

## Magnetic Translation Group. II. Irreducible Representations

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The physical irreducible representations of the magnetic translation group (M.T.G.) defined previously have been found. From these a set of solutions of Schrödinger's equation for a Bloch electron in a magnetic field has been constructed. In general the M.T.G. is non-Abelian. However, when the magnetic flux through areas enclosed by any vectors of the Bravais lattice become multiples of an elementary "fluxon"  $hc/e$ , the M.T.G. becomes isomorphic to the usual translation group.

### I. INTRODUCTION

IN a previous paper<sup>1</sup> a magnetic translation group was defined and its general properties were established. The elements of this group, which depend on both a point of the Bravais lattice and a path joining the origin of the lattice with this point, are given by

$$\tau(\mathbf{R} | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) = \exp\left\{ \frac{i}{\hbar} \mathbf{R}_n \cdot [\mathbf{p} + (e/c)\mathbf{A}] \right\} \times \exp\left\{ 2\pi i (n/bN)m \right\}, \quad (1)$$

where  $\mathbf{R}_n$  is a vector of the Bravais lattice,  $\mathbf{A}$  is the vector potential of the magnetic field  $\mathbf{H}$ ,  $m$  is the coefficient by the product  $\mathbf{a}_1 \times \mathbf{a}_2$  of the unit cell vectors  $\mathbf{a}_1, \mathbf{a}_2$  in the sum of ordered products

$$\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \dots + \mathbf{R}_1 \times \mathbf{R}_i + \mathbf{R}_2 \times \mathbf{R}_3 + \dots + \mathbf{R}_{i-1} \times \mathbf{R}_i, \quad (2)$$

$n, N$ , and  $b$  appear from the Born-von Karman conditions which turn the magnetic translation group into a finite one and impose the following condition on the magnetic field:

$$\frac{e\mathbf{H}}{\hbar c} = \frac{4\pi}{V} \frac{\mathbf{R}_n}{bN} = \frac{4\pi}{V} \frac{n}{bN} \mathbf{a}_3, \quad (3)$$

$V$  is the volume of the unit cell,  $V = \mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3$ , and  $b$  takes the values 1 or 2 for  $N$  odd or even, respectively.

The finite magnetic translation group  $\bar{G}$  is of the order  $b(N/p)N^3$ , where  $p$  is the largest common factor of  $N$  and  $n$ . For constructing the irreducible representations of  $\bar{G}$  we use the fact that it has an invariant subgroup  $\bar{F}$  consisting of elements

$$\tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) = \exp\left\{ \frac{i}{\hbar} \mathbf{r}_n \cdot \left( \mathbf{p} + \frac{e}{c}\mathbf{A} \right) \right\} \times \exp\left\{ 2\pi i \frac{n}{bN} m \right\}, \quad (4)$$

where

$$\mathbf{r}_n = n_1 \mathbf{a}_1 + n_3 \mathbf{a}_3. \quad (5)$$

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<sup>1</sup> J. Zak, Phys. Rev. **134**, A1602 (1964).

The group  $\bar{G}$  can therefore be written as

$$\bar{G} = \tau(\mathbf{a}_2 | \mathbf{a}_2) \bar{F} + \dots + \tau(N\mathbf{a}_2 | N\mathbf{a}_2) \bar{F}. \quad (6)$$

The invariant subgroup  $\bar{F}$  is a commutative group and its irreducible representations are well known. In order to find the irreducible representations of  $\bar{G}$  we use the method of Frobenius.<sup>2,3</sup> This method enables one to find all the irreducible representations of a group from the irreducible representations of its invariant subgroup.

In Sec. II the physical irreducible representations of the M.T.G. are constructed. They turn out to be the same in the case of the finite M.T.G. as the ray representations of the usual translation group that are given by Brown.<sup>4</sup> This result is not surprising because in the usual method for constructing ray representations of a finite group<sup>5,6</sup> one augments the group, finds the vector representations of the augmented group, and then chooses those representations which correspond to ray representations of the original group. It appears, however, more natural to define a group which commutes with the Hamiltonian for a Bloch electron in a magnetic field than to treat ray representations of a group (the usual translation group) which does *not* commute with this Hamiltonian. Moreover, by finding all the physical representations of the M.T.G., we are sure that we have all the possible symmetry types for the wave functions.<sup>7</sup>

For constructing the irreducible representations of the M.T.G., we first start with the finite group obtained by applying the boundary conditions. From the method of construction, it is possible to find a complete set of symmetry adapted functions for the problem under discussion.<sup>8</sup> These functions are presented in Sec. III. As shown in Ref. 1, the boundary conditions on the magnetic translation group lead to physical restrictions on the magnitude of the magnetic field. In Sec. IV we

<sup>2</sup> F. Seitz, Ann. Math. **37**, 17 (1936).

<sup>3</sup> J. Zak, J. Math. Phys. **1**, 165 (1960).

<sup>4</sup> E. Brown, Bull. Am. Phys. Soc. **8**, 257 (1963); Phys. Rev. **133**, A1038 (1964).

<sup>5</sup> I. Schur, J. Reine Aug. Math. **127**, 20 (1904); **132**, 85 (1907).

<sup>6</sup> W. Döring, Z. Naturforsch. **14**, 343 (1959).

<sup>7</sup> The statement used in Ref. 4 for showing the completeness of the irreducible representations, namely, that the sum of squares of the dimensions of nonequivalent irreducible ray representations equals the order of the group is, in general, not true. There are, for example, finite groups that have no ray representations at all.

<sup>8</sup> An alternative method for constructing symmetry adapted functions is discussed in Ref. 4.

remove these restrictions by dealing with an infinite M.T.G. Finally, in the same section, the significance of the elementary fluxon  $hc/e$  for the magnetic translation group is discussed.

## II. CONSTRUCTION OF THE IRREDUCIBLE REPRESENTATIONS OF $G$

The invariant subgroup  $\bar{F}$  of  $\bar{G}$  is a commutative group and its irreducible representations are

$$D^{(s, k_1, m_3)} \{ \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) \} \\ = \exp \left\{ 2\pi i \left[ \frac{n}{bN} m s + \frac{k_1 n_1}{N} + \frac{m_3 n_3}{N} \right] \right\}, \quad (7)$$

where  $s$  takes the values from 1 to  $bN/p$ , and  $k_1, m_3$  the values from 1 to  $N$ . Relation (7) thus defines  $(bN/p)N^2$  one-dimensional representations of  $\bar{F}$ . These are all the irreducible representations of  $\bar{F}$  because the order of the latter is just  $(bN/p)N^2$ . However, some of the representations (7) are nonphysical as may be seen by setting  $\mathbf{r}_n = \mathbf{o}$ . The element  $\tau(\mathbf{o} | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i)$  is a constant factor which will be represented by different constants if we take different values of  $s$  in (7). When the operator  $\tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i)$  itself operates in the functional space, the only physical representations in (7) will be those for  $s=1$ . We therefore consider the representations of  $\bar{F}$  only for  $s=1$  and from these we construct the irreducible representations of  $\bar{G}$ .

Let us first consider the case  $p=1$  (i.e., no common factor for  $N$  and  $n$ ) and denote the vector that spans representation (7) (for  $s=1$ ) by  $|k_1, m_3\rangle$ . Then

$$D^{(k_1, m_3)} \{ \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) \} |k_1, m_3\rangle \\ = \exp \left\{ 2\pi i \left[ \frac{n}{bN} m + \frac{2nk_1 n_1}{bN} + \frac{m_3 n_3}{N} \right] \right\} |k_1, m_3\rangle, \quad (8)$$

where a factor  $2n/b$  was introduced for convenience in front of  $k_1 n_1/N$ . (This is equivalent to an alternative numbering of the eigenvectors  $|k_1, m_3\rangle$ .) We now perform a similarity transformation:

$$\tau(-n_2 \mathbf{a}_2 | -n_2 \mathbf{a}_2) \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \\ = \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) \exp \{ 4\pi i (n/bN) n_1 n_2 \}. \quad (9)$$

It follows from (9) that

$$D \{ \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) D \{ \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \} |k_1, m_3\rangle \} \\ = \exp \left\{ 2\pi i \left[ \frac{n}{bN} m + \frac{2n(k_1 + n_2)n_1}{bN} + \frac{m_3 n_3}{N} \right] \right\} \\ \times D \{ \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \} |k_1, m_3\rangle. \quad (10)$$

It is seen that the vector  $D \{ \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \} |k_1, m_3\rangle$  is an eigenvector of  $D \{ \tau(\mathbf{r}_n | \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_i) \}$  corresponding to the eigenvalues  $k_1 + n_2, m_3$  ( $D$  now denotes a representation of  $\bar{G}$ ). Since we assumed that  $N$  and  $n$  have no common factor we get  $N$  vectors  $D \{ \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \}$

$\times |k_1, m_3\rangle$  for  $n_2 = 1, 2, \dots, N$ :

$$D \{ \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \} |k_1, m_3\rangle = |k_1 + n_2, m_3\rangle. \quad (11)$$

Let us show that relations (10) and (11) for each  $m_3$  define an irreducible representation of  $\bar{G}$ . According to (6) each operator  $\tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i)$  can be written as follows:

$$\tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \\ = \tau(n_2 \mathbf{a}_2 | n_2 \mathbf{a}_2) \tau(\mathbf{r}_n | -n_2 \mathbf{a}_2, \mathbf{R}_1, \dots, \mathbf{R}_i), \quad (12)$$

where  $\mathbf{R}_n = \mathbf{r}_n + n_2 \mathbf{a}_2$ ,  $\mathbf{r}_n = n_1 \mathbf{a}_1 + n_3 \mathbf{a}_3$ . Therefore,

$$D \{ \tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \} |k_1, m_3\rangle \\ = \exp \left\{ 2\pi i \left[ \frac{n}{bN} g + \frac{2nk_1 n_1}{bN} + \frac{m_3 n_3}{N} \right] \right\} |k_1 + n_2, m_3\rangle, \quad (13)$$

where  $g$  is the coefficient of the product  $\mathbf{a}_1 \times \mathbf{a}_2$  in

$$-n_2 \mathbf{a}_2 \times \mathbf{R}_n + \mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \dots + \mathbf{R}_{i-1} \times \mathbf{R}_i. \quad (14)$$

From (13) it follows that

$$D_{k'k}^{m_3} \{ \tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \} \\ = \langle m_3 k' | \tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) |k, m_3\rangle \\ = \delta_{k', k+n_2} \exp \left\{ 2\pi i \left[ \frac{n}{bN} g + \frac{2nk n_1}{bN} + \frac{m_3 n_3}{N} \right] \right\}, \quad (15)$$

where  $D_{k'k}^{m_3}$  denotes a matrix element  $k'k$  of the operator  $\tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i)$ ;  $k'$  and  $k$  take values from 1 to  $N$ , and  $k+n_2$  is taken modulo  $N$ .

We next show that for each  $m_3$  the matrices  $D^{m_3}$  form a representation of  $\bar{G}$ . To do this we first calculate the product of two matrices (15) corresponding to two elements  $\tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i)$  and  $\tau(\mathbf{R}_{n'} | \mathbf{R}'_1, \dots, \mathbf{R}'_i)$  and then the matrix which corresponds to the product  $\tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \tau(\mathbf{R}_{n'} | \mathbf{R}'_1, \dots, \mathbf{R}'_i)$ . The two results must be the same if (15) is to be a representation of  $\bar{G}$ . From (15) we have

$$\sum_{\alpha=1}^N D_{k' \alpha}^{m_3} \{ \tau(\mathbf{R}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \} D_{\alpha k}^{m_3} \{ \tau(\mathbf{R}_{n'} | \mathbf{R}'_1, \dots, \mathbf{R}'_i) \} \\ = \delta_{k', k+n_2+n_2'} \exp \left\{ 2\pi i \left[ \frac{n}{bN} (g+g') + \frac{2nk(n_1+n_1')}{bN} \right. \right. \\ \left. \left. + \frac{2nn_1 n_2'}{bN} + \frac{m_3(n_3+n_3')}{N} \right] \right\}. \quad (16)$$

On the other hand, the matrix corresponding to the product of the two elements is

$$D_{k'k}^{m_3} \{ \tau(\mathbf{R}_n + \mathbf{R}_{n'} | \mathbf{R}_1, \dots, \mathbf{R}_i, \dots, \mathbf{R}'_i) \} \\ = \delta_{k', k+n_2+n_2'} \exp \left\{ 2\pi i \left[ \frac{n}{bN} g'' + \frac{2nk(n_1+n_1')}{bN} \right. \right. \\ \left. \left. + \frac{m_3(n_3+n_3')}{N} \right] \right\}, \quad (17)$$

where  $g''$  is the coefficient by the product  $\mathbf{a}_1 \times \mathbf{a}_2$  in the expression

$$-(n_2+n_2')\mathbf{a}_2 \times (\mathbf{R}_n+\mathbf{R}_n')+\mathbf{R}_1 \times \mathbf{R}_2+\cdots \\ +\mathbf{R}_{i-1} \times \mathbf{R}_i+\mathbf{R}_1' \times \mathbf{R}_2'+\cdots+\mathbf{R}_{i-1}' \times \mathbf{R}_i'. \quad (18)$$

It is easily shown that

$$g''=g+g'+2n_1n_2'. \quad (19)$$

It therefore follows that expressions (16) and (17) are equal and thus that the matrices (15) for each  $m_3$  form a representation of  $\bar{G}$ . These representations are irreducible because all the vectors  $|km_3\rangle$  for a given  $m_3$  and different  $k(k=1, 2, \dots, N)$  form a closed subspace. An alternative way to check the irreducibility of (15) is to calculate the character for a given  $m_3$ ,

$$\chi^{m_3}\{\tau(\mathbf{R}_n|\mathbf{R}_1, \dots, \mathbf{R}_i)\} = \sum_{k=1}^N D_{kk}^{m_3} \\ = N \delta_{n_1 0} \delta_{n_2 0} \exp\left\{2\pi i \left[ \frac{n}{bN}g + \frac{m_3 n_3}{N} \right]\right\}, \quad (20)$$

and to find the sum

$$\sum_{\bar{G}} |\chi^{m_3}\{\tau(\mathbf{R}_n|\mathbf{R}_1, \dots, \mathbf{R}_i)\}|^2 = N^4. \quad (21)$$

Result (21) shows that the representation (15) with the character (20) is irreducible [for reducible representations the sum (21) is greater than the number of elements in  $\bar{G}$ ]. Note that the way of constructing irreducible representations here corresponds to the method of finding conjugate representations of the invariant subgroup  $\bar{F}$  by means of the elements of  $\bar{G}$  that do not belong<sup>3</sup> to  $\bar{F}$ . In the case when  $N$  and  $n$  have no common factor all the conjugate representations are nonequivalent and the representation of  $\bar{G}$  which they induce is thus irreducible.

According to the method of Froebenius, relation (15) gives us all the irreducible representations of the group<sup>2,3</sup> corresponding to  $s=1$ . Since we are interested only in the physical representations of  $\bar{G}$  these are all the representations of  $\bar{G}$ .

Let us now treat the case when the largest common factor of  $N$  and  $n$  is  $p$ . If we start with a vector  $|k_1, m_3\rangle$  [see (8)] and apply all the operators  $\tau(n_2\mathbf{a}_2|n_2\mathbf{a}_2)$  we shall get in general only  $N'=N/p$  independent vectors  $|k, m_3\rangle$  for  $k=1, 2, \dots, N'$ . According to Ref. 2 it again follows that we may assume

$$D\{\tau(n_2\mathbf{a}_2|n_2\mathbf{a}_2)\}|k, m_3\rangle \\ = \exp\{2\pi i(m_2n_2/N)\}|k+n_2, m_3\rangle \quad (22)$$

for  $n_2=1, 2, \dots, N'$  and  $m_2=0, 1, \dots, p-1$ . The representations induced by the vectors (22) can be

written as

$$D_{k', k}^{(m_1 m_2 m_3)}\{\tau(\mathbf{R}_n|\mathbf{R}_1, \dots, \mathbf{R}_i)\} \\ = \delta_{k', k+n_2} \exp\left\{2\pi i \left[ \frac{m_1 n_1}{N} + \frac{m_2 n_2}{N} + \frac{n}{bN}g \right. \right. \\ \left. \left. + \frac{\gamma n k n_1}{bN} + \frac{m_3 n_3}{N} \right]\right\}, \quad (23)$$

where the values of  $m_1, m_2$  range from 0 to  $p-1$ ;  $k, k'$  assume values from 1 to  $N'$  ( $k+n_2$  is defined modulo  $N'$ ), and  $m_3$  ranges from 1 to  $N$ . Relation (23) defines  $p^2N$  irreducible and nonequivalent  $N' \times N'$  representations of the group  $\bar{G}$  and again gives us all the physical representations of  $\bar{G}$ . Note that in this case when  $N$  and  $n$  have a common factor the conjugate representations of  $\bar{F}$ , constructed by means of elements of  $\bar{G}$  that do not belong to  $\bar{F}$ , will in general no longer be nonequivalent. The representations of  $\bar{G}$  induced by the conjugate representations of  $\bar{F}$  will be reducible; the irreducible parts are given in (23). In the case when  $p=1$ , representations (23) go over into (15). Hence, relation (23) gives all the irreducible physical representations of  $\bar{G}$ .

### III. SYMMETRY ADAPTED FUNCTIONS

We now use the irreducible representations of the magnetic translation group  $\bar{G}$  to construct symmetry adapted solutions of Schrödinger's equation for a Bloch electron in a magnetic field. By using the gauge

$$\mathbf{A} = \frac{1}{2}[\mathbf{H} \times \mathbf{r}], \quad (24)$$

we can write the elements (1) of the magnetic translation group as

$$\tau(\mathbf{R}_n|\mathbf{R}_1, \dots, \mathbf{R}_i) = \exp\left\{\frac{i}{\hbar}\mathbf{R}_n \cdot \mathbf{p} + i\frac{n}{bN}(n_2\mathbf{K}_1 - n_1\mathbf{K}_2) \cdot \mathbf{r}\right\} \\ \times \exp\left\{2\pi i\frac{n}{bN}m\right\}, \quad (25)$$

where  $\mathbf{K}_1$  and  $\mathbf{K}_2$  are vectors of the unit cell of the reciprocal lattice. Let

$$\psi(\mathbf{r}) = \exp\{i\mathbf{k} \cdot \mathbf{r}\}u(\mathbf{r}), \quad (26)$$

with

$$\mathbf{k} = \frac{1}{N} \left[ \left( m_1 + \frac{2nk_1}{b} \right) \mathbf{K}_1 + m_3 \mathbf{K}_3 \right], \\ m_1 = 0, 1, \dots, p-1; \quad k_1 = 1, \dots, N'; \quad (27)$$

and

$$\tau(\mathbf{r}_n|\mathbf{R}_1, \dots, \mathbf{R}_i)u(\mathbf{r}) = \exp\{2\pi i(n/bN)g\}u(\mathbf{r}).$$

The last condition on  $u(\mathbf{r})$  means that

$$u(\mathbf{r}+\mathbf{r}_n) = \exp\left\{i\frac{n}{bN}\mathbf{n}_1\mathbf{K}_2 \cdot \mathbf{r}\right\}u(\mathbf{r}), \quad (28)$$

in which case

$$\tau(\mathbf{r}_n | \mathbf{R}_1, \dots, \mathbf{R}_i) \psi(\mathbf{r}) = \exp \left\{ 2\pi i \left[ \frac{n}{bN} g + \frac{m_1 n_1}{N} + \frac{2nk_1 n_1}{bN} + \frac{m_3 n_3}{N} \right] \right\} \psi(\mathbf{r}). \quad (29)$$

In order to satisfy condition (28) and the boundary conditions, we choose  $u(\mathbf{r})$  as follows:

$$u(\mathbf{r}) = \exp \left\{ \frac{i}{2\pi} \frac{n}{bN} \mathbf{r} \cdot \mathbf{K}_1 \cdot \mathbf{K}_2 \right\} w(\mathbf{r}), \quad (30)$$

with

$$\begin{aligned} w(\mathbf{r} + \mathbf{r}_n) &= w(\mathbf{r}), \\ w(\mathbf{r} + N' \mathbf{a}_2) &= \exp \{ -iN' \mathbf{a}_2 \cdot \mathbf{h} \cdot \mathbf{r} \} w(\mathbf{r}). \end{aligned} \quad (31)$$

The function (26) will therefore be

$$\psi(\mathbf{r}) = \exp \{ i \mathbf{k} \cdot \mathbf{r} \} \exp \left\{ \frac{i}{2\pi} \frac{n}{bN} \mathbf{r} \cdot \mathbf{K}_1 \cdot \mathbf{K}_2 \right\} w(\mathbf{r}). \quad (32)$$

By using Eq. (32) and the relation (22) and by re-introducing the magnetic field according to Eq. (3) we get the functions

$$\begin{aligned} \psi_q^{(l, \mathbf{k})}(\mathbf{r}) &= \exp \{ i \mathbf{k} \cdot \mathbf{r} \} \\ &\times \exp \{ i [q + (1/4\pi) \mathbf{K}_2 \cdot \mathbf{r}] (\mathbf{a}_2 \times \mathbf{h}) \cdot \mathbf{r} \} w_{l\mathbf{k}}(\mathbf{r} + q\mathbf{a}_2), \end{aligned} \quad (33)$$

where  $\mathbf{k} = (1/N)(m_1 \mathbf{K}_1 + m_2 \mathbf{K}_2 + m_3 \mathbf{K}_3)$ ,  $m_1, m_2$  are integers which take values from 0 to  $p-1$  (with  $p$  again the common factor of  $N$  and  $n$ ),  $m_3$  is an integer whose values range from 1 to  $N$  and the integer  $q$  has values from 0 to  $N'-1$ . The functions  $w_{l\mathbf{k}}(\mathbf{r})$  satisfy conditions (31). The meaning of  $l$  will be given later. For fixed  $\mathbf{k}$  and  $l$  there are  $N'$  ( $=N/p$ ) functions in (33) which form a basis for an  $N' \times N'$  irreducible representation (23) of the magnetic translation group  $\bar{G}$ . For different  $\mathbf{k}$  we get nonequivalent representations of  $\bar{G}$ . The functions in (33) are thus the symmetry adapted functions for all the irreducible representations of  $\bar{G}$ . The physical picture connected with this description is the following. All the functions (33) with fixed  $l$  and  $\mathbf{k}$  (and varying  $q$ ) belong to the same energy. When  $\mathbf{k}$  also varies the energy will be in general varying and one obtains an energy band for each  $l$ . The number  $l$  was thus introduced to distinguish between different energy bands in the same way in which it is done in the case of the usual translation group.

From the fact that the function (33) form bases for irreducible unitary representations (23) of the magnetic translation group, it follows that functions (33) are orthogonal for different  $\mathbf{k}$  and  $q$ . [Note that the functions  $w_{l\mathbf{k}}(\mathbf{r})$  also depend on the vector  $\mathbf{k}$ . This dependence is obtained by substituting functions (33) into Schrödinger's equation.] By assuming (as is usual) the orthogonality of  $w_{l\mathbf{k}}(\mathbf{r})$  for different  $l$

$$\int w_{l' \mathbf{k}'}^*(\mathbf{r}) w_{l\mathbf{k}}(\mathbf{r}) dV = \delta_{l'l'}, \quad (34)$$

where the integration is over the volume of the crystal, we get

$$\int \psi_{q'}^{*(l' \mathbf{k}')}(\mathbf{r}) \psi_q^{(l, \mathbf{k})}(\mathbf{r}) dV = \delta_{q'q} \delta_{l'l'}. \quad (35)$$

Hence, the functions (33) form a complete orthonormal set.

#### IV. INFINITE MAGNETIC TRANSLATION GROUP

The construction of the representations of (23) of  $\bar{G}$  and of the symmetry adapted functions (33) was made possible by imposing the Born-von Karman boundary conditions. We know, however, that in the case of the usual translation group it is possible to write down the representations without using the boundary conditions, in which case the wave vector  $\mathbf{k}$  describing the representations varies continuously in the first Brillouin zone. One may expect the same to be valid also in the case of the magnetic translation group. The crucial point in deriving the irreducible representations of  $\bar{G}$  was the existence of an invariant Abelian subgroup  $\bar{F}$  of the group  $\bar{G}$ . The infinite magnetic translation group  $\bar{G}$  always has an invariant commutative subgroup  $F$  [Eq. (23), Ref. 1] when the magnetic field  $\mathbf{H}$  is in a direction of a lattice vector. The restriction imposed on the direction of the magnetic field only is a much weaker one and it leaves the group  $\bar{G}$  infinite. Since the Born-von Karman boundary conditions do not appear explicitly in the functions (33), it is easy to obtain a generalization of the functions in the case of an infinite M.T.G. (with the restriction that the magnetic field is in a direction of a lattice vector, say, again in the direction of  $\mathbf{a}_3$ ). We have, however, to distinguish the case

$$\mathbf{h} \neq (4\pi/V)(n/N)\mathbf{a}_3 \quad (36)$$

from the case

$$\mathbf{h} = (4\pi/V)(n/N)\mathbf{a}_3, \quad (37)$$

where  $n$  and  $N$  have no common factor. The integers  $n$  and  $N$  are no longer connected with the boundary conditions. In the case when (36) holds the symmetry adapted functions will be

$$\begin{aligned} \psi_q^{(l, m_3)}(\mathbf{r}) &= \exp \{ i m_3 \mathbf{K}_3 \cdot \mathbf{r} \} \exp \{ i [q + (1/4\pi) \mathbf{K}_2 \cdot \mathbf{r}] \\ &\times (\mathbf{a}_2 \times \mathbf{h}) \cdot \mathbf{r} \} w_{l m_3}(\mathbf{r} + q\mathbf{a}_2), \end{aligned} \quad (38)$$

where  $0 \leq m_3 < 1$  (continuously) and  $q$  takes on integer values from 0 to infinity. For the case (37) we get as in (33):

$$\begin{aligned} \psi_q^{(l, \mathbf{k})}(\mathbf{r}) &= \exp \{ i \mathbf{k} \cdot \mathbf{r} \} \exp \{ i [q + (1/4\pi) \mathbf{K}_2 \cdot \mathbf{r}] \\ &\times (\mathbf{a}_2 \times \mathbf{h}) \cdot \mathbf{r} \} w_{l\mathbf{k}}(\mathbf{r} + q\mathbf{a}_2), \end{aligned} \quad (39)$$

where

$$q = 0, 1, \dots, N-1 \quad [(N/2)-1] \text{ for odd (even) } N,$$

$$\mathbf{k} = \frac{m_1}{N} \mathbf{K}_1 + \frac{m_2}{N} \mathbf{K}_2 + m_3 \mathbf{K}_3, \quad (40)$$

$$0 \leq m_1, m_2 < 1 \quad (2) \text{ for odd (even) } N, \quad 0 \leq m_3 < 1,$$

and

$$w_{\mathbf{r}k}(\mathbf{r} + N\mathbf{a}_2) = \exp\{-iN\mathbf{a}_2 \times \mathbf{h} \cdot \mathbf{r}\} w_{\mathbf{r}k}(\mathbf{r})$$

for odd  $N$ , (41)

$$w_{\mathbf{r}k}[\mathbf{r} + (N/2)\mathbf{a}_2] = \exp\{-i(N/2)\mathbf{a}_2 \times \mathbf{h} \cdot \mathbf{r}\} w_{\mathbf{r}k}(\mathbf{r})$$

for even  $N$ .

One should note that the appearance of  $N/2$  for even  $N$  is in agreement with the distinction between even and odd  $N$  in the construction of the irreducible representations (23).

There are two interesting points connected with the generalization for an infinite M.T.G. The first point is that by changing the magnetic field *continuously* we can pass from case (37) to case (36). This means that by changing the magnetic field by an amount which can be as small as we like we change the degeneracy from a finite one (given by the number  $N$ ) to an infinite one. We thus see that the representations are very sensitive to the magnitude of the magnetic field. The relation (37) can also be written in a different way by multiplying both sides by  $\mathbf{a}_1 \times \mathbf{a}_2$ . We get (by using the definition of  $\mathbf{h}$ ):

$$\frac{\mathbf{H} \cdot \frac{1}{2}(\mathbf{a}_1 \times \mathbf{a}_2)}{hc/e} = \frac{n}{N}, \quad (42)$$

where  $h$  is Planck's constant. In the numerator on the left of (42) we have the flux of the magnetic field through an elementary area enclosed by the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  and  $-(\mathbf{a}_1 + \mathbf{a}_2)$ . The quantity  $hc/e$  is the elementary quantum of magnetic flux (fluxon) which is of great importance in superconductivity<sup>9</sup> and may have an influence on the significance of potentials in quantum mechanics.<sup>10</sup> From Eq. (42) it follows that the representations of the magnetic group are finite when the ratio of magnetic flux through areas enclosed by any vectors of the Bravais lattice to the elementary fluxon are given by rational numbers. Through Eq. (42) we come also to the second point, namely, when the ratio given by this equation is an integer, all the constant factors in the definition of the elements of the M.T.G. [Eq. (1)] will be unity. In this case the magnetic translation group will be isomorphic to the usual translation group and all the irreducible representations of the first will become one dimensional, and one has an energy band picture as in the Bloch case. In this connection, it is interesting to refer to the work of Azbel<sup>11</sup>

<sup>9</sup> M. Peshkin and W. Töbocman, Phys. Rev. **127**, 1865 (1962) and references given therein.

<sup>10</sup> Y. Aharonov and D. Bohm, Phys. Rev. **115**, 485 (1959); **123**, 1511 (1961).

<sup>11</sup> M. Y. Azbel, Zh. Eksperim. i Teor. Fiz. **44**, 980 (1963) [English transl.: Soviet Phys.—JETP **17**, 665 (1963)].

who shows that for a special Hamiltonian all physical properties of electrons in a magnetic field are periodic in the magnetic field with a period

$$\mathbf{h} = (4\pi/V)\mathbf{a}_3. \quad (43)$$

The relation (43) expressed in the form (42) is just a requirement on the magnetic flux through areas enclosed by any Bravais lattice vectors to be multiples of the fluxon  $hc/e$ . The fields satisfying condition (43) must be of the order of  $10^{10}$  G for  $a \approx 10^{-8}$  cm, and cannot be practically achieved. The fundamental significance of flux quantization in the problem under discussion is, however, of great interest and requires further investigation.

## V. CONCLUSION

We have indicated the usefulness of the magnetic translation group for investigating the dynamics of a Bloch electron in a magnetic field. From the irreducible representations of the M.T.G. a set of orthonormal functions was constructed. It turns out that when a magnetic field is present the imposition of boundary conditions leads to quantization of the field, i.e., by imposition of boundary conditions on crystals, even of dimensions of the order of 1 cm, the magnetic field can only take values which differ by about 10 G. (It has been usual to assume that the Born-von Karman boundary conditions have no influence on the physical description of an electron in a periodic potential.<sup>12</sup>) It was therefore important for us to remove the boundary conditions. By doing so, we found the irreducible representation of the M.T.G. (and the symmetry adapted functions) when the magnetic field is required to be along a lattice vector—without any restrictions on the magnitude of the magnetic field. It turns out that the representations are very sensitive to whether or not condition (42) holds.

It would be interesting to find the representations of the M.T.G. without any requirements on the magnetic field at all.

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<sup>12</sup> It is interesting to note that no boundary conditions can be introduced for different  $N_1$ ,  $N_2$ ,  $N_3$  (in directions  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$ , respectively) that have no common factor. In this case no ray representations exist for the usual translation group.