REVIEWS OF

MODERN PHYSICS

VOLUME 40, NUMBER 1 JANUARY 1968

Symmetry Properties of the Normal Vibrations of a Crystal

A. A. MARADUDIN*
Department of Physics, University of California, Irvine, California
S. H. VOSKO
Westinghouse Research Laboratories, Pittsburgh, Pennsylvania

A group-theoretic study is made of the degeneracies of the normal modes of vibration of a crystal and of the manner in which the polarization vectors describing these modes transform under the operations of the space group of the crystal. To describe the effects of the spatial symmetry operations a set of $3r$-dimensional matrices is constructed, where r is the number of atoms in a primitive unit cell of the crystal, each of which commutes with the Fourier-transformed dynamical matrix for each value of the wave vector labeling the modes. These matrices are shown to provide a multiplier representation of the point group of the wave vector. The reduction of this representation yields the degeneracies (due to spatial symmetry) and transformation properties of the polarization vectors corresponding to a given wave vector, while the forms of the eigenvectors are obtained by projection operator techniques. For appropriate wave vectors, the consequences of time-reversal symmetry on the degeneracies and polarization vectors are investigated by introducing an anti-unitary matrix operator which commutes with the Fourier-transformed dynamical matrix. A criterion for the existence of extra degeneracies due to time-reversal symmetry is presented. The symmetries of lattice vibrations and selection rules for two-phonon absorption processes corresponding to several values of **k** in the first Brillouin zone of diamond are determined to illustrate the methods developed in this paper.

1. INTRODUCTION

The normal modes of vibration of a crystal are labeled by a wave vector **k** and by a branch index j. The allowed values of the first index are determined by the cyclic boundary condition on the atomic displacements, and they are uniformly and densely distributed throughout the first Brillouin zone for the crystal. The second index differentiates among the $3r$ normal modes associated with the same value of **k**, where r is the number of atoms in a primitive unit cell of the crystal.[1]

The squares of the $3r$ normal mode frequencies $\{\omega_j^2(\mathbf{k})\}$ corresponding to a given value of **k** are the eigenvalues of a $3r\times 3r$ Hermitian matrix $\mathbf{D}(\mathbf{k})$ called the (Fourier-transformed) dynamical matrix, whose elements $\{D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k})\}$ are labeled by the Cartesian axes ($\alpha, \beta = x, y, z$) and by the indices of the atoms comprising the primitive unit cell ($\kappa, \kappa' = 1, 2, \cdots, r$). The eigenvectors $\{\mathbf{e}(\kappa \mid \mathbf{k}j)\}$ of this matrix describe the displacement pattern in space of the atoms comprising the crystal when the latter is vibrating in the mode ($\mathbf{k}j$). Knowledge of the forms of these eigenvectors and of their transformation properties under the symmetry operations which send the crystal into itself is often useful for the solution of certain types of lattice dynamical problems. Among these, for example, is the establishment of selection rules for processes such as two-phonon lattice absorption and the second-order Raman effect, or phonon-assisted electronic transitions in solids, in which normal modes associated with the same or with different wave vectors participate.

The use of group-theoretical arguments greatly simplifies the determination of the form of the dynamical matrix for a crystal and of its eigenvectors for values of **k** lying at points of symmetry inside or on the boundary of the Brillouin zone. The first application of group theory in this context seems to be due to Yanagawa,[2] who studied the vibrations of crystals of the rocksalt and diamond structures for values of **k** at symmetry points in the interior of the first Brillouin zone. He made use of the fact that the eigenvectors of

* This research was supported in part by the Air Force Office of Scientific Research, Office of Aerospace Research, U.S. Air Force, under AFOSR Grant No. 1080-66.

[1] It is assumed that the reader is acquainted with those elements of the theory of lattice dynamics which are discussed, for example, in (a) M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, Oxford, England, 1954); (b) A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Theory of Lattice Dynamics in the Harmonic Approximation* (Academic Press Inc., New York, 1963).

[2] S. Yanagawa, Progr. Theoret. Phys. (Kyoto) **10**, 83 (1953)

the dynamical matrix are basis vectors for the small representations[3] of $G_{\mathbf{k}}$, the space group of the wave vector $\mathbf{k}$, i.e., that space group whose purely rotational elements leave $\mathbf{k}$ invariant (modulo 2π times a translation vector of the reciprocal lattice). However, it is not clear that the method he used in this paper can be applied without modification to the determination of the forms of the eigenvectors associated with $\mathbf{k}$ vectors on the Brillouin zone boundary for crystals belonging to nonsymmorphic space groups, that is, to space groups among whose elements are found screw axes and/or glide planes. Subsequently, a similar kind of analysis, based on the theory of little groups,[4] was carried out by Raghavacharyulu[5] and was applied to the study of the dynamics of crystals of the diamond structure. More recently, Streitwolf[6] has considered this problem anew. He has given a detailed and general discussion of the symmetry properties of the dynamical matrix, but his discussion of the symmetry and transformation properties of the eigenvectors is rather brief. Streitwolf constructs a set of $3r$-dimensional matrices which commute with the dynamical matrix, and establishes that this set of matrices provides a representation of the group $G_{\mathbf{k}}$. Standard methods are used to reduce this representation into the irreducible representations which it contains, from which the transformation properties and the forms of the eigenvectors of $\mathbf{D}(\mathbf{k})$ can be obtained.

A group-theoretic method for determining the symmetry properties of the normal modes of vibration of a crystal, which resembles that of Streitwolf, has also recently been given by Chen.[7] The main difference between the two methods is that Chen uses a form for the dynamical matrix which is a periodic function of $\mathbf{k}$ with the periodicity of the reciprocal lattice while Streitwolf[6] does not. Chen's work contains the most thorough discussion of the transformation properties of the eigenvectors of the dynamical matrix which is presently available.

Despite the attention which has been devoted to the problem of determining the symmetry properties of the normal modes of vibration of a crystal labeled by a given wave vector $\mathbf{k}$, and the forms of the eigenvectors of the dynamical matrix corresponding to those modes, it was felt that the methods for dealing with these problems have not yet been formulated in as simple, explicit, and complete a manner as is possible. The desire to present a somewhat simpler and more explicit treatment of the symmetry properties of the dynamical matrix and of its eigenvectors than is to be found in preceding discussions motivated this paper.

In the present paper we describe a group-theoretical method for simplifying the dynamical matrix of an arbitrary crystal belonging to an arbitrary symmorphic or nonsymmorphic space group and for determining the forms of its eigenvectors. This method can be used as easily when the wave vector $\mathbf{k}$ lies on the Brillouin zone boundary as when it lies in the interior of the zone. It is based on the so-called multiplier or weighted representations of the point group of the wave vector $\mathbf{k}$, i.e., of that crystallographic point group whose operations applied to $\mathbf{k}$ leave it invariant (modulo 2π times a reciprocal lattice vector). These representations seem to have been used for the first time in the context of problems of solid state physics by Kovalev and Liubarskii[8] in their study of the degeneracies of electronic energy bands in crystals. The multiplier representations of the 32 crystallographic point groups were subsequently published by Döring,[9] and the use of these representations in problems of solid-state physics was described in some detail by Liubarskii.[10] Nevertheless, it is still true that the use of the multiplier representations of space groups is less widespread today than is the more conventional group-theoretical method due to Herring[11] which is based on the factor group $G_{\mathbf{k}}/T_{\mathbf{k}}$. Here $T_{\mathbf{k}}$ is the subgroup of all lattice translations through vectors $\mathbf{t}$ for which $\exp(-i\mathbf{k}\cdot\mathbf{t})=1$.

The reason for this comparative lack of interest in the use of multiplier representations may lie in the fact that until recently tables of the irreducible multiplier representations of the point groups of the wave vectors $\mathbf{k}$ associated with symmetry points of the Brillouin zone were not available in a form which permitted their direct application to problems such as the one considered here. However, the recent publication of a book by Kovalev[12] in which are tabulated the irreducible multiplier representations of the point groups of the wave vectors corresponding to most[13] of the symmetry points in the Brillouin zones for all 230 space groups now makes the multiplier representations practically useful as well as formally useful for the solution of solid-state problems in which space group symmetry plays the central role. Perhaps the application of these representations described here may

[3] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58 (1936).
[4] J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959).
[5] I. V. V. Raghavacharyulu, Can. J. Phys. **39**, 830 (1961).
[6] H. W. Streitwolf, Phys. Status Solidi **5**, 383 (1964).
[7] S. H. Chen, "Neutron Scattering Studies of Lattice Vibrations in Metals". Unpublished Ph.D. thesis, Physics Department, McMaster University, Hamilton, Canada (Sept. 1964).

[8] O. V. Kovalev and G. Ya. Liubarskii, Zh. Tekn. Fiz. **28**, 1151 (1958) [English transl.: Soviet Phys.—Tech. Phys. **3**, 1071 (1958)].
[9] W. Döring, Z. Naturforsch. **14a**, 343 (1959).
[10] G. Ya. Liubarskii, *The Application of Group Theory in Physics* (Pergamon Press, Inc., New York, 1960); see also P. Rudra, J. Math. Phys. **6**, 1273 (1965).
[11] C. Herring, J. Franklin Inst. **233**, 525 (1942).
[12] O. V. Kovalev, *Irreducible Representations of the Space Groups* (Academy of Sciences of the Ukrainian SSR, Kiev, 1961) [English transl.: (Gordon and Breach Science Publishers, New York, 1964).]
[13] In a private communication to one of the authors (A.A.M.) J. Zak has pointed out that Kovalev's tables are incomplete. $\mathbf{k}$ vectors corresponding to points of symmetry in the Brillouin zone whose point groups fall into certain crystal systems have been omitted from his tables. These omissions are rectified in a forthcoming book by Casher, Gluck, Gur, and Zak.

stimulate interest in their use in other solid-state physics problems.

The outline of the present paper is as follows. In Sec. 2, the Fourier-transformed dynamical matrix for an arbitrary crystal is introduced and some of its general properties are established. Also the fundamental vector field character of the atomic displacement vectors is exploited to derive a matrix representation for the transformation law of the eigenvectors of the dynamical matrix under crystal symmetry operations. In Sec. 3 the transformation properties of the dynamical matrix under the application of the operations of the space group of the crystal are established, and the multiplier representations of the point group of the wave vector are introduced. In addition, Sec. 3 contains a discussion of the effects on the dynamical matrix of combining space group operations and complex conjugation, for appropriate crystals and wave vectors, which lead to the introduction of a set of anti-unitary symmetry operations. In Sec. 4 the transformation properties of the dynamical matrix under space group operations are employed to determine the form and transformation properties of the eigenvectors of the dynamical matrix. A complete discussion of the consequences of time reversal symmetry for the eigenvectors and eigenvalues of the dynamical matrix is given in Sec. 5. Finally, Sec. 6 is devoted to the working out of several examples, illustrating the results obtained in the preceding sections.

2. FOURIER-TRANSFORMED DYNAMICAL MATRIX

The potential energy of an arbitrary crystal in the harmonic approximation can be written as

$$\Phi=\Phi_0+\tfrac{1}{2}\sum_{ll'}\sum_{\kappa\kappa'}\sum_{\alpha\beta}\Phi_{\alpha\beta}(l\kappa;\,l'\kappa')u_\alpha(l\kappa)u_\beta(l'\kappa'),\tag{2.1}$$

where Φ_0 is the potential energy of the static crystal, $u_\alpha(l\kappa)$ is the α-Cartesian component of the displacement of the κth atom in the lth unit cell from its equilibrium position, and the $\{\Phi_{\alpha\beta}(l\kappa;\,l'\kappa')\}$ are the atomic force constants of the crystal. From the formal definition of the latter coefficients, viz.,

$$\Phi_{\alpha\beta}(l\kappa;\,l'\kappa')=\partial^2\Phi/\partial u_\alpha(l\kappa)\partial u_\beta(l'\kappa')|_0,\tag{2.2}$$

where the subscript 0 indicates that the derivatives are evaluated in the configuration in which all atoms are occupying their equilibrium positions, it follows that they are symmetric in the indices $(l\kappa\alpha)$ and $(l'\kappa'\beta)$:

$$\Phi_{\alpha\beta}(l\kappa;\,l'\kappa')=\Phi_{\beta\alpha}(l'\kappa';\,l\kappa).\tag{2.3}$$

Let us now subject the crystal to an arbitrary operation of the space group G of the crystal. That we can do so implies that we are dealing with a crystal of infinite extent, and in all that follows we assume that this is the case. We represent such a symmetry operation in the Seitz[14] notation by $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$. Applied to the position vector of the equilibrium position of the κth atom in the lth unit cell, $\mathbf{x}(l\kappa)=\mathbf{x}(l)+\mathbf{x}(\kappa)$, where $\mathbf{x}(l)$ is the position vector of the origin of the lth unit cell and $\mathbf{x}(\kappa)$ is the position of the κth kind of atom relative to the origin of the cell, this operation transforms it according to the rule

$$\begin{aligned}\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}\mathbf{x}(l\kappa)&=\mathbf{S}\mathbf{x}(l\kappa)+\mathbf{v}(S)+\mathbf{x}(m),\\&\equiv\mathbf{x}(LK),\end{aligned}\tag{2.4}$$

which is to be interpreted in the active sense,[15] that is, as point transformations. $\mathbf{S}$ is a 3×3 real orthogonal matrix representation of one of the proper or improper rotations of the point group of the space group, $\mathbf{v}(S)$ is a vector which is smaller than any primitive translation vector of the crystal, and $\mathbf{x}(m)$ is a translation vector of the crystal. Nonzero values of the vector $\mathbf{v}(S)$ are associated with the symmetry elements called glide planes and screw axes. Space groups for which $\mathbf{v}(S)$ is identically zero for every rotation $\mathbf{S}$ of the point group of the space group are called symmorphic. All other space groups are called nonsymmorphic. The second equality in Eq. (2.4) expresses the fact that, because the operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ is one which sends the crystal into itself, the lattice site (lk) must be sent into an equivalent site which we label by (LK). Here, and where no confusion results from its use, we adopt the convention of labeling by capital letters the site into which a given site is transformed by the operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$.

With each operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ we associate a linear operator $O(\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$, which is defined[16] through its effect when applied to a scalar function of $\mathbf{x}(l\kappa)$:

$$\begin{aligned}O(\{\mathbf{S}\mid\mathbf{v}(S)&+\mathbf{x}(m)\})f(\mathbf{x}(l\kappa))\\&=f(\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(l\kappa)),\\&=f(\mathbf{S}^{-1}\mathbf{x}(l\kappa)-\mathbf{S}^{-1}\mathbf{v}(S)-\mathbf{S}^{-1}\mathbf{x}(m)).\end{aligned}\tag{2.5}$$

Under the space group operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$, the displacement vector $\mathbf{u}(l\kappa)$ is both rotated and transferred to the site (LK) into which $(l\kappa)$ is sent by this operation. Thus, at the site (LK), the new displacement vector $\mathbf{u}'(LK)$ is expressed in terms of the displacement vector $\mathbf{u}(l\kappa)$ according to[17]

$$\begin{aligned}u_\alpha'(LK)&=O(\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})u_\alpha(LK)\\&=\sum_\beta S_{\alpha\beta}u_\beta(l\kappa),\end{aligned}\tag{2.6}$$

which is just the transformation law for a vector field. Equation (2.6) is central to the discussion since it

[14] F. Seitz, Ann. Math. **37**, 17 (1936).

[15] S. L. Altmann and A. P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).

[16] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959).

[17] E. P. Wigner, Nachr. Akad. Wiss. Goettingen, Math.—Kl. Physik, p. 133 (1930) [English translation in R. S. Knox and A. Gold, *Symmetry in the Solid State* (W. A. Benjamin, Inc., New York, 1964)].

provides a matrix representation of the operations $\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}$.

The invariance of the potential energy under rotations, translations, and interchange of equivalent particles defines the transformation law for the atomic force constants when the crystal is subjected to a space group operation. According to Eq. (2.5) the new potential energy Φ', arising from the operation $\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}$, is defined in terms of Φ by

$$\begin{aligned}\Phi'(\cdots\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}\mathbf{x}(l\kappa)+\mathbf{S}\mathbf{u}(l\kappa)\cdots)\\ =\Phi(\cdots\mathbf{x}(l\kappa)+\mathbf{u}(l\kappa)\cdots),\\ =\Phi(\cdots\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}\mathbf{x}(l\kappa)+\mathbf{S}\mathbf{u}(l\kappa)\cdots),\end{aligned}\quad(2.7)$$

where the second equality follows from the invariance condition. Similarly, the invariance of Φ under interchange of equivalent particles requires that

$$\begin{aligned}\Phi(\mathbf{x}(l\kappa)+\mathbf{u}(l\kappa),\cdots,\mathbf{x}(LK)+\mathbf{u}(LK),\cdots)\\ =\Phi(\mathbf{x}(LK)+\mathbf{u}(LK),\cdots,\mathbf{x}(l\kappa)+\mathbf{u}(l\kappa),\cdots).\end{aligned}\quad(2.8)$$

It should be emphasized that Eqs. (2.7) and (2.8) are general invariance conditions on Φ for any rotation–translation operation and interchange of equivalent mass points. Making a Taylor series expansion of (2.7) and noting that the displacements $\mathbf{u}(l\kappa)$ are arbitrary leads to the condition

$$\Phi_{\alpha\beta}(l\kappa;l'\kappa')=\sum_{\mu\nu}\bar{\Phi}_{\mu\nu}(l\kappa;l'\kappa')S_{\mu\alpha}S_{\nu\beta},\quad(2.9)$$

where the bar on Φ indicates that the derivatives in Eq. (2.2) are evaluated with $\mathbf{x}(l\kappa)$ replaced by $\mathbf{x}(LK)$, $\mathbf{x}(l'\kappa')$ replaced by $\mathbf{x}(L'K')$, etc. Using the interchange symmetry (2.8) allows $\bar{\Phi}_{\mu\nu}(l\kappa;l'\kappa')$ to be replaced by $\Phi_{\mu\nu}(LK;L'K')$, so that (2.9) becomes

$$\Phi_{\alpha\beta}(l\kappa;l'\kappa')=\sum_{\mu\nu}\Phi_{\mu\nu}(LK;L'K')S_{\mu\alpha}S_{\nu\beta},\quad(2.10\text{a})$$

or, equivalently,

$$\Phi_{\mu\nu}(LK;L'K')=\sum_{\alpha\beta}S_{\mu\alpha}S_{\nu\beta}\Phi_{\alpha\beta}(l\kappa;l'\kappa').\quad(2.10\text{b})$$

Equation (2.10) is the fundamental transformation law for the atomic force constants under crystal symmetry operations, and it may be used to determine the independent force constants.[18]

From Eq. (2.10), when $\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}=\{\boldsymbol{\varepsilon} \mid \mathbf{x}(m)\}$ and where $\boldsymbol{\varepsilon}$ is the 3×3 unit matrix, we see that

$$\Phi_{\alpha\beta}(l+m,\kappa;l'+m,\kappa')=\Phi_{\alpha\beta}(l\kappa;l'\kappa').\quad(2.11\text{a})$$

By setting $m=-l$ or $m=-l'$, we see that $\Phi_{\alpha\beta}(l\kappa;l'\kappa')$ depends on l and l' only through their difference:

$$\begin{aligned}\Phi_{\alpha\beta}(l\kappa;l'\kappa')&=\Phi_{\alpha\beta}(0\kappa;l'-l\kappa'),\\ &=\Phi_{\alpha\beta}(l-l'\kappa;0\kappa').\end{aligned}\quad(2.11\text{b})$$

Because of the property of the atomic force constants expressed by Eq. (2.11), the equations of motion of the crystal,

$$\begin{aligned}M_\kappa\ddot{u}_\alpha(l\kappa)&=\partial\Phi/\partial u_\alpha(l\kappa),\\ &=-\sum_{l'\kappa'\beta}\Phi_{\alpha\beta}(l\kappa;l'\kappa')u_\beta(l'\kappa'),\end{aligned}\quad(2.12)$$

where M_κ is the mass of the κth kind of atom, can be simplified to a set of $3r$ equations in $3r$ unknowns by the substitution

$$u_\alpha(l\kappa)=[u_\alpha(\kappa)/(M_\kappa)^{1/2}]\exp[i\mathbf{k}\cdot\mathbf{x}(l)-i\omega t],\quad(2.13\text{a})$$

where the amplitude $u_\alpha(\kappa)$ is independent both of l and of the time t. The form of the solution (2.13) can be derived by use of group theory as follows: According to Eq. (2.11a), the equations of motion (2.12) are invariant under the translation operation $\{\boldsymbol{\varepsilon} \mid \mathbf{x}(m)\}$ which takes l into $L=l+m$. Therefore, we may require the solutions to transform according to the irreducible representations of the translation group, that is, we require the new displacement vector at LK, $\mathbf{u}'(LK)$, to be related to the old displacement vector at LK by

$$\begin{aligned}O(\{\boldsymbol{\varepsilon} \mid \mathbf{x}(m)\})\mathbf{u}(LK)\\ =\exp[-i\mathbf{k}\cdot\mathbf{x}(m)]\mathbf{u}(LK).\end{aligned}\quad(2.13\text{b})$$

On the other hand, from Eq. (2.6) we have

$$\begin{aligned}O(\{\boldsymbol{\varepsilon} \mid \mathbf{x}(m)\})\mathbf{u}(LK)&=\mathbf{u}(lK),\\ &=\mathbf{u}(L-mK),\end{aligned}\quad(2.13\text{c})$$

which when combined with Eq. (2.13b) gives

$$\mathbf{u}(LK)=\exp[i\mathbf{k}\cdot\mathbf{x}(m)]\mathbf{u}(L-mK).\quad(2.13\text{d})$$

Taking $m=L$ results in

$$\mathbf{u}(LK)=\exp[i\mathbf{k}\cdot\mathbf{x}(L)]\mathbf{u}(0K),\quad(2.13\text{e})$$

from which Eq. (2.13a) follows. Thus, if we start with solutions which transform according to the irreducible representations of the translation group, it is then reasonable—in fact, expected—that we will generate a representation of the group of the wave vector $\mathbf{k}$ by considering the transformation properties of the solutions under the crystal symmetry operations which leave the wave vector $\mathbf{k}$ invariant (modulo 2π times a reciprocal lattice vector). This will be explicitly demonstrated in the next section.

When we substitute Eq. (2.13a) into Eq. (2.12), the resulting equations for the amplitudes $\{u_\alpha(\kappa)\}$ can be written in the form

$$\omega^2u_\alpha(\kappa)=\sum_{\beta\kappa'}D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k})u_\beta(\kappa'),\qquad \alpha,\beta=x,y,z\qquad \kappa,\kappa'=1,2,\cdots,r,\quad(2.14)$$

where the elements of the $3r\times3r$ matrix $\mathbf{D}(\mathbf{k})$, called the Fourier-transformed dynamical matrix, are given

[18] G. Leibfried, in *Handbuch der Physik*, S. Flügge, Ed. (Springer–Verlag, Berlin, 1955), Vol. 7, Part I, p. 104.

explicitly by

$$D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) = (M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} \Phi_{\alpha\beta}(l\kappa; l'\kappa') \times \exp[-i\mathbf{k}\cdot(\mathbf{x}(l)-\mathbf{x}(l'))]. \quad (2.15)$$

Because of the property expressed by Eq. (2.11), the sum on l' on the right-hand side of this equation is independent of l.

The allowed values of the wave vector $\mathbf{k}$ appearing in Eqs. (2.13)–(2.15) are usually determined by postulating that the atomic displacement amplitudes $\{u_\alpha(l\kappa)\}$ obey the cyclic boundary condition, i.e., that they are periodic with the periodicity of a macrocrystal containing N atoms, which can be taken to be the crystal of physical interest. This postulate has the consequence that the allowed values of $\mathbf{k}$ are uniformly distributed throughout the first Brillouin zone of the crystal with a density equal to $V/(2\pi)^3$, where V is the crystal volume. We do not need the explicit values of $\mathbf{k}$ in the succeeding discussion.

The condition that the set of homogeneous linear equations (2.14) have nontrivial solutions for the amplitudes $\{u_\alpha(\kappa)\}$ is that the determinant of the coefficients vanish:

$$\det \mid \omega^2\delta_{\kappa\kappa'}\delta_{\alpha\beta} - D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) \mid = 0. \quad (2.16)$$

For each value of $\mathbf{k}$ Eq. (2.16) has $3r$ solutions for ω^2. We display the dependence of ω on $\mathbf{k}$ explicitly, label the solutions by an index j ($=1, 2, \cdots, 3r$), and adopt the ordered convention for the roots whereby $\omega_j^2(\mathbf{k}) \leq \omega_{j+1}^2(\mathbf{k})$. It is sometimes convenient to regard the $\{\omega_j^2(\mathbf{k})\}$ as the $3r$ branches of a multivalued function $\omega^2(\mathbf{k})$. From Eq. (2.14) we see that the $\{\omega_j^2(\mathbf{k})\}$ are the eigenvalues of the matrix $\mathbf{D}(\mathbf{k})$, and that the $\{u_\alpha(\kappa)\}$ are the corresponding eigenvectors. To make explicit the fact that a particular eigenvector $u_\alpha(\kappa)$ associated with a wave vector $\mathbf{k}$ has as its corresponding eigenvalue $\omega_j^2(\mathbf{k})$, we rewrite the former as $e_\alpha(\kappa \mid \mathbf{k}j)$, whereupon the eigenvalue equation (2.14), whose solutions they are, takes the form

$$\sum_{\kappa'\beta} D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) e_\beta(\kappa' \mid \mathbf{k}j) = \omega_j^2(\mathbf{k}) e_\alpha(\kappa \mid \mathbf{k}j). \quad (2.17)$$

Equations (2.10), (2.15), and (2.17) provide the starting point for the subsequent analysis.

The dynamical matrix $\mathbf{D}(\mathbf{k})$ has some general properties which are useful in what follows.

(A) From its definition, Eq. (2.15), together with the fact that

$$\mathbf{x}(l)\cdot\mathbf{b} = \text{integer}, \quad (2.18)$$

where $\mathbf{b}$ is an arbitrary translation vector of the reciprocal lattice, we see that $D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k})$ is a periodic function of $\mathbf{k}$ with the periodicity of the reciprocal lattice

$$D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}+2\pi\mathbf{b}) = D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}). \quad (2.19)$$

As a consequence of this result, the normal mode frequencies and the associated polarization vectors (with no loss of generality) can be chosen to have the periodicity of the reciprocal lattice:

$$\omega_j(\mathbf{k}+2\pi\mathbf{b}) = \omega_j(\mathbf{k}), \quad (2.20a)$$

$$\mathbf{e}(\kappa \mid \mathbf{k}+2\pi\mathbf{b}j) = \mathbf{e}(\kappa \mid \mathbf{k}j). \quad (2.20b)$$

The relation (2.20b) appears to be less fundamental than the relation (2.20a). Strictly speaking, if the normal modes associated with the wave vector $\mathbf{k}$ are degenerate, the right-hand side of Eq. (2.20a) should read $\omega_{j'}(\mathbf{k})$, where j' labels one of the modes whose frequency equals $\omega_j(\mathbf{k})$. We have merely made a natural choice in setting $j'=j$, since this convention allows us to treat points of degeneracy on an equal footing with points of no degeneracy. However, the fact that $e_\alpha(\kappa \mid \mathbf{k}+2\pi\mathbf{b}j)$ is an eigenvector of $\mathbf{D}(\mathbf{k})$ with an eigenvalue $\omega_j(\mathbf{k})$ does not permit us to conclude that $e_\alpha(\kappa \mid \mathbf{k}+2\pi\mathbf{b}j)$ equals $e_\alpha(\kappa \mid \mathbf{k}j)$, except to within an arbitrary phase factor of unit modulus (to assure preservation of normalization). We have chosen this phase factor to be unity purely for the sake of convenience.

(B) It follows directly from Eq. (2.15) that

$$D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) = D_{\alpha\beta}^*(\kappa\kappa' \mid -\mathbf{k}). \quad (2.21)$$

(C) If we combine Eqs. (2.3) and (2.15), we obtain

$$\begin{aligned} D_{\beta\alpha}(\kappa'\kappa \mid \mathbf{k}) &= (M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} \Phi_{\beta\alpha}(l\kappa'; l'\kappa) \times \exp[-i\mathbf{k}\cdot(\mathbf{x}(l)-\mathbf{x}(l'))], \\ &= (M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} \Phi_{\alpha\beta}(l'\kappa; l\kappa') \times \exp[i\mathbf{k}\cdot(\mathbf{x}(l')-\mathbf{x}(l))], \\ &= (M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} \Phi_{\alpha\beta}(l'-l\kappa; 0\kappa') \times \exp[i\mathbf{k}\cdot(\mathbf{x}(l')-\mathbf{x}(l))], \\ &= D_{\alpha\beta}^*(\kappa\kappa' \mid \mathbf{k}). \end{aligned} \quad (2.22)$$

Therefore, the matrix $\mathbf{D}(\mathbf{k})$ is Hermitian.

As corollaries to the last result it follows that the $\omega_j^2(\mathbf{k})$ are real, and that the eigenvectors $\{\mathbf{e}(\kappa \mid \mathbf{k}j)\}$ can be chosen to satisfy the orthonormality and closure conditions:

$$\sum_{\kappa\alpha} e_\alpha^*(\kappa \mid \mathbf{k}j) e_\alpha(\kappa \mid \mathbf{k}j') = \delta_{jj'}, \quad (2.23a)$$

$$\sum_j e_\alpha^*(\kappa \mid \mathbf{k}j) e_\beta(\kappa' \mid \mathbf{k}j) = \delta_{\kappa\kappa'}\delta_{\alpha\beta}. \quad (2.23b)$$

In terms of the eigenvectors $\mathbf{e}(\kappa \mid \mathbf{k}j)$ and corresponding eigenfrequencies $\omega_j(\mathbf{k})$, the atom displacements in Eq. (2.13) may be written as

$$u_\alpha(l\kappa) = [e_\alpha(\kappa \mid \mathbf{k}j)/(M_\kappa)^{1/2}] \exp\{i[\mathbf{k}\cdot\mathbf{x}(l) - \omega_j(\mathbf{k})t]\} \quad (2.24)$$

for the normal mode $(\mathbf{k}j)$. It is clear physically that if the crystal is subjected to a symmetry operation

$\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$, the normal mode (2.24) will now propagate with a wave vector $\mathbf{Sk}$. Because the relative atomic positions are not altered by a symmetry operation, the frequencies of the normal modes are not affected by such an operation, so that the frequency of the transformed mode remains $\omega_j(\mathbf{k})$. The new displacement at the (LK) site is given by Eq. (2.6). This interpretation is seen to be correct by noting that the equations of motion for the crystal in the new orientation are

$$M_K\ddot{u}_\mu'(LK)=-\sum_{L'K'\nu}\Phi_{\mu\nu}(LK;L'K')u_\nu'(L'K'),\qquad(2.25)$$

with solutions

$$u_\mu'(LK)=[e_\mu'(K\mid\mathbf{k}'j')/(M_K)^{1/2}]\times\exp\{i[\mathbf{k}'\cdot\mathbf{x}(L)-\omega_{j'}(\mathbf{k}')t]\},\qquad(2.26)$$

where $e_\mu'(K\mid\mathbf{k}'j')$ is a solution of Eq. (2.17) with α, β, l, κ, l', κ', $\mathbf{k}$, and j replaced by μ, ν, L, K, L', K', $\mathbf{k}'$, and j', respectively, in the appropriate places of Eqs. (2.15) and (2.17). On the other hand,

$$u_\mu'(LK)=\sum_\alpha S_{\mu\alpha}u_\alpha(l\kappa)\qquad(2.27)$$

is also a solution of (2.25) if $u_\alpha(l\kappa)$ is a solution of (2.12), since for a symmetry operation the atoms labeled by K and κ must be of the same kind, (i.e., $M_K=M_\kappa$); therefore

$$\begin{aligned}M_K\ddot{u}_\mu'(LK)&=M_\kappa\sum_\alpha S_{\mu\alpha}\ddot{u}_\alpha(l\kappa),\\&=-\sum_{\alpha\beta l'\kappa'}S_{\mu\alpha}\Phi_{\alpha\beta}(l\kappa;l'\kappa')u_\beta(l'\kappa'),\\&=-\sum_{\beta\nu\lambda L'K'}\Phi_{\mu\nu}(LK;L'K')S_{\nu\beta}S_{\beta\lambda}^{-1}u_\lambda'(L'K'),\\&=-\sum_{\nu L'K'}\Phi_{\mu\nu}(LK;L'K')u_\nu'(L'K'),\end{aligned}\qquad(2.28)$$

where Eqs. (2.12), (2.10), and (2.27) have been used. To write the solution (2.27) in the form (2.26), we note from (2.4) that

$$\mathbf{x}(l)=\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(LK)-\mathbf{x}(\kappa),\qquad(2.29\text{a})$$

$$=\mathbf{S}^{-1}\mathbf{x}(L)+\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa).\qquad(2.29\text{b})$$

Therefore

$$\exp[i\mathbf{k}\cdot\mathbf{x}(l)]=\exp[i\mathbf{Sk}\cdot\mathbf{x}(L)]\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa)])\qquad(2.30)$$

and

$$u_\mu'(LK)=[\sum_\alpha[S_{\mu\alpha}e_\alpha(\kappa\mid\mathbf{k}j)/(M_\kappa)^{1/2}]\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa)])]\times\exp\{i[\mathbf{Sk}\cdot\mathbf{x}(L)-\omega j(\mathbf{k})t]\}.\qquad(2.31)$$

Comparing Eqs. (2.26) and (2.31), we have

$$\mathbf{k}'=\mathbf{Sk};\qquad\omega_{j'}(\mathbf{Sk})=\omega_j(\mathbf{k})\qquad(2.32)$$

and

$$e_\mu'(K\mid\mathbf{S}\mathbf{k}j')=\sum_\alpha S_{\mu\alpha}e_\alpha(\kappa\mid\mathbf{k}j)\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa)]),\qquad(2.33)$$

which is what we anticipated above. Moreover, Eq. (2.33) provides us with a transformation law for the eigenvectors $\mathbf{e}(\mathbf{k}j)$ under crystal symmetry operations. With no loss of generality j' may be replaced by j in Eqs. (2.32) and (2.33) if $\mathbf{k}$ is a point at which $\omega(\mathbf{k})$ has no degenerate branches; by means of continuity the same identification can be made at points of degeneracy. This point is discussed further in Sec. 4.

The eigenvectors $\mathbf{e}(\mathbf{k}j)$ have $3r$ components, while the transformation law (2.33) does not emphasize this viewpoint. In order to cast (2.33) into the form of a relation between two vectors of $3r$ components, we introduce Kronecker symbols into the right-hand side of Eq. (2.33) in the following way:

$$e_\mu'(K\mid S\mathbf{k}j)=\sum_{\alpha\kappa_1}S_{\mu\alpha}\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa_1)])\delta(\kappa_1,F_0^{-1}(K;S))e_\alpha(\kappa_1\mid\mathbf{k}j),\qquad(2.34)$$

where the index κ was eliminated by writing

$$\kappa=F_0^{-1}(K;S),\qquad(2.35\text{a})$$

which expresses the fact that the index K uniquely labels the kind of atom κ that is brought into the K position by the symmetry operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$. That only the rotational element $\mathbf{S}$ of the operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ is required to specify uniquely the connection between κ and K follows from the fact that a pure translation of the crystal through the vector $\mathbf{x}(m)$ cannot affect the labeling of the constituent sublattices, and the vector $\mathbf{v}(S)$ is determined uniquely once the rotational element $\mathbf{S}$ is specified. To express the fact that κ is carried into K by $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$, we write

$$K=F_0(\kappa;S).\qquad(2.35\text{b})$$

Thus Eq. (2.34) can be written succinctly as

$$\mathbf{e}'(\mathbf{S}\mathbf{k}j)=\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{k}j), \tag{2.36}$$

where $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ is a $3r\times 3r$ matrix whose elements are given by

$$\Gamma_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})=S_{\alpha\beta}\delta(\kappa',F_0^{-1}(\kappa;S))\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]). \tag{2.37}$$

From (2.35) it is clear that $\delta(\kappa',F_0^{-1}(\kappa;S))=\delta(\kappa,F_0(\kappa';S))$, the form used in any particular application being dictated by convenience. It is often useful to write the exponent in the form

$$\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]=\mathbf{S}\mathbf{k}\cdot[\mathbf{x}(\kappa)-\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}\mathbf{x}(\kappa')]. \tag{2.38}$$

$\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ is a periodic function of $\mathbf{k}$ with periodicity of the reciprocal lattice,

$$\mathbf{\Gamma}(\mathbf{k}+2\pi\mathbf{b};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})=\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}), \tag{2.39}$$

since $[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa)]$ of Eqs. (2.29) and (2.33) is a lattice vector.

The matrix $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ plays a central role in our treatment. In the next section it is used to derive the transformation properties of the dynamical matrix $\mathbf{D}(\mathbf{k})$ under symmetry operations and to generate a matrix representation of the group of the wave vector $\mathbf{k}$, $G_{\mathbf{k}}$.

3. SYMMETRY OF THE DYNAMICAL MATRIX AND MULTIPLIER REPRESENTATIONS

In the previous section the transformation law for the polarization vectors $\mathbf{e}(\mathbf{k}j)$ under a crystal symmetry operation was deduced from the fundamental transformation laws of the displacement vectors (2.6), the atomic force constants (2.10), and the equations of motion (2.12). On the other hand, the polarization vectors and the normal mode frequencies are defined by the eigenvalue equation (2.17), and in many respects it is advantageous to work directly with this equation to derive the properties of the normal modes implied by symmetry. To bring the power of group-theoretical methods to bear on this problem it is helpful to have a set of matrices in the $3r$-dimensional space of the eigenvectors corresponding to the crystal symmetry operations which leave the dynamical matrix $\mathbf{D}(\mathbf{k})$ invariant under unitary transformations and provide a matrix representation of the relevant group. These matrices would then play a role similar to Wigner's[16] operators $\mathbf{P}_R$, which leave the Hamiltonian invariant under unitary transformations which correspond to symmetry operations of the physical system. In this section we show that the matrices $\mathbf{\Gamma}$, defined by (2.37), fulfill the above requirements if the crystal symmetry operations $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ are restricted to the operations which leave $\mathbf{k}$ invariant, i.e., to the elements of the space group of the wave vector $\mathbf{k}$, $G_{\mathbf{k}}$. These matrices are then used to derive a multiplier representation[8,10] of the point group $G_0(\mathbf{k})$ of the space group $G_{\mathbf{k}}$.

In addition, we see from Eq. (2.21) that taking the complex conjugate of $\mathbf{D}(\mathbf{k})$ is equivalent to reversing the wave vector $\mathbf{k}$. Thus, if the point group of the crystal contains an operation which reverses $\mathbf{k}$, it is possible to combine this operation with complex conjugation to produce an operation which commutes with the dynamical matrix. We will construct a number of such operators and consider their algebra at the end of this section. This type of operation is the analogue of Wigner's[16] time-reversal operator for a particle with spin.

From the definition of $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ given in Eq. (2.37), it is straightforward to show that $\mathbf{\Gamma}$ is unitary:

$$\Gamma_{\alpha\beta}^{+}(\kappa\kappa'\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})=\Gamma_{\beta\alpha}^{*}(\kappa'\kappa\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}), \tag{3.1a}$$

$$=S_{\beta\alpha}\delta(\kappa',F_0(\kappa;S))\exp(-i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(\kappa')-\mathbf{x}(\kappa)]), \tag{3.1b}$$

$$=\Gamma_{\alpha\beta}^{-1}(\kappa\kappa'\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}). \tag{3.1c}$$

In component form, a unitary transformation on $\mathbf{D}(\mathbf{k})$ with $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ is

$$\sum_{\alpha\kappa}\sum_{\beta\kappa'}\Gamma_{\mu\alpha}(K\kappa\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})\Gamma_{\beta\nu}^{+}(\kappa'K'\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$$
$$=\sum_{\alpha\kappa}\sum_{\beta\kappa'}S_{\mu\alpha}\delta(K,F_0(\kappa;S))\exp(i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K)-\mathbf{x}(\kappa)])(M_\kappa M_{\kappa'})^{-1/2}$$
$$\times\sum_{l'}\Phi_{\alpha\beta}(l\kappa;l'\kappa')\exp\{-i\mathbf{k}\cdot[\mathbf{x}(l)-\mathbf{x}(l')]\}S_{\nu\beta}\delta(K',F_0(\kappa';S))$$
$$\times\exp(-i\mathbf{k}\cdot[\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}^{-1}\mathbf{x}(K')-\mathbf{x}(\kappa')]), \tag{3.2}$$

$$=\sum_{\alpha\beta}\sum_{l'}\frac{S_{\mu\alpha}\Phi_{\alpha\beta}(lF_0^{-1}(K;S);l'F_0^{-1}(K';S))S_{\beta\nu}}{(M_K M_{K'})^{1/2}}\exp\{-i\mathbf{k}\cdot\mathbf{S}^{-1}[\mathbf{x}(L)-\mathbf{x}(L')]\}, \tag{3.3}$$

where we have used (2.29a), the analogous expression relating $(L'K')$ to $(l'\kappa')$, and the fact that in a symmetry operation the atoms labeled by K and κ must be of the same kind, so that M_K must equal M_κ, even when the space group operation $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ can interchange the sublattices of nonprimitive crystals so that K need not equal κ. The transformation law for the atomic force constants, Eq. (2.10), allows the right-hand side of Eq. (3.3) to be reduced to

$$(M_K M_{K'})^{-1/2}\sum_{L'}\Phi_{\mu\nu}(LK;L'K')\exp\{-i\mathbf{Sk}\cdot[\mathbf{x}(L)-\mathbf{x}(L')]\}=D_{\mu\nu}(KK'\mid\mathbf{Sk}),\tag{3.4}$$

where l' has been replaced by L' as a summation variable. In matrix notation the relation can be written compactly as

$$\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{D}(\mathbf{k})\mathbf{\Gamma}^{+}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})=\mathbf{D}(\mathbf{Sk}).\tag{3.5}$$

Thus the matrices $\mathbf{D}(\mathbf{k})$ and $\mathbf{D}(\mathbf{Sk})$ are related by a unitary transformation.

To investigate the group properties of the matrices $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ we must derive the relationship between the matrix corresponding to the product of two crystal symmetry operations and the matrices corresponding to the individual operations. Consider the product

$$\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}=\{\mathbf{S}_1\mathbf{S}_2\mid\mathbf{S}_1[\mathbf{v}(S_2)+\mathbf{x}(m_2)]+\mathbf{v}(S_1)+\mathbf{x}(m_1)\},\tag{3.6}$$

which must be a symmetry operation and can be interpreted as a point transformation according to

$$\mathbf{x}(l\kappa)=[\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}]\mathbf{x}(l''\kappa''),\tag{3.7a}$$

$$=\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}\mathbf{x}(l'\kappa').\tag{3.7b}$$

The corresponding matrix $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\})$ in component form is

$$\begin{aligned}&\Gamma_{\alpha\gamma}(\kappa\kappa''\mid\mathbf{k};\{\mathbf{S}_1\mid\mathbf{v}_1(S_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_2\mid\mathbf{v}_2(S_2)+\mathbf{x}(m_2)\})\\&\quad=(\mathbf{S}_1\mathbf{S}_2)_{\alpha\gamma}\delta(\kappa,F_0(\kappa'';S_1S_2))\exp(i\mathbf{k}\cdot[\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}^{-1}\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_2)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa'')]).\end{aligned}\tag{3.8}$$

The form of $\mathbf{\Gamma}$ in Eq. (2.37) suggests that the exponent in Eq. (3.8) be written in the form

$$\begin{aligned}&\mathbf{k}\cdot[\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}^{-1}\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa'')]\\&\quad=\mathbf{S}_2\mathbf{k}\cdot[\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]+\mathbf{k}\cdot[\mathbf{S}_2^{-1}\mathbf{x}(\kappa')-\mathbf{S}_2^{-1}\mathbf{v}(S_2)-\mathbf{S}_2\mathbf{x}(m_2)-\mathbf{x}(\kappa'')],\end{aligned}\tag{3.9a}$$

$$\quad=\mathbf{S}_2\mathbf{k}\cdot[\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]+\mathbf{k}\cdot[\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}^{-1}\mathbf{x}(\kappa')-\mathbf{x}(\kappa'')],\tag{3.9b}$$

where $\mathbf{S}_2\mathbf{k}\cdot\mathbf{x}(\kappa')=\mathbf{k}\cdot\mathbf{S}_2^{-1}\mathbf{x}(\kappa')$ has been added and subtracted. Also, according to Eq. (3.7), $\delta(\kappa,F_0(\kappa';S_1S_2))$ can be expressed as

$$\delta(\kappa;F_0(\kappa'';S_1S_2))=\sum_{\kappa'}\delta(\kappa;F_0(\kappa';S_1))\delta(\kappa';F_0(\kappa'';S_2)).\tag{3.10}$$

Substituting Eqs. (3.9b) and (3.10) in the right-hand side of Eq. (3.8) yields

$$\begin{aligned}&\sum_{\beta\kappa'}(\mathbf{S}_1)_{\alpha\beta}\delta(\kappa;F_0(\kappa';S_1))\exp(i\mathbf{S}_2\mathbf{k}\cdot[\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}^{-1}\mathbf{x}(\kappa)-\mathbf{x}(\kappa')])\\&\qquad\times(\mathbf{S}_2)_{\beta\gamma}\delta(\kappa';F_0(\kappa;S_2))\exp(i\mathbf{k}\cdot[\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}^{-1}\mathbf{x}(\kappa')-\mathbf{x}(\kappa)])\\&\qquad\quad=\sum_{\beta\kappa'}\Gamma_{\alpha\beta}(\kappa\kappa'\mid\mathbf{S}_2\mathbf{k};\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\})\Gamma_{\beta\gamma}(\kappa'\kappa''\mid\mathbf{k};\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}).\end{aligned}\tag{3.11}$$

Therefore we have established the result that

$$\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\})=\mathbf{\Gamma}(\mathbf{S}_2\mathbf{k};\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}).\tag{3.12}$$

It is important to note that $\mathbf{S}_2\mathbf{k}$ occurs in the first term on the right-hand side of (3.12). This is consistent with the transformation properties of the polarization vectors discussed in Sec. 2, as can be seen as follows: The operation $\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\}$ rotates the wave vector $\mathbf{k}$ to $\mathbf{S}_2\mathbf{k}$ and is represented by $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_2\mid\mathbf{v}(S_2)+\mathbf{x}(m_2)\})$. When the operation $\{\mathbf{S}_1\mid\mathbf{v}(S_1)+\mathbf{x}(m_1)\}$ is performed, it operates on a polarization vector whose wave vector is $\mathbf{S}_2\mathbf{k}$. Thus the matrix $\mathbf{\Gamma}$ for this operation depends on $\mathbf{S}_2\mathbf{k}$. Because of this $\mathbf{k}$ dependence, the matrices $\mathbf{\Gamma}$ do not form a representation of the whole space group G.

Let us now restrict ourselves to those operations which comprise the space group $G_{\mathbf{k}}$ of the wave vector $\mathbf{k}$. These are the operations[19] $\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\}$ which take the crystal into itself and whose purely rotational elements $\{\mathbf{R}\}$ have the property

$$\mathbf{Rk}=\mathbf{k}-2\pi\mathbf{b}(\mathbf{k},\mathbf{R}),\tag{3.13}$$

where $\mathbf{b}(\mathbf{k},\mathbf{R})$ is a translation vector of the reciprocal lattice. It is clear that $\mathbf{b}(\mathbf{k},\mathbf{R})$ vanishes if $\mathbf{k}$ lies inside

[19] Just as we have used $\mathbf{S}$ to denote a rotational element in the space group G, we will use $\mathbf{R}$ to denote a rotational element in the space group $G_{\mathbf{k}}$.

the first Brillouin zone of the crystal, and it can be nonzero only if $\mathbf{k}$ lies on the boundary of the zone. In view of Eqs. (2.19) and (3.13) we see that for the operations $\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\}$ Eq. (3.4) takes the form

$$\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})\mathbf{D}(\mathbf{k})\times\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})=\mathbf{D}(\mathbf{k}). \quad (3.14)$$

That is to say, the unitary matrices $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})$ commute with the Fourier-transformed dynamical matrix. Equation (3.14) can be used to determine the form of the matrix $\mathbf{D}(\mathbf{k})$, i.e., the independent, nonzero elements of this matrix. Moreover, these matrices provide a $3r$-dimensional unitary representation of the space group $G_{\mathbf{k}}$ as can be seen from Eqs. (3.5), (3.12), and (3.13); that is,

$$\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_1\mid\mathbf{v}(R_1)+\mathbf{x}(m_1)\}\{\mathbf{R}_2\mid\mathbf{v}(R_2)+\mathbf{x}(m_2)\})=\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_1\mid\mathbf{v}(R_1)+\mathbf{x}(m_1)\})\times\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_2\mid\mathbf{v}(R_2)+\mathbf{x}(m_2)\}). \quad (3.15)$$

Because the vector $[\mathbf{x}(\kappa)-\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}\mathbf{x}(\kappa')]$ of Eq. (2.38) is a translation vector of the crystal, if we combine Eqs. (2.37), (2.38), and (3.13) and make use of Eq. (2.18), we find that the elements of the matrix $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})$ are given explicitly by

$$\Gamma_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})=R_{\alpha\beta}\delta(\kappa,F_0(\kappa';R))\times\exp\left(i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\}\mathbf{x}(\kappa')]\right). \quad (3.16)$$

Rather than making the result expressed by Eq. (3.15) the basis for a discussion of the symmetry properties of the eigenvectors of $\mathbf{D}(\mathbf{k})$ as Streitwolf[6] and Chen[7] have done, we find it convenient to proceed somewhat differently. The purely rotational elements $\{\mathbf{R}\}$ in the space group $G_{\mathbf{k}}$ taken by themselves comprise a point group $G_0(\mathbf{k})$ called the point group of the wave vector $\mathbf{k}$. With each element $\mathbf{R}$ of the group $G_0(\mathbf{k})$ we associate a matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ which is defined in terms of the matrices $\{\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})\}$ by

$$\mathbf{T}(\mathbf{k};\mathbf{R})=\exp[i\mathbf{k}\cdot(\mathbf{v}(R)+\mathbf{x}(m))]\times\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\}), \quad (3.17a)$$

or

$$T_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k};\mathbf{R})=R_{\alpha\beta}\delta(\kappa,F_0(\kappa';R))\times\exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{R}\mathbf{x}(\kappa')]\}. \quad (3.17b)$$

This definition is clearly unique despite the fact that each rotational operation $\mathbf{R}$ is associated with an infinity of operations in the space group $G_{\mathbf{k}}$.

Although there is a one-to-one correspondence between the elements $\{\mathbf{R}\}$ of the point group $G_0(\mathbf{k})$ and the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, the latter, in general, do not provide a representation of the group $G_0(\mathbf{k})$ in the usual sense. To see this, let us determine the multiplication rule obeyed by the matrices associated with two elements $\mathbf{R}_i$ and $\mathbf{R}_j$ of the group:

$$\begin{aligned}\mathbf{T}(\mathbf{k};\mathbf{R}_i)\mathbf{T}(\mathbf{k};\mathbf{R}_j)&=\exp\{i\mathbf{k}\cdot[\mathbf{v}(R_i)+\mathbf{x}(m_i)]\}\exp\{i\mathbf{k}\cdot[\mathbf{v}(R_j)+\mathbf{x}(m_j)]\}\\&\quad\times\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_i\mid\mathbf{v}(R_i)+\mathbf{x}(m_i)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_j\mid\mathbf{v}(R_j)+\mathbf{x}(m_j)\}),\\&=\exp\{i\mathbf{k}\cdot[\mathbf{v}(R_i)+\mathbf{x}(m_i)]\}\exp\{i\mathbf{k}\cdot[\mathbf{v}(R_j)+\mathbf{x}(m_j)]\}\\&\quad\times\exp\{-i\mathbf{k}\cdot[\mathbf{R}_i\mathbf{v}(R_j)+\mathbf{R}_i\mathbf{x}(m_j)+\mathbf{v}(R_i)+\mathbf{x}(m_i)]\}\mathbf{T}(\mathbf{k};\mathbf{R}_i\mathbf{R}_j),\\&=\exp[i(\mathbf{k}-\mathbf{R}_i^{-1}\mathbf{k})\cdot(\mathbf{v}(R_j)+\mathbf{x}(m_j))]\mathbf{T}(\mathbf{k};\mathbf{R}_i\mathbf{R}_j).\end{aligned} \quad (3.18)$$

If we define a translation vector $\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1})$ of the reciprocal lattice by

$$\mathbf{R}_i^{-1}\mathbf{k}=\mathbf{k}-2\pi\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1}) \quad (3.19)$$

and use Eq. (2.18), we obtain for the multiplication rule obeyed by the matrices $\mathbf{T}(\mathbf{k};\mathbf{R}_i)$ and $\mathbf{T}(\mathbf{k};\mathbf{R}_j)$

$$\mathbf{T}(\mathbf{k};\mathbf{R}_i)\mathbf{T}(\mathbf{k};\mathbf{R}_j)=\exp[2\pi i\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1})\cdot\mathbf{v}(\mathbf{R}_j)]\mathbf{T}(\mathbf{k};\mathbf{R}_i\mathbf{R}_j). \quad (3.20)$$

A set of matrices $\{\mathbf{T}(\mathbf{R})\}$ in one-to-one correspondence with the elements $\{\mathbf{R}\}$ of a group and obeying a multiplication rule of the form

$$\mathbf{T}(\mathbf{R}_i)\mathbf{T}(\mathbf{R}_j)=\phi(\mathbf{R}_i,\mathbf{R}_j)\mathbf{T}(\mathbf{R}_i\mathbf{R}_j) \quad (3.21)$$

is said to provide a *multiplier* representation of the group; the scalar function $\phi(\mathbf{R}_i,\mathbf{R}_j)$ is called the multiplier. In the present context the multiplier $\phi(\mathbf{k};\mathbf{R}_i,\mathbf{R}_j)$ equals $\exp[2\pi i\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1})\cdot\mathbf{v}(\mathbf{R}_j)]$.

From Eqs. (3.17b), (3.20), and the result that

$$T_{\beta\alpha}^*(\kappa'\kappa\mid\mathbf{k};\mathbf{R})=T_{\alpha\beta}^{-1}(\kappa\kappa'\mid\mathbf{k};\mathbf{R}), \quad (3.22)$$

we can say that the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ provide a $3r$-dimensional unitary multiplier representation of the point group $G_0(\mathbf{k})$ of the wave vector $\mathbf{k}$. (Several properties of multiplier representations which will be useful in what follows are summarized in Refs. 8 and 10.) However, if $\mathbf{k}$ lies entirely within the Brillouin zone, the reciprocal lattice vector $\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1})$ is identically zero, and the multiplier $\exp[2\pi i\mathbf{b}(\mathbf{k},\mathbf{R}_i^{-1})\cdot\mathbf{v}(\mathbf{R}_j)]$ equals unity. Alternatively, if we are dealing with a crystal which has a symmorphic space group, so that $\mathbf{v}(R)$ is zero for every rotational element $\mathbf{R}$, this multiplier is also equal to unity. In each of these two cases, therefore, we see from Eq. (3.20) that the set of matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ provides an ordinary representation of the point group $G_0(\mathbf{k})$. Put another way, it is only when $\mathbf{k}$ is on the boundary of the Brillouin zone for a crystal that belongs to a nonsymmorphic space group that the representation of $G_0(\mathbf{k})$ provided by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ can differ from an ordinary representation of this point group, and even in such a case it need not differ from an ordinary representation.

If we combine Eqs. (3.7), (3.14), and (3.17a), we see that the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ also commute with the Fourier-transformed dynamical matrix $\mathbf{D}(\mathbf{k})$:

$$\mathbf{D}(\mathbf{k})=\mathbf{T}^{-1}(\mathbf{k};\mathbf{R})\mathbf{D}(\mathbf{k})\mathbf{T}(\mathbf{k};\mathbf{R}). \qquad (3.23)$$

Equations (3.14) and (3.23) are equivalent for determining the form of the matrix $\mathbf{D}(\mathbf{k})$.

So far we have considered the consequences of spatial symmetry alone for the form of the dynamical matrix $\mathbf{D}(\mathbf{k})$ of an arbitrary crystal. We conclude this section by considering the additional conditions imposed on the form of the dynamical matrix if the point group of the crystal contains a rotational element $\mathbf{S}_-$ such that $\mathbf{S}_-\mathbf{k}=-\mathbf{k}$, that is, if $-\mathbf{k}$ is in the star[10] of $\mathbf{k}$. (Recall that the star of $\mathbf{k}$ is defined as the set of inequivalent wave vectors generated by applying the point group operations $\mathbf{S}$ on a given wave vector $\mathbf{k}$.) If for some crystal $-\mathbf{k}$ is in the star of $\mathbf{k}$ only for special values of $\mathbf{k}$, then the following considerations are applicable to those values of $\mathbf{k}$ only. From Eqs. (3.2) and (3.4) we have

$$D_{\mu\nu}(\bar{\kappa}\bar{\kappa}'\mid-\mathbf{k})=\sum_{\alpha\beta}(\mathbf{S}_-)_{\mu\alpha}D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})(\mathbf{S}_-)_{\nu\beta}$$
$$\times\exp\{-i\mathbf{k}\cdot[\mathbf{x}(\bar{\kappa})+\mathbf{x}(\kappa)-\mathbf{x}(\kappa')-\mathbf{x}(\kappa')]\}, \qquad (3.24)$$

where $\bar{\kappa}$ and $\bar{\kappa}'$ are the labels of the atoms into which the atoms κ and κ' are sent by the operation $\{\mathbf{S}_-\mid v(S_-)\}$. Using the relation (2.21), Eq. (3.24) can be put into the form

$$\{\exp[-i\mathbf{k}\cdot\mathbf{x}(\bar{\kappa})]D_{\mu\nu}(\bar{\kappa}\bar{\kappa}'\mid\mathbf{k})\exp[i\mathbf{k}\cdot\mathbf{x}(\bar{\kappa}')]\}^*$$
$$=\sum_{\alpha\beta}(\mathbf{S}_-)_{\mu\alpha}\{\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})$$
$$\times\exp[i\mathbf{k}\cdot\mathbf{x}(\kappa')]\}(\mathbf{S}_-)_{\nu\beta}. \qquad (3.25)$$

When coupled with the fact that $\mathbf{D}(\mathbf{k})$ is Hermitian, Eq. (3.25) gives relations between elements of $\mathbf{D}(\mathbf{k})$ not contained in the symmetry conditions (3.14) [or, equivalently (3.23)], and therefore reduces the number of independent parameters in the dynamical matrix $\mathbf{D}(\mathbf{k})$.

The relation (3.25) is especially useful when the point group of the crystal contains the inversion, $\mathbf{i}$, since in this case $-\mathbf{k}$ is in the star of $\mathbf{k}$ for general $\mathbf{k}$. Taking $\mathbf{S}_-=\mathbf{i}$, Eq. (3.25) reduces to

$$\{\exp[-i\mathbf{k}\cdot\mathbf{x}(\bar{\kappa})]D_{\alpha\beta}(\bar{\kappa}\bar{\kappa}'\mid\mathbf{k})\exp[i\mathbf{k}\cdot\mathbf{x}(\bar{\kappa}')]\}^*$$
$$=\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})\exp[i\mathbf{k}\cdot\mathbf{x}(\kappa')]. \qquad (3.26)$$

In applying Eq. (3.26), it is helpful to note that if under the inversion operation κ is sent into $\bar{\kappa}$, then $\bar{\kappa}$ is simultaneously sent into κ. This follows from the property that applying the inversion operation twice in succession returns the crystal to its original configuration. We shall illustrate the consequences of (3.26) with a few examples.

(A) If every ion is at a center of inversion, so that $\bar{\kappa}=\kappa$ and $\bar{\kappa}'=\kappa'$, we see from Eq. (3.26) that the matrix $\mathbf{C}(\mathbf{k})$ whose elements are given by

$$C_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})=\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})$$
$$\times\exp[i\mathbf{k}\cdot\mathbf{x}(\kappa')] \qquad (3.27)$$

is a real symmetric matrix. This result can be used in conjunction with Eq. (3.23) to determine the form of $\mathbf{D}(\mathbf{k})$ or, equivalently, $\mathbf{C}(\mathbf{k})$. The eigenvalue equation (2.17) can be rewritten in terms of the matrix $\mathbf{C}(\mathbf{k})$ as

$$\sum_{\kappa'\beta}C_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})\{\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa')]e_\beta(\kappa'\mid\mathbf{k}j)\}$$
$$=\omega_j^2(\mathbf{k})\{\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]e_\alpha(\kappa\mid\mathbf{k}j)\}. \qquad (3.28)$$

Because the matrix $\mathbf{C}(\mathbf{k})$ is a real, symmetric matrix for crystals with each ion at a center of inversion, it follows from Eq. (3.28) that the eigenvector

$$w_\alpha(\kappa\mid\mathbf{k}j)=\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]e_\alpha(\kappa\mid\mathbf{k}j) \qquad (3.29)$$

can be chosen to be real for such crystals.

(B) If under the inversion operation κ is sent into $\bar{\kappa}$, then Eq. (3.26) gives useful relations between the elements labeled by κ and $\bar{\kappa}$. Take $\kappa'=\kappa$, then $\bar{\kappa}'=\bar{\kappa}$ and

$$D_{\alpha\beta}^*(\bar{\kappa}\bar{\kappa}\mid\mathbf{k})=D_{\alpha\beta}(\kappa\kappa\mid\mathbf{k}), \qquad (3.30)$$

that is, the elements of the dynamical matrix which are diagonal in κ and $\bar{\kappa}$ are complex conjugates of one another. A relation between the off-diagonal elements $(\kappa\alpha;\,\bar{\kappa}\beta)$ and $(\kappa\beta;\,\bar{\kappa}\alpha)$ can be obtained by taking $\kappa'=\bar{\kappa}$ in Eq. (3.26). It follows that $\bar{\kappa}'=\kappa$, so that

$$D_{\alpha\beta}^*(\bar{\kappa}\kappa\mid\mathbf{k})=D_{\alpha\beta}(\kappa\bar{\kappa}\mid\mathbf{k}), \qquad (3.31a)$$
$$=D_{\beta\alpha}^*(\bar{\kappa}\kappa\mid\mathbf{k}), \qquad (3.31b)$$

since $\mathbf{D}(\mathbf{k})$ is Hermitian. Thus $D_{\alpha\beta}(\kappa\bar{\kappa}\mid\mathbf{k})$ is symmetric in the indices α, β.

For the special case of two like atoms per primitive cell which are interchanged under the inversion operation, Eqs. (3.30) and (3.31) require the dynamical matrix to have the form

$$\mathbf{D}(\mathbf{k})=\begin{vmatrix}\mathbf{D}(11\mid\mathbf{k}) & \mathbf{D}(12\mid\mathbf{k})\\ \mathbf{D}^*(12\mid\mathbf{k}) & \mathbf{D}^*(11\mid\mathbf{k})\end{vmatrix}, \qquad (3.32)$$

where $\mathbf{D}(11\mid\mathbf{k})$ is Hermitian and $\mathbf{D}(12\mid\mathbf{k})$ is symmetric.

The analysis of the combined effect of the crystal symmetry element $\{\mathbf{S}_-\mid\mathbf{v}(S_-)\}$ and Eq. (2.21) on the eigenfrequencies and eigenvectors of the dynamical matrix is facilitated by recasting Eq. (3.24) into a form analogous to Eqs. (3.14) and (3.23). To this end we introduce the anti-unitary operator[16] $\mathbf{K}_0$ to represent the complex conjugate operation; we define it by its effect on an arbitrary vector $\mathbf{\Psi}$ in the $3r$-dimensional space:

$$\mathbf{K}_0\mathbf{\Psi} \equiv \mathbf{\Psi}^*. \tag{3.33}$$

Clearly $\mathbf{K}_0^2\mathbf{\Psi}=\mathbf{\Psi}$, and therefore $\mathbf{K}_0^{-1}=\mathbf{K}_0$. Using $\mathbf{K}_0$ to perform a similarity transformation on $\mathbf{D}(\mathbf{k})$ we have

$$\mathbf{K}_0\mathbf{D}(\mathbf{k})\mathbf{K}_0=\mathbf{D}^*(\mathbf{k}). \tag{3.34}$$

Thus, if $-\mathbf{k}$ is in the star of $\mathbf{k}$, combining Eqs. (3.4) and (3.34) with Eq. (2.21) results in

$$\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)\})\mathbf{D}(\mathbf{k})\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)\})\mathbf{K}_0 = \mathbf{K}_0\mathbf{D}(-\mathbf{k})\mathbf{K}_0=\mathbf{D}^*(-\mathbf{k})=\mathbf{D}(\mathbf{k}). \tag{3.35}$$

That is, the anti-unitary matrix operator $\mathbf{K}_0\mathbf{\Gamma}\times(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)\})$ commutes with the dynamical matrix $\mathbf{D}(\mathbf{k})$. Equation (3.35) is just a symbolic way of writing Eq. (3.25) in which the invariance of the dynamical matrix under the combined effects of the space group operation $\{\mathbf{S}_- \mid \mathbf{v}(S_-)\}$ and complex conjugation is expressed in a form in which the anti-unitary matrix operator $\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)\})$ plays a role completely analogous to that of the unitary matrix operator $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)\})$ in Eq. (3.14).

In order to proceed with a group-theoretical analysis, the products of the anti-unitary matrix operator $\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)\})$ with the matrices $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m)\})$ and $\mathbf{T}(\mathbf{k};\mathbf{R})$ are required. We first note that Eq. (3.35) remains valid when $\{\mathbf{S}_- \mid \mathbf{v}(S_-)\}$ is replaced by any of the following crystal symmetry operations: $\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m)\}$, $\{\mathbf{S}_-\mathbf{R} \mid \mathbf{v}(S_-R)+\mathbf{x}(m)\}$, and $\{\mathbf{R}\mathbf{S}_- \mid \mathbf{v}(RS_-)+\mathbf{x}(m)\}$, since either of the products $\mathbf{S}_-\mathbf{R}\mathbf{k}$ or $\mathbf{R}\mathbf{S}_-\mathbf{k}$ produces a vector equivalent to $-\mathbf{k}$. Using the definition of $\mathbf{K}_0$ and Eqs. (3.5), (3.12), and (3.13), we have

$$\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m_1)\})\cdot\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m_2)\})=\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m_1)\}\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m_2)\}) \tag{3.36}$$

and

$$\begin{aligned}\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m_2)\})\cdot\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m_1)\})&\\ =\mathbf{K}_0\mathbf{\Gamma}^*(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m_2)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m_1)\}),&\\ =\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m_2)\}\{\mathbf{S}_- \mid \mathbf{v}(S_-)+\mathbf{x}(m_1)\}),&\end{aligned} \tag{3.37}$$

where in the last step of Eq. (3.37) we have used the relation

$$\begin{aligned}\mathbf{\Gamma}^*(\mathbf{k};\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\})&=\mathbf{\Gamma}(-\mathbf{k};\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}),\\ &=\mathbf{\Gamma}(\mathbf{S}_-\mathbf{k};\{\mathbf{S} \mid \mathbf{v}(S)+\mathbf{x}(m)\}).\end{aligned} \tag{3.38}$$

We also find that

$$\begin{aligned}\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_1 \mid \mathbf{v}(S_-R_1)+\mathbf{x}(m_1)\})\cdot\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_2 \mid \mathbf{v}(S_-R_2)+\mathbf{x}(m_2)\})&\\ =\mathbf{\Gamma}^*(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_1 \mid \mathbf{v}(S_-R_1)+\mathbf{x}(m_1)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_2 \mid \mathbf{v}(S_-R_2)+\mathbf{x}(m_2)\}),&\\ =\mathbf{\Gamma}(\mathbf{S}_-\mathbf{R}_2\mathbf{k};\{\mathbf{S}_-\mathbf{R}_1 \mid \mathbf{v}(S_-R_1)+\mathbf{x}(m_1)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_2 \mid \mathbf{v}(S_-R_2)+\mathbf{x}(m_2)\}),&\\ =\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R}_1 \mid \mathbf{v}(S_-R_1)+\mathbf{x}(m_1)\}\{\mathbf{S}_-\mathbf{R}_2 \mid \mathbf{v}(S_-R_2)+\mathbf{x}(m_2)\}).&\end{aligned} \tag{3.39}$$

The product of two anti-unitary matrix operators is a unitary matrix corresponding to an element of $G_{\mathbf{k}}$, since $\mathbf{S}_-\mathbf{R}_1\mathbf{S}_-\mathbf{R}_2$ is an element of $G_0(\mathbf{k})$. Thus, the matrix operators $\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m)\})$ and $\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R} \mid \mathbf{v}(S_-R)+\mathbf{x}(m)\})$ form a symmetry group with a one-to-one relationship to the elements of the space group containing the crystal symmetry operations $\{\mathbf{R} \mid \mathbf{v}(R)+\mathbf{x}(m)\}$ and $\{\mathbf{S}_-\mathbf{R} \mid \mathbf{v}(S_-R)+\mathbf{x}(m)\}$. This space group, which is a sum of the space group $G_{\mathbf{k}}$ plus the coset $\{\mathbf{S}_- \mid \mathbf{v}(S_-)\}G_{\mathbf{k}}$, is designated by the symbol $G_{\mathbf{k};-\mathbf{k}}$. It should be noted that $G_{\mathbf{k}}$ is an invariant subgroup of $G_{\mathbf{k};-\mathbf{k}}$.

Equations (3.15), (3.36), (3.37), and (3.39) are the analogs of Wigner's[16] equations (26.18), (for an even number of electrons,) and could be used as the starting point for a group-theoretical analysis and a determination of the irreducible corepresentations[16] of the space group $G_{\mathbf{k};-\mathbf{k}}$. On the other hand, the purely rotational elements $\{\mathbf{R}\}$ and $\{\mathbf{S}_-\mathbf{R}\}$ in the space group $G_{\mathbf{k};-\mathbf{k}}$ taken by themselves form a point group $G_0(\mathbf{k};-\mathbf{k})$ in which $G_0(\mathbf{k})$ is an invariant subgroup. In analogy with Eq. (3.17), with each element $\mathbf{S}_-\mathbf{R}$ in the coset $\mathbf{S}_-G_0(\mathbf{k})$ we associate an anti-unitary matrix operator $\mathbf{T}(\mathbf{k};\mathbf{S}_-\mathbf{R})$ which is defined in terms of the matrix operators $\{\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_-\mathbf{R} \mid \mathbf{v}(S_-R)+

$\mathbf{x}(m)\})\}$ by

$$\mathbf{T}(\mathbf{k};\mathbf{S}_{-}\mathbf{R})=\mathbf{K}_0\exp\{-i\mathbf{k}\cdot[\mathbf{v}(S_{-}R)+\mathbf{x}(m)]\}\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_{-}\mathbf{R}\mid\mathbf{v}(S_{-}R)+\mathbf{x}(m)\}),\tag{3.40a}$$

$$=\exp\{+i\mathbf{k}\cdot[\mathbf{v}(S_{-}R)+\mathbf{x}(m)]\}\mathbf{K}_0\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}_{-}\mathbf{R}\mid\mathbf{v}(S_{-}R)+\mathbf{x}(m)\}).\tag{3.40b}$$

This definition is unique despite the fact that each rotational operation $\mathbf{S}_{-}\mathbf{R}_i$ is associated with an infinity of operations in the space group $G_{\mathbf{k};-\mathbf{k}}$. Moreover, since $G_0(\mathbf{k})$ is an invariant subgroup of $G_0(\mathbf{k};-\mathbf{k})$, to each element $\mathbf{S}_{-}\mathbf{R}_i$ there is associated a unique element $\mathbf{R}_j\mathbf{S}_{-}$, where $\mathbf{R}_j=\mathbf{S}_{-}\mathbf{R}_i\mathbf{S}_{-}^{-1}$ with $\mathbf{v}(R_jS_{-})=\mathbf{v}(S_{-}R_i)$. Therefore, from their definition the corresponding anti-unitary matrix operators $\mathbf{T}$ are equal:

$$\mathbf{T}(\mathbf{k};\mathbf{S}_{-}\mathbf{R}_i)=\mathbf{T}(\mathbf{k};\mathbf{R}_j\mathbf{S}_{-}).\tag{3.41}$$

To emphasize the anti-unitary aspect of the matrix operator $\mathbf{T}(\mathbf{k};\mathbf{S}_{-}\mathbf{R})$, a rotational element in the coset $\mathbf{S}_{-}G_0(\mathbf{k})$ will be denoted by $\mathbf{A}$ and the corresponding matrix operator by $\mathbf{T}(\mathbf{k};\mathbf{A})$.

The products of anti-unitary and unitary matrix operators $\mathbf{T}(\mathbf{k};\cdots)$ can be obtained with the aid of Eqs. (3.12), (3.37), (3.38), and (3.39) and their definitions (3.17) and (3.40). For example,

$$\mathbf{T}(\mathbf{k};\mathbf{A}_i)\mathbf{T}(\mathbf{k};\mathbf{R}_j)=\mathbf{K}_0\exp[-i\mathbf{k}\cdot\mathbf{v}(A_i)]\mathbf{\Gamma}(\mathbf{k};\{\mathbf{A}_i\mid\mathbf{v}(A_i)\})\exp[i\mathbf{k}\cdot\mathbf{v}(R_j)]\mathbf{\Gamma}(\mathbf{k};\{\mathbf{R}_j\mid\mathbf{v}(R_j)\}),$$
$$=\exp\{i\mathbf{k}\cdot[\mathbf{v}(A_i)-\mathbf{v}(R_j)]\}\exp\{-i\mathbf{k}\cdot[\mathbf{v}(A_i)+\mathbf{A}_i\mathbf{v}(R_j)]\}\mathbf{T}(\mathbf{k};\mathbf{A}_i\mathbf{R}_j),$$
$$=\exp\{-i[\mathbf{k}+\mathbf{A}_i^{-1}\mathbf{k}]\cdot\mathbf{v}(R_j)\}\mathbf{T}(\mathbf{k};\mathbf{A}_i\mathbf{R}_j).\tag{3.42}$$

Similarly,

$$\mathbf{T}(\mathbf{k};\mathbf{R}_j)\mathbf{T}(\mathbf{k};\mathbf{A}_i)=\exp\{i[\mathbf{k}-\mathbf{R}_j^{-1}\mathbf{k}]\cdot\mathbf{v}(A_i)\}\mathbf{T}(\mathbf{k};\mathbf{R}_j\mathbf{A}_i)\tag{3.43}$$

and

$$\mathbf{T}(\mathbf{k};\mathbf{A}_i)\mathbf{T}(\mathbf{k};\mathbf{A}_j)=\exp\{-i[\mathbf{k}+\mathbf{A}_i^{-1}\mathbf{k}]\cdot\mathbf{v}(A_j)\}\mathbf{T}(\mathbf{k};\mathbf{A}_i\mathbf{A}_j).\tag{3.44}$$

A product of rotational elements containing an even or odd number of $\mathbf{A}$'s is a member of $G_0(\mathbf{k})$ or $\mathbf{S}_{-}G_0(\mathbf{k})$, respectively. This property is essential in deriving Eqs. (3.42)–(3.44). Comparing Eqs. (3.42) and (3.44) with Eqs. (3.18) and (3.43), we see that the multiplier has a different form if the anti-unitary matrix operator is the first factor in a product. Introducing $\bar{\mathbf{R}}$ to denote an element in the point group $G_0(\mathbf{k};-\mathbf{k})$, then Eqs. (3.18), (3.42)–(3.44) can be combined into a single equation:

$$\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_i)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_j)=\phi(\mathbf{k};\bar{\mathbf{R}}_i,\bar{\mathbf{R}}_j)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_i\bar{\mathbf{R}}_j),\tag{3.45}$$

where for $\bar{\mathbf{R}}_i=\mathbf{R}_i$

$$\phi(\mathbf{k};\mathbf{R}_i,\bar{\mathbf{R}}_j)=\exp\{i[\mathbf{k}-\mathbf{R}_i^{-1}\mathbf{k}]\cdot\mathbf{v}(\bar{\mathbf{R}}_j)\},\tag{3.46}$$

and for $\bar{\mathbf{R}}_i=\mathbf{A}_i$

$$\phi(\mathbf{k};\mathbf{A}_i,\bar{\mathbf{R}}_j)=\exp\{-i[\mathbf{k}+\mathbf{A}_i^{-1}\mathbf{k}]\cdot\mathbf{v}(\bar{\mathbf{R}}_j)\}.\tag{3.47}$$

If either $\mathbf{k}$ lies entirely within the Brillouin zone or the space group $G_{\mathbf{k};-\mathbf{k}}$ of the crystal is symmorphic, so that $\mathbf{v}(\mathbf{R})$ is zero, then the multiplier $\phi(\mathbf{k};\mathbf{R}_i,\mathbf{R}_j)$ is unity.

It is clear from Eqs. (3.35) and (3.40) that the anti-unitary matrix operators $\mathbf{T}(\mathbf{k};\mathbf{S}_{-}\mathbf{R})$ commute with the Fourier-transformed dynamical matrix $\mathbf{D}(\mathbf{k})$. In terms of the $\bar{\mathbf{R}}$ notation this result and Eq. (3.23) may be expressed as a single equation:

$$\mathbf{D}(\mathbf{k})=\mathbf{T}^{-1}(\mathbf{k};\bar{\mathbf{R}})\mathbf{D}(\mathbf{k})\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}).\tag{3.48}$$

As has been emphasized by Wigner,[16] the matrices which transform the eigenvectors of an eigenvalue equation that is invariant under the operations of a group which contains anti-unitary operators do not form a representation (ordinary or multiplier) in the usual sense. In Sec. 5 it will be necessary to introduce the multiplier corepresentation matrices to describe the transformations of the eigenvectors of $\mathbf{D}(\mathbf{k})$ under the group of matrix operations $\mathbf{T}(\mathbf{k};\bar{\mathbf{R}})$, where $\bar{\mathbf{R}}$ is a rotational element of $G_0(\mathbf{k};-\mathbf{k})$. In particular, it is shown there that the irreducible multiplier corepresentations of the point group $G_0(\mathbf{k};-\mathbf{k})$ can be expressed in terms of the irreducible multiplier representations of the point group $G_0(\mathbf{k})$ (which is discussed in the next section).

In the above discussion the extension of the group of symmetry operations that commute with the dynamical matrix $\mathbf{D}(\mathbf{k})$ to include the anti-unitary operations was dependent on the $\mathbf{k}$ vector and crystal symmetry in that the existence of a rotational element $\mathbf{S}_{-}$ was required. In this context the special case where the wave vector $\mathbf{k}$ is equivalent to $-\mathbf{k}$ (i.e., $\mathbf{k}=\pi$ times a reciprocal lattice vector $=\pi\mathbf{b}$) should be singled out in that here there always exists a set of anti-unitary symmetry operations which commute with the dynamical matrix, since $\mathbf{D}(\pi\mathbf{b})$ is real:

$$\mathbf{D}(\pi\mathbf{b})=\mathbf{D}(\pi\mathbf{b}-2\pi\mathbf{b})=\mathbf{D}(-\pi\mathbf{b})=\mathbf{D}^*(\pi\mathbf{b}).\tag{3.49}$$

Similarly, from Eq. (2.39) it is clear that the matrix $\mathbf{\Gamma}(\pi\mathbf{b};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})$ is real. Combining Eqs. (3.23) and (3.49) and expressing the result in operator form yields

$$\mathbf{K}_0\mathbf{T}(\pi\mathbf{b};\mathbf{R})\mathbf{D}(\pi\mathbf{b})\mathbf{T}^{-1}(\pi\mathbf{b};\mathbf{R})\mathbf{K}_0=\mathbf{K}_0\mathbf{D}(\pi\mathbf{b})\mathbf{K}_0=\mathbf{D}^*(\pi\mathbf{b})=\mathbf{D}(\pi\mathbf{b}).\tag{3.50}$$

Therefore the group of matrix operators that commute with the dynamical matrix $\mathbf{D}(\pi\mathbf{b})$ are $\mathbf{T}(\pi\mathbf{b};\mathbf{R})$ and $\mathbf{K}_0\mathbf{T}(\pi\mathbf{b};\mathbf{R})$ regardless of whether the crystal point group does or does not contain an element $\mathbf{S}_-$. Even though the anti-unitary elements $\mathbf{K}_0\mathbf{T}(\pi\mathbf{b};\mathbf{R})$ are not given by Eqs. (3.40), we continue to use the notation $\mathbf{T}(\pi\mathbf{b},\mathbf{A})$ for them, and denote the group made up of the operations $\mathbf{T}(\pi\mathbf{b},\mathbf{R})$ and $\mathbf{K}_0\mathbf{T}(\pi\mathbf{b},\mathbf{R})$ by $G_0(\pi\mathbf{b};-\pi\mathbf{b})$. The wave vector $\pi\mathbf{b}$ is sufficient to distinguish this case from the others. The analogs of Eqs. (3.42), (3.43), and (3.44) for products involving anti-unitary operators are

$$\mathbf{T}(\pi\mathbf{b};\mathbf{A}_i)\mathbf{T}(\pi\mathbf{b};\mathbf{R}_j)=\phi^*(\pi\mathbf{b};\mathbf{R}_i,\mathbf{R}_j)\mathbf{T}(\pi\mathbf{b};\mathbf{A}_i\mathbf{R}_j), \tag{3.51}$$

$$\mathbf{T}(\pi\mathbf{b};\mathbf{R}_j)\mathbf{T}(\pi\mathbf{b};\mathbf{A}_i)=\exp[i2\pi\mathbf{b}\cdot\mathbf{v}(R_j)]\times\phi^*(\pi\mathbf{b};\mathbf{R}_j,\mathbf{R}_i)\mathbf{T}(\pi\mathbf{b};\mathbf{R}_j\mathbf{A}_i), \tag{3.52}$$

$$\mathbf{T}(\pi\mathbf{b};\mathbf{A}_i)\mathbf{T}(\pi\mathbf{b};\mathbf{A}_j)=\exp[-i2\pi\mathbf{b}\cdot\mathbf{v}(R_i)]\times\phi(\pi\mathbf{b};\mathbf{R}_i,\mathbf{R}_j)\mathbf{T}(\pi\mathbf{b};\mathbf{R}_i\mathbf{R}_j). \tag{3.53}$$

The multipliers in these equations are not the same as those given in Eqs. (3.46) and (3.47). However, this does not affect the results of the general theory given in Sec. 5.

Another important case in which the dynamical matrix is real is for the wave vector at the center of the Brillouin zone, i.e., $\mathbf{k}=\mathbf{0}$, as is clear from Eq. (2.21). Setting $\mathbf{k}=\mathbf{0}$ in Eqs. (3.16) and (3.17) we see that the matrices $\mathbf{\Gamma}(\mathbf{0};\{\mathbf{R}\mid\mathbf{v}(R)+\mathbf{x}(m)\})$ and $\mathbf{T}(\mathbf{0};\mathbf{R})$ are equal and real. The comments and results of the previous paragraph are applicable here except that all the multipliers are unity, since $\pi\mathbf{b}$ is replaced by the wave vector $\mathbf{0}$. In this special case the point group $G_0(\mathbf{0})$ of the space group of the wave vector is the point group of the crystal symmetry group.

Henceforth, the invariance of the dynamical matrix $\mathbf{D}(\mathbf{k})$ with respect to unitary and anti-unitary symmetry operations will be distinguished by referring to the former as invariance with respect to spatial symmetry [e.g., Eqs. (3.14) and (3.23)], and to the latter as invariance with respect to time-reversal symmetry, [e.g., Eqs. (3.35), (3.48), and (3.50)].

4. TRANSFORMATION PROPERTIES OF THE EIGENVECTORS OF THE DYNAMICAL MATRIX

We are now in a position to determine the transformation properties of the eigenvector $\mathbf{e}(\kappa\mid\mathbf{k}j)$ under the operations of the space group G of the crystal and of the space group $G_{\mathbf{k}}$ of the wave vector $\mathbf{k}$. We begin by establishing several general properties of the eigenvectors $\{\mathbf{e}(\kappa\mid\mathbf{k}j)\}$ and of the eigenvalues $\{\omega_j^2(\mathbf{k})\}$ which are independent of the specific space group to which the crystal belongs. The consequences of extending the group operations to include time-reversal symmetry are discussed in Sec. 5.

If we replace $\mathbf{k}$ by $-\mathbf{k}$ in Eq. (2.17), take the complex conjugate of the resulting equation, and make use of Eq. (2.21), we obtain the result that

$$\sum_{\kappa'\beta} D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})e_\beta^*(\kappa'\mid-\mathbf{k}j)=\omega_j^2(-\mathbf{k})e_\alpha^*(\kappa\mid-\mathbf{k}j), \tag{4.1}$$

where we have used the fact that $\omega_j^2(\mathbf{k})$ is real because $\mathbf{D}(\mathbf{k})$ is a Hermitian matrix. From Eq. (4.1) we see that the squared frequencies $\{\omega_j^2(-\mathbf{k})\}$ and the squared frequencies $\{\omega_j^2(\mathbf{k})\}$ are eigenvalues of the same matrix $\mathbf{D}(\mathbf{k})$. If $\mathbf{k}$ is not a point in the first Brillouin zone at which $\mathbf{D}(\mathbf{k})$ has degenerate eigenvalues, we therefore obtain the result that

$$\omega_j^2(-\mathbf{k})=\omega_j^2(\mathbf{k}). \tag{4.2}$$

By continuity we extend this result to points of degeneracy, since in such cases Eq. (4.2) merely gives us a prescription for labeling the modes at $-\mathbf{k}$ in terms of those at $\mathbf{k}$.

Because the vector $\mathbf{e}^*(-\mathbf{k}j)$ satisfies the same equation as the eigenvector $\mathbf{e}(\mathbf{k}j)$, then, as long as $\mathbf{k}$ is not a point of degeneracy, the two vectors can differ at most by an arbitrary factor of modulus unity (to preserve normalization):

$$\mathbf{e}^*(-\mathbf{k}j)=e^{i\phi}\mathbf{e}(\mathbf{k}j). \tag{4.3}$$

Two choices for the phase factor $e^{i\phi}$ are in common use. Leibfried[18] makes the choice $e^{i\phi}=-1$, while Born and Huang[20] make the choice $e^{i\phi}=1$. Clearly, no result of any calculation of a physical property of a crystal can be affected by the choice of one value for this phase factor in preference to another. In what follows we follow Born and Huang and choose the phase factor to equal unity:

$$e_\alpha^*(\kappa\mid-\mathbf{k}j)=e_\alpha(\kappa\mid\mathbf{k}j). \tag{4.4}$$

Equation (4.4) was derived on the assumption that $\mathbf{k}$ is not a point of degeneracy. When $\mathbf{k}$ is a point of degeneracy, the most we can infer from Eq. (4.1) is that $e_\alpha^*(\kappa\mid-\mathbf{k}j)$ is an arbitrary linear combination of the eigenvectors $\{e_\alpha(\kappa\mid\mathbf{k}j')\}$ for which $\omega_{j'}^2(\mathbf{k})=\omega_j^2(\mathbf{k})$. However, it has become conventional to choose this linear combination in such a way that Eq. (4.4) remains valid at such points as well if the degeneracy is due to spatial symmetry only. For these points Eq. (4.4) gives us a convention for labeling the normal modes at $-\mathbf{k}$ in terms of the labeling at $\mathbf{k}$, which is consistent with that given by Eq. (4.2).

The eigenvalue equation (2.17), associated with the wave vector $\mathbf{Sk}$, can be written in matrix form as

$$\mathbf{D}(\mathbf{Sk})\mathbf{e}(\mathbf{Sk}j)=\omega_j^2(\mathbf{Sk})\mathbf{e}(\mathbf{Sk}j). \tag{4.5}$$

If we multiply both sides of this equation from the left by the matrix $\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})$ and make use

---

[20] Reference 1a, p. 298.

of Eq. (3.4), we obtain the result that

$$\mathbf{D}(\mathbf{k})\{\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{S}\mathbf{k}j)\}$$
$$=\omega_j^2(\mathbf{S}\mathbf{k})\{\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{S}\mathbf{k}j)\}. \quad (4.6)$$

Comparing Eq. (4.6) with Eq. (2.17), we see that the $\{\omega_j^2(\mathbf{Sk})\}$ are eigenvalues of the matrix of which the $\{\omega_j^2(\mathbf{k})\}$ are also eigenvalues. If $\mathbf{k}$ is a point at which none of the eigenvalues of $\mathbf{D}(\mathbf{k})$ are degenerate, then clearly we must have the relation

$$\omega_j^2(\mathbf{k})=\omega_j^2(\mathbf{Sk}). \quad (4.7)$$

If $\mathbf{k}$ is a point at which two or more eigenvalues $\{\omega_j^2(\mathbf{k})\}$ are equal, then, in general, the most we may say is that

$$\omega_j^2(\mathbf{Sk})=\omega_{j'}^2(\mathbf{k}),$$

where $\omega_{j'}^2(\mathbf{k})$ is one of the eigenvalues at $\mathbf{k}$ which equals $\omega_j^2(\mathbf{k})$. However, with no loss of generality we may replace j' by j on the right-hand side of this equation, since all that this does is to give us a particularly convenient way of labeling the modes at $\mathbf{Sk}$ in terms of those at $\mathbf{k}$. Put another way, by continuity we extend Eq. (4.7), which was established on the assumption that $\mathbf{k}$ is not a point at which $\mathbf{D}(\mathbf{k})$ has degenerate eigenvalues, to points of degeneracy as well. Equation (4.7) states that $\omega_j^2(\mathbf{k})$ has the full symmetry of the point group of the crystal. However, from Eq. (4.2) $\omega_j^2(\mathbf{k})$ is an even function of $\mathbf{k}$ even if the point group of the crystal does not contain the inversion.

If $\mathbf{k}$ is not at a point of degeneracy, the vector $\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{Sk}j)$ can differ from the eigenvector $\mathbf{e}(\mathbf{k}j)$ by a complex phase factor of unit modulus (to preserve normalization),

$$\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{Sk}j)=e^{i\theta}\mathbf{e}(\mathbf{k}j),$$

or, using (3.12),

$$\mathbf{e}(\mathbf{Sk}j)=e^{i\theta}\mathbf{\Gamma}(\mathbf{Sk};\{\boldsymbol{\varepsilon}\mid\mathbf{x}(m)\})\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)\})\mathbf{e}(\mathbf{k}j). \quad (4.8)$$

Because the effect on the displacement field of translating the crystal through one of its periods enters only through the factor $\exp[i\mathbf{k}\cdot\mathbf{x}(l)]$ on the right side of Eq. (2.13) and not through the eigenvector $\mathbf{e}(\mathbf{k}j)$, it is convenient to choose for the phase angle θ in Eq. (4.8) the value $\mathbf{Sk}\cdot\mathbf{x}(m)$. The motivation for this somewhat arbitrary choice is that the law of transformation for the eigenvector $\mathbf{e}(\mathbf{k}j)$ becomes

$$\mathbf{e}(\mathbf{Sk}j)=\mathbf{\Gamma}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)\})\mathbf{e}(\mathbf{k}j), \quad (4.9a)$$

or, in component form,

$$\exp[-i\mathbf{Sk}\cdot\mathbf{x}(F_0(\kappa;S))]e_\alpha(F_0(\kappa;S)\mid\mathbf{Sk}j)$$
$$=\sum_\beta S_{\alpha\beta}\exp[-i\mathbf{Sk}\cdot\mathbf{v}(S)]$$
$$\times\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]e_\beta(\kappa\mid\mathbf{k}j). \quad (4.9b)$$

The transformation law given by Eq. (4.9) is convenient in that as the left-hand side of Eq. (4.8) is independent of the translation vector $\mathbf{x}(m)$, it is natural to insist that the right-hand side be independent of this vector as well.

When $\mathbf{k}$ is a point at which $\mathbf{D}(\mathbf{k})$ has degenerate eigenvalues, the most we can infer from Eq. (4.6) is that $\mathbf{\Gamma}^{-1}(\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})\mathbf{e}(\mathbf{Sk}j)$ is some linear combination of the eigenvectors $\{\mathbf{e}(\mathbf{k}j')\}$, where j' labels those branches of $\omega^2(\mathbf{k})$ for which $\omega_{j'}^2(\mathbf{k})=\omega_j^2(\mathbf{k})$. However, with no loss of generality we can take the point of view that once we know the vector $\mathbf{e}(\mathbf{k}j)$ associated with a point of degeneracy, then Eq. (4.9) describes how this vector transforms when the vector $\mathbf{k}$ is taken into the vector $\mathbf{Sk}$ by one of the symmetry operations of the crystal, provided that the symmetry operation is not such that $\mathbf{Sk}=\mathbf{k}-2\pi\mathbf{b}(\mathbf{k},\mathbf{S})$, where $\mathbf{b}(\mathbf{k},\mathbf{S})$ is a translation vector of the reciprocal lattice. It only remains to determine the forms of the eigenvectors $\{\mathbf{e}(\mathbf{k}j)\}$ associated with a point of degeneracy in the first Brillouin zone. These are determined by the symmetry operations (spatial) which leave the wave vector $\mathbf{k}$ invariant (modulo 2π times a reciprocal lattice vector) in a way which will be described below.

We will make one exception to the transformation law for eigenvectors given by Eq. (4.9). If the rotational element $\mathbf{S}_-$ is in the point group of the crystal, we will make a different choice for the phase factor in Eq. (4.8) than that which leads to Eqs. (4.9) for $\mathbf{S}=\mathbf{S}_-$. Taking $\mathbf{x}(m)=0$ and $\mathbf{S}=\mathbf{S}_-$ in Eq. (4.8), we obtain

$$e_\alpha(\bar\kappa\mid-\mathbf{k}j)=e^{i\theta}\exp\{-i\mathbf{k}\cdot[\mathbf{x}(\bar\kappa)-\mathbf{S}_-\mathbf{x}(\kappa)-\mathbf{v}(S_-)]\}$$
$$\times\sum_\beta(\mathbf{S}_-)_{\alpha\beta}e_\beta(\kappa\mid\mathbf{k}j), \quad (4.10)$$

where the atom labeled by κ is sent into $\bar\kappa$ by the crystal symmetry operation $\{\mathbf{S}_-\mid\mathbf{v}(S_-)\}$. Comparing Eq. (4.10) with Eqs. (4.3), one might be tempted to replace the left-hand side of Eq. (4.10) with $e^{-i\phi}e_\alpha^*(\bar\kappa\mid\mathbf{k}j)$; however, this is not always possible, as will become clear in the next section. On the other hand, in cases where it is possible Eq. (4.10) yields a valuable relation in that it relates the components of $\mathbf{e}(\mathbf{k}j)$ to $\mathbf{e}^*(\mathbf{k}j)$. With this in mind, it is convenient to choose the phase factor according to

$$e^{i\theta}=-e^{-i\phi}\exp[-i\mathbf{k}\cdot\mathbf{v}(S_-)], \quad (4.11)$$

and obtain the transformation law

$$e_\alpha(\bar\kappa\mid-\mathbf{k}j)=-e^{-i\phi}\exp\{-i\mathbf{k}\cdot[\mathbf{x}(\bar\kappa)-\mathbf{S}_-\mathbf{x}(\kappa)]\}$$
$$\times\sum_\beta(\mathbf{S}_-)_{\alpha\beta}e_\beta(\kappa\mid\mathbf{k}j). \quad (4.12)$$

When $e_\alpha(\bar\kappa\mid-\mathbf{k}j)$ can be replaced by $e^{-i\phi}e_\alpha^*(\bar\kappa\mid\mathbf{k}j)$, then the choice of phase in Eq. (4.11) corresponds to choosing the vectors $\mathbf{e}(\mathbf{k}j)$ to be eigenvectors of the anti-unitary matrix operator $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ of Eq. (3.40) with eigenvalue equal to -1. Also in this case, if $\mathbf{S}_-$ is the inversion operator $\mathbf{i}$ and every ion is at a center of inversion symmetry, so that $\bar{\kappa}=\kappa$, it follows directly that $\exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]\mathbf{e}(\mathbf{k}j)$ is real.

We now turn to a determination of the transformation properties of the eigenvectors $\{\mathbf{e}(\mathbf{k}j)\}$ associated with $\mathbf{k}$ vectors which correspond to points of symmetry in the first Brillouin zone. Such points are points for which the group of the wave vector $\mathbf{k}$, $G_{\mathbf{k}}$ is larger than the invariant subgroup of pure translations, or, equivalently, they are points for which the point group of the wave vector $\mathbf{k}$, $G_0(\mathbf{k})$ contains more than the identity.

Our starting point is the eigenvalue equation (2.17) together with Eq. (3.23). Multiplying both sides of Eq. (2.17) from the left by the matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ and using the fact that $\mathbf{T}(\mathbf{k};\mathbf{R})$ commutes with $\mathbf{D}(\mathbf{k})$, we obtain

$$\mathbf{D}(\mathbf{k})\{\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}j)\}=\omega_j^2(\mathbf{k})\{\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}j)\}. \quad (4.13)$$

This result tells us that if $\mathbf{e}(\mathbf{k}j)$ is an eigenvector of $\mathbf{D}(\mathbf{k})$ with an eigenvalue $\omega_j^2(\mathbf{k})$, then so is $\mathbf{T}(\mathbf{k};\mathbf{R})\times\mathbf{e}(\mathbf{k}j)$, for every operation $\mathbf{R}$ of the point group $G_0(\mathbf{k})$. Consequently $\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}j)$ is a linear combination of the eigenvectors of $\mathbf{D}(\mathbf{k})$ whose eigenvalues are equal to $\omega_j^2(\mathbf{k})$. To express this result conveniently we replace the single index j by a double index $\sigma\lambda$, where σ labels the *distinct* values of $\omega_j^2(\mathbf{k})$ for a given wave vector $\mathbf{k}$, and $\lambda(=1, 2, \cdots, f_\sigma)$ labels the linearly independent eigenvectors associated with the eigenvalue $\omega_\sigma^2(\mathbf{k})$. Therefore f_σ is the degeneracy of the normal mode whose frequency is $\omega_\sigma^2(\mathbf{k})$. The eigenvalue equation (2.17) in this notation takes the form

$$\mathbf{D}(\mathbf{k})\mathbf{e}(\mathbf{k}\sigma\lambda)=\omega_\sigma^2(\mathbf{k})\mathbf{e}(\mathbf{k}\sigma\lambda) \qquad \lambda=1, 2, \cdots, f_\sigma. \quad (4.14)$$

In view of Eq. (4.13) and the discussion following it, we can write

$$\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}\sigma\lambda)=\sum_{\lambda'=1}^{f_\sigma}\tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}\sigma\lambda') \quad (4.15)$$

for every operation $\mathbf{R}$ of the point group $G_0(\mathbf{k})$.

The f_σ dimensional matrices $\{\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})\}$ can be shown to provide a multiplier representation of $G_0(\mathbf{k})$. For if we multiply both sides of Eq. (4.15) by the matrix $\mathbf{T}(\mathbf{k};\mathbf{R}')$, where $\mathbf{R}'$ is an arbitrary operation of the group $G_0(\mathbf{k})$, we obtain

$$\begin{aligned}\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}\sigma\lambda)&=\sum_{\lambda'=1}^{f_\sigma}\tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{e}(\mathbf{k}\sigma\lambda'),\\&=\sum_{\lambda'=1}^{f_\sigma}\sum_{\lambda''=1}^{f_\sigma}\tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R})\tau_{\lambda''\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R}')\mathbf{e}(\mathbf{k}\sigma\lambda'').\end{aligned} \quad (4.16)$$

Using Eq. (3.20) and the fact that Eq. (4.15) must hold for every element of the group $G_0(\mathbf{k})$, because $\mathbf{R}'\mathbf{R}$ is in this group, we rewrite the left-hand side of Eq. (4.16) as

$$\phi(\mathbf{k};\mathbf{R}',\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{R}'\mathbf{R})\mathbf{e}(\mathbf{k}\sigma\lambda)=\phi(\mathbf{k};\mathbf{R}',\mathbf{R})\sum_{\lambda''=1}^{f_\sigma}\tau_{\lambda''\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R}'\mathbf{R})\mathbf{e}(\mathbf{k}\sigma\lambda''). \quad (4.17)$$

Equating the right-hand sides of Eqs. (4.16) and (4.17), we obtain

$$\sum_{\lambda'=1}^{f_\sigma}\tau_{\lambda''\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R}')\tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R})=\phi(\mathbf{k};\mathbf{R}',\mathbf{R})\tau_{\lambda''\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R}'\mathbf{R}). \quad (4.18)$$

We now establish one additional useful property of the matrices $\{\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})\}$. From Eq. (4.15) and the orthonormality of the eigenvectors $\{\mathbf{e}(\mathbf{k}\sigma\lambda)\}$, Eq. (2.23a), we find that

$$\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R})=\sum_{\kappa\alpha}\sum_{\kappa'\beta}e_\alpha^*(\kappa\,|\,\mathbf{k}\sigma\lambda)\times T_{\alpha\beta}(\kappa\kappa'\,|\,\mathbf{k};\mathbf{R})e_\beta(\kappa'\,|\,\mathbf{k}\sigma\lambda'). \quad (4.19)$$

Now let $\mathbf{R}$ be the identity transformation $\mathbf{R}=\boldsymbol{\varepsilon}$, where $\boldsymbol{\varepsilon}$ is the 3×3 unit matrix. From Eq. (3.17b) we see in this case that

$$T_{\alpha\beta}(\kappa\kappa'\,|\,\mathbf{k};\boldsymbol{\varepsilon})=\delta_{\alpha\beta}\delta(\kappa,\kappa'), \quad (4.20)$$

from which it follows that

$$\begin{aligned}\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\boldsymbol{\varepsilon})&=\sum_{\kappa\alpha}\sum_{\kappa'\beta}e_\alpha^*(\kappa\,|\,\mathbf{k}\sigma\lambda)\delta_{\alpha\beta}\delta(\kappa,\kappa')e_\beta(\kappa'\,|\,\mathbf{k}\sigma\lambda'),\\&=\sum_{\kappa\alpha}e_\alpha^*(\kappa\,|\,\mathbf{k}\sigma\lambda)e_\alpha(\kappa\,|\,\mathbf{k}\sigma\lambda'),\\&=\delta_{\lambda\lambda'}.\end{aligned} \quad (4.21)$$

Thus the matrix $\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\boldsymbol{\varepsilon})$ is the $f_\sigma\times f_\sigma$ unit matrix.

Combining the results given by Eqs. (4.18) and (4.20), we find that

$$\sum_{\lambda'=1}^{f_\sigma}\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R})\tau_{\lambda'\lambda''}^{(\sigma)}(\mathbf{k};\mathbf{R}^{-1})=\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})\delta_{\lambda\lambda''}, \quad (4.22)$$

so that

$$\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R}^{-1})=\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})^{-1}. \quad (4.23)$$

Let us now take the complex conjugate of both sides of Eq. (4.19):

$$\begin{aligned}\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R})^*&=\sum_{\kappa\alpha}\sum_{\kappa'\beta}e_\alpha(\kappa\,|\,\mathbf{k}\sigma\lambda)T_{\alpha\beta}^*(\kappa\kappa'\,|\,\mathbf{k};\mathbf{R})e_\beta^*(\kappa'\,|\,\mathbf{k}\sigma\lambda'),\\&=\sum_{\kappa\alpha}\sum_{\kappa'\beta}e_\alpha^*(\kappa\,|\,\mathbf{k}\sigma\lambda')T_{\beta\alpha}^*(\kappa'\kappa\,|\,\mathbf{k};\mathbf{R})e_\beta(\kappa'\,|\,\mathbf{k}\sigma\lambda),\\&=\sum_{\kappa\alpha}\sum_{\kappa'\beta}e_\alpha^*(\kappa\,|\,\mathbf{k}\sigma\lambda')T_{\alpha\beta}^{-1}(\kappa\kappa'\,|\,\mathbf{k};\mathbf{R})e_\beta(\kappa'\,|\,\mathbf{k}\sigma\lambda),\end{aligned} \quad (4.24)$$

where we have used the fact that $\mathbf{T}(\mathbf{k};\mathbf{R})$ is a unitary matrix. In just the same way that Eq. (4.23) was established we can prove the result that

$$T_{\alpha\beta}^{-1}(\kappa\kappa' \mid \mathbf{k};\mathbf{R}) = [\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})]^{-1} T_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k};\mathbf{R}^{-1}). \tag{4.25}$$

Substituting this result into Eq. (4.24), we find that

$$\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R})^* = [\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})]^{-1} \tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R}^{-1}). \tag{4.26}$$

Combining Eqs. (4.23) and (4.26), we finally obtain the desired result:

$$\tau_{\lambda\lambda'}^{(\sigma)}(\mathbf{k};\mathbf{R})^{-1} = \tau_{\lambda'\lambda}^{(\sigma)}(\mathbf{k};\mathbf{R})^*, \tag{4.27}$$

i.e., that $\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})$ is a unitary matrix.

It is a well-known result of group theory that in the absence of accidental degeneracy, the eigenfunctions corresponding to each eigenvalue of an operator transform irreducibly under the symmetry transformations which leave the operator invariant.[21] In other words, the f_σ eigenvectors $\{\mathbf{e}(\mathbf{k}\sigma\lambda)\}$ ($\lambda = 1, 2, \cdots, f_\sigma$), which correspond to the eigenvalue $\omega_\sigma^2(\mathbf{k})$ and which are sent into linear combinations of themselves under multiplication by the set of matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, cannot be divided into two or more groups such that the members of any group are sent only into linear combinations of each other by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ and do not mix with the members of the other groups. This means that in the absence of accidental degeneracy the set of matrices $\{\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})\}$ constitute an f_σ-dimensional irreducible multiplier representation of the point group $G_0(\mathbf{k})$.

Let us now assume that we know all the eigenvectors $\{\mathbf{e}(\mathbf{k}\sigma\lambda)\}$ of $\mathbf{D}(\mathbf{k})$ for a given value of $\mathbf{k}$. From Eq. (4.15) it follows that if we construct a $3r \times 3r$ matrix $\mathbf{e}(\mathbf{k})$ whose columns are just the vectors $\{\mathbf{e}(\mathbf{k}\sigma\lambda)\}$, so that the $(\alpha\kappa;\sigma\lambda)$ element of this matrix is given by

$$e_{\alpha\kappa;\sigma\lambda}(\mathbf{k}) = e_\alpha(\kappa \mid \mathbf{k}\sigma\lambda), \tag{4.28}$$

we obtain as the equation for $\mathbf{e}(\mathbf{k})$

$$\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}) = \mathbf{e}(\mathbf{k})\boldsymbol{\Delta}(\mathbf{k};\mathbf{R}), \tag{4.29}$$

where the $3r \times 3r$ matrix $\boldsymbol{\Delta}(\mathbf{k};\mathbf{R})$ has the form

$$\boldsymbol{\Delta}(\mathbf{k};\mathbf{R}) = \begin{pmatrix} \boldsymbol{\tau}^{(1)}(\mathbf{k};\mathbf{R}) & 0 & 0 & \cdot \\ 0 & \boldsymbol{\tau}^{(2)}(\mathbf{k};\mathbf{R}) & 0 & \cdot \\ 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{4.30}$$

In Eq. (4.30) $\boldsymbol{\tau}^{(1)}(\mathbf{k};\mathbf{R})$, $\boldsymbol{\tau}^{(2)}(\mathbf{k};\mathbf{R})$, $\cdots$, are the matrices of the irreducible multiplier representations of $G_0(\mathbf{k})$ corresponding to the frequencies $\omega_1^2(\mathbf{k})$, $\omega_2^2(\mathbf{k})$, $\cdots$, respectively, in the sense of Eq. (4.15).

From Eq. (4.29) we see that the matrix $\mathbf{e}(\mathbf{k})$ is the matrix which block-diagonalizes every matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ corresponding to one of the operations of $G_0(\mathbf{k})$ into the form given by Eq. (4.30) by a similarity transformation

$$\begin{aligned} \boldsymbol{\Delta}(\mathbf{k};\mathbf{R}) &= \mathbf{e}^{-1}(\mathbf{k})\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}), \\ &= \mathbf{e}^T(\mathbf{k})^*\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}). \end{aligned} \tag{4.31}$$

[The unitarity of the matrix $\mathbf{e}(\mathbf{k})$ is an immediate consequence of Eqs. (2.23).] In other words, the matrix of the eigenvectors of $\mathbf{D}(\mathbf{k})$ reduces the reducible representation of $G_0(\mathbf{k})$ provided by the $3r \times 3r$ matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ into its irreducible representations.

It may be found that some irreducible representation, i.e., some matrix $\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})$, appears more than once, say c times, in the reduction of the representation of $G_0(\mathbf{k})$ given by the set of matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, as expressed by Eq. (4.30). This means that there are that many distinct sets of f_σ eigenvectors $\{\mathbf{e}(\mathbf{k}\sigma\lambda)\}$, each of which corresponds to a different value of $\omega^2(\mathbf{k})$, (since σ labels the distinct eigenvalues) which have the property that the eigenvectors comprising a given set transform into linear combinations of each other under the operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ in the same way as do the eigenvectors comprising each of the remaining $c-1$ sets. This circumstance [that c sets of matrices (where $c>1$) $\{\boldsymbol{\tau}^{(\sigma)}(\mathbf{k};\mathbf{R})\}$ are, in fact, identical] has the consequence that σ is not a unique label for the irreducible representations of $G_0(\mathbf{k})$ contained in the reducible representation provided by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$. Therefore it is convenient to generalize our notation still further. We will use the index s to label the irreducible representations of $G_0(\mathbf{k})$ and will add to it a "repetition" index a which differentiates among the different eigenvalues whose associated eigenvectors transform according to the same irreducible representation of $G_0(\mathbf{k})$. The index a takes on the values $1, 2, \cdots, c_s$, where c_s is the number of times the sth irreducible representation of $G_0(\mathbf{k})$ is contained in the representation given by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$.

In the new notation the eigenvalue equation (2.17) takes the form

$$\mathbf{D}(\mathbf{k})\mathbf{e}(\mathbf{k}sa\lambda) = \omega_{sa}^2(\mathbf{k})\mathbf{e}(\mathbf{k}sa\lambda)$$
$$\lambda = 1, 2, \cdots, f_s,\ a = 1, 2, \cdots, c_s. \tag{4.32}$$

At the same time Eq. (4.15) takes the form

$$\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda) = \sum_{\lambda'=1}^{f_s} \tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda'). \tag{4.33}$$

The irreducible representation matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ have been tabulated for all 230 space groups by Kovalev,[12] and are therefore known. (However, see Ref. 13.)

The reduction of the reducible representation of $G_0(\mathbf{k})$ provided by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ into its irreducible representations is carried out by standard methods.[10] If we denote the characters of the reducible represen-

[21] See, for example, V. Heine, *Group Theory in Quantum Mechanics* (Pergamon Press, Inc., New York, 1960), p. 44.

tation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ by $\chi(\mathbf{k};\mathbf{R})$,

$$\chi(\mathbf{k};\mathbf{R})=\mathrm{Tr}\,\mathbf{T}(\mathbf{k};\mathbf{R}),$$
$$=\sum_{\kappa\alpha} R_{\alpha\alpha}\delta(\kappa, F_0(\kappa;R))\times\exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{R}\mathbf{x}(\kappa)]\}, \quad (4.34)$$

and if we denote the characters of the sth irreducible representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ by $\chi^{(s)}(\mathbf{k};\mathbf{R})$,

$$\chi^{(s)}(\mathbf{k};\mathbf{R})=\mathrm{Tr}\,\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}), \quad (4.35)$$

then the number of times the sth irreducible representation is contained in the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ is[10]

$$c_s=h^{-1}\sum_R \chi(\mathbf{k};\mathbf{R})\chi^{(s)}(\mathbf{k};\mathbf{R})^* \quad (4.36)$$

where h is the order of the group $G_0(\mathbf{k})$.

The forms of the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ can be obtained by projection operator techniques. The analog of the usual projection operator[10] in our $3r$-dimensional space is the $3r\times 3r$ matrix $\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})$ defined as

$$\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})=(f_s/h)\sum_R \tau_{\lambda\lambda'}^{(s)}(\mathbf{k};\mathbf{R})^*\mathbf{T}(\mathbf{k};\mathbf{R}). \quad (4.37)$$

If we denote by $\boldsymbol{\Psi}$ an arbitrary $3r$-component vector whose elements are $\{\psi_\alpha(\kappa)\}$, then it is straightforward to show that the vector

$$\mathbf{E}(\mathbf{k};s\lambda)=\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})\,\boldsymbol{\psi} \quad (4.38)$$

for any fixed λ' transforms under the application of the matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ in exactly the same way as the eigenvector $\mathbf{e}(\mathbf{k}sa\lambda)$ does. Let us apply the matrix $\mathbf{T}(\mathbf{k};\mathbf{R}')$ to both sides of Eq. (4.38):

$$\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{E}(\mathbf{k};s\lambda)=(f_s/h)\sum_R \tau_{\lambda\lambda'}^{(s)}(\mathbf{k};\mathbf{R})^*\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{T}(\mathbf{k};\mathbf{R})\,\boldsymbol{\psi}. \quad (4.39)$$

Using Eqs. (4.26) and (4.18), we can write

$$\tau_{\lambda\lambda'}^{(s)}(\mathbf{k};\mathbf{R})^*=[\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})]^{-1}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R}^{-1}),$$
$$=[\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})\phi(\mathbf{k};\mathbf{R}^{-1}\mathbf{R}'^{-1},\mathbf{R}')]^{-1}\sum_{\lambda_1}\tau_{\lambda'\lambda_1}^{(s)}(\mathbf{k};\mathbf{R}^{-1}\mathbf{R}'^{-1})\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R}'),$$
$$=\frac{\phi(\mathbf{k};\mathbf{R}'\mathbf{R},\mathbf{R}^{-1}\mathbf{R}'^{-1})}{\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})\phi(\mathbf{k};\mathbf{R}^{-1}\mathbf{R}'^{-1},\mathbf{R}')}\sum_{\lambda_1}\tau_{\lambda_1\lambda'}^{(s)}(\mathbf{k};\mathbf{R}'\mathbf{R})^*\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R}'). \quad (4.40)$$

Substituting this result into Eq. (4.39), we obtain

$$\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{E}(\mathbf{k};s\lambda)=\sum_{\lambda_1}\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R}')\left\{\frac{f_s}{h}\sum_R\frac{\phi(\mathbf{k};\mathbf{R}',\mathbf{R})\phi(\mathbf{k};\mathbf{R}'\mathbf{R},\mathbf{R}^{-1}\mathbf{R}'^{-1})}{\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})\phi(\mathbf{k};\mathbf{R}^{-1}\mathbf{R}'^{-1},\mathbf{R}')}\tau_{\lambda_1\lambda'}^{(s)}(\mathbf{k};\mathbf{R}'\mathbf{R})^*\mathbf{T}(\mathbf{k};\mathbf{R}'\mathbf{R})\,\boldsymbol{\psi}\right\}. \quad (4.41)$$

We now use the general results that[10]

$$\phi(\mathbf{k};\mathbf{R}_1,\mathbf{R}_2)\phi(\mathbf{k};\mathbf{R}_1\mathbf{R}_2,\mathbf{R}_3)=\phi(\mathbf{k};\mathbf{R}_1,\mathbf{R}_2\mathbf{R}_3)\phi(\mathbf{k};\mathbf{R}_2,\mathbf{R}_3), \quad (4.42a)$$

$$\phi(\mathbf{k};\mathbf{R},\mathbf{R}^{-1})=\phi(\mathbf{k};\mathbf{R}^{-1},\mathbf{R}) \quad (4.42b)$$

to establish the result that

$$\phi(\mathbf{k};\mathbf{R}^{-1}\mathbf{R}'^{-1},\mathbf{R}')\phi(\mathbf{k};\mathbf{R}^{-1},\mathbf{R})=\phi(\mathbf{k};\mathbf{R}'\mathbf{R},\mathbf{R}^{-1}\mathbf{R}'^{-1})\phi(\mathbf{k};\mathbf{R}',\mathbf{R}). \quad (4.43)$$

It follows, therefore, that

$$\mathbf{T}(\mathbf{k};\mathbf{R}')\mathbf{E}(\mathbf{k};s\lambda)=\sum_{\lambda_1}\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R}')\{\mathbf{P}_{\lambda_1\lambda'}^{(s)}(\mathbf{k})\boldsymbol{\psi}\},$$
$$=\sum_{\lambda_1}\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R}')\mathbf{E}(\mathbf{k};s\lambda_1), \quad (4.44)$$

which is the result we set out to establish. To prove that $\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})$ is a projection operator, we apply it to the eigenvector $\mathbf{e}(\mathbf{k}s'a\lambda)$. Then, using Eq. (4.33), we have

$$\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})\mathbf{e}(\mathbf{k}s'a\lambda_1)=(f_s/h)\sum_R\sum_{\lambda_2}\tau_{\lambda\lambda'}^{(s)}(\mathbf{k};\mathbf{R})^*\times\tau_{\lambda_2\lambda_1}^{(s')}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}s'a\lambda_2). \quad (4.45)$$

The orthogonality[10] of the matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ expressed by

$$\sum_R\tau_{\lambda\lambda'}^{(s)}(\mathbf{k};\mathbf{R})^*\tau_{\lambda_2\lambda_1}^{(s')}(\mathbf{k};\mathbf{R})=(h/f_s)\delta_{ss'}\delta_{\lambda\lambda_2}\delta_{\lambda'\lambda_1} \quad (4.46)$$

allows Eq. (4.45) to be reduced to

$$\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})\mathbf{e}(\mathbf{k}s'a\lambda_1)=\delta_{ss'}\delta_{\lambda'\lambda_1}\mathbf{e}(\mathbf{k}sa\lambda). \quad (4.47)$$

Thus $\mathbf{P}_{\lambda\lambda'}^{(s)}(\mathbf{k})$ is a projection operator. In some applications it is useful to deal with the matrix

$$\mathbf{P}^{(s)}(\mathbf{k})=\sum_\lambda \mathbf{P}_{\lambda\lambda}^{(s)}(\mathbf{k}),$$
$$=(f_s/h)\sum_R\chi^{(s)}(\mathbf{k};\mathbf{R})^*\mathbf{T}(\mathbf{k};\mathbf{R}), \quad (4.48)$$

which projects out of an arbitrary vector that part which transforms according to the sth irreducible representation, for example

$$\mathbf{P}^{(s)}(\mathbf{k})\mathbf{e}(\mathbf{k}s'a\lambda)=\delta_{ss'}\mathbf{e}(\mathbf{k}sa\lambda). \quad (4.49)$$

In the special case that the sth irreducible representation appears only once in the reduction of the representation of $G_0(\mathbf{k})$ provided by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, so that c_s and the corresponding repetition index "a" both equal unity, the vector $\mathbf{E}(\mathbf{k};\,s\lambda)$, constructed according to Eq. (4.38) and normalized to unity, can be taken to be the eigenvector $\mathbf{e}(\mathbf{k};\,sa\lambda)$ of $\mathbf{D}(\mathbf{k})$.

In the case that the sth irreducible representation of $G_0(\mathbf{k})$ appears more than once, the vector $\mathbf{E}(\mathbf{k};\,s\lambda)$ is no longer an (un-normalized) eigenvector of $\mathbf{D}(\mathbf{k})$. Rather, in general, it is some linear combination of the c_s eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ $(a=1,\,2,\,\cdots,\,c_s)$ corresponding to the distinct eigenfrequencies $\{\omega_{sa}^2(\mathbf{k})\}$. In this case, multiplication of the vector $\mathbf{E}(\mathbf{k};\,s\lambda)$ by the matrix $\mathbf{D}(\mathbf{k})$ yields the c_s complex homogeneous equations in the c_s unknown complex components of this vector which suffice to determine the c_s eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and the associated eigenfrequencies $\{\omega_{sa}^2(\mathbf{k})\}$. In terms of real quantities one has $2c_s$ homogeneous real equations in $2c_s$ real unknowns. Actually, since the equations are homogeneous, one must only solve for $2(c_s-1)$ real quantities and then normalize the eigenvector to unity.

If for a particular wave vector or crystal point group the symmetry group of the dynamical matrix can be enlarged to include anti-unitary operations, the problem of determining the eigenvectors is simplified further. For example, if time-reversal symmetry does not introduce additional degeneracies, it is possible to reduce the number of unknown real quantities in $\mathbf{E}(\mathbf{k};\,s\lambda)$ from $2(c_s-1)$ to (c_s-1) when $c_s>1$. A complete discussion, including conditions for determining when additional degeneracies occur from the properties of the irreducible multiplier representations of the point group $G_0(\mathbf{k})$, is given in the next section. On the other hand, since additional degeneracy due to time-reversal symmetry is the exception rather than the rule, it is useful to derive a few simple properties of the irreducible multiplier representations under the assumption that additional degeneracy does not occur, without recourse to the general theory of corepresentations. This allows the interested reader to turn to the applications of the above results in Sec. 6 before studying Sec. 5.

If time-reversal symmetry does not produce additional degeneracy for the wave vector $\pi\mathbf{b}$ where Eq. (3.50) is applicable, then it is always possible to require $\mathbf{e}(\pi\mathbf{b}sa\lambda)$ to be real, i.e., to be an eigenvector of the anti-unitary operator $\mathbf{T}(\pi\mathbf{b};\,\mathbf{A})=\mathbf{K}_0$:

$$\begin{aligned}\mathbf{K}_0\mathbf{e}(\pi\mathbf{b}sa\lambda)&=\mathbf{e}^*(\pi\mathbf{b}sa\lambda),\\&=\mathbf{e}(\pi\mathbf{b}sa\lambda).\end{aligned}\tag{4.50a}$$

In the general case governed by Eq. (3.45), even when time-reversal symmetry does not produce additional degeneracy, it does not necessarily follow that the $\mathbf{e}(\mathbf{k}sa\lambda)$ can be chosen to be eigenvectors of one of the anti-unitary matrix operators $\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-}\mathbf{R})$ when $f_s>2$. In this section, for purposes of simplicity, we limit outselves to cases where it can be done and choose the phases according to Eqs. (4.4) and (4.12) so that

$$\begin{aligned}\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})\mathbf{e}(\mathbf{k}sa\lambda)&\equiv\mathbf{K}_0\exp[-i\mathbf{k}\cdot\mathbf{v}(S_{-})]\\&\times\boldsymbol{\Gamma}(\mathbf{k};\,\{\mathbf{S}_{-}\mid\mathbf{v}(S_{-})\})\mathbf{e}(\mathbf{k}sa\lambda)=-\mathbf{e}(\mathbf{k}sa\lambda),\end{aligned}\tag{4.50b}$$

or, applying $\mathbf{K}_0$ to both sides of Eq. (4.50b) and writing the result out in component form, we have

$$\begin{aligned}e_\alpha^*(\bar{\kappa}\mid\mathbf{k}sa\lambda)&=-\exp\{-i\mathbf{k}\cdot[\mathbf{x}(\bar{\kappa})-\mathbf{S}_{-}\mathbf{x}(\kappa)]\}\\&\times\sum_\beta(\mathbf{S}_{-})_{\alpha\beta}e_\beta(\kappa\mid\mathbf{k}sa\lambda),\end{aligned}\tag{4.50c}$$

where $\bar{\kappa}$ and κ are related as in Eq. (4.12). In the special case that the sth irreducible representation appears only once in the reduction of the representation of $G_0(\mathbf{k})$ provided by the matrices $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, the eigenvector $\mathbf{e}(\mathbf{k}sa\lambda)$, as given by Eq. (4.38) and Eqs. (4.50), simply serves to specify a convenient form for the eigenvectors. On the other hand, if the sth irreducible multiplier representation is multidimensional, $f_s\geq 2$, and appears more than once in the reduction, $c_s\geq 2$, the form of the eigenvector $\mathbf{E}(\mathbf{k};\,s\lambda)$ constructed according to Eq. (4.38) may be incompatible with Eqs. (4.50). To avoid duplication Eq. (4.50a) will be considered to be a special case of Eq. (4.50b). The following theorem provides a useful necessary condition on the form of the irreducible multiplier representation matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ for $\mathbf{E}(\mathbf{k};\,s\lambda)$ to be compatible with Eqs. (4.50):

If the matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ commutes with the anti-unitary matrix-operator $\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})$ and the vectors $\mathbf{e}(\mathbf{k}sa\lambda)$ are eigenvectors of $\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})$, then the irreducible representation matrix $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ of $\mathbf{T}(\mathbf{k};\mathbf{R})$ must be real.

The proof is straightforward. From Eqs. (4.50) and (4.33) we have

$$\begin{aligned}\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})\mathbf{e}(\mathbf{k}sa\lambda)&=-\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda),\\&=-\sum_{\lambda'}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda')\end{aligned}\tag{4.51a}$$

and

$$\begin{aligned}&\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda)\\&\quad=\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})\sum_{\lambda'}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda'),\\&\quad=-\sum_{\lambda'}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})^*\mathbf{e}(\mathbf{k}sa\lambda').\end{aligned}\tag{4.51b}$$

If $\mathbf{T}(\mathbf{k};\mathbf{R})$ and $\mathbf{T}(\mathbf{k};\,\mathbf{S}_{-})$ commute, since the vectors $\mathbf{e}(\mathbf{k}sa\lambda')$ are orthogonal, the coefficients of each $\mathbf{e}(\mathbf{k}sa\lambda')$ on the right-hand sides of Eqs. (4.51) must be equal:

$$\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})=\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})^*,\tag{4.52}$$

which is what we set out to prove.

Also, a condition on the representation matrix

$\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{S}_-^2)$ follows from

$$\mathbf{T}(\mathbf{k};\mathbf{S}_-)\mathbf{T}(\mathbf{k};\mathbf{S}_-)\mathbf{e}(\mathbf{k}sa\lambda)$$
$$=\phi(\mathbf{k};\mathbf{S}_-,\mathbf{S}_-)\mathbf{T}(\mathbf{k};\mathbf{S}_-^2)\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi(\mathbf{k};\mathbf{S}_-,\mathbf{S}_-)\sum_{\lambda'}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{S}_-^2)\mathbf{e}(\mathbf{k}sa\lambda').$$

But if $\mathbf{e}(\mathbf{k}sa\lambda)$ is an eigenvector of $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$, so that

$$\mathbf{T}(\mathbf{k};\mathbf{S}_-)\mathbf{T}(\mathbf{k};\mathbf{S}_-)\mathbf{e}(\mathbf{k}sa\lambda)=\mathbf{e}(\mathbf{k}sa\lambda),$$

we obtain the condition

$$\phi(\mathbf{k};\mathbf{S}_-,\mathbf{S}_-)\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{S}_-^2)=\delta_{\lambda'\lambda}.$$

Often this condition is an identity in that for certain crystals it can occur that

$$\mathbf{T}(\mathbf{k};\mathbf{S}_-)\mathbf{T}(\mathbf{k};\mathbf{S}_-)=\mathbf{T}(\mathbf{k};\boldsymbol{\varepsilon}).$$

This is the case, for example, when $\mathbf{S}_-=\mathbf{i}$.

The irreducible multiplier representations $\{\tau^{(s)}(\mathbf{k};\mathbf{R})\}$ of $G_0(\mathbf{k})$ do not necessarily satisfy Eq. (4.52). However, since the matrices $\{\boldsymbol{\tau}(\mathbf{k};\mathbf{R})\}$ may be defined in terms of the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$, it is always possible to obtain an equivalent irreducible multiplier representation which does satisfy Eq. (4.52) when $\mathbf{e}(\mathbf{k}sa\lambda)$ may be chosen to be an eigenvector of $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$. The important conclusion is that if we wish the vector $\mathbf{E}(\mathbf{k};s\lambda)$ in Eq. (4.38) to be an eigenvector of $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ the projection operator (4.37) must be constructed from an irreducible multiplier representation in which all the matrices $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ corresponding to $\mathbf{T}(\mathbf{k};\mathbf{R})$'s which commute with $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ are real. This is not a sufficient condition for the vectors $\mathbf{E}(\mathbf{k};s\lambda)$ to be compatible with Eqs. (4.50). For example, the irreducible multiplier representation ($f_s\geq 2$) may be real with matrices $\boldsymbol{\tau}(\mathbf{k};\mathbf{R})$ corresponding to elements $\mathbf{T}(\mathbf{k};\mathbf{R})$ which do not commute with $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ in diagonal form, while matrices $\boldsymbol{\tau}(\mathbf{k};\mathbf{R})$ corresponding to elements $\mathbf{T}(\mathbf{k};\mathbf{R})$ which do commute with $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ in nondiagonal form. Clearly this is incompatible with $\mathbf{E}(\mathbf{k};s\lambda)$ being an eigenvector of $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$. Thus the irreducible multiplier representation used in Eq. (4.37) should be chosen according to the following: (i) The matrices $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ corresponding to $\mathbf{T}(\mathbf{k};\mathbf{R})$'s which commute with $\mathbf{T}(\mathbf{k};\mathbf{S}_-)$ must be real; (ii) As many as possible of these $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ should be in diagonal form. Given any irreducible multiplier representation of $G_0(\mathbf{k})$, it is a trivial matter to find an equivalent representation which conforms with these requirements.

The results given by Eqs. (4.36) and Eqs. (4.38) formally solve the problem posed in this paper, except for additional degeneracy due to time-reversal symmetry. From Eq. (4.36) we can obtain the symmetries of the normal modes described by the wave vector $\mathbf{k}$, i.e., the irreducible multiplier representations of $G_0(\mathbf{k})$ according to which they transform; the dimensionalities of the irreducible representations contained in the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ give the degeneracies of the modes corresponding to the wave vector $\mathbf{k}$ due to spatial symmetry. From Eq. (4.38) we can obtain the forms of these eigenvectors. Examples of the use of these results are given in Sec. 6.

We conclude this section by deriving a result which may be useful in determining the frequencies of individual normal modes. It is the extension to the lattice dynamical case of a theorem first established by Wigner[17] in the context of molecular vibrations.

Repeated application of the matrix $\mathbf{D}(\mathbf{k})$ to both sides of the eigenvalue equation, Eq. (2.17) yields the result that

$$\mathbf{D}^n(\mathbf{k})\mathbf{e}(\mathbf{k}sa\lambda)=\omega_{sa}^{2n}(\mathbf{k})\mathbf{e}(\mathbf{k}sa\lambda). \qquad (4.53)$$

Introducing the column vector and row vector notation for $\mathbf{e}(\mathbf{k}sa\lambda)$ and its Hermitian conjugate $\mathbf{e}^+(\mathbf{k}sa\lambda)$, the closure relation (2.23b) can be recast into the matrix form:

$$\sum_{sa\lambda}\mathbf{e}(\mathbf{k}sa\lambda)\mathbf{e}^+(\mathbf{k}sa\lambda)=\boldsymbol{\varepsilon}_r, \qquad (4.54)$$

where $\boldsymbol{\varepsilon}_r$ is the $3r\times 3r$ unit matrix, and (4.53) can be rewritten as

$$\mathbf{D}^n(\mathbf{k})=\sum_{sa\lambda}\omega_{sa}^{2n}(\mathbf{k})\mathbf{e}(\mathbf{k}sa\lambda)\mathbf{e}^+(\mathbf{k}sa\lambda). \qquad (4.55)$$

To focus on the frequencies associated with the s' irreducible representation we project onto this subspace by applying the projection operator $\mathbf{P}^{(s')}(\mathbf{k})$ defined in Eq. (4.48) to both sides of Eq. (4.55) and obtain

$$\mathbf{P}^{(s')}(\mathbf{k})\mathbf{D}^n(\mathbf{k})=\sum_{a\lambda}\omega_{s'a}^{2n}(\mathbf{k})\mathbf{e}(\mathbf{k}s'a\lambda)\mathbf{e}^+(\mathbf{k}s'a\lambda). \qquad (4.56)$$

The eigenvectors on the right-hand side can be eliminated by taking the trace of both sides of (4.56) with respect to "$\kappa\alpha$" and using the normalization condition (2.23a), that is,

$$\mathrm{Tr}\{\sum_{a\lambda}\omega_{sa}^{2n}(\mathbf{k})\mathbf{e}(\mathbf{k}s\lambda a)\mathbf{e}^+(\mathbf{k}s\lambda a)\}$$
$$=\sum_{a\lambda}\omega_{sa}^{2n}(\mathbf{k})\sum_{\alpha\kappa}e_\alpha(\kappa\,|\,\mathbf{k}sa\lambda)e_\alpha^*(\kappa\,|\,\mathbf{k}sa\lambda),$$
$$=\sum_{a\lambda}\omega_{sa}^{2n}(\mathbf{k}),$$
$$=f_s\sum_a\omega_{sa}^{2n}(\mathbf{k}). \qquad (4.57)$$

Writing the $\kappa'\beta$; $\kappa\alpha$ element of the matrix $\mathbf{D}^n(\mathbf{k})$ as $[\mathbf{D}^n(\mathbf{k})]_{\beta\alpha}{}^{\kappa'\kappa}$, the diagonal elements of the matrix on the left-hand side of Eq. (4.56) are

$$\sum_{\kappa'\beta}(f_s/h)\sum_{\mathbf{R}}\chi^{(s)}(\mathbf{k};\mathbf{R})^*T_{\alpha\beta}(\kappa\kappa'\,|\,\mathbf{k};\mathbf{R})[\mathbf{D}^n(\mathbf{k})]_{\beta\alpha}{}^{\kappa'\kappa}$$
$$=(f_s/h)\sum_{\mathbf{R}}\sum_{\beta}\chi^{(s)}(\mathbf{k};\mathbf{R})^*$$
$$\times\exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{R}\mathbf{x}(F_0^{-1}(\kappa;R))]\}R_{\alpha\beta}$$
$$\times[\mathbf{D}^n(\mathbf{k})]_{\beta\alpha}{}^{F_0^{-1}(\kappa;R)\kappa} \qquad (4.58)$$

where the explicit form (3.17b) has been used for $T_{\alpha\beta}(\kappa\kappa'\,|\,\mathbf{k};\mathbf{R})$. Equating the trace of (4.58) to (4.57), we have finally the result that the sum of the $2n$th powers of the frequencies whose associated eigenvectors transform according to the sth irreducible multiplier representation of $G_0(\mathbf{k})$ is given by

$$\sum_{a=1}^{c_s} \omega_{sa}^{2n}(\mathbf{k}) = h^{-1} \sum_{\mathrm{R}} \sum_{\kappa\alpha\beta} \chi^{(s)}(\mathbf{k};\mathbf{R})^* \times \exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa) - \mathbf{R}\mathbf{x}(F_0^{-1}(\kappa;R))]\} \times R_{\alpha\beta}[\mathbf{D}^n(\mathbf{k})]_{\beta\alpha}{}^{F_0^{-1}(\kappa;R)\kappa} \tag{4.59}$$

In the special case that the sth irreducible representation occurs only once in the representation of $G_0(\mathbf{k})$ generated by the $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, so that the repetition index a can be suppressed, we obtain the simple result that

$$\omega_s^2(\mathbf{k}) = h^{-1} \sum_{\mathrm{R}} \sum_{\kappa\alpha\beta} \chi^{(s)}(\mathbf{k};\mathbf{R})^* \times \exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa) - \mathbf{R}\mathbf{x}(F_0^{-1}(\kappa;R))]\} \times R_{\alpha\beta} D_{\beta\alpha}(F_0^{-1}(\kappa;R)\kappa\mid\mathbf{k}). \tag{4.60}$$

The result given by Eq. (4.59) is also useful if the sth irreducible representation appears twice in the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$. If we denote the two frequencies associated with this representation by $\omega_{s1}^2(\mathbf{k})$ and $\omega_{s2}^2(\mathbf{k})$, then from Eq. (4.59) we have that

$$\omega_{s1}^2(\mathbf{k}) + \omega_{s2}^2(\mathbf{k}) = a_s(\mathbf{k}),$$
$$\omega_{s1}^4(\mathbf{k}) + \omega_{s2}^4(\mathbf{k}) = b_s(\mathbf{k}), \tag{4.61}$$

where $a_s(\mathbf{k})$ and $b_s(\mathbf{k})$ are obtained by setting $n=1$ and $n=2$ in the right-hand side of Eq. (4.59), respectively. Solving the pair of equations (4.61) we find that

$$\omega_{s1}^2(\mathbf{k}) = \tfrac{1}{2}\{a_s(\mathbf{k}) - [2b_s(\mathbf{k}) - a_s^2(\mathbf{k})]^{1/2}\},$$
$$\omega_{s2}^2(\mathbf{k}) = \tfrac{1}{2}\{a_s(\mathbf{k}) + [2b_s(\mathbf{k}) - a_s^2(\mathbf{k})]^{1/2}\}. \tag{4.62}$$

If a particular irreducible representation occurs more than twice in the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, this method of computing the $\{\omega_{sa}^2(\mathbf{k})\}$ loses its simplicity.

5. CONSEQUENCES OF TIME-REVERSAL SYMMETRY

The fact that, under special circumstances, time-reversal symmetry can produce extra degeneracies in the lattice vibration frequencies in addition to those due to the multidimensionality of the irreducible representations of the space group $G_{\mathbf{k}}$ was pointed out by Herring[22] in a classic paper on the effects of time-reversal symmetry on energy bands. Herring's treatment was based on Wigner's[23] early work on time-reversal in which the reality of the Hamiltonian and the property that the operation of complex conjugation commutes with the spatial symmetry operations play an essential role. To apply this approach to our problem would in essence require us to deal with the eigenvalue problem in real form, for example, by use of Eq. (2.12) and the irreducible representations of the space group G of the crystal, even though the final conditions for the existence of extra degeneracies could be expressed in terms of the irreducible representations of the space group $G_{\mathbf{k}}$. Rather than taking this approach, we prefer to use Wigner's more recent method of corepresentations,[16] modified to include the multipliers of Eq. (3.45), which allows us to deal with the eigenvalue problem in terms of the dynamical matrix and the symmetry operations $\mathbf{T}(\mathbf{k};\mathbf{R})$ of the point group $G_0(\mathbf{k};-\mathbf{k})$. This modification of Wigner's method will be referred to as the multiplier corepresentation method. The conditions for the existence of extra degeneracies due to extending the group of unitary symmetry operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k})$ to form the enlarged symmetry group $\{\mathbf{T}(\mathbf{k};\bar{\mathbf{R}})\}$, containing unitary and anti-unitary operations, of the group $G_0(\mathbf{k};-\mathbf{k})$ will be expressed entirely in terms of the known irreducible multiplier representations[12] $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k})$ which is an invariant subgroup of $G_0(\mathbf{k};-\mathbf{k})$. In particular, we will see that under the influence of an anti-unitary symmetry operation the irreducible multiplier representations separate into three types with properties which are similar to those of the analogous ordinary irreducible representations.[16] With one type are associated no additional degeneracies; with the other, there are two. The method of multiplier correpresentations has been used recently to study the electron energy spectrum in crystals.[24,25] In the following analysis we assume that we are dealing either with a crystal whose symmetry is such that $-\mathbf{k}$ is in the star of $\mathbf{k}$ or with a wave vector which equals π times a reciprocal lattice vector, so that Eq. (3.50) applies. The latter case will be treated as a special case of the former, keeping in mind that for a product involving an anti-unitary operation the multipliers in Eqs. (3.46) and (3.47) are altered according to Eqs. (3.51), (3.52) and (3.53).

Before beginning the general analysis we wish to derive a few results which will prove useful in the following. From the definition of the matrix operators $\mathbf{T}(\mathbf{k};\mathbf{R})$ we see that multiplication is associative for unitary and anti-unitary operations:

$$[\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_1)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_2)]\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_3) = \mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_1)[\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_2)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_3)]. \tag{5.1}$$

Carrying out the multiplications according to Eq.

[22] C. Herring, Phys. Rev. **52**, 361 (1937).

[23] E. Wigner, Nachr. Akad. Wiss. Goettingen, Math.—Kl. Physik, p. 546 (1932) [English translation in *Group Theory and Solid State Physics: I.* P. H. Meijer, Ed. (Gordon and Breach Science Publishers, New York, 1964)].

[24] G. F. Karavaev, N. V. Kudryavtseva, and V. A. Chaldzskev, Fiz. Tverd. Tela **4**, 3471 (1962) [English transl.: Soviet Phys.—Solid State **4**, 2540 (1963)].

[25] N. V. Kudryavtseva, Fiz. Tverd. Tela **7**, 998 (1965) [English transl.: Soviet Phys.—Solid State **7**, 803 (1965)].

(3.45), we obtain

$$\phi(\mathbf{k};\bar{\mathbf{R}}_1,\bar{\mathbf{R}}_2)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_1,\bar{\mathbf{R}}_2)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_3)$$
$$=\phi(\mathbf{k};\bar{\mathbf{R}}_1,\bar{\mathbf{R}}_2)\phi(\mathbf{k};\bar{\mathbf{R}}_1\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_1\bar{\mathbf{R}}_2\bar{\mathbf{R}}_3),$$
$$=\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_1)\phi(\mathbf{k};\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3)\mathbf{T}(\mathbf{k};\bar{\mathbf{R}}_2\bar{\mathbf{R}}_3). \tag{5.2}$$

To reduce the last term in Eq. (5.2) further it is necessary to distinguish the unitary and the anti-unitary possibilities for $\mathbf{T}(\mathbf{k};\mathbf{R}_1)$. Using the notation $\mathbf{R}_1$ and $\mathbf{A}_1$ for $\mathbf{R}_1$ to distinguish the two cases, it follows directly from Eq. (5.2) that the multipliers $\phi(\mathbf{k};\mathbf{R}_i,\bar{\mathbf{R}}_j)$ satisfy the functional equations

$$\phi(\mathbf{k};\mathbf{R}_1,\bar{\mathbf{R}}_2)\phi(\mathbf{k};\mathbf{R}_1\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3)=\phi(\mathbf{k};\mathbf{R}_1,\bar{\mathbf{R}}_2\bar{\mathbf{R}}_3)\phi(\mathbf{k};\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3), \tag{5.3a}$$

$$\phi(\mathbf{k};\mathbf{A}_1,\bar{\mathbf{R}}_2)\phi(\mathbf{k};\mathbf{A}_1\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3)=\phi(\mathbf{k};\mathbf{A}_1,\mathbf{R}_2\mathbf{R}_3)\phi^*(\mathbf{k};\bar{\mathbf{R}}_2,\bar{\mathbf{R}}_3). \tag{5.3b}$$

A second useful result concerns the inverse of $\mathbf{T}(\mathbf{k};\mathbf{A})$. From Eq. (3.45) we see that

$$\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{T}(\mathbf{k};\mathbf{A}^{-1})=\phi(\mathbf{k};\mathbf{A},\mathbf{A}^{-1})\mathbf{T}(\mathbf{k};\varepsilon), \tag{5.4}$$

so that multiplying both sides of Eq. (5.4) from the left with $\mathbf{T}^{-1}(\mathbf{k};\mathbf{A})$ gives

$$\mathbf{T}(\mathbf{k};\mathbf{A}^{-1})=\phi^*(\mathbf{k};\mathbf{A},\mathbf{A}^{-1})\mathbf{T}^{-1}(\mathbf{k};\mathbf{A}) \tag{5.5a}$$

or

$$\mathbf{T}^{-1}(\mathbf{k};\mathbf{A})=\phi(\mathbf{k};\mathbf{A},\mathbf{A}^{-1})\mathbf{T}(\mathbf{k};\mathbf{A}^{-1}). \tag{5.5b}$$

Setting $\mathbf{A}_1=\mathbf{R}_3=\mathbf{A}$ and $\mathbf{R}_2=\mathbf{A}^{-1}$ in Eq. (5.3b) yields the useful relation

$$\phi(\mathbf{k};\mathbf{A},\mathbf{A}^{-1})=\phi^*(\mathbf{k};\mathbf{A}^{-1},\mathbf{A}). \tag{5.6}$$

The extension of the analysis that leads from Eqs. (4.13) to (4.33) to include anti-unitary matrix operators is straightforward. Operating on both sides of Eq. (4.32) from the left with the matrix operator $\mathbf{T}(\mathbf{k};\mathbf{A})$ and using the fact that $\mathbf{T}(\mathbf{k};\mathbf{A})$ commutes with $\mathbf{D}(\mathbf{k})$, we obtain

$$\mathbf{D}(\mathbf{k})\{\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)\}=\omega_{sa}^2(\mathbf{k})\{\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)\}. \tag{5.7}$$

Therefore, if $\mathbf{e}(\mathbf{k}sa\lambda)$ is an eigenvector of $\mathbf{D}(\mathbf{k})$ with eigenvalue $\omega_{sa}^2(\mathbf{k})$, then so is $\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)$ for every operation $\mathbf{A}$ of the coset $\mathbf{S}\_G_0(\mathbf{k})$ of the point group $G_0(\mathbf{k};-\mathbf{k})$. Consequently, $\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)$ is a linear combination of the eigenvectors of $\mathbf{D}(\mathbf{k})$ whose eigenvalues are equal to $\omega_{sa}^2(\mathbf{k})$.

Instead of introducing the concept of corepresentations at this juncture we prefer to derive the conditions for the existence of additional degeneracies due to time-reversal symmetry by a direct investigation of the linear dependence of the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)$. Clearly, if the two sets of eigenvectors are required to be linearly independent by time-reversal symmetry, there is an additional degeneracy. To proceed we define

$$\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\equiv\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda), \tag{5.8}$$

and consider the transformation properties of the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ under the spatial symmetry operations $\mathbf{T}(\mathbf{k};\mathbf{R})$ of the point group $G_0(\mathbf{k})$. The $\mathbf{A}_0$ is an arbitrary element of the coset $\mathbf{S}\_G_0(\mathbf{k})$, the choice being governed by convenience only. Recall from Eq. (4.33) that

$$\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda)=\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{R})\mathbf{e}(\mathbf{k}sa\lambda'). \tag{5.9}$$

To obtain the effect of $\mathbf{T}(\mathbf{k};\mathbf{R})$ on $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ we make use of the matrix-operator identity [see Eqs. (3.45) and (5.3)]

$$\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{A}_0)=\mathbf{T}(\mathbf{k};\mathbf{A}_0\mathbf{A}_0^{-1}\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{A}_0),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{A}_0),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0), \tag{5.10a}$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)\phi(\mathbf{k};\mathbf{R},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0) \tag{5.10b}$$

and the fact that $\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0$ is an element of $G_0(\mathbf{k})$. Therefore, using the form in Eq. (5.10a), we have

$$\mathbf{T}(\mathbf{k};\mathbf{R})\bar{\mathbf{e}}(\mathbf{k}sa\lambda)=\mathbf{T}(\mathbf{k};\mathbf{R})\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda'),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*\bar{\mathbf{e}}(\mathbf{k}sa\lambda'). \tag{5.11}$$

That is, the f_s eigenvectors $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ transform into linear combinations of themselves under a unitary operation $\mathbf{T}(\mathbf{k};\mathbf{R})$ according to the unitary irreducible multiplier representation $\{\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k})$, where, according to Eqs. (5.11) and (5.3),

$$\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\equiv\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*, \tag{5.12a}$$

$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)\phi(\mathbf{k};\mathbf{R},\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*. \tag{5.12b}$$

The unitarity and the irreducibility of the $\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ are direct consequences of the unitarity and the irreducibility of the $\tau^{(s)}(\mathbf{k};\mathbf{R})$.

We now prove that the matrices $\{\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ defined by Eqs. (5.12) form a multiplier representation of $G_0(\mathbf{k})$ with the same factor system (i.e., multipliers) as occur in the representation provided by the $\{\tau^{(s)}(\mathbf{k};\mathbf{R})\}$. Taking the complex conjugate of Eq. (4.18) to evaluate the product of the matrices $\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_1)$ and $\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_2)$ gives [the choice made of (a) and (b) forms is for convenience only]:

$$\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_1)\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_2)=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_1)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0)$$
$$\times\phi(\mathbf{k};\mathbf{R}_2,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2\mathbf{A}_0)^*, \tag{5.13}$$

which must be related to

$$\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_1\mathbf{R}_2)=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2\mathbf{A}_0)^*. \tag{5.14}$$

By repeated application of Eqs. (5.3) it can be shown that

$$\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0)=\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{A}_0\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0)\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0) \tag{5.15}$$

and

$$\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{A}_0\mathbf{A}_0^{-1}\mathbf{R}_2\mathbf{A}_0)=\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{R}_2)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{R}_2,\mathbf{A}_0),$$
$$=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_1)\phi(\mathbf{k};\mathbf{A}_0\mathbf{A}_0^{-1}\mathbf{R}_1,\mathbf{R}_2)\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2)$$
$$\times\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{R}_2,\mathbf{A}_0). \tag{5.16}$$

Substituting Eqs. (5.15) and (5.16) for the appropriate multiplier in Eq. (5.13) and performing the obvious cancellations yields

$$\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_1)\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_2)=\phi(\mathbf{k};\mathbf{R}_1,\mathbf{R}_2)\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2)\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}_1\mathbf{R}_2\mathbf{A}_0)^*,$$
$$=\phi(\mathbf{k};\mathbf{R}_1,\mathbf{R}_2)\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R}_1\mathbf{R}_2), \tag{5.17}$$

which is the desired result.

For later reference it is useful to record the results of applying an anti-unitary matrix operator $\mathbf{T}(\mathbf{k};\mathbf{A})$ to the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$. From Eqs. (3.45), (5.8), and (5.9) we obtain

$$\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda)$$
$$=\mathbf{T}(\mathbf{k};\mathbf{A}_0\mathbf{A}_0^{-1}\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{A})\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{A})\mathbf{T}(\mathbf{k};\mathbf{A}_0)\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{A})\mathbf{e}(\mathbf{k}sa\lambda'),$$
$$=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{A})\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{A})^*\bar{\mathbf{e}}(\mathbf{k}sa\lambda') \tag{5.18}$$

and

$$\mathbf{T}(\mathbf{k};\mathbf{A})\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$$
$$=\mathbf{T}(\mathbf{k};\mathbf{A})\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi(\mathbf{k};\mathbf{A},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda),$$
$$=\phi(\mathbf{k};\mathbf{A},\mathbf{A}_0)\sum_{\lambda'=1}^{f_s}\tau_{\lambda'\lambda}^{(s)}(\mathbf{k};\mathbf{A}\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda'). \tag{5.19}$$

$\mathbf{A}_0^{-1}$ and $\mathbf{A}\mathbf{A}_0$ are elements of $G_0(\mathbf{k})$, so that the corresponding $\tau^{(s)}$ matrices in Eqs. (5.18) and (5.19) are well-defined.

We now turn our attention to the question of the linear dependence of the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\mathbf{e}(\mathbf{k}sa\lambda)$. This question can be resolved by considering the relationship between the irreducible multiplier representations $\{\tau^{(s)}(\mathbf{k};\mathbf{R})\}$ and $\{\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k})$ which define the transformation properties of the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$, respectively, under the operations of the unitary matrices $\mathbf{T}(\mathbf{k};\mathbf{R})$. Noting that the irreducible multiplier representations $\tau^{(s)}$ and $\bar{\tau}^{(s)}$ belong to the same factor system, they can be either equivalent or inequivalent. The latter of these two possibilities is simpler and will be treated first.

If the irreducible multiplier representations $\tau^{(s)}$ and $\bar{\tau}^{(s)}$ are not equivalent (such representations will be referred to as of the third type) the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ are orthogonal, since they belong to different irreducible multiplier representations of the point group $G_0(\mathbf{k})$. Since $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ are eigenvectors of the dynamical matrix $\mathbf{D}(\mathbf{k})$ with equal eigenvalues $\omega_{sa}^2(\mathbf{k})$, the f_s-fold degeneracy is doubled to $2f_s$ by time-reversal symmetry for this case.

In the alternative situation $\boldsymbol{\tau}^{(s)}$ and $\bar{\boldsymbol{\tau}}^{(s)}$ are equivalent. At first sight one might expect that the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ could not be linearly independent. However, Wigner[16] has shown that it is possible under special circumstances to have additional degeneracies in this case. The analysis for multiplier representations is very similar to that for ordinary representations.[16] For the sake of completeness we carry out the analysis for multiplier representations and derive a criterion for determining whether the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ are linearly independent or whether they are linearly dependent.

Since $\boldsymbol{\tau}^{(s)}$ and $\bar{\boldsymbol{\tau}}^{(s)}$ are equivalent and belong to the same factor system, they are related by a similarity transformation:

$$\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\times\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*=\boldsymbol{\beta}^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta}, \quad (5.20)$$

where $\boldsymbol{\beta}$ is a unitary matrix. We now show that the property of the irreducible multiplier representation that causes the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ to be linearly independent is reflected in the "structure" [see comment below Eqs. (5.33)] of the unitary matrix $\boldsymbol{\beta}$ and is expressible as a condition on the matrix $\boldsymbol{\beta}\boldsymbol{\beta}^*$. To gain some insight into the way in which this comes about we begin by showing that the matrix $\boldsymbol{\beta}$ is unique up to a phase factor and that it may be expressed in terms of the irreducible multiplier representation matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$.

The uniqueness of form for $\boldsymbol{\beta}$ follows from the irreducibility of the matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$, since, if $\boldsymbol{\gamma}$ is a second matrix which connects $\bar{\boldsymbol{\tau}}^{(s)}$ and $\boldsymbol{\tau}^{(s)}$ as in Eq. (5.20), then

$$\boldsymbol{\gamma}^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\gamma}=\boldsymbol{\beta}^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta} \quad (5.21)$$

for all elements $\mathbf{R}$ of $G_0(\mathbf{k})$. Multiplying Eq. (5.21) by $\boldsymbol{\gamma}$ from the left and $\boldsymbol{\beta}^{-1}$ from the right gives

$$\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\gamma}\boldsymbol{\beta}^{-1}=\boldsymbol{\gamma}\boldsymbol{\beta}^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}), \quad (5.22)$$

that is, the matrix $\boldsymbol{\gamma}\boldsymbol{\beta}^{-1}$ commutes with all the matrices of an irreducible multiplier representation of the group $G_0(\mathbf{k})$. It follows from Schur's Lemmas[10,16] that the matrix $\boldsymbol{\gamma}\boldsymbol{\beta}^{-1}$ is proportional to the unit matrix, so that

$$\boldsymbol{\gamma}=c\boldsymbol{\beta}, \quad (5.23)$$

where $|c|=1$. Furthermore, Eq. (5.20) may be rewritten as a condition on $\boldsymbol{\beta}$, namely that $\boldsymbol{\beta}$ is a matrix that satisfies the relation

$$\boldsymbol{\beta}=\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta}\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})^{\dagger}. \quad (5.24)$$

It follows from the above discussion that any non-null matrix that satisfies Eq. (5.24) is proportional to $\boldsymbol{\beta}$. In particular, the matrix

$$\boldsymbol{\beta}=c'\sum_{\mathbf{R}'}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}')\mathbf{X}\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R}')^{\dagger} \quad (5.25)$$

satisfies (5.24) for arbitrary $\mathbf{X}$. Thus, since the matrices $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ are determined by Eqs. (5.12) once the matrices $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and $\mathbf{A}_0$ are given, the matrix $\boldsymbol{\beta}$ is defined up to a phase factor by the irreducible multiplier representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and the element $\mathbf{A}_0$. The matrix defined by Eq. (5.25) is a null matrix if the representations $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ are inequivalent, as can be seen from the orthogonality theorem as expressed in Eq. (4.46). Thus these results are consistent with irreducible multiplier representations of the third type.

In the last paragraph we emphasized that not only the existence but also the "form" of the matrix $\boldsymbol{\beta}$ is a unique property of an irreducible multiplier representation. We now show that the structure of the matrix $\boldsymbol{\beta}$ characterizes the irreducible multiplier representations which satisfy Eq. (5.20) by deriving a condition on the matrix $\boldsymbol{\beta}\boldsymbol{\beta}^*$. Substituting the rotational element $\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0$ for $\mathbf{R}$ in the complex conjugate of Eq. (5.20) and using Eq. (5.12a) we obtain

$$\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*=\boldsymbol{\beta}^{-1*}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*\boldsymbol{\beta}^*, \quad (5.26a)$$
$$=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\times\boldsymbol{\beta}^{-1*}\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta}^*,$$
$$=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\times\boldsymbol{\beta}^{-1*}\boldsymbol{\beta}^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta}\boldsymbol{\beta}^*, \quad (5.26b)$$

where Eq. (5.20) has been used in the last step. On the other hand, replacing $\mathbf{R}$ by $\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0$ in Eq. (5.12a) and taking the complex conjugate of the resulting equation yields

$$\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-2}\mathbf{R}\mathbf{A}_0)\times\phi(\mathbf{k};\mathbf{A}_0^{-2}\mathbf{R}\mathbf{A}_0,\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2}\mathbf{R}\mathbf{A}_0^2). \quad (5.27)$$

Noting that $\mathbf{A}_0^{-2}$ and $\mathbf{A}_0^2$ are elements of $G_0(\mathbf{k})$, then $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2}\mathbf{R}\mathbf{A}_0^2)$ may be written as a product of three $\boldsymbol{\tau}^{(s)}$ matrices by applying Eq. (4.33) twice:

$$\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2}\mathbf{R}\mathbf{A}_0^2)=\phi^*(\mathbf{k};\mathbf{A}_0^{-2},\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-2}\mathbf{R},\mathbf{A}_0^2)\times\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2). \quad (5.28)$$

Substituting Eq. (5.28) in Eq. (5.27), after repeated application of Eqs. (5.3) on the multipliers, one obtains

$$\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*=\phi^*(\mathbf{k};\mathbf{A}_0^2,\mathbf{A}_0^{-2})\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\times\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2). \quad (5.29)$$

Equating the right-hand sides of Eqs. (5.26) and (5.29) yields the important result

$$(\boldsymbol{\beta}\boldsymbol{\beta}^*)^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\beta}\boldsymbol{\beta}^*=\phi^*(\mathbf{k};\mathbf{A}_0^2,\mathbf{A}_0^{-2})\times\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2). \quad (5.30)$$

Clearly, the matrix $\boldsymbol{\beta}\boldsymbol{\beta}^*\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2})$ commutes with all the matrices $\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})$ of an irreducible multiplier representation, and therefore must be proportional to the unit matrix. It follows that

$$\beta\beta^* = c\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2). \tag{5.31}$$

Since all the matrices in Eq. (5.31) are unitary, $cc^*=1$. To obtain c, set $\mathbf{R}=\mathbf{A}_0^2$ in Eq. (5.20) and use Eq. (5.31) to express $\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2)$:

$$\begin{aligned}\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2)^* &= \phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)^2 c\beta^*\beta,\\ &= \beta^{-1}\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2)\beta,\\ &= c^{-1}\beta^{-1}\beta\beta^*\beta = c^{-1}\beta^*\beta.\end{aligned} \tag{5.32}$$

Therefore $c=\pm\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)$ and

$$\beta\beta^* = \phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2) \tag{5.33a}$$

or

$$\beta\beta^* = -\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2). \tag{5.33b}$$

These two cases are referred to as being of the first and second types, respectively. If (as is often the case) the element $\mathbf{A}_0$ is such that $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2)$ is equal to the unit matrix, that is, Eqs. (5.33) become $\beta\beta^*=\pm\mathbf{1}$, then the matrix β is symmetric or antisymmetric, respectively. This is an example of what was meant by the "structure" of the matrix β in the paragraph below Eq. (5.20). It is shown below that the eigenvectors $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ are linearly independent when the matrix β satisfies Eq. (5.33b), and thus time-reversal symmetry produces an additional degeneracy. If Eq. (5.33a) applies, time-reversal symmetry does not affect the degeneracy.

An important feature of Eqs. (5.33) is that their form is invariant under a unitary transformation on the representation matrices. To see this, let the representation $\tau^{(s)}$ undergo a unitary transformation with a matrix $\mathbf{U}$:

$$\tau'^{(s)}(\mathbf{k};\mathbf{R}) = \mathbf{U}^{-1}\tau^{(s)}(\mathbf{k};\mathbf{R})\mathbf{U}. \tag{5.34}$$

Then there exists a set of matrices $\{\bar{\tau}'^{(s)}(\mathbf{k};\mathbf{R})\}$ that is related to the set $\{\tau'^{(s)}(\mathbf{k};\mathbf{R})\}$ in the same way as the sets $\{\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and $\{\tau^{(s)}(\mathbf{k};\mathbf{R})\}$ are related—that is, according to Eq. (5.20) with β replaced by a new matrix β':

$$\bar{\tau}'^{(s)}(\mathbf{k};\mathbf{R}) = \phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\times\tau'^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*, \tag{5.35a}$$

$$= \beta'^{-1}\tau'^{(s)}(\mathbf{k};\mathbf{R})\beta'. \tag{5.35b}$$

Using Eqs. (5.20) and (5.34) in Eq. (5.35a), we obtain

$$\bar{\tau}'^{(s)}(\mathbf{k};\mathbf{R}) = \mathbf{U}^{-1*}\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\mathbf{U}^*, \tag{5.36a}$$

$$= \mathbf{U}^{-1*}\beta^{-1}\mathbf{U}\tau'^{(s)}(\mathbf{k};\mathbf{R})\mathbf{U}^{-1}\beta\mathbf{U}^*. \tag{5.36b}$$

Therefore

$$\beta' = \mathbf{U}^{-1}\beta\mathbf{U}^*, \tag{5.37}$$

where we have set the arbitrary phase factor equal to unity. The important feature of Eq. (5.37) is that, in general, β' and β are *not* related by a similarity transformation even though $\tau'^{(s)}$ and $\tau^{(s)}$ are. Thus, from Eqs. (5.33), (5.34), and (5.37), we have

$$\begin{aligned}\beta'\beta'^* &= \mathbf{U}^{-1}\beta\mathbf{U}^*\mathbf{U}^{-1*}\beta^*\mathbf{U} = \mathbf{U}^{-1}\beta\beta^*\mathbf{U},\\ &= \pm\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\mathbf{U}^{-1}\tau^{(s)}(\mathbf{k};\mathbf{A}_0^2)\mathbf{U},\\ &= \pm\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau'^{(s)}(\mathbf{k};\mathbf{A}_0^2),\end{aligned} \tag{5.38}$$

which is the result we wished to demonstrate. Thus the "type" of the irreducible multiplier representation cannot be changed by a similarity transformation.

Let us now turn our attention to the problem of the linear independence of $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}(\mathbf{k}sa\lambda)$ for Eq. (5.33b). For convenience we introduce a bra-ket type of notation for scalar products. Let φ and ψ be 2 arbitrary vectors in the $3r$-dimensional space. Then the (Hermitian) scalar product [see Eq. (2.23a)] is denoted by

$$\langle\varphi,\psi\rangle \equiv \sum_{\alpha,\kappa}\varphi_\alpha^*(\kappa)\psi_\alpha(\kappa). \tag{5.39}$$

It is important to distinguish the effect on the scalar product of a unitary and an anti-unitary transformation on the vectors φ and ψ. In particular,

$$\langle\mathbf{T}(\mathbf{k};\mathbf{R})\varphi,\mathbf{T}(\mathbf{k};\mathbf{R})\psi\rangle = \langle\varphi,\psi\rangle \tag{5.40}$$

while

$$\langle\mathbf{T}(\mathbf{k};\mathbf{A})\varphi,\mathbf{T}(\mathbf{k};\mathbf{A})\psi\rangle = \langle\psi,\varphi\rangle. \tag{5.41}$$

Instead of dealing with the eigenvectors $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$ which transform according to $\{\bar{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}=\{\beta^{-1}\times\tau^{(s)}(\mathbf{k};\mathbf{R})\beta\}$ under the operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$, it is convenient to introduce a linear combination of $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$ which transforms according to $\{\tau^{(s)}(\mathbf{k};\mathbf{R})\}$. Let us denote this combination by $\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)$, and define it by

$$\bar{\mathbf{e}}'(\mathbf{k}sa\lambda) = \sum_{\mu=1}^{f_s}\beta_{\mu\lambda}^{-1}\bar{\mathbf{e}}(\mathbf{k}sa\mu), \tag{5.42a}$$

$$= \mathbf{T}(\mathbf{k};\mathbf{A}_0)\sum_{\mu=1}^{f_s}\beta_{\mu\lambda}^{-1*}\mathbf{e}(\mathbf{k}sa\mu). \tag{5.42b}$$

Then, from Eqs. (5.11), (5.12), and (5.20), it follows that

$$\mathbf{T}(\mathbf{k};\mathbf{R})\bar{\mathbf{e}}'(\mathbf{k}sa\lambda) = \sum_{\lambda''=1}^{f_s}\tau_{\lambda''\lambda}^{(s)}(\mathbf{k};\mathbf{R})\bar{\mathbf{e}}'(\mathbf{k}sa\lambda''). \tag{5.42c}$$

Also, by inverting Eq. (5.42a) we obtain

$$\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda) \equiv \bar{\mathbf{e}}(\mathbf{k}sa\lambda) = \sum_{\mu=1}^{f_s}\beta_{\mu\lambda}\bar{\mathbf{e}}'(\mathbf{k}sa\mu). \tag{5.42d}$$

The effect of $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ on $\bar{\mathbf{e}}'(\mathbf{k}sa\lambda')$ can be expressed in terms of the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ by use of Eqs.

(5.42b), (3.45), and (5.9):

$$\mathbf{T}(\mathbf{k};\mathbf{A}_0)\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)=\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)\sum_{\mu=1}^{f_s}\beta_{\mu\lambda}{}^{-1*}\mathbf{e}(\mathbf{k}sa\mu),$$
$$=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0{}^2)\sum_{\mu=1}^{f_s}\beta_{\mu\lambda}{}^{-1*}\times\mathbf{e}(\mathbf{k}sa\mu),$$
$$=\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\sum_{\mu,\mu'=1}^{f_s}\beta_{\mu\lambda}{}^{-1*}\times\tau_{\mu'\mu}{}^{(s)}(\mathbf{k};\mathbf{A}_0{}^2)\mathbf{e}(\mathbf{k}sa\mu'). \quad (5.43)$$

Therefore, depending on whether $\beta\beta^*$ satisfies Eq. (5.33a) or (5.33b), we obtain

$$\mathbf{T}(\mathbf{k};\mathbf{A}_0)\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)=\sum_{\mu,\mu'=1}^{f_s}\beta_{\mu\lambda}{}^{-1*}[\beta\beta^*]_{\mu'\mu}\mathbf{e}(\mathbf{k}sa\mu'),$$
$$=\sum_{\mu'=1}^{f_s}\beta_{\mu'\lambda}\mathbf{e}(\mathbf{k}sa\mu') \quad (5.44a)$$

or

$$\mathbf{T}(\mathbf{k};\mathbf{A}_0)\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)=-\sum_{\mu,\mu'=1}^{f_s}\beta_{\mu\lambda}{}^{-1*}[\beta\beta^*]_{\mu'\mu}\mathbf{e}(\mathbf{k}sa\mu'),$$
$$=-\sum_{\mu'=1}^{f_s}\beta_{\mu'\lambda}\mathbf{e}(\mathbf{k}sa\mu'). \quad (5.44b)$$

Now consider the scalar product of $\bar{\mathbf{e}}'(\mathbf{k}sa\lambda')$ with $\mathbf{e}(\mathbf{k}sa\lambda)$. Since these eigenvectors belong to the same irreducible multiplier representation, it follows from Eqs. (4.46) and (5.40) that

$$\langle\bar{\mathbf{e}}'(\mathbf{k}sa\lambda'),\mathbf{e}(\mathbf{k}sa\lambda)\rangle$$
$$=\delta_{\lambda\lambda'}[f_s{}^{-1}\sum_{\mu_1=1}^{f_s}\langle\bar{\mathbf{e}}'(\mathbf{k}sa\mu_1),\mathbf{e}(\mathbf{k}sa\mu_1)\rangle]. \quad (5.45a)$$

On the other hand, from Eqs. (5.41), (5.42d), (5.44), (5.45a), and the unitarity of the matrix β we obtain

$$\langle\bar{\mathbf{e}}'(\mathbf{k}sa\lambda'),\mathbf{e}(\mathbf{k}sa\lambda)\rangle$$
$$=\langle\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{e}(\mathbf{k}sa\lambda),\mathbf{T}(\mathbf{k};\mathbf{A}_0)\bar{\mathbf{e}}'(\mathbf{k}sa\lambda')\rangle,$$
$$=\pm\sum_{\mu,\mu'=1}^{f_s}\beta_{\mu\lambda}{}^*\beta_{\mu'\lambda'}\langle\bar{\mathbf{e}}'(\mathbf{k}sa\mu),\mathbf{e}(\mathbf{k}sa\mu')\rangle,$$
$$=\pm\delta_{\lambda\lambda'}[f_s{}^{-1}\sum_{\mu_1=1}^{f_s}\langle\bar{\mathbf{e}}'(\mathbf{k}sa\mu_1),\mathbf{e}(\mathbf{k}sa\mu_1)\rangle]. \quad (5.45b)$$

Clearly, if $\beta\beta^*$ satisfies Eq. (5.35b) so that the minus sign in Eq. (5.45b) is appropriate, then

$$\langle\bar{\mathbf{e}}'(\mathbf{k}sa\lambda'),\mathbf{e}(\mathbf{k}sa\lambda)\rangle=0. \quad (5.46)$$

Also, the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$ are orthogonal, since the latter may be expressed as linear combinations of $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$. It is worth emphasizing that this orthogonality does not depend on the details of the way in which the set $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ is chosen, but requires only that the set transform according to an irreducible multiplier representation of the second type under the symmetry operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$. For example, the vectors $\{[\mathbf{e}(\mathbf{k}sa\lambda)+c\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)]\}$ and $\{\mathbf{T}(\mathbf{k};\mathbf{A}_0)[\mathbf{e}(\mathbf{k}sa\lambda)+c\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)]\}$ are orthogonal if they belong to the second type of irreducible multiplier representation. Thus, the minimum dimension of the subspace that is invariant under the operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k};-\mathbf{k})$ is $2f_s$ if $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ is of the second type.

If the matrix β satisfies Eq. (5.33a) (that is, the irreducible multiplier representation is of the first type) then Eqs. (5.45) do not say anything about the linear dependence of the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$, and we must consider the two possibilities. If they are linearly dependent, then from Eq. (5.45a) they can differ by at most an arbitrary phase factor, and there is no additional degeneracy. On the other hand, if they are linearly independent, this situation can be referred to as an accidental degeneracy, since the $2f_s$-dimensional subspace consisting of the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ is reducible into two f_s-dimensional subspaces each of which is invariant under the symmetry operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k};-\mathbf{k})$. If the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ are linearly independent, then the eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)+\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ and $\{\mathbf{e}(\mathbf{k}sa\lambda)-\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ are also. In fact, the latter two sets can be made orthogonal by adjusting the arbitrary phase factor in the set $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ so that $\langle\mathbf{e}(\mathbf{k}sa\lambda),\mathbf{e}'(\mathbf{k}sa\lambda)\rangle$ is real, since

$$\langle\mathbf{e}(\mathbf{k}sa\lambda)-\bar{\mathbf{e}}'(\mathbf{k}sa\lambda),\mathbf{e}(\mathbf{k}sa\lambda)+\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\rangle$$
$$=\langle\mathbf{e}(\mathbf{k}sa\lambda),\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\rangle-\langle\bar{\mathbf{e}}'(\mathbf{k}sa\lambda),\mathbf{e}(\mathbf{k}sa\lambda)\rangle.$$

Clearly, each set transforms according to the irreducible multiplier representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ under the symmetry operations $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ of the point group $G_0(\mathbf{k})$. Also from Eqs. (5.42d) and (5.44a) we find that

$$\mathbf{T}(\mathbf{k};\mathbf{A}_0)[\mathbf{e}(\mathbf{k}sa\lambda)\pm'\bar{\mathbf{e}}(\mathbf{k}sa\lambda)]$$
$$=\pm\sum_{\mu}\beta_{\mu\lambda}[\mathbf{e}(\mathbf{k}sa\mu)\pm\bar{\mathbf{e}}'(\mathbf{k}sa\mu)]. \quad (5.47)$$

And since

$$\mathbf{T}(\mathbf{k};\mathbf{A})=\phi^*(\mathbf{k};\mathbf{A}\mathbf{A}_0{}^{-1},\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}\mathbf{A}_0{}^{-1})\mathbf{T}(\mathbf{k};\mathbf{A}_0), \quad (5.48)$$

there is no mixing of the eigenvectors from the two sets for any operation of the point group $G_0(\mathbf{k};-\mathbf{k})$. Therefore, each of the sets of eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)+\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ and $\{\mathbf{e}(\mathbf{k}sa\lambda)-\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ individually is a set of basis vectors for the symmetry operations $\{\mathbf{T}(\mathbf{k};\bar{\mathbf{R}})\}$ of the point group $G_0(\mathbf{k};-\mathbf{k})$ and thus symmetry does not require the two linearly independent sets to exist. This completes our proof that for the first type of irreducible multiplier representation time-reversal symmetry does not produce any additional degeneracy; if it did occur, it would be considered accidental.

From the above results it is a simple matter to determine the irreducible multiplier corepresentations. We begin by introducing the corepresentation concept for a group of symmetry operations, some of which are anti-unitary. Returning for a moment to the "j" index of Eq. (2.17) for labeling the branches of $\omega(\mathbf{k})$, since for any element $\bar{\mathbf{R}}$ of the point group $G_0(\mathbf{k}; -\mathbf{k})$ the matrix operator $\mathbf{T}(\mathbf{k}; \bar{\mathbf{R}})$ commutes with the dynamical matrix $\mathbf{D}(\mathbf{k})$, the effect of applying this operator to the eigenvector $\mathbf{e}(\mathbf{k}j)$ can be expressed as

$$\mathbf{T}(\mathbf{k}; \bar{\mathbf{R}})\mathbf{e}(\mathbf{k}j) = \sum_{j'} \Theta_{j'j}(\mathbf{k}; \bar{\mathbf{R}})\mathbf{e}(\mathbf{k}j'), \quad (5.49)$$

where the sum over j' extends over all branches of the phonon spectrum at the point $\mathbf{k}$ for which $\omega_{j'}^2(\mathbf{k}) = \omega_j^2(\mathbf{k})$. It follows directly from Eqs. (5.40) and (5.41) that $\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}})$ is a unitary matrix. Applying a unitary operation $\mathbf{T}(\mathbf{k}; \mathbf{R})$ to both sides of Eq. (5.49) from the left and following the same steps that lead to Eq. (4.18), we obtain

$$\mathbf{\Theta}(\mathbf{k}; \mathbf{R})\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}}) = \phi(\mathbf{k}; \mathbf{R}, \bar{\mathbf{R}})\mathbf{\Theta}(\mathbf{k}; \mathbf{R}\bar{\mathbf{R}}), \quad (5.50a)$$

where $\phi(\mathbf{k}; \mathbf{R}, \mathbf{R})$ is defined in Eq. (3.46). Alternatively, performing the same type of analysis with an anti-unitary operator $\mathbf{T}(\mathbf{k}; \mathbf{A})$ instead of with $\mathbf{T}(\mathbf{k}; \mathbf{R})$, we have

$$\begin{aligned} T(\mathbf{k}; \mathbf{A})\mathbf{T}(\mathbf{k}; \bar{\mathbf{R}})\mathbf{e}(\mathbf{k}j) &= \phi(\mathbf{k}; \mathbf{A}, \mathbf{R})\mathbf{T}(\mathbf{k}; \mathbf{A}\bar{\mathbf{R}})\mathbf{e}(\mathbf{k}j), \\ &= \phi(\mathbf{k}; \mathbf{A}, \bar{\mathbf{R}}) \sum_{j''} \Theta_{j''j}(\mathbf{k}; \mathbf{A}\bar{\mathbf{R}})\mathbf{e}(\mathbf{k}j''), \quad (5.51a) \\ &= \sum_{j'} \Theta_{j'j}(\mathbf{k}; \bar{\mathbf{R}})^* \mathbf{T}(\mathbf{k}; \mathbf{A})\mathbf{e}(\mathbf{k}j'), \\ &= \sum_{j'j''} \Theta_{j'j}(\mathbf{k}; \bar{\mathbf{R}})^* \Theta_{j''j'}(\mathbf{k}; \mathbf{A})\mathbf{e}(\mathbf{k}j''). \quad (5.51b) \end{aligned}$$

Comparing Eqs. (5.51a) and (5.51b), we are led to the result that

$$\mathbf{\Theta}(\mathbf{k}; \mathbf{A})\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}})^* = \phi(\mathbf{k}; \mathbf{A}, \bar{\mathbf{R}})\mathbf{\Theta}(\mathbf{k}; \mathbf{A}\bar{\mathbf{R}}), \quad (5.50b)$$

where $\phi(\mathbf{k}; \mathbf{A}, \bar{\mathbf{R}})$ is defined in Eq. (3.47). Note the complex conjugate in Eq. (5.50b). Clearly, the unitary matrices $\{\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}})\}$ which satisfy Eqs. (5.50) are not a representation of the group of unitary and anti-unitary symmetry operations $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$ in the usual sense. For this reason they are called multiplier corepresentations.[16,24]

In the preceding analysis it was shown that the dimensions of the subspaces of eigenvectors, which are invariant under the symmetry operations $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$ of the point group $G_0(\mathbf{k}; -\mathbf{k})$, are f_s or $2f_s$, depending upon the irreducible multiplier representation to which they belong for unitary symmetry operations. Therefore, the dimensions of the irreducible matrices $\{\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}})\}$ are either f_s or $2f_s$. By using the appropriate eigenvectors $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$, $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$, and $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$ as basis vectors, it is straightforward to construct an irreducible multiplier corepresentation that satisfies Eqs. (5.50) for each type of irreducible multiplier representation. The corresponding irreducible multiplier corepresentations will be referred to as being of the first, second, or third types also, and will be denoted by $\{\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{R})\}$. We now summarize the results.

First type. The irreducible multiplier representations $\{\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R})\}$ and

$$\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k}; \mathbf{R})\} = \{\phi^*(\mathbf{k}; \mathbf{A}_0, \mathbf{A}_0^{-1}\mathbf{R}) \times \phi^*(\mathbf{k}; \mathbf{A}_0^{-1}\mathbf{R}, \mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*\}$$

are equivalent. The unitary matrix $\boldsymbol{\beta}$ which transforms $\boldsymbol{\tau}^{(s)}$ into $\bar{\boldsymbol{\tau}}^{(s)}$ satisfies the equation $\boldsymbol{\beta}\boldsymbol{\beta}^* = \phi(\mathbf{k}; \mathbf{A}_0, \mathbf{A}_0) \times \boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}_0^2)$. The invariant subspace has f_s dimensions, and the basis vectors are $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$. In this case from the definition of $\mathbf{\Theta}(\mathbf{k}; \bar{\mathbf{R}})$ in Eq. (5.49) we have

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{R}) = \boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R}), \quad (5.52a)$$

while, from Eqs. (5.42d) and (5.44a),

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{A}_0) = \boldsymbol{\beta}, \quad (5.52b)$$

and combining Eqs. (5.48), (5.52a), and (5.52b) gives

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{A}) = \phi^*(\mathbf{k}; \mathbf{A}\mathbf{A}_0^{-1}, \mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}\mathbf{A}_0^{-1})\boldsymbol{\beta}. \quad (5.52c)$$

Second type. The irreducible multiplier representations $\{\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R})\}$ and $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k}; \mathbf{R})\}$ are equivalent as in the first case, but in this case $\boldsymbol{\beta}$ satisfies the equation $\boldsymbol{\beta}\boldsymbol{\beta}^* = -\phi(\mathbf{k}; \mathbf{A}_0, \mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}_0^2)$. The invariant subspace has $2f_s$ dimensions. The first f_s basis vectors are $\{\mathbf{e}(\mathbf{k}sa\lambda)$ and the second f_s basis vectors are $\{\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)\}$, defined by Eq. (5.42a). For convenience we partition the $2f_s \times 2f_s$ irreducible multiplier corepresentation matrices $\{\mathbf{\Theta}^{(s)}(\mathbf{k}; \bar{\mathbf{R}})\}$ into four $f_s \times f_s$ blocks. Then from Eqs. (5.9), (5.42c), and (5.49) it follows that

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{R}) = \begin{pmatrix} \boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R}) & 0 \\ 0 & \boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R}) \end{pmatrix}, \quad (5.53a)$$

while from Eqs. (5.42d), (5.44b), and (5.49), we have that

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{A}_0) = \begin{pmatrix} 0 & -\boldsymbol{\beta} \\ \boldsymbol{\beta} & 0 \end{pmatrix}, \quad (5.53b)$$

and combining Eqs. (5.48), (5.42d), and (5.44b) with Eq. (5.49) gives

$$\mathbf{\Theta}^{(s)}(\mathbf{k}; \mathbf{A}) = \phi^*(\mathbf{k}; \mathbf{A}\mathbf{A}_0^{-1}, \mathbf{A}_0) \times \begin{pmatrix} 0 & -\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}\mathbf{A}_0^{-1})\boldsymbol{\beta} \\ \boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{A}\mathbf{A}_0^{-1})\boldsymbol{\beta} & 0 \end{pmatrix}. \quad (5.53c)$$

Third type. The irreducible multiplier representations

$\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and

$$\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}=\{\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\times\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*\}$$

are inequivalent. The invariant subspace has $2f_s$ dimensions; the first f_s basis vectors are $\{\mathbf{e}(\mathbf{k}sa\lambda)\}$ and the second f_s basis vectors are $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$ [see Eq. (5.8)]. If for convenience we partition the $2f_s\times 2f_s$ irreducible multiplier corepresentation matrices $\{\boldsymbol{\Theta}^{(s)}(\mathbf{k};\bar{\mathbf{R}})\}$ into four $f_s\times f_s$ blocks, then, from Eqs. (5.9), (5.11), (5.12), and (5.49), it follows that

$$\boldsymbol{\Theta}^{(s)}(\mathbf{k};\mathbf{R})=\begin{pmatrix}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}) & 0\\ 0 & \bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\end{pmatrix}\tag{5.54a}$$

while, from Eqs. (5.18), (5.19), and (5.49),

$$\boldsymbol{\Theta}^{(s)}(\mathbf{k};\mathbf{A}_0)=\begin{pmatrix}0 & \phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2)\\ 1 & 0\end{pmatrix}\tag{5.54b}$$

and

$$\boldsymbol{\Theta}^{(s)}(\mathbf{k};\mathbf{A})=\begin{pmatrix}0 & \phi(\mathbf{k};\mathbf{A},\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}\mathbf{A}_0)\\ \phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{A})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{A})^* & 0\end{pmatrix}.\tag{5.54c}$$

The relation between the irreducible multiplier representations $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ and $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ is reciprocal in that if we had started the analysis that leads from Eq. (5.8) to Eq. (5.12) with eigenvectors $\{\bar{\bar{\mathbf{e}}}(\mathbf{k}sa\lambda)\}\equiv\{\mathbf{T}(\mathbf{k};\mathbf{A}_0)\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$, where $\{\bar{\mathbf{e}}(\mathbf{k}sa\lambda)\}$ belongs to $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$, then we would have found that $\{\bar{\bar{\mathbf{e}}}(\mathbf{k}sa\lambda)\}$ belongs to the irreducible multiplier representation $\{\bar{\bar{\boldsymbol{\tau}}}^{(s)}(\mathbf{k};\mathbf{R})\}$, which is equivalent to $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$. To see this we note that $\bar{\bar{\boldsymbol{\tau}}}^{(s)}$ must be related to $\bar{\boldsymbol{\tau}}^{(s)}$ in precisely the same way that $\bar{\boldsymbol{\tau}}^{(s)}$ is related to $\boldsymbol{\tau}^{(s)}$. Accordingly, from Eqs. (5.12) and (5.29), we have

$$\begin{aligned}\bar{\bar{\boldsymbol{\tau}}}^{(s)}(\mathbf{k};\mathbf{R})&=\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*,\\ &=\phi^*(\mathbf{k};\mathbf{A}_0^2,\mathbf{A}_0^{-2})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-2})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2),\\ &=\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2)^{-1}\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2).\end{aligned}\tag{5.55}$$

The consequences of time-reversal symmetry on the number of times the sth irreducible multiplier representation is contained in the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ [see Eq. (4.36)] follow directly from the above results: Irreducible multiplier representations of the first type may occur any number of times, while the second type must occur an even number of times, and irreducible multiplier representations of the third type always occur in pairs. Therefore the existence of anti-unitary symmetry operations in the symmetry group of the dynamical matrix $\mathbf{D}(\mathbf{k})$ reduces the labor involved in determining the eigenvectors by a factor of two. For eigenvectors which belong to representations of type one, the number of unknown real quantities in $\mathbf{E}(\mathbf{k};s\lambda)$ of Eq. (4.38) may be reduced from $2(c_s-1)$ to (c_s-1) when $c_s>1$ by use of Eqs. (5.49) and (5.52b). This case is especially simple if the matrix $\boldsymbol{\beta}$ is diagonal or has one nonzero element in each row. For eigenvectors which belong to representations of type two, $\mathbf{E}(\mathbf{k};s\lambda)$ will contain $(c_s/2)$ pairs $\mathbf{e}(\mathbf{k}sa\lambda)$ and $\bar{\mathbf{e}}'(\mathbf{k}sa\lambda)$, where c_s is an even integer. By use of the operator $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ one can again reduce the number of unknowns from $2(c_s-1)$ to (c_s-1). In the case of type three, after finding the eigenvectors that belong to $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ we can obtain the ones that belong to $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ by applying $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ to the former.

In principle, the above results describe the effects of time-reversal symmetry on the eigenvalues and eigenvectors of the dynamical matrix. However, the criteria for establishing the type of representation one is dealing with are cumbersome in that they require the irreducible multiplier representation $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ to be constructed by use of Eq. (5.12); then its relation to $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$ must be determined from an orthogonality theorem. If they turn out to be equivalent, then the matrix $\boldsymbol{\beta}$ which connects them must be found [e.g., Eq. (5.25)] and its "structure" determined by use of Eqs. (5.33). On the other hand, it is well known that there is a criterion due to Frobenius and Schur (see for example Refs. 21, 22, or 23) which allows ordinary irreducible representations to be classified in a manner which is very similar to the types used here and involves only the characters of the ordinary irreducible representations. We shall now derive the analogous criterion for irreducible multiplier representations. This criterion will also clarify the close connection between Herring's[22] results and ours.

To derive the criterion we note the fundamental difference between equivalent and inequivalent types of irreducible multiplier representations in terms of the orthogonality theorem (4.46) and Eq. (5.20):

$$\sum_{\mathbf{R}} \bar{\tau}_{\mu\mu'}{}^{(s)}(\mathbf{k};\mathbf{R})^{*}\tau_{\nu\nu'}{}^{(s)}(\mathbf{k};\mathbf{R})$$

$$=(h/f_s)\beta_{\mu\nu}{}^{-1*}\beta_{\nu'\mu'}{}^{*} \quad \text{first or second type,} \quad (5.56\text{a})$$

$$=0, \quad \text{third type.} \quad (5.56\text{b})$$

Using the definition of $\bar{\tau}^{(s)}$ in Eq. (5.12a), which is valid for all three types, the left-hand side of Eq. (5.56) may be written as

$$\sum_{\mathbf{R}} \phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\tau_{\mu\mu'}{}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)\times\tau_{\nu\nu'}{}^{(s)}(\mathbf{k};\mathbf{R}).$$

Substituting this form in Eqs. (5.56) and summing over ν (after setting μ' equal to ν) yields

$$\sum_{\mathbf{R}} \phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\times\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0,\mathbf{R})\tau_{\mu\nu'}{}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0\mathbf{R})$$

$$=(h/f_s)[(\boldsymbol{\beta}\boldsymbol{\beta}^{*})^{-1}]_{\mu\nu'}, \quad \text{first or second type,} \quad (5.57\text{a})$$

$$=0, \quad \text{third type,} \quad (5.57\text{b})$$

where the unitary property of $\boldsymbol{\beta}$ has been used to simplify the right-hand side of Eq. (5.57a). A comparison of Eqs. (5.33) and (5.57) suggests how the first and second types of irreducible multiplier representations may be distinguished; namely, multiply both sides of Eqs. (5.57) by $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\tau_{\lambda\mu}{}^{(s)}(\mathbf{k};\mathbf{A}_0^2)$, sum over μ, and use Eqs. (5.33) to simplify the right-hand side. After a little algebra we arrive at the interesting result:

$$\sum_{\mathbf{R}} \phi(\mathbf{k};\mathbf{A}_0\mathbf{R},\mathbf{A}_0\mathbf{R})\tau_{\lambda\lambda'}{}^{(s)}(\mathbf{k};\mathbf{A}_0\mathbf{R}\mathbf{A}_0\mathbf{R})$$

$$=+(h/f_s)\delta_{\lambda\lambda'}, \quad \text{first type,} \quad (5.58\text{a})$$

$$=-(h/f_s)\delta_{\lambda\lambda'}, \quad \text{second type,} \quad (5.58\text{b})$$

$$=0, \quad \text{third type,} \quad (5.58\text{c})$$

where the left-hand side has been simplified by use of the identity

$$\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\times\phi(\mathbf{k};\mathbf{A}_0^2,\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0\mathbf{R})\phi(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0,\mathbf{R})=\phi(\mathbf{k};\mathbf{A}_0\mathbf{R},\mathbf{A}_0\mathbf{R}), \quad (5.59)$$

which may be demonstrated by repeated application of Eqs. (5.3). Although Eqs. (5.58) may be used to identify the type of irreducible multiplier representation one is dealing with, it is customary to express the criterion in terms of the characters $\chi^{(s)}$ of Eq. (4.35) by setting $\lambda'=\lambda$ and summing over λ. Thus

$$\sum_{\mathbf{R}} \phi(\mathbf{k};\mathbf{A}_0\mathbf{R},\mathbf{A}_0\mathbf{R})\chi^{(s)}(\mathbf{k};\mathbf{A}_0\mathbf{R}\mathbf{A}_0\mathbf{R})$$

$$=h, \quad \text{first type,} \quad (5.60\text{a})$$

$$=-h, \quad \text{second type,} \quad (5.60\text{b})$$

$$=0, \quad \text{third type.} \quad (5.60\text{c})$$

Also, instead of summing over the rotational elements $\mathbf{R}$ of the point group $G_0(\mathbf{k})$ as in Eqs. (5.58) and (5.60), one can express the criterion as a sum over the rotational elements $\mathbf{A}$ of the coset $S_{-}G_0(\mathbf{k})$ (or $\mathbf{A}_0G_0(\mathbf{k})$) since $\mathbf{A}_0\mathbf{R}$ corresponds to a unique element $\mathbf{A}$. For example, Eq. (5.60) becomes

$$\sum_{\mathbf{A}} \phi(\mathbf{k};\mathbf{A},\mathbf{A})\chi^{(s)}(\mathbf{k};\mathbf{A}^2)$$

$$=h, \quad \text{first type,} \quad (5.61\text{a})$$

$$=-h, \quad \text{second type,} \quad (5.61\text{b})$$

$$=0, \quad \text{third type.} \quad (5.61\text{c})$$

If either $\mathbf{k}$ lies entirely within the Brillouin zone or the space group $G_{\mathbf{k};-\mathbf{k}}$ of the crystal is symmorphic (so that $\mathbf{v}(\bar{R})$ is zero) then the multiplier $\phi(\mathbf{k};\mathbf{R}_i,\bar{\mathbf{R}}_j)$ is unity. In the special case the criterion takes the form that the wave vector is equal to $\pi\mathbf{b}$, so that Eqs. (3.49) to (3.53) apply. Equations (5.12) are replaced by

$$\bar{\boldsymbol{\tau}}^{(s)}(\pi\mathbf{b};\mathbf{R})=\exp[i2\pi\mathbf{b}\cdot\mathbf{v}(R)]\boldsymbol{\tau}^{(s)}(\pi\mathbf{b};\mathbf{R})^{*}, \quad (5.62)$$

and from Eq. (3.53) the multiplier $\phi(\mathbf{k};\mathbf{A},\mathbf{A})$ must be replaced by $\exp[-i2\pi\mathbf{b}\cdot\mathbf{v}(R)]\phi(\pi\mathbf{b};\mathbf{R},\mathbf{R})$. Thus in this special case the criterion (5.61) becomes

$$\sum_{\mathbf{R}} \exp\{-i\pi[\mathbf{b}+\mathbf{R}^{-1}\mathbf{b}]\cdot\mathbf{v}(R)]\chi^{(s)}(\pi\mathbf{b};\mathbf{R}^2)$$

$$=h, \quad \text{first type,} \quad (5.63\text{a})$$

$$=-h, \quad \text{second type,} \quad (5.63\text{b})$$

$$=0, \quad \text{third type.} \quad (5.63\text{c})$$

The special case of the wave vector at the center of the Brillouin zone (i.e., $\mathbf{k}=\mathbf{0}$) is covered by Eqs. (5.63) with $\pi\mathbf{b}$ set equal to $\mathbf{0}$.

In comparing these criteria with Herring's work,[22] it should be noted that we have followed Wigner's[16] more recent classification, so that the second and third types of the present work correspond to Herring's cases "c" and "b", respectively. With this in mind, the equivalence of the two methods is clear. The above criteria provide a complete solution to the problem of determining the additional degeneracies due to time-reversal symmetry in terms of the characters $\{\chi^{(s)}(\mathbf{k};\mathbf{R})\}$, the rotational element $\mathbf{A}_0$, and the multiplier $\phi(\mathbf{k};\mathbf{A}_0\mathbf{R},\mathbf{A}_0\mathbf{R})$ without recourse to either the representation $\{\bar{\boldsymbol{\tau}}^{(s)}(\mathbf{k};\mathbf{R})\}$ or the matrix $\boldsymbol{\beta}$. For determining the eigenvectors which belong to the first and second type of irreducible multiplier representations it is helpful to have the matrix $\boldsymbol{\beta}$ available. Fortunately, the matrix $\boldsymbol{\beta}$ is often known from the type of representation alone. We conclude this section by examining the matrix $\boldsymbol{\beta}$ in these special cases.

Consider the situation where $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2)$ is equal to the unit matrix. This occurs quite often since in many crystals there exists an element $\mathbf{A}_0$ such that $\mathbf{T}(\mathbf{k};\mathbf{A}_0)\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ is equal to $\mathbf{T}(\mathbf{k};\boldsymbol{\varepsilon})$. Important examples are: (1) The point group of the crystal contains the inversion, i.e., $\mathbf{A}_0=\mathbf{i}$; (2) The dynamical matrix is real, so that $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ may be taken to be $\mathbf{K}_0$.

First type. According to Eq. (5.33a), $\beta\beta^*=\mathbf{1}$; and since β is unitary, it must be symmetric. Therefore it can be put into diagonal form by the bilinear transformation (5.37). In particular, with $\mathbf{U}=\beta^{1/2}$, where $\beta^{1/2}$ is a symmetric unitary matrix and $\beta^{1/2}\beta^{1/2}=\beta$, we have

$$\beta'=\beta^{-1/2}\beta\beta^{1/2*}=\beta^{1/2}\beta^{1/2*}=\mathbf{1}. \quad (5.64)$$

In Sec. 4 we commented that in certain cases it was possible for $\mathbf{e}(\mathbf{k}sa\lambda)$ to be an eigenvector of the anti-unitary matrix operator $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$. The necessary and sufficient condition for this to be possible is now clear: The irreducible multiplier representation must be of the first type and $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2)=\mathbf{1}$.

Let us now assume that the irreducible multiplier representation has been transformed so that β is diagonal. Then, from Eq. (5.20), the representation must satisfy

$$\phi^*(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0^{-1}\mathbf{R})\phi^*(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R},\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^{-1}\mathbf{R}\mathbf{A}_0)^*=\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}). \quad (5.65)$$

This is the generalization of Eq. (4.52) to include all elements $\mathbf{R}$ of $G_0(\mathbf{k})$.

Second type. According to Eq. (5.33b), $\beta\beta^*=-\mathbf{1}$; and since β is unitary, it must be anti-symmetric. Therefore the dimension f_s of the representation must be even. In this case it is always possible to find a unitary matrix $\mathbf{U}$ such that [see Eq. (5.37)]

$$\beta'=\mathbf{U}^{-1}\beta\mathbf{U}=\begin{pmatrix}0 & -\mathbf{1}'\\ \mathbf{1}' & 0\end{pmatrix}, \quad (5.66)$$

where β' has been written in a partitioned form, with $\mathbf{1}'$ being a $(f_s/2)\times(f_s/2)$ unit matrix. β' can be substituted into Eq. (5.53b) to obtain the effect of $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ on the eigenvectors.

Finally, if $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{A}_0^2)$ is equal to minus the unit matrix, then clearly (5.64) and (5.66) are interchanged. For example, this could come about if $\mathbf{A}_0^2=\boldsymbol{\varepsilon}$ and $\phi(\mathbf{k};\mathbf{A}_0,\mathbf{A}_0)=-1$. It should be emphasized that $\mathbf{e}(\mathbf{k}sa\lambda)$ cannot be made an eigenvector of $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$ for either the first or second types in this situation.

6. EXAMPLES

To illustrate the applications of the results to specific lattice dynamical problems, we consider the normal modes propagating in the [110] and [001] directions (including the points on the Brillouin zone boundary) and the selection rules for two phonon processes in a crystal of the diamond structure. The notation and classification of Kovalev[12] is used (except that the rotational elements will be designated by $\mathbf{R}$ instead of $\mathbf{h}$); where possible, it is related to Herring's[11] notation.

The space group of diamond is O_h^7. The translation vectors of the crystal can be chosen to be

$$\mathbf{x}(l)=l_1\mathbf{a}_1+l_2\mathbf{a}_2+l_3\mathbf{a}_3, \quad (6.1a)$$

$$\mathbf{a}_1=\tau(0,1,1),\quad \mathbf{a}_2=\tau(1,0,1),\quad \mathbf{a}_3=\tau(1,1,0), \quad (6.1b)$$

where l_1, l_2, l_3 are three integers which are positive, negative, or zero and $2\tau(=a)$ is the lattice parameter. The positions of the two atoms in a primitive unit cell are given by the two basis vectors

$$\mathbf{x}(\kappa=1)=0, \quad (6.2a)$$

$$\mathbf{x}(\kappa=2)=(\tau/2)(1,1,1). \quad (6.2b)$$

Following Kovalev,[12] in this section the factor 2π is included in the definition of the reciprocal lattice vectors:

$$\mathbf{b}_1=(\pi/\tau)(-1,1,1),\qquad \mathbf{b}_2=(\pi/\tau)(1,-1,1),$$
$$\mathbf{b}_3=(\pi/\tau)(1,1,-1). \quad (6.3)$$

To save writing where possible 6-vectors and the 6×6 transformation matrices will be written in the abbreviated forms

$$\boldsymbol{\psi}=\begin{pmatrix}\boldsymbol{\psi}(1)\\ \boldsymbol{\psi}(2)\end{pmatrix},$$

where

$$\boldsymbol{\psi}(\kappa)=\begin{pmatrix}\psi_x(\kappa)\\ \psi_y(\kappa)\\ \psi_z(\kappa)\end{pmatrix} \quad (6.4)$$

and

$$T(k;R)=\begin{pmatrix}\Lambda(1,1)\mathbf{R} & \Lambda(1,2)\mathbf{R}\\ \Lambda(2,1)\mathbf{R} & \Lambda(2,2)\mathbf{R}\end{pmatrix}, \quad (6.5a)$$

where, according to Eq. (3.17b),

$$\Lambda(\kappa,\kappa')=\delta(\kappa,F_0(\kappa';R))\exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{R}\cdot\mathbf{x}(\kappa')]\} \quad (6.5b)$$

and $\mathbf{R}$ is a 3×3 matrix. The particular rotational elements $\mathbf{R}$, with their corresponding $\mathbf{v}(R)$ and their effects on the sublattices, required for the present work are given in the appendix. It is worth noting that the transformation matrix $\mathbf{T}(\mathbf{k};\mathbf{R})$ in Eq. (6.5a) is diagonal or off-diagonal in the indices (κ,κ'). Since the point group for diamond structure contains the inversion operation, we may invoke time-reversal symmetry for all wave vectors. If $\mathbf{A}_0$ is taken to be the inversion, then $\mathbf{A}_0\mathbf{R}\mathbf{A}_0\mathbf{R}$ in Eqs. (5.60) reduces to $\mathbf{R}^2$. Also, from results of Sec. 5, eigenvectors which belong to the first type of irreducible multiplier representations may be chosen to be eigenvectors of $\mathbf{T}(\mathbf{k};\mathbf{A}_0)$.

The wave vector $\mathbf{k}$ for propagation in the [110] direction in a fcc crystal is designated by $\mathbf{k}_4$ in Kovalev's[12] classification (Σ in Herring's[11]):

$$\mathbf{k}_4=(2\pi/\tau)(\mu,\mu,0),\qquad 0<\mu\leq\tfrac{3}{8}. \quad (6.6)$$

TABLE I. Irreducible multiplier representations[a] of the group $G_0(\mathbf{k}_4)$.

	$\mathbf{R}_1$	$\mathbf{R}_{16}$	$\mathbf{R}_{28}$	$\mathbf{R}_{37}$	Ref. 11
$\boldsymbol{\tau}^{(1)}$	1	1	1	1	Σ_1
$\boldsymbol{\tau}^{(2)}$	1	1	−1	−1	Σ_2
$\boldsymbol{\tau}^{(3)}$	1	−1	1	−1	Σ_4
$\boldsymbol{\tau}^{(4)}$	1	−1	−1	1	Σ_3

[a] See Ref. 12.

The point group of the wave vector $\mathbf{k}_4$, $G_0(\mathbf{k}_4)$ is the group C_{2v}. The four rotational elements are $\mathbf{R}_1$, $\mathbf{R}_{16}$, $\mathbf{R}_{28}$, and $\mathbf{R}_{37}$. The point $\mu=\frac{3}{8}$ on the Brillouin zone boundary does not introduce any additional symmetry elements. Using the notation (6.5), the matrices $\{\mathbf{T}(\mathbf{k}_4;\mathbf{R})\}$ are found from Eqs. (3.17b), (6.2), and (6.6) to be

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_1)=\begin{pmatrix}\mathbf{R}_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{R}_1\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{16})=\begin{pmatrix}\mathbf{0} & \rho_4^*\mathbf{R}_{16}\\ \rho_4\mathbf{R}_{16} & \mathbf{0}\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{28})=\begin{pmatrix}\mathbf{0} & \rho_4^*\mathbf{R}_{28}\\ \rho_4\mathbf{R}_{28} & \mathbf{0}\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{37})=\begin{pmatrix}\mathbf{R}_{37} & \mathbf{0}\\ \mathbf{0} & \mathbf{R}_{37}\end{pmatrix}, \tag{6.7}$$

where $\rho_4=\exp[i\mathbf{k}_4\cdot\mathbf{x}(2)]=\exp(i2\pi\mu)$. From these matrices we obtain the characters $\chi(\mathbf{k}_4;\mathbf{R})$:

$$\chi(\mathbf{k}_4;\mathbf{R}_1)=6,\qquad \chi(\mathbf{k}_4;\mathbf{R}_{16})=0,$$
$$\chi(\mathbf{k}_4;\mathbf{R}_{28})=0,\qquad \chi(\mathbf{k}_4;\mathbf{R}_{37})=2. \tag{6.8}$$

The irreducible multiplier representations[12] of the group $G_0(\mathbf{k}_4)$ are all one-dimensional and are given in Table I. Clearly, the elements of the representation matrices in this case are also the characters $\{\chi^{(s)}(\mathbf{k}_4;\mathbf{R})\}$. These characters together with those given by Eq. (6.8) when used in Eq. (4.36) yield the following results for the number of times, c_s, that the sth irreducible representation of $G_0(\mathbf{k}_4)$ is contained in the representation $\{\mathbf{T}(\mathbf{k}_4;\mathbf{R})\}$:

$$c_1=2,\qquad c_2=1,\qquad c_3=1,\qquad c_4=2. \tag{6.9}$$

Because all the irreducible representations of $G_0(\mathbf{k}_4)$ are one-dimensional, there is no degeneracy of the normal modes for the wave vector $\mathbf{k}_4$, which is required by spatial symmetry. The criterion (5.60) is trivial to apply in this case, since $\mathbf{R}^2=\mathbf{R}_1=\boldsymbol{\varepsilon}$ for all $\mathbf{R}$ and $\phi(\mathbf{k};\mathbf{A},\mathbf{A})=1$. Therefore all irreducible multiplier representations of $G_6(\mathbf{k}_4)$ are the first type; thus time-reversal symmetry does not produce any degeneracy either. In order to obtain the frequencies and the polarization vectors of the modes which transform according to the irreducible representations $\boldsymbol{\tau}^{(1)}$ and $\boldsymbol{\tau}^{(4)}$ it is necessary to diagonalize two 2×2 matrices ($c_1=c_4=2$). This is a considerably simpler problem than having to diagonalize the 6×6 matrix $\mathbf{D}(\mathbf{k})$ with which we originally started. This result seems to have been pointed out first by Yanagawa.[2] If only the frequencies are required, the results derived in Eqs. (4.59)–(4.62) may be used.

The effects of the matrices $\{\mathbf{T}(\mathbf{k}_4;\mathbf{R})\}$ on an arbitrary six-dimensional vector $\boldsymbol{\psi}$ are found to be

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_1)\,\boldsymbol{\psi}=\begin{pmatrix}\psi_x(1)\\ \psi_y(1)\\ \psi_z(1)\\ \psi_x(2)\\ \psi_y(2)\\ \psi_z(2)\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{16})\,\boldsymbol{\psi}=\begin{pmatrix}\rho_4^*\psi_y(2)\\ \rho_4^*\psi_x(2)\\ -\rho_4^*\psi_z(2)\\ \rho_4\psi_y(1)\\ \rho_4\psi_x(1)\\ -\rho_4\psi_z(1)\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{28})\,\boldsymbol{\psi}=\begin{pmatrix}\rho_4^*\psi_x(2)\\ \rho_4^*\psi_y(2)\\ -\rho_4^*\psi_z(2)\\ \rho_4\psi_x(1)\\ \rho_4\psi_y(1)\\ -\rho_4\psi_z(1)\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_4;\mathbf{R}_{37})\,\boldsymbol{\psi}=\begin{pmatrix}\psi_y(1)\\ \psi_x(1)\\ \psi_z(1)\\ \psi_y(2)\\ \psi_x(2)\\ \psi_z(2)\end{pmatrix}.$$

Substitution of these results (together with Table I) into Eqs. (4.37) and (4.38) leads to the following results for the vectors $\mathbf{E}(\mathbf{k};s)$. (Because the irreducible representations $\boldsymbol{\tau}^{(1)},\cdots\boldsymbol{\tau}^{(4)}$ are all one-dimensional, we can suppress the index λ):

$$\mathbf{E}(\mathbf{k}_4;1)=\begin{pmatrix}a_1\\a_1\\b_1\\\rho_4a_1\\\rho_4a_1\\-\rho_4b_1\end{pmatrix},\qquad \mathbf{E}(\mathbf{k}_4;2)=\begin{pmatrix}a_2\\-a_2\\0\\-\rho_4a_2\\\rho_4a_2\\0\end{pmatrix},$$

$$\mathbf{E}(\mathbf{k}_4;3)=\begin{pmatrix}a_3\\-a_3\\0\\\rho_4a_3\\-\rho_4a_3\\0\end{pmatrix},\qquad \mathbf{E}(\mathbf{k}_4;4)=\begin{pmatrix}a_4\\a_4\\b_4\\-\rho_4a_4\\-\rho_4a_4\\\rho_4b_4\end{pmatrix},\tag{6.10}$$

where the quantities a_n and b_n are complex. According to Eq. (6.9), the representations $\boldsymbol{\tau}^{(2)}$ and $\boldsymbol{\tau}^{(3)}$ occur once. Thus the eigenvectors $\mathbf{e}(\mathbf{k}_421)$ and $\mathbf{e}(\mathbf{k}_431)$, after normalization, can be taken to be $\mathbf{E}(\mathbf{k}_4;2)$ and $\mathbf{E}(\mathbf{k}\ ;3)$, respectively. On the other hand, the representations $\boldsymbol{\tau}^{(1)}$ and $\boldsymbol{\tau}^{(4)}$ each occur twice. Thus in the form of $\mathbf{E}(\mathbf{k}\ s)$ in (6.10) two real quantities for each eigenvalue must be determined from the eigenvector equation to specify the corresponding eigenvectors $\mathbf{e}(\mathbf{k}_4sa)$. (The normalization and the arbitrariness of the phase has been used to reduce the number of undetermined real quantities from 4 to 2.) The problem can be simplified further. Because the eigenvectors belong to the first type of irreducible multiplier representation, we may invoke Eq. (4.50c) with $\mathbf{S}_-=\mathbf{A}_0=\mathbf{i}$, [see Eq. (4.12)], which in the present case takes the form

$$e_\alpha^*(1\mid\mathbf{k}_4sa)=\rho_4^*e_\alpha(2\mid\mathbf{k}_4sa).$$

This condition requires the elements a_1, a_3, and b_4 to be real, while b_1, a_2, and a_4 must be pure imaginary. Using these results, the determination of the eigenvectors $\mathbf{e}(\mathbf{k}_411)$, $\mathbf{e}(\mathbf{k}_412)$ and $\mathbf{e}(\mathbf{k}_441)$, $\mathbf{e}(\mathbf{k}_442)$ reduces to the trivial problem of solving a single linear equation for the ratios (ib_1/a_1) and (b_4/ia_4), respectively. This linear equation is obtained by multiplying the vectors $\mathbf{E}(\mathbf{k}_4;1)$ and $\mathbf{E}(\mathbf{k}_4;4)$, respectively, by $[\mathbf{D}(\mathbf{k}_4)-\omega^2\mathbf{I}_{3r}]$ and equating the result to zero. It is worth remarking that $\mathbf{D}(\mathbf{k}_4)$ is of the form (3.32) in this case.

The lattice vibration modes are often labeled as Longitudinal-Acoustic (or Optic) or Transverse-Acoustic (or Optic), depending on the orientation of the polarization vectors relative to the wave vector $\mathbf{k}$ and the frequency of the mode as $\mathbf{k}\to0$. According to this classification it is clear from Eq. (6.10) that $\mathbf{E}(\mathbf{k}_4;1)$ is LA+TO, $\mathbf{E}(\mathbf{k}_4;2)$ is TO, $\mathbf{E}(\mathbf{k}_4;3)$ is TA, and $\mathbf{E}(\mathbf{k}_4;4)$ is LO+TA.

For waves propagating in the [001] direction the wave vector on the Brillouin zone boundary must be treated separately from the interior points. In Kovalev's[12] classification the interior wave vector is designated by

$$\mathbf{k}_6=(2\pi/\tau)(0,0,\mu),\qquad 0<\mu<\tfrac{1}{2},\tag{6.11}$$

(Δ in Herring's[11] notation). The point group of the wave vector $\mathbf{k}_6$, $G_0(\mathbf{k}_6)$ is C_{4v} with eight rotational elements: $\mathbf{R}_1$, $\mathbf{R}_4$, $\mathbf{R}_{14}$, $\mathbf{R}_{15}$, $\mathbf{R}_{26}$, $\mathbf{R}_{27}$, $\mathbf{R}_{37}$, $\mathbf{R}_{40}$. From Eqs. (3.17b), (5.2), and (6.11) the matrices $\{\mathbf{T}(\mathbf{k}_6;\mathbf{R})\}$ are found to be

$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_1)=\begin{pmatrix}\mathbf{R}_1&\mathbf{0}\\\mathbf{0}&\mathbf{R}_1\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_4)=\begin{pmatrix}\mathbf{R}_4&\mathbf{0}\\\mathbf{0}&\mathbf{R}_4\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{14})=\begin{pmatrix}\mathbf{0}&\rho_6^*\mathbf{R}_{14}\\\rho_6\mathbf{R}_{14}&\mathbf{0}\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{15})=\begin{pmatrix}\mathbf{0}&\rho_6^*\mathbf{R}_{15}\\\rho_6\mathbf{R}_{15}&\mathbf{0}\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{26})=\begin{pmatrix}\mathbf{0}&\rho_6^*\mathbf{R}_{26}\\\rho_6\mathbf{R}_{26}&\mathbf{0}\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{27})=\begin{pmatrix}\mathbf{0}&\rho_6^*\mathbf{R}_{27}\\\rho_6\mathbf{R}_{27}&\mathbf{0}\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{37})=\begin{pmatrix}\mathbf{R}_{37}&\mathbf{0}\\\mathbf{0}&\mathbf{R}_{37}\end{pmatrix},$$
$$\mathbf{T}(\mathbf{k}_6;\mathbf{R}_{40})=\begin{pmatrix}\mathbf{R}_{40}&\mathbf{0}\\\mathbf{0}&\mathbf{R}_{40}\end{pmatrix},\tag{6.12}$$

where $\rho_6=\exp(i\mathbf{k}_6\cdot\mathbf{x}(2))=\exp(i\mu\pi)$. From these matrices we obtain the characters $\chi(\mathbf{k}_6;\mathbf{R})$:

$$\chi(\mathbf{k}_6;\mathbf{R}_1)=6,\qquad \chi(\mathbf{k}_6;\mathbf{R}_4)=-2,$$
$$\chi(\mathbf{k}_6;\mathbf{R}_{14})=0,\qquad \chi(\mathbf{k}_6;\mathbf{R}_{15})=0,$$
$$\chi(\mathbf{k}_6;\mathbf{R}_{26})=0,\qquad \chi(\mathbf{k}_6;\mathbf{R}_{27})=0,$$
$$\chi(\mathbf{k}_6;\mathbf{R}_{37})=2,\qquad \chi(\mathbf{k}_6;\mathbf{R}_{40})=2.\tag{6.13}$$

There are five irreducible multiplier representations[12] of the group $G_0(\mathbf{k}_6)$, (four one-dimensional and one two-dimensional) and they are given in Table II. The representation matrices for the two-dimensional case are expressed in terms of the 2×2 Pauli spin matrices:

$$\boldsymbol{\varepsilon}=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \boldsymbol{\sigma}_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},$$
$$\boldsymbol{\sigma}_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \boldsymbol{\sigma}_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\tag{6.14a}$$

which satisfy the relations

$$\boldsymbol{\sigma}_x^2=\boldsymbol{\sigma}_y^2=\boldsymbol{\sigma}_z^2=\boldsymbol{\varepsilon},\tag{6.14b}$$

$$\boldsymbol{\sigma}_x\boldsymbol{\sigma}_y=-\boldsymbol{\sigma}_y\boldsymbol{\sigma}_x=i\boldsymbol{\sigma}_z,\qquad \text{etc.}\tag{6.14c}$$

The characters for the two-dimensional representation are also listed. Using Table II and the characters (6.13) in Eq. (4.36) yields the following results for the number of times, c_s, that the sth irreducible representation of $G_0(\mathbf{k}_6)$ is contained in the representation $\{\mathbf{T}(\mathbf{k}_6;\mathbf{R})\}$:

$$c_1=1,\quad c_2=0,\quad c_3=0,\quad c_4=1,\quad c_5=2.\tag{6.15}$$

Since $\boldsymbol{\tau}^{(5)}$ is two-dimensional, two lattice vibration normal modes of the wave vector $\mathbf{k}_6$ are required to be twofold degenerate by spatial symmetry. Since $\mathbf{R}_{14}^2=\mathbf{R}_{15}^2=\mathbf{R}_4$ and $\mathbf{R}^2=\mathbf{R}_1$ for the remainder of the elements of $G_0(\mathbf{k}_6)$, it follows from Eqs. (5.60) and Table II that the irreducible multiplier representations are of the first type; thus time-reversal symmetry does not require any additional degeneracy.

Following the procedure leading to Eq. (6.10), we find the following vectors $\mathbf{E}(\mathbf{k}_6;s\lambda)$:

$$\mathbf{E}(\mathbf{k}_6;11)=\begin{pmatrix}0\\0\\a_1\\0\\0\\\rho_6a_1\end{pmatrix},\quad \mathbf{E}(\mathbf{k}_6;41)=\begin{pmatrix}0\\0\\a_4\\0\\0\\-\rho_6a_4\end{pmatrix},$$

$$\mathbf{E}(\mathbf{k}_6;51)=\begin{pmatrix}a_5\\b_5\\0\\i\rho_6b_5\\-i\rho_6a_5\\0\end{pmatrix},\quad \mathbf{E}(\mathbf{k}_6;52)=\begin{pmatrix}-ib_5\\-ia_5\\0\\-\rho_6a_5\\\rho_6b_5\\0\end{pmatrix}.\tag{6.16}$$

In the present case Eqs. (4.12) and (4.50c) take the form

$$e_\alpha^*(1\mid\mathbf{k}sa\lambda)=\rho_6^*e_\alpha(2\mid\mathbf{k}sa\lambda).\tag{6.17}$$

Therefore a_1 is real and a_4 is pure imaginary. Also, $\mathbf{E}(\mathbf{k}_6;11)$ and $\mathbf{E}(\mathbf{k}_6;41)$ are LA and LO, respectively. If one attempts to simplify the vectors $\mathbf{E}(\mathbf{k}_6;51)$ and $\mathbf{E}(\mathbf{k}_6;52)$ by invoking Eq. (6.17), one arrives at the absurd results that $a_5=b_5=0$. The source of the difficulty is that we have not taken the precaution to insure that the irreducible representation $\boldsymbol{\tau}^{(5)}$ conforms with Eq. (4.52). Taking $\mathbf{S}_-=\mathbf{R}_{25}=\mathbf{i}$, the anti-unitary symmetry operator $\mathbf{T}(\mathbf{k}_6;\mathbf{S}_-)$, according to Eqs. (2.37) and (3.40), is

$$\mathbf{T}(\mathbf{k}_6;\mathbf{S}_-)=\rho_6\mathbf{K}_0\begin{pmatrix}\mathbf{0}&\mathbf{R}_{25}\\\mathbf{R}_{25}&\mathbf{0}\end{pmatrix},$$
$$=\rho_6\begin{pmatrix}\mathbf{0}&\mathbf{R}_{25}\\\mathbf{R}_{25}&\mathbf{0}\end{pmatrix}\mathbf{K}_0.\tag{6.18}$$

It is straightforward to show that $\mathbf{T}(\mathbf{k}_6;\mathbf{S}_-)$ commutes with all the matrices $\mathbf{T}(\mathbf{k}_6;\mathbf{R})$ given in Eq. (6.12). Therefore, according to Eq. (4.52), the irreducible multiplier representation $\boldsymbol{\tau}^{(5)}$ can be put into real form by a similarity transformation with a unitary matrix. From an examination of $\boldsymbol{\tau}^{(5)}$ in Table II and the Pauli spin matrices in Eq. (6.14a) it is clear that a satisfactory transformation should take $\boldsymbol{\sigma}_z$ into $\pm\boldsymbol{\sigma}_y$, and $\boldsymbol{\sigma}_y$ into $\pm\boldsymbol{\sigma}_z$. Recalling that the Pauli spin matrices transform like the components of a 3-vector under rotations,[16] a rotation of 90° about the x axis gives the desired result; that is, $\boldsymbol{\sigma}_x\to\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y\to\boldsymbol{\sigma}_z$, and $\boldsymbol{\sigma}_z\to-\boldsymbol{\sigma}_y$. The new $\boldsymbol{\tau}^{(5)}$ representation is designated by $\boldsymbol{\tau}'^{(5)}$ in Table II, and the corresponding vectors $\mathbf{E}'(\mathbf{k}_6;5\lambda)$ are

$$\mathbf{E}'(\mathbf{k}_6;51)=\begin{pmatrix}\bar{a}_5\\\bar{a}_5\\0\\\bar{b}_5\\\bar{b}_5\\0\end{pmatrix},\quad \mathbf{E}'(\mathbf{k}_6;52)=\begin{pmatrix}-\rho_6^*\bar{b}_5\\\rho_6^*\bar{b}_5\\0\\-\rho_6\bar{a}^5\\\rho_6\bar{a}_5\\0\end{pmatrix}.\tag{6.19}$$

Clearly $\mathbf{E}'(\mathbf{k}_6;5\lambda)$ is TA+TO, each being twofold degenerate. Applying Eq. (6.17), we have $\bar{a}_5^*=\rho_6^*\bar{b}_5$ or $\bar{b}_5=\rho_6\bar{a}_5^*$. Thus the two atoms vibrate with equal amplitudes, their relative phase being the only unknown quantity to be determined from the eigenvector equation. If we write $\bar{a}_5$ in the form $|\bar{a}_5|\exp[i\alpha(\mathbf{k}_6)]$, the phase $\alpha(\mathbf{k}_6)$ is determined by multiplying $\mathbf{E}'(\mathbf{k}_6;51)$ by $[\mathbf{D}(\mathbf{k}_6)-\omega^2\mathbf{I}_3|]$ and equating the result to zero. In the limit $\mathbf{k}_6\to0$, $\alpha(\mathbf{k}_6)\to0$, and $\pi/2$, corresponding to the TA and TO modes, respectively.

TABLE II. Irreducible multiplier representations[a] of the group $G_0(\mathbf{k}_6)$.

	$\mathbf{R}_1$	$\mathbf{R}_4$	$\mathbf{R}_{14}$	$\mathbf{R}_{15}$	$\mathbf{R}_{26}$	$\mathbf{R}_{27}$	$\mathbf{R}_{37}$	$\mathbf{R}_{40}$	Ref. 11[b]
$\boldsymbol{\tau}^{(1)}$	1	1	1	1	1	1	1	1	Δ_1
$\boldsymbol{\tau}^{(2)}$	1	1	1	1	−1	−1	−1	−1	Δ_1'
$\boldsymbol{\tau}^{(3)}$	1	1	−1	−1	1	1	−1	−1	Δ_2
$\boldsymbol{\tau}^{(4)}$	1	1	−1	−1	−1	−1	1	1	Δ_2'
$\boldsymbol{\tau}^{(5)}$	$\boldsymbol{\varepsilon}$	$-\boldsymbol{\varepsilon}$	$i\boldsymbol{\sigma}_z$	$-i\boldsymbol{\sigma}_z$	$\boldsymbol{\sigma}_x$	$-\boldsymbol{\sigma}_x$	$\boldsymbol{\sigma}_y$	$-\boldsymbol{\sigma}_y$	Δ_5
$\chi^{(5)}$	2	−2	0	0	0	0	0	0	
$\boldsymbol{\tau}'^{(5)}$	$\boldsymbol{\varepsilon}$	$-\boldsymbol{\varepsilon}$	$-i\boldsymbol{\sigma}_y$	$i\boldsymbol{\sigma}_y$	$\boldsymbol{\sigma}_x$	$-\boldsymbol{\sigma}_x$	$-\boldsymbol{\sigma}_z$	$-\boldsymbol{\sigma}_z$	Δ_5

[a] See Ref. 12.
[b] It should be noted that Herring (Ref. 11) deals with the factor group $G_\mathbf{k}/T_\mathbf{k}$, which contains twice as many elements; however, the connection can still be made.

The wave vector on the Brillouin zone boundary for the [001] direction in Kovalev's[12] classification is designated by

$$\mathbf{k}_{10}=(\pi/\tau)(0,0,1), \tag{6.20}$$

(X in Herring's[11] notation). The point group of the wave vector $\mathbf{k}_{10}$, $G_0(\mathbf{k}_{10})$ is D_{4h} with sixteen rotational elements: $\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{R}_3$, $\mathbf{R}_4$, $\mathbf{R}_{13}$, $\mathbf{R}_{14}$, $\mathbf{R}_{15}$, $\mathbf{R}_{16}$, $\mathbf{R}_{25}$, $\mathbf{R}_{26}$ $\mathbf{R}_{27}$, $\mathbf{R}_{28}$, $\mathbf{R}_{37}$, $\mathbf{R}_{38}$, $\mathbf{R}_{39}$, $\mathbf{R}_{40}$. Here we see an advantage of the multiplier representation approach in that there is no need to extend the point group as in the $G_\mathbf{k}/T_\mathbf{k}$ method.[11] The matrices $\{\mathbf{T}(\mathbf{k}_{10};\mathbf{R})\}$ are found from Eqs. (3.17b), (6.2), and (6.20) to be

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_1)=\begin{pmatrix}\mathbf{R}_1 & 0\\ 0 & \mathbf{R}_1\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_2)=\begin{pmatrix}\mathbf{R}_2 & 0\\ 0 & -\mathbf{R}_2\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_3)=\begin{pmatrix}\mathbf{R}_3 & 0\\ 0 & -\mathbf{R}_3\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_4)=\begin{pmatrix}\mathbf{R}_4 & 0\\ 0 & \mathbf{R}_4\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{13})=\begin{pmatrix}0 & i\mathbf{R}_{13}\\ i\mathbf{R}_{13} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{14})=\begin{pmatrix}0 & -i\mathbf{R}_{14}\\ i\mathbf{R}_{14} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{15})=\begin{pmatrix}0 & -i\mathbf{R}_{15}\\ i\mathbf{R}_{15} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{16})=\begin{pmatrix}0 & i\mathbf{R}_{16}\\ i\mathbf{R}_{16} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{25})=\begin{pmatrix}0 & i\mathbf{R}_{25}\\ i\mathbf{R}_{25} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{26})=\begin{pmatrix}0 & -i\mathbf{R}_{26}\\ i\mathbf{R}_{26} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{27})=\begin{pmatrix}0 & -i\mathbf{R}_{27}\\ i\mathbf{R}_{27} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{28})=\begin{pmatrix}0 & i\mathbf{R}_{28}\\ i\mathbf{R}_{28} & 0\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{37})=\begin{pmatrix}\mathbf{R}_{37} & 0\\ 0 & \mathbf{R}_{37}\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{38})=\begin{pmatrix}\mathbf{R}_{38} & 0\\ 0 & -\mathbf{R}_{38}\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{39})=\begin{pmatrix}\mathbf{R}_{39} & 0\\ 0 & -\mathbf{R}_{39}\end{pmatrix},$$

$$\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{40})=\begin{pmatrix}\mathbf{R}_{40} & 0\\ 0 & \mathbf{R}_{40}\end{pmatrix}. \tag{6.21}$$

The characters obtained from these matrices are listed in the last row of Table III.

There are four two-dimensional irreducible multiplier representations[12] of the group $G_0(\mathbf{k}_{10})$. The representation matrices are given in Table III in terms of the Pauli spin matrices (6.14) along with the characters. Using the characters of the $\{\mathbf{T}(\mathbf{k}_{10};\mathbf{R})\}$ matrices and the characters of the irreducible representations given in Table III in Eq. (4.36), we find the number of times, c_s, that sth irreducible multiplier representation of $G_0(\mathbf{k}_{10})$ is contained in the representation $\{\mathbf{T}(\mathbf{k}_{10};\mathbf{R})\}$:

$$c_1=1, \quad c_2=1, \quad c_3=1, \quad c_4=0. \tag{6.22}$$

Since $\mathbf{k}_{10}=\frac{1}{2}(\mathbf{b}_1+\mathbf{b}_2+\mathbf{b}_3)$, the dynamical matrix $\mathbf{D}(\mathbf{k}_{10})$ is real, and the consequences of time-reversal symmetry are described by Eqs. (3.49)–(3.53). The criterion for determining the type of representation is given in Eq. (5.63), from which it is easy to see that only the first type occurs for $G_0(\mathbf{k}_{10})$. [Note the difference in defi-

TABLE III. Irreducible multiplier representations[a] of $G_0(\mathbf{k}_{10})$ and the characters of $\mathbf{T}(\mathbf{k}_{10};\mathbf{R})$.

	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_4$	$\mathbf{R}_{13}$	$\mathbf{R}_{14}$	$\mathbf{R}_{15}$	$\mathbf{R}_{16}$	$\mathbf{R}_{25}$	$\mathbf{R}_{26}$	$\mathbf{R}_{27}$	$\mathbf{R}_{28}$	$\mathbf{R}_{37}$	$\mathbf{R}_{38}$	$\mathbf{R}_{39}$	$\mathbf{R}_{40}$	Ref. 11
$\boldsymbol{\tau}^{(1)}$	ε	σ_z	$-\sigma_z$	$-\varepsilon$	$i\varepsilon$	$-i\sigma_z$	$i\sigma_z$	$-i\varepsilon$	$i\sigma_y$	$-\sigma_x$	σ_x	$-i\sigma_y$	σ_y	$-i\sigma_x$	$i\sigma_x$	$-\sigma_y$	X_4
$\boldsymbol{\tau}'^{(1)}$	ε	σ_z	$-\sigma_z$	$-\varepsilon$	$i\varepsilon$	$-i\sigma_z$	$i\sigma_z$	$-i\varepsilon$	$-i\sigma_x$	$-\sigma_y$	σ_y	$i\sigma_x$	$-\sigma_x$	$-i\sigma_y$	$i\sigma_y$	σ_x	
$\chi^{(1)}$	2	0	0	-2	$i2$	0	0	$-i2$	0	0	0	0	0	0	0	0	
$\boldsymbol{\tau}^{(2)}$	ε	$-\sigma_z$	σ_z	$-\varepsilon$	$-i\varepsilon$	$-i\sigma_z$	$i\sigma_z$	$i\varepsilon$	$i\sigma_y$	σ_x	$-\sigma_x$	$-i\sigma_y$	$-\sigma_y$	$-i\sigma_x$	$i\sigma_x$	σ_y	X_3
$\boldsymbol{\tau}'^{(2)}$	ε	$-\sigma_z$	σ_z	$-\varepsilon$	$-i\varepsilon$	$-i\sigma_z$	$i\sigma_z$	$i\varepsilon$	$-i\sigma_x$	σ_y	$-\sigma_y$	$i\sigma_x$	σ_x	$-i\sigma_y$	$i\sigma_y$	$-\sigma_x$	
$\chi^{(2)}$	2	0	0	-2	$-i2$	0	0	$i2$	0	0	0	0	0	0	0	0	
$\boldsymbol{\tau}^{(3)}$	ε	σ_x	σ_x	ε	$i\sigma_y$	σ_z	σ_z	$i\sigma_y$	$i\sigma_y$	σ_z	σ_z	$i\sigma_y$	ε	σ_x	σ_x	ε	X_1
$\boldsymbol{\tau}'^{(3)}$	ε	σ_z	σ_z	ε	$i\sigma_x$	σ_y	σ_y	$i\sigma_x$	$i\sigma_x$	σ_y	σ_y	$i\sigma_x$	ε	σ_z	σ_z	ε	
$\chi^{(3)}$	2	0	0	2	0	0	0	0	0	0	0	0	2	0	0	2	
$\boldsymbol{\tau}^{(4)}$	ε	σ_x	σ_x	ε	$i\sigma_x$	σ_z	σ_z	$i\sigma_y$	$-i\sigma_y$	$-\sigma_z$	$-\sigma_z$	$-i\sigma_y$	$-\varepsilon$	$-\sigma_x$	$-\sigma_x$	$-\varepsilon$	X_2
$\boldsymbol{\tau}'^{(4)}$	ε	σ_z	σ_z	ε	$i\sigma_x$	σ_y	σ_y	$i\sigma_x$	$-i\sigma_x$	$-\sigma_y$	$-\sigma_y$	$-i\sigma_x$	$-\varepsilon$	$-\sigma_z$	$-\sigma_z$	$-\varepsilon$	
$\chi^{(4)}$	2	0	0	2	0	0	0	0	0	0	0	0	-2	0	0	-2	
χ	6	0	0	-2	0	0	0	0	0	0	0	0	2	0	0	2	

[a] See Ref. 12.

nition of reciprocal lattice vectors in Eqs. (5.63) and (6.3).] Therefore each lattice vibration normal mode is twofold degenerate for the wave vector $\mathbf{k}_{10}$ and the eigenvectors may be chosen to be real, (i.e., eigenvectors of $\mathbf{K}_0$). From Eq. (6.21) we see that the matrices $\mathbf{T}(\mathbf{k}_{10};\mathbf{R})$ for $\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{R}_3$, $\mathbf{R}_4$, $\mathbf{R}_{37}$, $\mathbf{R}_{38}$, $\mathbf{R}_{39}$, and $\mathbf{R}_{40}$ commute with $\mathbf{K}_0$. Therefore, according to Eq. (4.52), the corresponding irreducible representation matrices $\boldsymbol{\tau}(\mathbf{k};\mathbf{R})$ must be real to insure that the eigenvectors are compatible with Eq. (4.12b). From Table III we see that the Kovalev[12] form of $\boldsymbol{\tau}^{(1)}$ and $\boldsymbol{\tau}^{(2)}$ do not satisfy Eq. (4.52) for $\mathbf{R}_{37}$, $\mathbf{R}_{38}$, $\mathbf{R}_{39}$, and $\mathbf{R}_{40}$. It is clear that a similarity transformation corresponding to a rotation of 90° about the z axis which transforms $\sigma_x \rightarrow \sigma_y$, $\sigma_y \rightarrow -\sigma_x$, and $\sigma_z \rightarrow \sigma_z$ produces an irreducible representation of the required form. These representations are designated by $\boldsymbol{\tau}'^{(1)}$ and $\boldsymbol{\tau}'^{(2)}$. Using $\boldsymbol{\tau}'^{(1)}$ and $\boldsymbol{\tau}'^{(2)}$ in Eqs. (4.37) and (4.38), we obtain the eigenvectors:

$$\mathbf{e}(\mathbf{k}_{10}111) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \quad \mathbf{e}(\mathbf{k}_{10}112) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad (6.23a)$$

and

$$\mathbf{e}(\mathbf{k}_{10}211) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{e}(\mathbf{k}_{10}212) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}. \qquad (6.23b)$$

Clearly the eigenvectors in Eqs. (6.23a) and (6.23b) each represent a two-fold degenerate transverse mode. However, it is not possible to decide which is acoustical or optical on the basis of symmetry alone.

The situation for $\boldsymbol{\tau}^{(3)}$ in Table III corresponds to the discussion below Eq. (4.52). Namely, Kovalev's irreducible representation $\boldsymbol{\tau}^{(3)}$ is real; however, it is two-dimensional ($f_s=2$), and a number of the irreducible representation matrices which correspond to elements which do not commute with $\mathbf{K}_0$ are diagonal, while the matrices representing $\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_2)$, $\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_3)$, $\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{38})$, and $\mathbf{T}(\mathbf{k}_{10};\mathbf{R}_{39})$ which do commute with $\mathbf{K}_0$ are non-diagonal. Since the matrices $\mathbf{T}(\mathbf{k}_{10};\mathbf{R})$ for $\mathbf{R}=\mathbf{R}_{13}$, $\mathbf{R}_{14}$, $\mathbf{R}_{15}$, $\mathbf{R}_{16}$, $\mathbf{R}_{25}$, $\mathbf{R}_{26}$, $\mathbf{R}_{27}$, and $\mathbf{R}_{28}$ are imaginary, they must be represented by imaginary $\boldsymbol{\tau}(\mathbf{k};R)$ when the basis vectors are real. An examination of $\boldsymbol{\tau}^{(3)}$ in Table III shows that we must transform $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y$, $\boldsymbol{\sigma}_z$ into $\pm\boldsymbol{\sigma}_z$, $\pm\boldsymbol{\sigma}_x$, $\pm\boldsymbol{\sigma}_y$, respectively, to obtain a representation of the desired form. This is accomplished by a unitary transformation corresponding to a 240° rotation about the (1, 1, 1) axis. The new equivalent irreducible representation is designated by $\boldsymbol{\tau}'^{(3)}$ in Table III, and the corresponding eigenvectors are

$$\mathbf{e}(\mathbf{k}_{10}311)=\begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix},\quad \mathbf{e}(\mathbf{k}_{10}312)=\begin{pmatrix}0\\0\\1\\0\\0\\0\end{pmatrix},\quad (6.24)$$

which clearly describe longitudinal vibration modes. That is, the LA and LO modes for propagation in the [001] direction become degenerate at the zone boundary in a crystal of the diamond structure.

Another type of application is the determination of selection rules. We illustrate this application with an example. The μ-Cartesian component of the dipole moment operator for a crystal can be expanded in powers of the nuclear displacements according to[26]

Table IV. The form of the matrices $M_\mu(\mathbf{k}_4 sas'a')$.

sa	$s'a'$ 11	12	21	31	41	42
			$\mu=x$:			
11	0	a_1	0	a_2	0	0
12	$-a_1$	0	0	a_3	0	0
21	0	0	0	0	a_4	a_5
31	$-a_2$	$-a_3$	0	0	0	0
41	0	0	$-a_4$	0	0	a_6
42	0	0	$-a_5$	0	$-a_6$	0
			$\mu=y$:			
11	0	a_1	0	$-a_2$	0	0
12	$-a_1$	0	0	$-a_3$	0	0
21	0	0	0	0	$-a_4$	$-a_5$
31	a_2	a_3	0	0	0	0
41	0	0	a_4	0	0	a_6
42	0	0	a_5	0	$-a_6$	0
			$\mu=z$:			
11	0	0	0	0	b_1	b_2
12	0	0	0	0	b_3	b_4
21	0	0	0	b_5	0	0
31	0	0	$-b_5$	0	0	0
41	$-b_1$	$-b_3$	0	0	0	0
42	$-b_2$	$-b_4$	0	0	0	0

$$M_\mu=M_\mu^{(0)}+\sum_{l\kappa\alpha}M_{\mu,\alpha}(l\kappa)u_\alpha(l\kappa)+\tfrac{1}{2}\sum_{l\kappa\alpha}\sum_{l'\kappa'\beta}M_{\mu,\alpha\beta}(l\kappa;l'\kappa')u_\alpha(l\kappa)u_\beta(l'\kappa')+\cdots. \quad (6.25)$$

It is the second-order terms comprising $M_\mu^{(2)}$ with which we are particularly concerned here. If we make the transformation to phonon field operators according to

$$u_\alpha(l\kappa)=(\hbar/2NM_\kappa)^{1/2}\sum_{\mathbf{k}j}[e_\alpha(\kappa\mid\mathbf{k}j)/(\omega_j(\mathbf{k}))^{1/2}]\exp[i\mathbf{k}\cdot\mathbf{x}(l)]A_{\mathbf{k}j}, \quad (6.26a)$$

where

$$A_{-\mathbf{k}j}=A_{\mathbf{k}j}^{+}, \quad (6.26b)$$

then we may write $M_\mu^{(2)}$ in the form

$$M_\mu^{(2)}=\tfrac{1}{2}\sum_{\mathbf{k}j_1j_2}M_\mu(\mathbf{k}j_1j_2)A_{\mathbf{k}j_1}{}^{+}A_{\mathbf{k}j_2} \quad (6.27)$$

with

$$M\ (\mathbf{k}j_1j_2)=\tfrac{1}{2}\hbar(\omega_{j_1}(\mathbf{k})\omega_{j_2}(\mathbf{k}))^{-1/2}\sum_{l'}\sum_{\kappa\kappa'}\sum_{\alpha\beta}M_{\mu,\alpha\beta}(l\kappa;l'\kappa')$$
$$\times[e_\alpha^*(\kappa\mid\mathbf{k}j_1)/(M_\kappa)^{1/2}][e_\beta(\kappa'\mid\mathbf{k}j_2)/(M_{\kappa'})^{1/2}]\exp[-i\mathbf{k}\cdot(\mathbf{x}(l)-\mathbf{x}(l'))], \quad (6.28)$$

where the invariance of $M_{\mu,\alpha\beta}(l\kappa;l'\kappa')$ under translations has been used,[26] that is,

$$M_{\mu,\alpha\beta}(l\kappa;l'\kappa')=M_{\mu,\alpha\beta}(l-l'\kappa;0\kappa'),$$
$$=M_{\mu,\alpha\beta}(0\kappa;l'-l\kappa'). \quad (6.29)$$

Regarding the coefficient $M_\mu(kj_1j_2)$ as a $3r\times3r$ matrix in the branch indices j_1 and j_2, we ask: Which are the nonzero elements of this matrix when $\mathbf{k}$ is a point of symmetry in the first Brillouin zone of the crystal? The interest in this question stems from the fact that the coefficient $M_\mu(\mathbf{k}j_1j_2)$ enters multiplicatively into the expression for the strength of the infrared lattice vibration absorption[27] by two phonon processes in which the incident photon interacts with two phonons of equal and opposite wave vectors $\mathbf{k}$ and $-\mathbf{k}$ which belong to the branches j_1 and j_2

[26] Reference 1a, p. 219.
[27] Reference 1a, p. 363 ff.

of $\omega^2(\mathbf{k})$. Knowing the nonzero elements of $M_\mu(\mathbf{k}j_1j_2)$, we know between which branches of the phonon spectrum at $\mathbf{k}$ phonon transitions can occur.

From Eq. (6.28) we see first that $M_\mu(\mathbf{k}j_1j_2)$ has the following two general properties:

$$M_\mu(-\mathbf{k}j_1j_2)=M_\mu^*(\mathbf{k}j_1j_2), \tag{6.30}$$

$$M_\mu(-\mathbf{k}j_1j_2)=M_\mu(\mathbf{k}j_2j_1), \tag{6.31}$$

so that it is a Hermitian matrix.

To determine the restrictions placed on $M_\mu(\mathbf{k}j_1j_2)$ by the symmetry and structure of the crystal we require the result that under a space group operation, Eq. (2.4), the crystal dipole moment transforms as a polar vector with the result that the coefficients $\{M_{\mu,\alpha\beta}(l\kappa;l'\kappa')\}$ transform according to the law[26]

$$M_{\mu,\alpha\beta}(LK;L'K')=\sum_{\nu\rho\sigma} S_{\mu\nu}S_{\alpha\rho}S_{\beta\sigma}M_{\nu,\rho\sigma}(l\kappa;l'\kappa'). \tag{6.32}$$

If the point group of the space group G contains the inversion, and if we denote by $(\bar{l}\bar{\kappa})$ the lattice site into which $(l\kappa)$ is taken by a space group operation containing the inversion, then we can rewrite Eq. (6.28) as

$$M_\mu(\mathbf{k}j_1j_2)=-\tfrac{1}{2}\hbar(\omega_{j_1}(\mathbf{k})\omega_{j_2}(\mathbf{k}))^{-1/2}\sum_{l'}\sum_{\kappa\kappa'}\sum_{\alpha\beta}M_{\mu,\alpha\beta}(\bar{l}\bar{\kappa};\bar{l}'\bar{\kappa}')[e_\alpha(\bar{\kappa}\mid\mathbf{k}j_1)/(M_{\bar{\kappa}})^{1/2}]$$
$$\times\exp\{-i\mathbf{k}\cdot[\mathbf{x}(\bar{\kappa})+\mathbf{x}(\kappa)]\}[e_\beta^*(\bar{\kappa}'\mid\mathbf{k}j_2)/(M_{\bar{\kappa}'})^{1/2}]\exp\{i\mathbf{k}\cdot[\mathbf{x}(\bar{\kappa}')+\mathbf{x}(\kappa')]\}$$
$$\times\exp\{i\mathbf{k}\cdot[\mathbf{x}(\bar{l})+\mathbf{x}(\bar{\kappa})+\mathbf{x}(\kappa)-\mathbf{x}(\bar{l}')-\mathbf{x}(\bar{\kappa}')-\mathbf{x}(\kappa')]\}=-M_\mu^*(\mathbf{k}j_1j_2). \tag{6.33}$$

It follows from comparing this result with that given by Eq. (6.30) that for crystals which possess a center of inversion

$$M_\mu(\mathbf{k}j_1j_2)=-M_\mu(\mathbf{k}j_2j_1).$$

Consequently, for such crystals

$$M_\mu(\mathbf{k}jj)=0, \tag{6.34}$$

a well-known result.[28]

If we make use of Eqs. (6.32), (3.3), and (3.7), we can rewrite Eq. (6.28) for an arbitrary crystal as

$$M_\mu(\mathbf{k}j_1j_2)=\tfrac{1}{2}\hbar(\omega_{j_1}(\mathbf{Sk})\omega_{j_2}(\mathbf{Sk}))^{-1/2}\sum_\nu S_{\nu\mu}\sum_{l'}\sum_{\kappa\kappa'}\sum_{\rho\sigma}[M_{\nu,\rho\sigma}(l\kappa;l'\kappa')/(M_\kappa M_{\kappa'})^{1/2}]\exp[-i\mathbf{Sk}\cdot(\mathbf{x}(l)-\mathbf{x}(l'))]$$
$$\times\{\sum_{\kappa_1\alpha}\Gamma_{\rho\alpha}^*(\kappa\kappa_1\mid\mathbf{k};\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})e_\alpha^*(\kappa_1\mid\mathbf{k}j_1)\}\{\sum_{\kappa_2\beta}\Gamma_{\sigma\beta}(\kappa'\kappa_2\mid k;\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\})e_\beta(\kappa_2\mid\mathbf{k}j_2)\}. \tag{6.35}$$

If $\mathbf{S}$ is not a rotation in the group of the wave vector and is not the inversion, then, according to Eq. (4.9a), we have the transformation law

$$M_\mu(\mathbf{k}j_1j_2)=\sum_\nu S_{\nu\mu}M_\nu(\mathbf{Sk}j_1j_2). \tag{6.36}$$

Let us now restrict the symmetry operations $\{\mathbf{S}\mid\mathbf{v}(S)+\mathbf{x}(m)\}$ to be those belonging to the space group of the wave vector $\mathbf{k}$. In this case, we can rewrite Eq. (6.35) in the form

$$M_\mu(\mathbf{k}j_1j_2)=\tfrac{1}{2}\hbar(\omega_{j_1}(\mathbf{k})\omega_{j_2}(\mathbf{k}))^{-1/2}\sum_\nu R_{\nu\mu}\sum_{l'}\sum_{\kappa\kappa'}\sum_{\rho\sigma}[M_{\nu,\rho\sigma}(l\kappa;l'\kappa')/(M_\kappa M_{\kappa'})^{1/2}]\exp[-i\mathbf{k}\cdot(\mathbf{x}(l)-\mathbf{x}(l'))]$$
$$\times\{\sum_{\kappa_1\alpha}T_{\rho\alpha}^*(\kappa\kappa_1\mid\mathbf{k};\mathbf{R})e_\alpha^*(\kappa_1\mid\mathbf{k}j_1)\}\{\sum_{\kappa_2\beta}T_{\sigma\beta}(\kappa'\kappa_2\mid\mathbf{k};\mathbf{R})e_\beta(\kappa_2\mid\mathbf{k}j_2)\}. \tag{6.37}$$

To proceed beyond this point we introduce the more general notation of the preceding section and obtain

$$M_\mu(\mathbf{k}sa\lambda s'a'\lambda')=\sum_\nu R_{\nu\mu}\sum_{\lambda_1\lambda_2}\tau_{\lambda_1\lambda}^{(s)}(\mathbf{k};\mathbf{R})^*\tau_{\lambda_2\lambda'}^{(s')}(\mathbf{k};\mathbf{R})M_\nu(\mathbf{k}sa\lambda_1s'a'\lambda_2). \tag{6.38}$$

From this result one can determine the form of the coefficient $M_\mu(\mathbf{k}sa\lambda s'a'\lambda')$ regarded as a $3r\times3r$ matrix in the indices $(sa\lambda)$ and $(s'a'\lambda')$.

For example, if $\mathbf{k}$ is a vector lying along the [110] direction in the first Brillouin zone of a crystal possessing the diamond structure, Eq. (6.38) together with the results obtained in the first part of this section enables us to establish that the matrices $M_\mu(\mathbf{k}_4sas'a')$ $(\mu=x, y, z)$ have the forms summarized in Table IV. In obtaining these results, we have made use of the fact that crystals of the diamond structure possess a center of inversion, so that Eq. (6.34) applies.

The result expressed by Eq. (6.38) contains more information than merely between which branches of the phonon spectrum at the point $\mathbf{k}$ in the first Brillouin zone two-phonon absorption can occur. This is equivalent

[28] L. E. Gurevich and I. P. Ipatova, Proceedings of the International Conference on Semiconductor Physics, Exeter (1962); R. Loudon, Phys. Rev. **137**, A1784 (1965); and M. Lax, *ibid.* **138**, A793 (1965).

to knowing which are the nonzero elements of the tensor $M_\mu(\mathbf{k}sa\lambda s'a'\lambda')$. From Eq. (6.38) the complete form of this tensor can be obtained, including any relations among its components.

ACKNOWLEDGMENT

It is a pleasure to thank Sandra Cooke for doing an excellent job of typing the manuscript.

APPENDIX

This appendix contains the rotational elements $\mathbf{R}$ in matrix form, and the $\mathbf{v}(R)$ for a crystal of the diamond structure which enter the particular applications discussed in Sec. 6. The corresponding symbols used by Herring[11] are given. For the choice of origin (6.2) it is straightforward to show that for all cases where $\mathbf{v}(R)=0$ the sublattices go into themselves under a crystal symmetry operation, while for $\mathbf{v}(R)\neq 0$ the sublattices are interchanged ($\kappa=1\to 2$, $\kappa=2\to 1$). Therefore, we separate the rotational elements $\mathbf{R}$ accordingly.

$\mathbf{v}(R)=0$:

$$\mathbf{R}_1=\boldsymbol{\varepsilon}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\qquad \mathbf{R}_2=\boldsymbol{\delta}_{2x}=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},$$

$$\mathbf{R}_3=\boldsymbol{\delta}_{2y}=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\qquad \mathbf{R}_4=\boldsymbol{\delta}_{2z}=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},$$

$$\mathbf{R}_{37}=\boldsymbol{\rho}_{xy}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix},\qquad \mathbf{R}_{38}=\boldsymbol{\sigma}_{4z}=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix},$$

$$\mathbf{R}_{39}=\boldsymbol{\sigma}_{4z}^{-1}=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&-1\end{pmatrix},\qquad \mathbf{R}_{40}=\boldsymbol{\rho}_{xy}=\begin{pmatrix}0&-1&0\\-1&0&0\\0&0&1\end{pmatrix};$$

$\mathbf{v}(R)=\mathbf{x}(2)=(\tau/2)(1,1,1)$:

$$\mathbf{R}_{13}=\boldsymbol{\delta}_{2\bar{x}y}=\begin{pmatrix}0&-1&0\\-1&0&0\\0&0&-1\end{pmatrix},\qquad \mathbf{R}_{14}=\boldsymbol{\delta}_{4z}=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix},$$

$$\mathbf{R}_{15}=\boldsymbol{\delta}_{4z}^{-1}=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix},\qquad \mathbf{R}_{16}=\boldsymbol{\delta}_{2xy}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&-1\end{pmatrix},$$

$$\mathbf{R}_{25}=\mathbf{i}=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\qquad \mathbf{R}_{26}=\boldsymbol{\rho}_{x}=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&1\end{pmatrix},$$

$$\mathbf{R}_{27}=\boldsymbol{\rho}_{y}=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\qquad \mathbf{R}_{28}=\boldsymbol{\rho}_{z}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}.$$