aligned}B_{k_x,k_y}{}^n&=\sum_{m=-\infty}^{\infty}e^{imk_yNb}T_y(mNb)\psi_{k_x}{}^n\\ &=\textstyle\sum_m e^{imk_yNb}\psi_{k_x-2\pi ml/a}{}^n,\end{aligned} \quad (40a)$$

satisfies the relation,

$$T_y(Nb)B_{k_x,k_y}=e^{-ik_yNb}B_{k_x,k_y} \quad (40b)$$

as well as Eqs. (37a), and (37c). In Eq. (40a) the domain of k_x can be easily seen to be from zero to $l(2\pi/a)$, whereas the domain of k_y is zero to $2\pi/Nb$, corresponding to an effective translation distance Nb.

It should be noted that it is only in the empty lattice that a meaning can be attached to a value of k_x greater than $2\pi/a$. Those differing by $(2\pi/a)$ are in different but equivalent representations. We thus have each representation appearing l times with a single energy. In other words, we have l sub-bands clustered. In this special case, all the states in a cluster, as well as the clusters themselves are degenerate. The functions $B_{k_x,k_y}{}^n$ are of the type described in the previous section, satisfying periodic boundary conditions. For a given value of n there are lN_1N_2/N degenerate states. The coarse grained density of states associated with the

x-y motion is thus $lN_1N_2/(2N\beta)$. Using Eq. (38) it is found that $g(E)=(N_1a)(N_2b)/4\pi$, which agrees with that of the zero-field case. Thus, the magnetic periodic boundary conditions do not cause difficulties in this respect.

It is worth noting that the infinite-fold degeneracy of the energy eigenvalues in a magnetic field in empty space can be demonstrated simply from the group properties. Since we can pick the lattice constant arbitrarily, we can select a and b for a given field such that $\beta ab=2\pi/N$, where N is an arbitrarily large integer. Each representation is then N-fold degenerate, so that in the limit as (ab) is made arbitrarily small the degeneracy becomes infinite.

5. EFFECTIVE HAMILTONIAN

An effective Hamiltonian can be most easily derived by showing the existence of a set of functions which are the magnetic analog of Wannier functions. Denoting a particular one of these functions by $A(\mathbf{r})$ we define

$$A(\mathbf{R}_n;\mathbf{r})=T(\mathbf{R}_n)A(\mathbf{r}). \tag{41}$$

It will be shown that there exist functions $A(\mathbf{R}_n;\mathbf{r})$ which form an orthonormal set, and which also span the space of the eigenfunctions of the magnetic-field Hamiltonian arising from a single band. Once this is done, the demonstration that an effective Hamiltonian exists, follows the procedure of Wannier.[6]

It should be remembered that in the magnetic field all representations are N by N. Also, each representation appears N times in the states arising from a single band. Using the notation of Eq. (30) the various eigenfunctions can be denoted by $\psi_{m,n}{}^{\mathbf{q}}$. The first subscript designates the partner in the $\mathbf{q}$ representation and n labels the magnetic band. Both m and n take on N different values. Let

$$A(\mathbf{r})=(N/N_1N_2N_3)^{1/2}\sum_{m,\mathbf{q}}\psi_{m,m}{}^{\mathbf{q}}. \tag{42}$$

Then from Eq. (31) it follows that

$$A(\mathbf{R}_n;\mathbf{r})=(N/N_1N_2N_3)^{1/2}\sum_{m,\mathbf{q}}\times\exp\{-i[\mathbf{q}+(m-n_2/2)(\boldsymbol{\beta}\times\mathbf{a}_2)]\cdot\mathbf{R}_n\}\psi_{m-n_2,m}{}^{\mathbf{q}} \tag{43}$$

and the orthonormalcy can be seen from

$$\begin{aligned}I_{n,n'}&=\int A^*(\mathbf{R}_{n'};\mathbf{r})A(\mathbf{R}_n;\mathbf{r})d^3r\\&=N/(N_1N_2N_3)\sum_{m,m',\mathbf{q},\mathbf{q}'}\times\exp\{i[\mathbf{q}+(m-n_2'/2)(\boldsymbol{\beta}\times\mathbf{a}_2)]\cdot R_{n'}\\&\quad-i[\mathbf{q}'+(m'-n_2/2)(\boldsymbol{\beta}\times\mathbf{a}_2)]\cdot\mathbf{R}_n\}\times\delta_{\mathbf{q},\mathbf{q}'}\delta_{m,m'}\delta_{n_2,n_2'}.\end{aligned} \tag{44}$$

The Kronecker delta $\delta_{n_2,n_2'}$ is to be interpreted modulo N. The domain of $\mathbf{q}$ is the magnetic zone. Thus,

$$\begin{aligned}I_{n,n'}&=N/(N_1N_2N_3)\sum_{m,\mathbf{q}}\times\exp\{i[\mathbf{q}+m(\boldsymbol{\beta}\times\mathbf{a}_2)]\cdot(\mathbf{R}_{n'}-\mathbf{R}_n)\}\delta_{n_2,n_2'}\times\exp[i(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot(n_2\mathbf{R}_n-n_2'\mathbf{R}_{n'})/2]\\&=N/(N_1N_2N_3)\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_{n'}-\mathbf{R}_n)}\delta_{n_2,n_2'}\times\exp[i(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot(n_2\mathbf{R}_n-n_2'\mathbf{R}_{n'})/2].\end{aligned} \tag{45}$$

This clearly vanishes if $\mathbf{R}_n\neq\mathbf{R}_{n'}$. The domain of $\mathbf{k}$ is shorter than the Brillouin zone by a factor N in the $\mathbf{a}_2{}^*$ direction, and thus contains $N_1N_2N_3/N$ states, yielding

$$I_{n,n'}=\delta_{\mathbf{R}_n,\mathbf{R}_{n'}}, \tag{46}$$

which is the orthonormality condition. The number of functions is clearly the same as the number of states in a single band, neglecting the factor of two for spin. They are thus capable of playing the same role as Wannier functions, in the construction of an effective Hamiltonian.

Let

$$\psi=\sum f(\mathbf{R}_n)A(\mathbf{R}_n;\mathbf{r}). \tag{47}$$

The coefficients $f(\mathbf{R}_n)$ must satisfy

$$\sum H_{m,n}f(\mathbf{R}_n)=Ef(\mathbf{R}_m), \tag{48}$$

in the absence of a perturbation. In the above equation $H_{m,n}$ is the matrix element of the Hamiltonian between two functions $A(\mathbf{R}_m;\mathbf{r})$ and $A(\mathbf{R}_n;\mathbf{r})$,

$$H_{m,n}=(T(\mathbf{R}_m)A(\mathbf{r}),HT(\mathbf{R}_n)A(\mathbf{r})). \tag{49}$$

Making use of the unitary and commutative properties of the magnetic translations one obtains

$$\begin{aligned}H_{m,n}&=(A(\mathbf{R}_m-\mathbf{R}_n;\mathbf{r}),HA(\mathbf{r}))\times\exp[i\boldsymbol{\beta}\cdot(\mathbf{R}_m\times\mathbf{R}_n)/2]\\&=\epsilon(\mathbf{R}_m-\mathbf{R}_n)\exp[i\boldsymbol{\beta}\cdot(\mathbf{R}_m\times\mathbf{R}_n)/2],\end{aligned} \tag{50}$$

where $\epsilon(\mathbf{R}_m)=(A(\mathbf{R}_m;\mathbf{r}),HA(\mathbf{r}))$. Thus Eq. (48) takes the form

$$\begin{aligned}&\sum_n\epsilon(\mathbf{R}_m-\mathbf{R}_n)\exp[i\boldsymbol{\beta}\cdot(\mathbf{R}_m\times\mathbf{R}_n)/2]f(\mathbf{R}_n)\\&\quad=\sum_{n'}\epsilon(\mathbf{R}_{n'})\exp[i\boldsymbol{\beta}\cdot(\mathbf{R}_{n'}\times\mathbf{R}_m)/2]f(\mathbf{R}_m-\mathbf{R}_{n'})\\&\quad=\sum_n\epsilon(\mathbf{R}_n)T_-(\mathbf{R}_n)f(\mathbf{R}_m)=Ef(\mathbf{R}_m).\end{aligned} \tag{51}$$

In the above equation $T_-(\mathbf{R}_n)$ is the operator obtained from $T(\mathbf{R}_n)$ by replacing the vector potential by its negative. In using Eq. (51), $f(\mathbf{R}_m)$ is to be interpreted as a function of a continuous variable $\mathbf{r}$, and the expression evaluated at $\mathbf{r}=\mathbf{R}_m$.

From the definition of $T_-(\mathbf{R}_n)$ Eq. (51) becomes

$$\begin{aligned}\{\sum_n\epsilon(\mathbf{R}_n)\exp[-i\mathbf{R}_n\cdot(\mathbf{P}+e\mathbf{A}/c)/\hbar]\}f(\mathbf{R}_m)&=Ef(\mathbf{R}_m),\\H_{\text{eff}}(\mathbf{P}+e\mathbf{A}/c)f(\mathbf{r})&=Ef(\mathbf{r}).\end{aligned} \tag{52}$$

It is a straightforward procedure to incorporate the effect of a perturbation, as is done in the usual effective Hamiltonians. One drawback to the utility of the effective Hamiltonian as defined in Eq. (22), is that the

coefficients $\epsilon(\mathbf{R}_n)$ depend on the field. As was noted by Kohn[3] this prevents one from taking experimental information at zero field and applying it directly to the magnetic problem.

6. DISCUSSION

Although group theory, by itself, cannot yield the energy spectrum of quantum mechanical systems, it does provide a useful tool in such an investigation when applicable.

It is significant that group theory is still applicable when a solid is subject to a uniform magnetic field. In addition to establishing the essential degeneracies, and classifying states according to symmetry it can be used in connection with selection rules. Moreover, explicit numerical computations on level structure are usually greatly simplified by its application.

There is no reason why the method must be restricted to the one electron approximation, since the Hamiltonian for the many-electron system is invariant under a similar ray group of operations. These operators are just those which shift all the electronic coordinates and momenta simultaneously. It should also be possible to extend the theory to include spin and the effects of uniform electric fields.

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APPENDIX

The theorems which lead up to the orthogonality relations for the irreducible representations of a group are here derived for the ray representations encountered in this work.

Theorem 1. Any ray representation by nonsingular matrices is equivalent to one by unitary matrices.

Let the matrices $D(i)$ be a ray representation, so that

$$D(i)D(j)=\omega(i,j)D(k), \tag{A1}$$

where $\omega(i,j)$ is a complex number of magnitude unity. Define the positive definite matrix K,

$$K=\sum D(i)D^\dagger(i). \tag{A2}$$

Let

$$\bar{D}(i)=K^{-1/2}D(i)K^{1/2}. \tag{A3a}$$

Then, making use of Eq. (A1) and (A2), it is found that

$$\begin{aligned}\bar{D}(i)\bar{D}^\dagger(i)&=K^{-1/2}D(i)KD^\dagger(i)K^{-1/2}\\&=K^{-1/2}\textstyle\sum_j D(i)D(j)D^\dagger(j)D^\dagger(i)K^{-1/2}\\&=K^{-1/2}KK^{-1/2}=1.\end{aligned} \tag{A3b}$$

The matrices $\bar{D}(i)$ thus form a unitary representation.

Theorem 2. Every matrix M commuting with all the matrices $D(i)$ of an irreducible representation is a multiple of the unit matrix.

The proof of this for ray representations is identical with that for ordinary representations.[15]

Theorem 3. If λ_1 and λ_2 are two irreducible representations of dimensions l_1 and l_2, respectively, and if there exists a matrix X such that $XD^{\lambda_1}(i)=D^{\lambda_2}(i)X$ for each i then either (a) *X is the null matrix or* (b) *$l_1=l_2$, and the two representations are equivalent.*

The proof of this also is identical with that for ordinary representations.

Theorem 4. (Orthogonality relations) *For two irreducible unitary ray representations λ_1, λ_2,*

$$\textstyle\sum_k D_{ij}^{*\lambda_1}(k)D_{lm}^{\lambda_2}(k)=\delta_{i,l}\delta_{j,m}\delta_{\lambda_1,\lambda_2}g/l, \tag{A4}$$

where g is the order of the group, and l is the dimensionality of either representation.

Let

$$M=\textstyle\sum_R D^{\lambda_1}(R)XD^{\lambda_2}(R^{-1}), \tag{A5}$$

where R labels a group element, and X is an arbitrary l_1 by l_2 matrix. Then,

$$M=\textstyle\sum_R D^{\lambda_1}(SR)XD^{\lambda_2}((SR)^{-1}), \tag{A6}$$

since (SR) takes on all the elements of the group as R does, if S is an arbitrary element.

From Eq. (A5),

$$D^{\lambda_1}(S)M=\textstyle\sum_R \omega(S,R)D^{\lambda_1}(SR)XD^{\lambda_2}(R^{-1}). \tag{A7}$$

From Eq. (A6),

$$MD^{\lambda_1}(S)=\textstyle\sum_R D^{\lambda_1}(SR)XD^{\lambda_2}(R^{-1})\omega((SR)^{-1},R^{-1}). \tag{A8}$$

In the ray representation for the magnetic-field problem $\omega(S,R)$ is given by $\exp[i\boldsymbol{\beta}\cdot(\mathbf{R}_R\times\mathbf{R}_S)/2]$ so that

$$\begin{aligned}&\omega((SR)^{-1},R^{-1})\\&\quad=\exp\{i\boldsymbol{\beta}\cdot[-\mathbf{R}_R\times(-\mathbf{R}_R-\mathbf{R}_S)/2]\}\\&\quad=\omega(S,R).\end{aligned} \tag{A9}$$

Thus, for these representations,

$$D^{\lambda_1}(S)M=MD^{\lambda_2}(S), \tag{A10}$$

so that M satisfies the conditions of Theorem 3. The remainder of the proof is identical with that for ordinary representations.

The projection methods of representation theory may be derived in similar fashion.