

nucleus, and M_s is saturation magnetization. We observe first that the ratio (H_n/M_s) is nearly the same for Fe, Ni, and Co so that a difference in η must come from a difference in domain and domain-wall structure. Fe and cubic Co have very similar magnetic properties and, as expected, their enhancement factors are about the same (for Co, $\eta \approx 1500$).² The magnetic properties of Ni are different. Nonetheless a rough calculation indicates that $D(d\theta/dZ)$ should be nearly the same for Ni as for Fe. The dimension D for the underlying domain structure of a ferromagnetic particle is determined by competition between domain-wall energy and surface energy. Since our filings have surfaces which are randomly oriented with respect to the crystalline axes, either free magnetic poles will form on the surface or domains of closure must form along hard directions of magnetization. For materials, like Fe and Ni, having weak anisotropy, we expect the surface energy will be of the form $E_s \propto K_1 D \{1 + C(K_1/M_s^2)\}$, where K_1 is the anisotropy constant and C is a number of order of magnitude 1 or smaller. (The simple closure structure described by Friedel and deGennes²⁰ leads to values for $C < 0.1$. Since K_1/M_s^2 is small and only changes by a factor of about 0.7 on going from Ni to Fe, the closure structure will be similar in the two

²⁰ J. Friedel and P. G. deGennes, *Compt. Rend.* **251**, 1283 (1960).

materials and the details of closure are not very important. An elementary calculation then gives $D(d\theta/dZ) \propto (K_1/JS^2)^{1/4}$, where J is the exchange constant and S the ion spin. This expression for $D(d\theta/dZ)$ is about 20% smaller for Ni than for Fe.)

Finally, we would like to point out the advantages in observing this kind of resonance in the fast-passage mode at 90° phase setting. Not only is the quantity $h(\omega, \omega_0)$ more easily interpreted than the derivative of the susceptibility, but the 90° phase setting makes for an improved signal-to-noise ratio because of the high stability.

Note added in proof. (1) Professor A. M. Portis has informed us that the paper, A. C. Gossard, A. M. Portis, M. Rubenstein, and R. H. Lindquist, *Phys. Rev.* **138**, A1415 (1965) contains a theoretical discussion of the mode mixing in ferromagnetic materials. The analysis suggests that $\beta_0 = 2\omega\tau$, where τ is the relaxation time of the domain wall.

Note added in proof. (2) Dr. R. L. Streever has informed us that in an unpublished extension of the work reported in R. L. Streever, *Phys. Rev.* **134**, A1612 (1964) he has measured T_1 in pure well-annealed Ni metal at room temperature and found that T_1 is about 0.16 msec although the accuracy of the measurement was poor. In addition he has found T_1 to depend on the state of anneal of the metal. He has found T_1 to be 0.35 msec in a sample which was not carefully annealed.

Electric and Magnetic Translation Group

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(Received 14 December 1964)

A set of translation operators is defined which commute with the combination of operators occurring in the time-dependent Schrödinger equation for an electron in potentials periodic in time and space, with uniform applied electric and magnetic fields in arbitrary directions. It is shown that the operators form a group. The group is made finite by imposing periodic boundary conditions, and restrictions on the electric and magnetic fields are obtained. All irreducible representations of the group, and corresponding basis functions are generated. The limit of these functions is found as the distance between boundaries becomes infinite and the restrictions on the fields disappear.

I. INTRODUCTION

WHEN there are no applied fields, the Hamiltonian for an electron in the periodic potential of a crystal lattice is invariant under a symmetry translation \mathbf{R}_n of the lattice. A group of translation operators of the form $\exp(\mathbf{R}_n \cdot \nabla)$ may then be defined, and it may be shown that the wave functions take the form of Bloch functions, $\exp(i\mathbf{k} \cdot \mathbf{r})u_{\mathbf{k}}(\mathbf{r})$, where \mathbf{k} is a wave vector and $u_{\mathbf{k}}(\mathbf{r})$ has the period of the lattice. However, when uniform electric or magnetic fields are present, the Hamiltonian may contain terms linear in \mathbf{r} or t and hence

it no longer retains the translational symmetry of the lattice.

It was pointed out by Wannier and Fredkin¹ that a uniform field physically does not destroy the translational invariance of the crystal, since the physical environment of the electron is the same at all sites whose positions differ by a lattice vector \mathbf{R}_n . Thus it follows, as noted by Brown,² that a type of translation

¹ G. H. Wannier and D. R. Fredkin, *Phys. Rev.* **125**, 1910 (1962).

² E. Brown, *Bull. Am. Phys. Soc.* **8**, 259 (1963); *Phys. Rev.* **133**, A1038 (1964).

operator should exist under which the Hamiltonian is invariant. In transporting a charge e through a lattice displacement \mathbf{R}_n in the time T_n in the presence of electric and magnetic fields \mathbf{E} and \mathbf{B} , an impulse \mathbf{I} must be supplied which is given by

$$\mathbf{I} = -e\mathbf{R}_n \times \mathbf{B}/c - e\mathbf{E}T_n$$

and work W must be done of amount

$$W = -e\mathbf{E} \cdot \mathbf{R}_n.$$

Thus in addition to a shift in position and time there must be a shift in the kinetic momentum $\mathbf{p} + e\mathbf{A}/c$ and in the energy H in order to leave the electron in an invariant condition. In the quantum mechanical formalism, the translation operators which commute with the Hamiltonian should incorporate these momentum and energy shifts as well as the shifts in position and time.

For an electron in a crystal lattice with a magnetic field, Brown² has defined a set of translation operators which form a ray group. Zak³ has recently shown, for this same physical situation, how to define a set of operators which form a group and which commute with the Hamiltonian, and he has obtained irreducible representations and basis functions for this group.

By assuming that the Hamiltonian contains time-dependent terms which may be arbitrarily small and which are periodic in the time, we may generalize to a group which includes the effect of a uniform applied electric field in addition to the uniform magnetic field. The periodicity in time is assumed in order that the group may be made finite. The period may at the end of the calculation be made to approach zero, to obtain an infinite group corresponding to infinitesimal translations in the time.

In Sec. II, the operators of the group are defined. Born-von Karman boundary conditions are applied and the finite electric and magnetic translation group is obtained in Sec. III. Irreducible representations and basis functions are generated in Secs. IV and V.

II. DEFINITION OF GROUP OPERATORS

The time-dependent wave equation for a particle in uniform electric and magnetic fields may be written in the form

$$S\Psi \equiv [i\hbar\partial/\partial t + \frac{1}{2}e\mathbf{E} \cdot \mathbf{r} - eA^0(\mathbf{r},t) - \mathcal{H}(\mathbf{p} + \frac{1}{2}e\mathbf{E}t - \frac{1}{2}e\mathbf{B} \times \mathbf{r}/c - e\mathbf{A}(\mathbf{r},t)/c)]\Psi(\mathbf{r},t) = E_0\Psi, \quad (1)$$

where the vector and scalar potentials have been chosen in a convenient gauge for the uniform electric and magnetic fields. The eigenvalues E_0 simply correspond to different choices of the zero of energy. The potentials A^0 and \mathbf{A} are functions periodic in the

coordinates \mathbf{r} and time. The primitive translation in ct will be assumed to have the period a_0 . The primitive spatial translation vectors are \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 . A general translation will be of the form

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad cT_n = n_0a_0 \quad (2)$$

where n_0, n_1, n_2, n_3 are integers.

The periodic spatial potential of a crystal is a special case of these potentials where

$$A^0(\mathbf{r},t) = V(\mathbf{r}), \quad \mathbf{A} = 0 \\ V(\mathbf{r} + \mathbf{R}_n) = V(\mathbf{r}).$$

We wish to define a set of operators which commute with the operator S acting on $\psi(\mathbf{r},t)$ in Eq. (1). These operators will be chosen to form a group, and to reduce to the ordinary translation operators when there are no applied electric or magnetic fields.

Brown² and Zak³ have introduced operators which commute with the Hamiltonian when no electric field is present. This may be immediately generalized to obtain an operator that commutes with S . Consider the operators

$$\pi_0 = (i\partial/\partial t - \frac{1}{2}e\mathbf{E} \cdot \mathbf{r}/\hbar)/c, \\ \pi = -i\nabla + (e/2\hbar c)(\mathbf{B} \times \mathbf{r} - c\mathbf{E}t). \quad (3)$$

It is easy to verify that these four operators commute with the operators

$$i\hbar\partial/\partial t + \frac{1}{2}e\mathbf{E} \cdot \mathbf{r} \quad \text{and} \quad -i\hbar\nabla - (e/2c)(\mathbf{B} \times \mathbf{r} - c\mathbf{E}t),$$

which occur in S .

Operators which also commute with the periodic functions A^0 and \mathbf{A} , and thus with S , are defined by

$$T(\mathbf{R}_n, T_n) = \exp(i\mathbf{R}_n \cdot \pi - icT_n\pi_0), \quad (4)$$

where R_n and T_n are translations of the lattice, as defined in Eq. (2).

The combination of the differential operators, $\mathbf{R}_n \cdot \nabla + T_n\partial/\partial t$, in the exponent of Eq. (4) commutes with the rest of the exponent. Then the operator $T(\mathbf{R}_n, T_n)$ may be written as

$$T(\mathbf{R}_n, T_n) = \exp\{(ie/2\hbar c)[\mathbf{R}_n \cdot (\mathbf{B} \times \mathbf{r}) + cT_n\mathbf{E} \cdot \mathbf{r} - \mathbf{R}_n \cdot \mathbf{E}ct]\} \exp(\mathbf{R}_n \cdot \nabla) \exp(T_n\partial/\partial t). \quad (5)$$

The product of two such operators, $T(\mathbf{R}_1, T_1)$ and $T(\mathbf{R}_2, T_2)$ is

$$T(\mathbf{R}_1, T_1)T(\mathbf{R}_2, T_2) = T(\mathbf{R}_1 + \mathbf{R}_2, T_1 + T_2) \exp\{(ie/2\hbar c) \times ([\mathbf{R}_1 \times \mathbf{R}_2] \cdot \mathbf{B} + c[T_2\mathbf{R}_1 - T_1\mathbf{R}_2] \cdot \mathbf{E})\}. \quad (6)$$

Therefore the operators $T(\mathbf{R}_n, T_n)$ do not form a group because the product of two such operators does not form another operator of the same type. However, by analogy with the work of Zak,³ a group of operators

$$\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \mathbf{R}_2 T_2; \dots; \mathbf{R}_l T_l)$$

³ J. Zak, Phys. Rev. **134**, A1602 (1964); **134**, A1607 (1964); **136**, A776 (1964); **136**, A1647 (1964).

may be defined as follows:

$$\begin{aligned} \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \mathbf{R}_2 T_2; \cdots; \mathbf{R}_l T_l) \\ \equiv \exp\left\{\frac{1}{2}i \sum_{i < j}^l [(\mathbf{R}_i \times \mathbf{R}_j) \cdot \mathbf{h} \right. \\ \left. - c(T_i \mathbf{R}_j - T_j \mathbf{R}_i) \cdot \mathbf{e}]\right\} T(\mathbf{R}_n, T_n), \quad (7) \end{aligned}$$

where

$$\mathbf{h} = e\mathbf{B}/\hbar c, \quad \mathbf{e} = e\mathbf{E}/\hbar c. \quad (8)$$

The ordered set of translations $\mathbf{R}_1 T_1, \mathbf{R}_2 T_2, \cdots, \mathbf{R}_l T_l$ form a path in four-dimensional space which joins the

$$\begin{aligned} \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l) \tau(\mathbf{R}_n' T_n' | \mathbf{R}_1' T_1'; \cdots; \mathbf{R}_k' T_k') \\ = \exp\left\{\frac{1}{2}i \left[\sum_{i < j}^l [(\mathbf{R}_i \times \mathbf{R}_j) \cdot \mathbf{h} - c(T_i \mathbf{R}_j - T_j \mathbf{R}_i) \cdot \mathbf{e}] \right] + \frac{1}{2}i \left[\sum_{i=1}^l \sum_{j=1}^k [(\mathbf{R}_i \times \mathbf{R}_j') \cdot \mathbf{h} - c(T_i \mathbf{R}_j' - T_j' \mathbf{R}_i) \cdot \mathbf{e}] \right] \right. \\ \left. + \frac{1}{2}i \left[\sum_{i < j}^k [(\mathbf{R}_i' \times \mathbf{R}_j') \cdot \mathbf{h} - c(T_i' \mathbf{R}_j' - T_j' \mathbf{R}_i') \cdot \mathbf{e}] \right] \right\} T(\mathbf{R}_n + \mathbf{R}_n', T_n + T_n') \\ = \tau(\mathbf{R}_n + \mathbf{R}_n', T_n + T_n' | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l; \mathbf{R}_1' T_1'; \cdots; \mathbf{R}_k' T_k'), \quad (10) \end{aligned}$$

which is another member of the same set of τ operators. It is easy to see that the operator inverse to

$$\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l)$$

is simply $\tau(-\mathbf{R}_n - T_n | -\mathbf{R}_l - T_l; \cdots; -\mathbf{R}_1 - T_1)$. Thus the τ 's form a group. We will call this group the electric and magnetic translation group (EMTG).

III. FINITE GROUP

When the electric and magnetic fields are zero, the translation group is ordinarily rendered finite by imposing Born-von Karman boundary conditions, which imply that the operators T act in a function space such that

$$\begin{aligned} T(N\mathbf{a}_1, O) = T(N\mathbf{a}_2, O) = T(N\mathbf{a}_3, O) \\ = T(O, Na_0/c) = T(O, O), \quad (11) \end{aligned}$$

where N is a large integer. As shown by Zak, a generalization of this set of conditions for the group of operators τ is to require that the operators

$$\begin{aligned} \tau(O, Na_0/c | R_1 T_1; \cdots; R_l T_l), \\ \tau(N\mathbf{a}_k, O | R_1 T_1; \cdots; R_l T_l) \quad k=1, 2, 3 \quad (12) \end{aligned}$$

are constant factors.

From Eq. (10), if $\mathbf{R}_n = 0$, and $T_n = Na_0/c$, then in order for the operator $\tau(O, Na_0/c | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l)$ to act as a constant factor, the exponential,

$$\exp\left\{\frac{1}{2}i[-Na_0 \mathbf{R}_n' \cdot \mathbf{e}]\right\},$$

must be unity. Therefore,

$$Na_0 \mathbf{R}_n' \cdot \mathbf{e} = 4\pi l', \quad (13)$$

origin to the point $\mathbf{R}_n T_n$. Thus,

$$\mathbf{R}_n = \sum_{i=1}^l \mathbf{R}_i \quad \text{and} \quad T_n = \sum_{i=1}^l T_i. \quad (9)$$

Clearly the operators τ commute with S since T commutes with S .

To show that the operators τ form a group, let us form the product of the two operators

$$\begin{aligned} \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l), \\ \tau(\mathbf{R}_n' T_n' | \mathbf{R}_1' T_1'; \cdots; \mathbf{R}_k' T_k'). \end{aligned}$$

Their product is

where l' is an integer or zero. The reciprocal lattice vectors are defined in the usual way:

$$\mathbf{K}_i = 2\pi(\mathbf{a}_j \times \mathbf{a}_k)/V, \quad (14)$$

where i, j, k are in the cyclic order (1,2,3) and V is the volume of the unit cell in three dimensions. Condition (13) then immediately implies that \mathbf{e} must be in the direction of a reciprocal lattice vector:

$$\mathbf{e} = 2(\zeta_1 \mathbf{K}_1 + \zeta_2 \mathbf{K}_2 + \zeta_3 \mathbf{K}_3)/Na_0, \quad (15)$$

where $\zeta_1, \zeta_2, \zeta_3$ are integers.

Further, if $\mathbf{R}_n = N\mathbf{a}_k$ and $T_n = 0$, the exponential factor from Eq. (10) which must be set equal to unity is $\exp\left\{\frac{1}{2}i[(N\mathbf{a}_k \times \mathbf{R}_n') \cdot \mathbf{h} + cT_n' \mathbf{R}_n \cdot \mathbf{e}]\right\}$, giving the condition

$$(N\mathbf{a}_k \times \mathbf{R}_n') \cdot \mathbf{h} + cT_n' N\mathbf{a}_k \cdot \mathbf{e} = 4\pi l'', \quad (16)$$

where l'' is an integer. The term involving \mathbf{e} in Eq. (16) is 4π times an integer, from Eq. (15), and therefore we find

$$(N\mathbf{a}_k \times \mathbf{R}_n') \cdot \mathbf{h} = 4\pi l, \quad (17)$$

where l is an integer. The factor $\mathbf{a}_k \times \mathbf{R}_n'$ is a sum of reciprocal lattice vectors times $V/2\pi$ and therefore \mathbf{h} must be in the direction of a lattice vector:

$$\mathbf{h} = 4\pi(\xi_1 \mathbf{a}_1 + \xi_2 \mathbf{a}_2 + \xi_3 \mathbf{a}_3)/VN, \quad (18)$$

where ξ_1, ξ_2, ξ_3 are integers. Thus imposition of periodic boundary conditions limits the possible directions and magnitudes of both \mathbf{e} and \mathbf{h} .

To simplify our further development, we shall from now on choose new basis vectors $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$ of the unit cell such that \mathbf{R}_3 is the smallest lattice vector in the

direction of \mathbf{B} .

$$n\mathbf{R}_3 = NV\mathbf{h}/4\pi, \quad (19)$$

where n is an integer. We choose \mathbf{R}_1 to be a vector of the lattice which is perpendicular to \mathbf{e} , and \mathbf{R}_2 is chosen so that $\mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3) = V$. There are many choices for \mathbf{R}_1 and \mathbf{R}_2 which satisfy these conditions. We may also define new reciprocal lattice vectors by $\mathbf{K}_i = 2\pi(\mathbf{R}_j \times \mathbf{R}_k)/V$ where i, j, k are in the cyclic order (1,2,3).

Since \mathbf{R}_1 is perpendicular to \mathbf{e} , and since any vector of the lattice can be written in the form $l_1\mathbf{R}_1 + l_2\mathbf{R}_2 + l_3\mathbf{R}_3$, Eq. (15) is of the form

$$\mathbf{e} = 4\pi\eta(l_2\mathbf{R}_2 + l_3\mathbf{R}_3) \times \mathbf{R}_1 / VN a_0 \\ = 2\eta(-l_2\mathbf{K}_3 + l_3\mathbf{K}_2) / Na_0, \quad (20)$$

where l_2, l_3 are integers which are relatively prime and η is an integer.

The group of operators τ is now finite. To prove this, we note that with the above choices for \mathbf{e} and \mathbf{h} , the extra exponential factor multiplying T in the definition of τ , Eq. (7), is

$$\exp\left\{\frac{1}{2}i \sum_{i < j} [4\pi n\mathbf{R}_3 \cdot (\mathbf{R}_i \times \mathbf{R}_j) - 4\pi\eta(l_2\mathbf{R}_2 + l_3\mathbf{R}_3) \times \mathbf{R}_1 \cdot c(T_i\mathbf{R}_j - T_j\mathbf{R}_i)/a_0] / VN\right\} \\ = \exp[2\pi i(nm + \eta\mu)/N], \quad (21)$$

where m and μ are positive or negative integers or zero. Suppose that n, η and N have a common factor p' . Then the number of independent values of $(nm + \eta\mu)/N$ as m and μ vary, which lead to different values of the exponential in Eq. (21), is N/p' . Thus the set of inequivalent values of m and μ is finite. Since there are N^4 translations which are independent of the path, the total number of elements of the finite group is N^3/p' .

IV. IRREDUCIBLE REPRESENTATIONS

We shall base the construction of the irreducible representations of the finite group on the fact that if the resultant translational parts of the operators τ are confined to the two-dimensional subspace formed by multiples of the lattice vectors \mathbf{R}_1 and a_0 , the resulting group of operators τ form an invariant subgroup of the total group. We then augment the invariant subgroup by adding separately translations in the \mathbf{R}_2 direction, and then in the \mathbf{R}_3 direction. We then show that the representations obtained by combining the results of these two augmentations gives all the irreducible representations of the full EMTG.

Consider the subgroup of all operators

$$\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l)$$

such that

$$\mathbf{R}_n = \mathbf{r}_n \equiv n_1 \mathbf{R}_1, \quad cT_n = ct_n \equiv n_0 a_0. \quad (22)$$

The paths by which the resultant \mathbf{r}_n, t_n is reached are not assumed to lie in the 1,0 subspace necessarily, but

may include \mathbf{R}_2 and \mathbf{R}_3 components. Such elements are denoted by

$$\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l) \\ = \exp\{(2\pi i/N)(nm + \eta\mu)\} T(\mathbf{r}_n, t_n), \quad (23)$$

where $T(\mathbf{r}_n, t_n)$ is given by Eqs. (4) or (5).

It is easily seen that this subgroup is an invariant subgroup; for if $\tau' = \tau(\mathbf{R}_n' T_n' | \mathbf{R}_1' T_1'; \cdots; \mathbf{R}_l' T_l')$, then from Eq. (12) the product,

$$\tau' \tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l) (\tau')^{-1},$$

is equal to an operator $\tau(\mathbf{r}_n t_n | \cdots)$ where the resultant is still $\mathbf{r}_n t_n$ but the path may be different. Therefore the resulting operator is an element of the subgroup, and the subgroup is an invariant subgroup.

Further, it is a commutative subgroup, for $(\mathbf{r}_n \times \mathbf{r}_n') \cdot \mathbf{h} = 0$ and $(t_n \mathbf{r}_n' - t_n' \mathbf{r}_n) \cdot \mathbf{e} = 0$ since $\mathbf{r}_n, \mathbf{r}_n'$ are normal to \mathbf{e} , for all $\mathbf{r}_n t_n$ and $\mathbf{r}_n' t_n'$ in the 1-0 subspace. The irreducible representations are well known. They are

$$D^{(s, \sigma, k_0'', k_1'')} [\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l)] \\ = \exp\{2\pi i[nms + \eta\mu\sigma + k_0'' n_0 + k_1'' n_1] / N\}, \quad (24)$$

where n_1 and n_0 are defined by Eq. (22). The parameters s and σ are integers, and the number of independent sets of values of s and σ such that $\exp[2\pi i(nms + \eta\mu\sigma)/N]$ takes on all possible different values, is N/p' . The quantities k_1'' and k_0'' are integers which take on the values 1 through N . The total number of such representations is N^3/p' . Because $\exp[2\pi i(nm + \eta\mu)]$ occurs in the actual operators τ , it is sufficient in a physical problem to consider only the representations for which $s = \sigma = 1$. This reduces the number of representations we consider to N^2 . It will be convenient to relabel the representations D so that

$$k_0'' = 2\eta k_0 + m_0, \\ k_1'' = 2n k_1 + m_1. \quad (25)$$

With this relabeling, as the integers k_0 and k_1 vary, in general we do not obtain N independent values for each of k_0'' and k_1'' , and thus the integers m_0 and m_1 are introduced to give the complete set of independent values. The ranges of the values of m_0 and m_1 are found in the appendix. The representations are then

$$D^{(k_0, m_0, k_1, m_1)} [\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_n T_n)] \\ = \exp\{2\pi i[nm + \eta\mu + 2\eta n_0 k_0 + 2n m_1 k_1 \\ + m_0 n_0 + m_1 n_1] / N\}. \quad (26)$$

We augment first by adding to the translations $\mathbf{r}_n t_n$ of the subgroup, translations whose resultants lie in the \mathbf{R}_2 direction. Consider the similarity transformation

$$\tau(-n_2 \mathbf{R}_2, 0 | -n_2 \mathbf{R}_2, 0) \tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l) \\ \times \tau(n_2 \mathbf{R}_2, 0 | n_2 \mathbf{R}_2, 0) \\ = \tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_l T_l) \\ \times \exp\{4\pi i[nm_1 n_2 - \eta l_3 n_0 n_2] / N\}, \quad (27)$$

which follows from Eq. (10). Let $|k_0, m_0, k_1, m_1\rangle$ be a

column eigenvector representation of an eigenfunction of the operator $\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)$, and let D now be a representation of the augmented group. Then the matrix representation of Eq. (27) yields

$$\begin{aligned} & D[\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)] \\ & \quad \times D[\tau(n_2 \mathbf{R}_2, O | n_2 \mathbf{R}_2, O)] | k_0, m_0, k_1, m_1 \rangle \\ & = \exp\{2\pi i[nm + \eta\mu + 2\eta(k_0 - l_3 n_2)n_0 \\ & \quad + 2n(k_1 + n_2)n_1 + m_0 n_0 + m_1 n_1]/N\} \\ & \quad \times D[\tau(n_2 \mathbf{R}_2, O | n_2 \mathbf{R}_2, O)] | k_0, m_0, k_1, m_1 \rangle. \end{aligned} \quad (28)$$

It is clear that the vector $D[\tau(n_2 \mathbf{R}_2, O | n_2 \mathbf{R}_2, O)] \times |k_0, m_0, k_1, m_1\rangle$ is an eigenvector of

$$D[\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)]$$

corresponding to the eigenvalues labelled by $k_0 - l_3 n_2$, $k_1 + n_2$.

The operator $\tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O)$ commutes with $\tau(n_2 \mathbf{R}_2, O | n_2 \mathbf{R}_2, O)$, because $(\mathbf{R}_2 \times \mathbf{R}_3) \cdot \mathbf{h} = 0$. Thus the order of augmentation of the subgroup by these two operators is immaterial. Augmentation by

$$\tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O)$$

using a procedure similar to the one above yields

$$\begin{aligned} & D[\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)] \\ & \quad \times D[\tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O)] | k_0 m_0 k_1 m_1 \rangle \\ & = \exp\{2\pi i[nm + \eta\mu + 2\eta(k_0 + l_2 n_3)n_0 \\ & \quad + 2nk_1 n_1 + m_0 n_0 + m_1 n_1]/N\} \\ & \quad \times D[\tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O)] | k_0 m_0 k_1 m_1 \rangle. \end{aligned} \quad (29)$$

Thus the vector $D[\tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O)] | k_0 m_0 k_1 m_1 \rangle$ is an eigenvector of $D[\tau(\mathbf{r}_n t_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)]$ corresponding to the eigenvalues labelled by $k_0 + l_2 n_3$, k_1 .

Any element of the total finite group may be written

$$D_{(k_0' k_1' | k_0 k_1)}^{(m_0 m_1 m_2 m_3)} [\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)]$$

$$= \delta_{k_0', k_0 + l_2 n_3 - l_3 n_2} \delta_{k_1', k_1 + n_2} \exp\{2\pi i[nG + \eta\Gamma + 2\eta k_0 n_0 + 2nk_1 n_1 + m_0 n_0 + m_1 n_1 + m_2 n_2 + m_3 n_3]/N\}. \quad (36)$$

Let us now prove that the matrix given in Eq. (36) is indeed a representation of the group. Using Eq. (36), the matrix representation of the product of two operators, $\tau(\mathbf{R}_n' T_n' | \mathbf{R}_1' T_1'; \dots; \mathbf{R}_k' T_k') \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)$, is found to be

$$\begin{aligned} & \sum_{\alpha, \beta} D_{(k_0' k_1' | \alpha \beta)}^{(m_0 m_1 m_2 m_3)} [\tau(\mathbf{R}_n' T_n' | \mathbf{R}_1' T_1'; \dots; \mathbf{R}_k' T_k')] D_{(\alpha \beta | k_0 k_1)}^{(m_0 m_1 m_2 m_3)} [\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)] \\ & = \delta_{k_0', k_0 + l_2(n_3 + n_3') - l_3(n_2 + n_2')} \delta_{k_1', k_1 + n_2 + n_2'} \exp\{2\pi i[n(G + G') + \eta(\Gamma + \Gamma') + 2\eta k_0(n_0 + n_0') + 2nk_1(n_1 + n_1') \\ & \quad + m_0(n_0 + n_0') + m_1(n_1 + n_1') + m_2(n_2 + n_2') + m_3(n_3 + n_3') + 2\eta n_0'(l_2 n_3 - l_3 n_2) + 2nn_2 n_1']/N\}. \end{aligned} \quad (37)$$

The matrix corresponding to the product of the two operators is

$$\begin{aligned} & D_{(k_0' k_1' | k_0 k_1)}^{(m_0 m_1 m_2 m_3)} [\tau(\mathbf{R}_n' + \mathbf{R}_n, T_n' + T_n | \mathbf{R}_1' T_1'; \dots; \mathbf{R}_k' T_k'; \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)] \\ & = \delta_{k_0', k_0 + l_2(n_3 + n_3') - l_3(n_2 + n_2')} \delta_{k_1', k_1 + n_2 + n_2'} \exp\{2\pi i[nG'' + \eta\Gamma'' + 2\eta k_0(n_0 + n_0') + 2nk_1(n_1 + n_1') \\ & \quad + m_0(n_0 + n_0') + m_1(n_1 + n_1') + m_2(n_2 + n_2') + m_3(n_3 + n_3')]/N\}, \end{aligned} \quad (38)$$

in the form

$$\begin{aligned} & \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l) \\ & = \tau(n_2 \mathbf{R}_2, O | n_2 \mathbf{R}_2, O) \tau(n_3 \mathbf{R}_3, O | n_3 \mathbf{R}_3, O) \\ & \quad \times \tau(\mathbf{r}_n t_n | -n_2 \mathbf{R}_2, O; -n_3 \mathbf{R}_3, O; \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l). \end{aligned} \quad (30)$$

Therefore, the matrix representation of Eq. (30) may be written in the form

$$\begin{aligned} & D[\tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \dots; \mathbf{R}_l T_l)] | k_0 m_0 k_1 m_1 \rangle \\ & = \exp[2\pi i(m_2 n_2 + m_3 n_3)/N] \exp\{2\pi i[nG + \eta\Gamma \\ & \quad + 2\eta k_0 n_0 + 2nk_1 n_1 + m_0 n_0 + m_1 n_1]/N\} \\ & \quad \times |k_0 + l_2 n_3 - l_3 n_2, m_0, k_1 + n_2, m_1 \rangle. \end{aligned} \quad (31)$$

Here m_2 and m_3 are integers, and clearly if this is a representation when $m_2 = m_3 = 0$, then it is also a representation when m_2 and m_3 are integers. The range of inequivalent values of m_2 and m_3 will be found in the appendix. The quantities G and Γ are given by

$$\begin{aligned} 2\pi nG/N & = \frac{1}{2}(-n_2 \mathbf{R}_2 \times \mathbf{r}_n) \cdot \mathbf{h} + 2\pi nm/N \\ & = 2\pi n(m + n_1 n_2)/N, \end{aligned} \quad (32)$$

and

$$\begin{aligned} 2\pi \eta \Gamma/N & = \frac{1}{2} c T_n (-n_2 \mathbf{R}_2 - n_3 \mathbf{R}_3) \cdot \mathbf{e} + 2\pi \eta \mu/N \\ & = 2\pi \eta [\mu + n_0(-l_3 n_2 + l_2 n_3)]/N, \end{aligned} \quad (33)$$

where from Eq. (21), the integers m and μ are given as

$$2\pi nm/N = \frac{1}{2} \sum_{i < j} (\mathbf{R}_i \times \mathbf{R}_j) \cdot \mathbf{h}, \quad (34)$$

$$2\pi \eta \mu/N = -\frac{1}{2} \sum_{i < j} c(T_i \mathbf{R}_j - T_j \mathbf{R}_i) \cdot \mathbf{e}. \quad (35)$$

The matrix of the assumed representation is

where G'' is given by

$$\begin{aligned} 2\pi nG''/N &= 2\pi(nm+nm')/N + \frac{1}{2}\{-(n_2+n_2')[\mathbf{R}_2 \times (\mathbf{r}_n' + \mathbf{r}_n)] \cdot \mathbf{h}\} + \frac{1}{2}(\mathbf{R}_n' \times \mathbf{R}_n) \cdot \mathbf{h} \\ &= 2\pi n[m+n_1n_2+m'+n_1'n_2'+2n_1'n_2]/N \\ &= 2\pi n[G+G'+2n_1'n_2]/N. \end{aligned} \quad (39)$$

The number Γ'' is given by a similar calculation:

$$\begin{aligned} 2\pi\eta\Gamma''/N &= 2\pi(\eta\mu+\eta\mu')/N - \frac{1}{2}c(T_n'\mathbf{R}_n - T_n\mathbf{R}_n') \cdot \mathbf{e} + \frac{1}{2}c(T_n+T_n')[-(n_2+n_2')\mathbf{R}_2 - (n_3+n_3')\mathbf{R}_3] \cdot \mathbf{e} \\ &= 2\pi\eta[\mu+n_0(-l_3n_2+l_2n_3)+\mu'+n_0'(-l_3n_2'+l_2n_3')+2n_0'(l_2n_3-l_3n_2)]/N \\ &= 2\pi\eta[\Gamma+\Gamma'+2n_0'(l_2n_3-l_3n_2)]/N. \end{aligned} \quad (40)$$

Upon comparison of these results with Eq. (37), it is seen that the matrix $D_{\binom{m_0m_1m_2m_3}{k_0k_1|k_0k_1}}$ is indeed a representation of the group of operators τ .

In the appendix the ranges of values of the integers m_i are found. For that argument, it is necessary to define common factors of N , $2n$, $2\eta l_2$, and $2\eta l_3$ as follows:

$$\begin{aligned} N &= puv\alpha\beta\gamma A a^2, \\ 2n &= puvr\alpha\delta\sigma B a, \\ 2\eta l_2 &= puwr\beta\delta\nu C a, \\ 2\eta l_3 &= pvwr\gamma\sigma\nu D, \end{aligned} \quad (41)$$

where p is the largest common factor of all four quantities; (ua) , r , v , and w are the remaining largest common factors of the quantities taken three at a time; α , β , γ , ν , σ , and δ are the remaining largest common factors of the quantities taken two at a time, and (Aa) , B , C

and D are the remaining factors. Also a is the largest common factor of (ua) and (Aa) . If N is odd, p is the same as the p' of Sec. III. If N is even, p is either the same as p' or is $2p'$ depending on the number of factors of 2 in n and η .

The result, which is proved in the appendix, is that the dimension of the representation (the number of independent combinations of k_0 and k_1) is $N\gamma A/p$. The integer m_0 can be chosen to include all integers in the range from 0 through $puv\alpha a-1$; m_1 then ranges from 0 through $puv\alpha a-1$; m_2 can be chosen to range from 0 through $pv\alpha a-1$, and m_3 from 0 through $pv\alpha\beta a-1$.

To prove that these representations are irreducible, we calculate the character for a particular representation, which is a sum over independent combinations of the set of integers $\{k_0, k_1\}$. With the definition, $\Delta(n)=1$ if n is an integral multiple of N and $\Delta(n)=0$ otherwise, the character is

$$\begin{aligned} \chi^{m_0m_1m_2m_3}\{\tau(\mathbf{R}_nT_n | \mathbf{R}_1T_1; \dots; \mathbf{R}_lT_l)\} &= \sum_{\{k_0, k_1\}} D_{\binom{m_0m_1m_2m_3}{k_0k_1|k_0k_1}} = \sum_{\{k_0, k_1\}} \Delta(2nn_2)\Delta(2\eta[l_2n_3-l_3n_2]) \\ &\quad \times \exp\{2\pi i(nG+\eta\Gamma+2\eta k_0n_0+2nk_1n_1+m_0n_0+m_1n_1+m_2n_2+m_3n_3)/N\}, \end{aligned} \quad (42)$$

where, when we take a diagonal element, it is necessary to note that n_2 and n_3 can take on more than one value each. The total number of values that n_2 and n_3 can have in this case is $N^2/(N\gamma A/p) = Np/\gamma A$ since the number of independent combinations of k_0 and k_1 is $N\gamma A/p$. In performing the summation over the independent set of values of k_0 and k_1 , the exponential factor $\exp\{2\pi i(2\eta k_0n_0+2nk_1n_1)/N\}$ will give zero unless n_0 and n_1 take on special values:

$$\begin{aligned} \Delta(2\eta l_2n_0) &= 1, \\ \Delta(2nn_1-2\eta l_3n_0) &= 1. \end{aligned}$$

The total number of such values of n_0 and n_1 is $N^2/(N\gamma A/p) = Np/\gamma A$. If n_0 and n_1 take on any of such values, then the sum over $\{k_0, k_1\}$ gives $N\gamma A/p$ equal terms, so

$$\begin{aligned} \chi^{m_0m_1m_2m_3} &= \Delta(2nn_2)\Delta(2\eta[l_2n_3-l_3n_2])\Delta(2\eta l_2n_0) \\ &\quad \times \Delta(2nn_1-2\eta l_3n_0)(N\gamma A/p)\exp\{2\pi i(nG \\ &\quad +\eta\Gamma+m_0n_0+m_1n_1+m_2n_2+m_3n_3)/N\}. \end{aligned} \quad (43)$$

Since there are N/p' independent values of $\exp\{2\pi i \times (nG+\eta\Gamma)/N\}$ for varying G and Γ , the sum of the squares of the characters over the elements of the finite group is

$$\begin{aligned} \sum |\chi^{m_0m_1m_2m_3}|^2 &= (N/p')(Np/\gamma A)^2(N\gamma A/p)^2 = N^5/p', \end{aligned} \quad (44)$$

which is just the number of elements of the finite group. If these representations were reducible, we would have obtained in the sum a number greater than N^5/p' . The representations in Eq. (36) therefore are irreducible. Further, these give all the irreducible representations since it is easily seen that the sum over all representations (including those for which $s \neq 1$, $\sigma \neq 1$) of the squares of the dimensions just gives N^5/p' .

V. BASIS FUNCTIONS

In this section we will use the properties of the matrices of the irreducible representations to guide us in constructing the general form of the solutions of

Eq. (1), which are basis functions for the representations. The general expression for an operator of the finite EMTG may be written:

$$\begin{aligned} \tau(\mathbf{R}_n T_n | \mathbf{R}_1 T_1; \cdots; \mathbf{R}_i T_i) \\ = \exp[2\pi i(nm + \eta\mu)/N] \exp\{[in(n_2 \mathbf{K}_1 - n_1 \mathbf{K}_2) \\ + i\eta n_0(l_3 \mathbf{K}_2 - l_2 \mathbf{K}_3)] \cdot \mathbf{r}/N\} \exp[2\pi i\eta \\ \times (l_2 n_3 - l_3 n_2)ct/N a_0] \exp[\mathbf{R}_n \cdot \nabla + T_n \partial/\partial t]. \end{aligned} \quad (45)$$

We take the solutions $\psi(\mathbf{r}, t)$ to be of the form

$$\psi(\mathbf{r}, t) = \Phi(\mathbf{r}, t) e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t} W_{\kappa\omega}(\mathbf{r}, t), \quad (46)$$

where

$$\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3,$$

with

$$\begin{aligned} \mathbf{k}_1 &= (2nk_1 + m_1) \mathbf{K}_1/N, \\ \mathbf{k}_2 &= m_2 \mathbf{K}_2/N, \\ \mathbf{k}_3 &= m_3 \mathbf{K}_3/N, \end{aligned} \quad (47)$$

and where

$$\omega = -2\pi c(2\eta k_0 + m_0)/N a_0. \quad (48)$$

The solutions are chosen so that $\Phi(\mathbf{r}, t)$ does not depend on \mathbf{k} or ω . The operator $\tau(n_2 \mathbf{R}_2, 0 | n_2 \mathbf{R}_2, 0)$ acting on ψ should change k_1 to $k_1 + n_2$, and k_0 to $k_0 - l_3 n_2$. The function $W_{\kappa\omega}(\mathbf{r}, t)$ is assumed to depend on k_0 and k_1 , and is thereby changed by τ , and $\Phi(\mathbf{r}, t)$, which is assumed to be independent of k_0 and k_1 , should give an additional factor $\exp\{i2\pi n_2 \mathbf{K}_1 \cdot \mathbf{r}/N - i4\pi \eta l_3 n_2 ct/N a_0\}$. Further, the operator $\tau(n_3 \mathbf{R}_3, 0 | n_3 \mathbf{R}_3, 0)$ acting on ψ should give the exponential factor $\exp\{4\pi i \eta l_2 n_3 ct/N a_0\}$. A function which has these properties is

$$\begin{aligned} \Phi(\mathbf{r}, t) = \exp\{(i/2\pi)((n/N) \mathbf{K}_1 \cdot \mathbf{r} \mathbf{K}_2 \cdot \mathbf{r}) \\ - (i\eta/N)(-l_2 \mathbf{K}_3 + l_3 \mathbf{K}_2) \cdot \mathbf{r}(ct/a_0)\}. \end{aligned} \quad (49)$$

It is easily verified that any operator τ acting on $e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t} \Phi(\mathbf{r}, t)$ has the same effect as the matrix $D(\tau)$ acting on the column eigenvectors $|k_0, m_0, k_1, m_1\rangle$, except that the set of values of \mathbf{k} and ω do not form a closed set. By choosing $W_{\kappa\omega}(\mathbf{r}, t)$ to satisfy appropriate boundary conditions, the set of values of \mathbf{k} and ω will be the same as those obtained for the matrix representations.

If a translation by an amount corresponding to Δn_2 and Δn_3 is such that the changes in $2\eta k_0/N$ and $2nk_1/N$ satisfy the simultaneous conditions

$$2\eta(l_2 \Delta n_3 - l_3 \Delta n_2)/N = \text{integer} = L_0 \quad (50)$$

and

$$2n \Delta n_2/N = \text{integer} = L_1, \quad (51)$$

then the new k_0 and k_1 are equivalent to the original k_0 and k_1 . In the Appendix, it is shown that if N_2 and N_3 are particular integer solutions to the equation

$$N_3 \delta C - N_2 (\sigma w D \gamma) = 1, \quad (52)$$

then the solutions of Eqs. (50) and (51) for Δn_2 and Δn_3 are

$$\Delta n_2 = N_2(N/pv)L_2 + l_2 w \gamma A L_3, \quad (53)$$

$$\Delta n_3 = N_3 v \gamma A \alpha L_2 + l_3 w \gamma A L_3, \quad (54)$$

where L_3 is any integer and L_0 is related to the integer L_2 by $L_0 = v r L_2$. The various coefficients are defined in Eq. (41). Therefore, in order to give a closed set of independent values of k_0 and k_1 , the function $W_{\kappa\omega}(\mathbf{r}, t)$ must satisfy the periodicity conditions:

$$W_{\kappa\omega}(\mathbf{r} + \mathbf{R}_1, t) = W_{\kappa\omega}(\mathbf{r}, t), \quad (55)$$

$$W_{\kappa\omega}(\mathbf{r}, t + a_0/c) = W_{\kappa\omega}(\mathbf{r}, t), \quad (56)$$

$$\begin{aligned} W_{\kappa\omega}(\mathbf{r} + N_3 v \gamma A \alpha L_3 + N_2 [N/pv] \mathbf{R}_2, t) \\ = \exp\{-(2inN_2/pv) \mathbf{K}_1 \cdot \mathbf{r} - 2\pi i r v c t/a_0\} W_{\kappa\omega}(\mathbf{r}, t), \end{aligned} \quad (57)$$

$$\begin{aligned} W_{\kappa\omega}(\mathbf{r} + w \gamma A l_3 \mathbf{R}_3 + w \gamma A l_2 \mathbf{R}_2) \\ = \exp\{-i w r \delta^2 \sigma B C \mathbf{K}_1 \cdot \mathbf{r}\} W_{\kappa\omega}(\mathbf{r}, t). \end{aligned} \quad (58)$$

Also as shown in the appendix, alternate equivalent conditions for Eqs. (53) and (54) are

$$\Delta n_2 = (N/pv)L_4 + w \gamma A l_2 L_5, \quad (59)$$

$$\Delta n_3 = v \gamma A \alpha L_6 + w \gamma A l_3 L_5, \quad (60)$$

where L_4 , L_5 , and L_6 are arbitrary integers. For these conditions Eqs. (55), (56), and (58) would remain unchanged while Eq. (57) is replaced by the two equations,

$$\begin{aligned} W_{\kappa\omega}(\mathbf{r} + [N/pv] \mathbf{R}_2, t) = \exp\{-2in \mathbf{K}_1 \cdot \mathbf{r}/pv \\ + 4\pi i \eta c l_3/pv a_0\} W_{\kappa\omega}(\mathbf{r}, t), \end{aligned} \quad (61)$$

$$\begin{aligned} W_{\kappa\omega}(\mathbf{r} + v \gamma A \alpha L_3, t) = \exp\{-2\pi i c t(r \delta v C)/a_0\} \\ \times W_{\kappa\omega}(\mathbf{r}, t). \end{aligned} \quad (62)$$

The resulting expression for $\psi(\mathbf{r}, t)$ can be put in the form

$$\begin{aligned} \psi(\mathbf{r}, t) = e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t} \exp\{i(q_2 + \mathbf{K}_2 \cdot \mathbf{r}/4\pi)(\mathbf{R}_2 \times \mathbf{h}) \cdot \mathbf{r} \\ - i(q_2 \mathbf{R}_2 + q_3 \mathbf{R}_3 + \frac{1}{2} \mathbf{r}) \cdot \mathbf{e} c t\} \\ \times W(\mathbf{r} + q_2 \mathbf{R}_2 + q_3 \mathbf{R}_3, t), \end{aligned} \quad (63)$$

where q_2 and q_3 are integers corresponding to translations in the 2 and 3 directions. These functions ψ are described by eigenvalues $m_0, m_1, m_2, m_3, k_0 + l_2 q_3 - l_3 q_2$, and $k_1 + q_2$ arising from group theory; further eigenvalues would be obtained by solving the wave equation. The usual orthogonality relations hold for these functions.

VI. INFINITE EMTG

In order to accommodate all possible electric and magnetic fields, it is convenient to let N approach infinity, and thus we obtain an infinite group. The actual wavefunctions in the interior of a reasonably large crystal should still be similar to functions of the type of Eq. (63), since boundary conditions should have little effect on the general form of wave functions in the interior.

In letting N approach infinity, there are several possibilities, depending on whether $2n/N$, $2\eta/N$, l_2/N , and l_3/N approach rational or irrational numbers. If these are all rational numbers, we obtain an infinite

number of finite-dimensional representations. If some are irrational and some rational, we find an infinite number of infinite-dimensional representations. If all are irrational, we find one infinite-dimensional representation, and $m_0=m_1=m_2=m_3=0$. We shall consider explicitly only the latter, most simple, case. The various cases differ only by infinitesimal changes in the electric and magnetic fields, so the phenomena of physical interest may be discussed with the aid of any one of the cases.

To obtain the case in which all these numbers are irrational, we assume that $N=A$, $2n=B$, $2\eta l_2=\nu C$, $2\eta l_3=\nu D$, [all other factors in Eq. (41) being unity], and let A , B , and ω approach infinity so that the ratios $2n/N$, $2\eta l_2/N$, $2\eta l_3/N$, and thus the electric and magnetic fields, remain finite. For convenience we assume that C and D remain finite.

Redefining k_0 and k_1 so that

$$\lim(2n/N)k_1 \rightarrow k_1, \quad (64)$$

$$\lim(2\eta/N)k_0 \rightarrow k_0, \quad (65)$$

we have

$$\begin{aligned} \psi = \exp[ik_1\mathbf{K}_1 \cdot \mathbf{r} + i2\pi k_0 ct/a_0] \exp\{i(q_2 + \mathbf{K}_2 \cdot \mathbf{r}/4\pi) \\ \times (\mathbf{R}_2 \times \mathbf{h}) \cdot \mathbf{r} - i(q_2\mathbf{R}_2 + q_3\mathbf{R}_3 + \frac{1}{2}\mathbf{r}) \cdot \mathbf{e}ct\} \\ \times W(\mathbf{r} + q_2\mathbf{R}_2 + q_3\mathbf{R}_3, t), \quad (66) \end{aligned}$$

where q_2 and q_3 are integers which range from 0 to infinity. Thus k_0 and k_1 may have any values we please. The function W now satisfies only the periodicity conditions

$$\begin{aligned} W(\mathbf{r} + \mathbf{R}_1, t) = W(\mathbf{r}, t), \\ W(\mathbf{r}, t + a_0/c) = W(\mathbf{r}, t). \quad (67) \end{aligned}$$

An interesting special case is that in which there is no time dependence of the periodic potentials. To treat this case, we let a_0 approach zero in such a way that k_0/a_0 , \mathbf{e} and \mathbf{h} remain finite. Then we may assume that k_0 has been chosen so that W approaches a function independent of the time. Thus the basis function is of the form

$$\begin{aligned} \psi = \exp[ik_1\mathbf{K}_1 \cdot \mathbf{r} - i\omega t] \exp\{i(q_2 + \mathbf{K}_2 \cdot \mathbf{r}/4\pi)(\mathbf{R}_2 \times \mathbf{h}) \cdot \mathbf{r} \\ - i(q_2\mathbf{R}_2 + q_3\mathbf{R}_3 + \frac{1}{2}\mathbf{r}) \cdot \mathbf{e}ct\} W(\mathbf{r} + q_2\mathbf{R}_2 + q_3\mathbf{R}_3). \quad (68) \end{aligned}$$

This is similar to the usual time-separated solution to the wave function, but with an additional phase factor corresponding to our choice of gauge. The factor, $\exp\{-i(q_2\mathbf{R}_2 + q_3\mathbf{R}_3) \cdot \mathbf{e}ct\}$, corresponds to the shift in potential energy under a translation parallel to the electric field.

VII. CONCLUSION

We have defined a group of electric and magnetic translation operators which commute with the operator S , and have shown how a set of basis functions suitable for describing an electron in a lattice, with applied uniform electric and magnetic fields, may be derived.

As Zak pointed out, for a crystal of dimensions of the order of 1 cm, the imposition of boundary conditions restricts the magnetic field only to values which can differ by about 10 G. If we also choose $a_0=10^{-8}$ cm, then the electric field is restricted to values which differ by about 10^4 V/cm. However, for a periodic applied field, of frequency 3×10^{15} sec $^{-1}$, corresponding to $a_0=1000$ Å, the electric field values may differ by about 10 V/cm, a more reasonable value. The longer the period in time, the more closely the allowed values of the electric field are spaced. For the magnetic field there is no such possibility of choice because the spatial configuration of a crystal lattice is fixed. However, it is presumed that these field spacings are without much physical significance since they arose from the arbitrary imposition of periodic boundary conditions.

The representations of the group were seen to be very sensitive to the common factors of $2n$, $2\eta l_2$, $2\eta l_3$, and N . On the other hand one would not expect the important physical characteristics of the wavefunction to be sensitive to these factors. Thus one could probably choose any one of the possibilities to describe a given physical situation. The various possibilities were discussed in detail because in a particular problem one of them might be easier to treat mathematically than the others. Also, the number of independent solutions for a given periodic function $W(\mathbf{r}, t)$ is given by the dimension of the matrix representations, $N\gamma A/p$. Changing the size of the sample by a small amount (say, changing N by unity) or changing the fields (n or η) by a very small amount, can change the number of solutions by a large amount. Therefore, it is useful to have the representations for the cases when the quantities N , $2n$, $2\eta l_2$, and $2\eta l_3$ have various common factors, in order to be able to calculate the number of solutions.

APPENDIX

In this Appendix we will derive the number of independent combinations of the integers k_0 and k_1 introduced in Eq. (25) and the corresponding ranges of the integers m_0 , m_1 , m_2 , and m_3 . In addition the related question of the conditions imposed on the function $W(\mathbf{r}, t)$ of Eqs. (55)–(58) for changes in n_2 and n_3 will be discussed. For these discussions a knowledge of the common factors of the various integers involved is important. We therefore introduce common factors of N , $2n$, $2\eta l_2$, $2\eta l_3$ as follows:

$$\begin{aligned} N &= p(ua)v\omega\alpha\beta\gamma(Aa), \\ 2n &= p(ua)v\omega\alpha\delta\sigma B, \\ 2\eta l_2 &= p(ua)\omega r\beta\delta\nu C, \\ 2\eta l_3 &= p\omega r\gamma\sigma\nu D. \end{aligned} \quad (A1)$$

Here all the symbols represent integers with p the largest common factor of all four quantities, ua the largest remaining common factor of N , $2n$, and $2\eta l_2$, ν the largest remaining common factor of N , $2n$, and

$2\eta l_3$, etc. Some of these integers in the same quantity, such as B and r for instance, may still have some common factors. However, the only one of these that is important in the discussion below is the possible common factor a between ua and Aa .

The quantities that generate k_0 and k_1 are $l_2n_3 - l_3n_2$ and n_2 , respectively. The combination of k_0 and k_1 within the exponent thus starts repeating when the changes in n_2 and n_3 are such that the following relations are satisfied simultaneously:

$$(2\eta/N)(l_2\Delta n_3 - l_3\Delta n_2) = L_0, \tag{A2}$$

$$(2n/N)\Delta n_2 = L_1, \tag{A3}$$

where L_0 and L_1 are integers. After using Eq. (A1) and cancelling common factors, we find from Eq. (A3) the relation

$$(r\delta\sigma B)\Delta n_2 = (w\beta\gamma Aa)L_1. \tag{A4}$$

Thus $\Delta n_2 = w\beta\gamma AaL_1'$, where L_1' is another integer. Substitution of this Δn_2 into Eq. (A2) and cancellation of common factors leads to

$$r\nu(u\delta C\Delta n_3 - v\omega\gamma^2 A\sigma DL_1') / (u\omega\alpha\gamma Aa) = L_0. \tag{A5}$$

Thus the number of different values less than $r\nu$ that the left side of this expression may have is $u\omega\alpha\gamma Aa$. This times $w\beta\gamma Aa$, which from Eq. (A4) is the number of values $2\eta\Delta n_2/N$ can have less than $r\delta\sigma B$, gives the number of independent combinations of k_0 and k_1 . It is $u\omega\alpha\beta\gamma^2 A^2 a^2 = N\gamma A/p$.

To find the specific values of Δn_2 and Δn_3 such that k_0 and k_1 start repeating, set $\Delta n_3 = v\gamma AL_7$, $L_1' = uL_8$, $L_0 = r\nu L_2$ where all the L 's are integers and where we have factored out of Δn_3 , L_1' , and L_0 all possible factors which Eq. (A5) forces them to contain. Then Eq. (A5) becomes

$$(\delta C)L_7 - (w\gamma\sigma D)L_8 = (\alpha a)L_2. \tag{A6}$$

Thus, if $L_7 = \alpha a N_3$ and $L_8 = \alpha a N_2$ give a particular set of integers which satisfy Eq. (A6) for $L_2 = 1$, the general solution of Eq. (A6) for a given L_2 is $L_7 = L_2\alpha a N_3 + L_3 w\gamma\sigma D$, $L_8 = L_2\alpha a N_2 + L_3\delta C$ where L_3 is another arbitrary integer. Thus

$$\Delta n_2 = w\omega\beta\gamma AaL_8 = w\omega\beta\gamma Aa(L_2\alpha a N_2 + L_3\delta C) \tag{A7}$$

and

$$\Delta n_3 = v\gamma AL_7 = v\gamma A(L_2\alpha a N_3 + L_3 w\gamma\sigma D). \tag{A8}$$

The basis functions for the representations should then have their k_0 and k_1 periodic for a change in n_2 and n_3 corresponding to $L_2 = 1$ and $L_3 = 0$ and also for $L_2 = 0$ and $L_3 = 1$.

The conditions (A7) and (A8) on the changes Δn_2 and Δn_3 may be written in an equivalent, and sometimes more convenient form by choosing L_2 and L_3 in Eqs. (A7) and (A8) so that

$$L_2 = \delta CL_6 - w\gamma\sigma DL_4, \tag{A9}$$

$$L_3 = -\alpha a N_2 L_6 + \alpha a N_3 L_4 + L_5, \tag{A10}$$

where L_4 , L_5 , and L_6 are arbitrary integers. Then it may easily be shown that

$$\Delta n_2 = u\omega\beta\gamma Aa(\alpha a L_4 + \delta CL_5), \tag{A11}$$

$$\Delta n_3 = v\gamma A(\alpha a L_6 + w\gamma\sigma L_5). \tag{A12}$$

Although three arbitrary integers appear in these latter expressions, different choices of L_4 , L_5 , and L_6 do not all give independent conditions on Δn_2 and Δn_3 . In some cases, however, it may be more convenient to use Eqs. (A11), (A12) rather than the equivalent Eqs. (A7), (A8) where only two arbitrary integers occur.

The choice of the ranges of m_0 and m_1 is not unique. One choice is made by noting that the number of k_0 's for each k_1 is $N\gamma A/p$ divided by the number of k_1 's or $u\omega\alpha\gamma Aa$, so that for a given k_1 , the range of m_0 is $0, 1, \dots, (N/u\omega\alpha\gamma Aa) - 1$ or $0, 1, \dots, p\omega\beta a - 1$. Then since the number of k_1 's is $w\beta\gamma Aa$, the range of m_1 is $0, 1, \dots, (N/w\beta\gamma Aa) - 1$ or $0, 1, \dots, p\nu\alpha a - 1$. Alternatively, one could start with the number of k_1 's for each k_0 and divide this into N to find the number of m_1 's, and divide N by the number of k_0 's to find the number of m_0 's. These choices would give different ranges, but the product of the number of m_1 's and m_0 's is the same, $Np/\gamma A$. The different choices simply correspond to a relabeling of rows and columns of the representation matrices.

In finding the matrices of the irreducible representations, we could have started with matrices which are diagonal for operators corresponding to translations in the 2,3 space. Augmentation with $\tau(0, T_n | 0, T_n)$ and $\tau(\mathbf{R}_1 n_1, 0 | \mathbf{R}_1 n_1, 0)$ would then have generated matrices whose rows and columns would be labeled by k_2 and k_3 rather than the k_0 and k_1 previously. The number of combinations of k_2 and k_3 would be the same as the previous number of combinations of k_0 and k_1 , $N\gamma A/p$. This corresponds to the fact that the dimension of the matrix remains unchanged under a similarity transformation. Since under a similarity transformation, the labels of the different representations, m_0 , m_1 , m_2 , and m_3 , can be taken to be unchanged, we can now use the procedure, followed above in finding the ranges of m_0 and m_1 , to find the ranges of m_2 and m_3 . The result is not unique; one choice is: $m_2 = 0, 1, \dots, p\nu\alpha a - 1$ and $m_3 = 0, 1, \dots, p\nu\omega\beta a - 1$.