The representation group and its application to space groups

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A so-called representation (rep) group $\mathbf{G}$ is introduced which is formed by all the $|\mathbf{G}|$ distinct operators (or matrices) of an abstract group $\hat{\mathbf{G}}$ in a rep space L and which is an m-fold covering group of another abstract group $\mathbf{g}$. $\mathbf{G}$ forms a rep of $\hat{\mathbf{G}}$. The rep group differs from an abstract group in that its elements are not linearly independent and thus the number n of its linearly independent class operators is less than its class number N. A systematic theory is established for the rep group based on Dirac's CSCO (complete set of commuting operators) approach in quantum mechanics. This theory also comprises the rep theory for abstract groups as a special case of $m=1$. Three kinds of CSCO, the CSCO-I, -II, and -III, are defined which are the analogies of J^2, (J^2,J_z), and $(J^2,J_z,\bar{J}_z)$, respectively, for the rotation group SO_3, where $\bar{J}_z$ is the component of angular momentum in the intrinsic frame. The primitive characters, the irreducible basis and Clebsch-Gordan coefficients, and the irreducible matrices of the rep group $\mathbf{G}$ in any subgroup symmetry adaptation can be found by solving the eigenequations of the CSCO-I, -II, and -III of $\mathbf{G}$, respectively, in appropriate vector spaces. It is shown that the rep group $\mathbf{G}$ has only n instead of N inequivalent irreducible representations (irreps), which are just the allowable irreps of the abstract group $\hat{\mathbf{G}}$ in the space L. Therefore, the construction of the irreps of $\hat{\mathbf{G}}$ in L can be replaced by that of $\mathbf{G}$. The labor involved in the construction of the irreps of the rep group $\mathbf{G}$ with order $|\mathbf{G}|$ is no more than that for the group $\mathbf{g}$ with order $|\mathbf{g}|=|\mathbf{G}|/m$, and thus tremendous labor can be saved by working with the rep group $\mathbf{G}$ instead of the abstract group $\hat{\mathbf{G}}$. Based on the rep-group theory, a new approach to the space-group rep theory is proposed, which is distinguished by its simplicity and applicability. Corresponding to each little group $\mathbf{G}(\mathbf{k})$, there is a rep group $\mathbf{G}'_{\mathbf{k}}$. The n inequivalent irreps of $\mathbf{G}'_{\mathbf{k}}$ are essentially just the acceptable irreps of the little group $\mathbf{G}(\mathbf{k})$. Consequently the construction of the irreps of $\mathbf{G}(\mathbf{k})$ is almost as easy as that of the little co-group $\mathbf{G}_0(\mathbf{k})$. An easily programmable algorithm is established for computing the Clebsch-Gordan series and Clebsch-Gordan coefficients of a space group simultaneously.

CONTENTS

GLOSSARY

C_i	the ith class operator
C $(C(i))$	complete set of commuting operators (CSCO or CSCO-I) of $\mathbf{G}$ $(\mathbf{G}(i))$
CGC	Clebsch-Gordan coefficient
$C(s)=(C(1),C(2),\ldots)$	complete set of commuting operators of $\mathbf{G}(s)$
$\overline{C}(s)=(\overline{C}(1),\overline{C}(2),\ldots)$	complete set of commuting operators of $\overline{\mathbf{G}}(s)$
CSCO	complete set of commuting operators
$D^{(\nu)}(R_i)$	the irreducible matrix for the group element R_i
EFM	eigenfunction method
$\mathbf{g}$	abstract group
g_i	number of elements in the ith class
$\mathbf{G}$	representation group (in Secs. I—VIII), space group (in Secs. IX—XX)
$\hat{\mathbf{G}}$	abstract group
$\overline{\mathbf{G}}$	the intrinsic group of $\mathbf{G}$
$\lvert\mathbf{G}\rvert$ $(\lvert\mathbf{g}\rvert)$	order of the group $\mathbf{G}$ $(\mathbf{g})$
$\mathbf{G_k}, \mathbf{G'_k}$	representation groups
$\hat{\mathbf{G}}'_\mathbf{k}$	the abstract group isomorphic to $\mathbf{G'_k}$
$\mathbf{G}(\mathbf{k})$	little group
$\mathbf{G}_0$	isogonal point group of the space group $\mathbf{G}$
$\mathbf{G}_0(\mathbf{k})$	little co-group
$\mathbf{G}_0(\mathbf{k})^*$	central extension of $\mathbf{G}_0(\mathbf{k})$
$\mathbf{G}(s)=\mathbf{G}(1)\supset\mathbf{G}(2)\supset\cdots$	subgroup chain
h_ν	dimension of the irreducible representation ν
IRB	irreducible basis
irrep	irreducible representation
ISF	isoscalar factor
L	the representation space of $\hat{\mathbf{G}}$ associated with the representation group $\mathbf{G}$, space lattice, $L=\{\mathbf{R}_n\}$ (in Secs. IX—XX)
L_g	group space of the representation group $\mathbf{G}$
$L(\mathbf{k})$	group space of the representation group $\mathbf{G'_k}$
L_ν	eigenspace of the CSCO of the representation group $\mathbf{G}$
$\mathscr{L}_\mathbf{k}$	eigenspace of the translation operator $\{\varepsilon\,\vert\,\mathbf{R}_n\}$
$\mathscr{L}(*\mathbf{k})$	the representation space of the space group $\mathbf{G}$
n	number of linearly independent class operators of $\mathbf{G}$
N	number of classes of the representation group $\mathbf{G}$
$\mathbf{P}$	holosymmetric point group of the crystal system
$\mathbf{P}(\mathbf{k})$	symmetric group of $\mathbf{k}$
$P_{ab}^{(\nu)}$	the generalized projection operator of the representation group $\mathbf{G}$
$P_a^{(\nu)b}$	the normalized generalized projection

	operator of the representation group **G**
rep	representation
T	translation group
(ν,a,b)	eigenvalue of $(C,C(s),\bar{C}(s))$
$(\nu_1 a_1 \nu_2 a_2 \mid \nu\theta a)$	Clebsch-Gordan coefficient
$\left(\begin{smallmatrix}\nu\mathbf{k}\nu'\mathbf{k}'\\ \sigma a\sigma' a'\end{smallmatrix}\middle\vert \begin{smallmatrix}\nu''\mathbf{k}''\\ \sigma'' a''\end{smallmatrix}\theta\right)$, $U^{(\theta)}_{\sigma a\sigma' a',\sigma'' a''}$	the space-group Clebsch-Gordan coefficient
θ	multiplicity index
$\psi_a^{(\nu)b}$	the ath vector for the bth irreducible representation ν

Genealogical relation for the space group and its point group

$$\mathbf{G}\supset\mathbf{G}(\mathbf{k})\supset\mathbf{G}(s)\supset\mathbf{T},$$
$$\mathbf{P}\supset\mathbf{G}_0\supset\mathbf{G}_0(\mathbf{k}),$$
$$\mathbf{P}\supset\mathbf{P}(\mathbf{k}),$$
$$\mathbf{G}_0(\mathbf{k})=\mathbf{P}(\mathbf{k})\cap\mathbf{G}_0$$

Coset decomposition

$$\mathbf{G}=\sum_\sigma{}^{q}_{1}\oplus\{\beta_\sigma\mid\mathbf{V}_\sigma\mid\}\mathbf{G}(\mathbf{k}),$$
$$\mathbf{G}_0=\sum_\sigma{}^{q}_{1}\oplus\beta_\sigma\mathbf{G}_0(\mathbf{k})$$

TABLE I. Space-group elements, IRB and irrep.

	$\mathbf{G}$	$\mathbf{G}(\mathbf{k})$[a]	$\mathbf{T}$	$\mathbf{G}'_\mathbf{k}$[b]	$\mathbf{G}_0(\mathbf{k})$[c]
group element	$\{\alpha_i\mid\mathbf{V}(\alpha_i)+\mathbf{R}_n\}$	$\{\gamma_i\mid\mathbf{V}(\gamma_i)+\mathbf{R}_n\}$	$\{\varepsilon\mid\mathbf{R}_n\}$	$\{\gamma_i\mid\mathbf{V}(\gamma_i)\}'$	γ
basis vector	$\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\{\beta_\sigma\mid\mathbf{V}_\sigma\}\psi^{(\nu)}_{\mathbf{k},a}$	$\psi^{(\nu)}_{\mathbf{k},a}$	$\psi_\mathbf{k}=e^{i(\mathbf{k}+\mathbf{K}_m)\cdot r}$	$\psi^{(\nu)}_{\mathbf{k},a}$	
irrep	$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}$	$D^{(\mathbf{k})(\nu)}_{ba}$	$\exp(-i\mathbf{k}\cdot\mathbf{R}_n)$	$D^{(\mathbf{k})(\nu)}_{ba}$	$\Delta^{(\nu)}_{ba}$
dimension	qh_ν	h_ν	1	h_ν	h_ν

[a]The irrep of $\mathbf{G}(\mathbf{k})$ is $D^{(\mathbf{k})(\nu)}(\{\gamma\mid\mathbf{c}\})=\exp(-i\mathbf{k}\cdot\mathbf{c})\Delta^{(\nu)}(\gamma)$.
[b]$\{\gamma_j\mid\mathbf{V}(\gamma_j)\}'=R_j=\exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_j)]\,\{\gamma_j\mid\mathbf{V}(\gamma_j)\}$, $j=1,2,\ldots,\mid\mathbf{G}_0(\mathbf{k})\mid$, are the active elements of the rep group $\mathbf{G}'_\mathbf{k}$.
[c]$\Delta^{(\nu)}$ is the projective irrep of the little co-group $\mathbf{G}_0(\mathbf{k})$ and $\Delta^{(\nu)}(\gamma)=D^{(\mathbf{k})(\nu)}(\{\gamma\mid V(\gamma)\}')$.

I. INTRODUCTION

A. Historical retrospect

Group representation (rep) theory plays a very important role in physics and quantum chemistry, and its importance has increased with modern developments. The rep theory for both finite groups and compact Lie groups is rather mature and is treated extensively in numerous books and articles (e.g., Eisenhart, 1933; Murnaghan, 1938; Weyl, 1950; Racah, 1951; Burnside, 1955; Lyubarskii, 1957; Littlewood, 1958; Wigner, 1959; Hamermesh, 1962; Boerner, 1963; Löwdin, 1967; Miller, 1972; Wybourne, 1974). This theory, which we call the traditional group representation theory, seems to be perfect from the mathematical point of view. However, it is not totally satisfying from a practical, or physical, point of view. First, as pointed out by Salam (1963), it is unphysical. Group theory was introduced into mathematics as early as 1810, and the theory of group rep was developed mainly by mathematicians during the 1920s, before quantum mechanics was established; in this it is unlike calculus, which was invented at about the same time as the discovery of Newton's law. As a result, many sophisticated physicists who are quite at home in their own fields seem to be afraid of group theory (Lipkin, 1966). Second, there is no general method for treating various kinds of problems in group rep. Any given technique applies only to a particular problem for a particular group. Not only do the methods for dealing with point groups, permutation groups, space groups, and Lie groups all differ drastically, but the methods for finding the characters, irreducible basis (IRB), irreducible matrices, and Clebsch-Gordan coefficients (CGC, or CG coefficients) also vary from one to another. Therefore, in many cases, these methods are more of an art than a science.

In physical applications, we often need to construct an IRB adapted to a hierarchy of groups, the so-called symmetry-adapted IRB, starting with a high-symmetry group that approximately represents the structure of the system under investigation, down to the actual symmetry group of the system, and terminating in an Abelian group (Butler and Wybourne, 1976b). The analysis due to Devine (1967) of the spectroscopic properties of the rare-earth double nitrates via the group chain $SO_3\supset I_h\supset T_h\supset\mathscr{C}_3$ affords a beautiful example of the application of descending symmetry. The symmetry-adapted IRB is also required in dealing with a system having the so-called dynamical symmetries (Arima and Iachello, 1979, and references therein).

The standard method for constructing an IRB adapted to a group chain $\mathbf{G}\supset\mathbf{G}(s)$, $\mathbf{G}(s)=\mathbf{G}(1)\supset\mathbf{G}(2)\supset\cdots$ is to use the generalized projection operator (Elliott and Dawber, 1979),

$$P^{(\nu)}_{ab}=\frac{h_\nu}{\mid\mathbf{G}\mid}\sum_{i=1}^{\mid\mathbf{G}\mid}D^{(\nu)}_{ab}(R_i)^*R_i\ , \tag{1.1a}$$

where $\mid\mathbf{G}\mid$ is the order of $\mathbf{G}$, h_ν the dimension of the irreducible representation (irrep) (ν), and $D^{(\nu)}_{ab}(R_i)$ the irreducible matrix elements in the $\mathbf{G}\supset\mathbf{G}(s)$ classification. Notice that here a or b is no longer merely an index enumerating the basis, but denotes a set of quantum numbers $a=(\lambda_1,\lambda_2,\ldots)$, λ_i being the irrep label of the subgroup $\mathbf{G}(i)$. Supposing that φ is one of the reducible basis vectors of $\mathbf{G}$, an IRB might be obtained by applying $P^{(\nu)}_{ab}$ to φ,

$$\psi^{(\nu)}_a=\text{const}\times P^{(\nu)}_{ab}\varphi\ . \tag{1.1b}$$

The question is how to get the irreducible matrices $D^{(\nu)}$ in the given $\mathbf{G}\supset\mathbf{G}(s)$ classification. If the $\mathbf{G}\supset\mathbf{G}(s)$ IRB $\psi^{(\nu)}_a$ were known, then

$$D^{(\nu)}_{ab}(R_i)=\langle\psi^{(\nu)}_a\mid R_i\mid\psi^{(\nu)}_b\rangle\ . \tag{1.2}$$

The trouble is that the IRB in the $\mathbf{G}\supset\mathbf{G}(s)$ scheme is not known yet. It is seen that Eqs. (1.1) and (1.2) are two interdependent problems; the solving of one is prerequisite for the solving of the other. Therefore, we are at an impasse when both the matrices and the IRB are unknown. One might use the successive induction technique to construct the $\mathbf{G}\supset\mathbf{G}(s)$ IRB (Boerner, 1963; Bradley and Cracknell, 1972; Altmann, 1977; Dirl, 1977); however, this technique is rather intricate, and a systematic induction procedure can be developed only for invariant subgroups.

The situation is similar for the space-group rep theory. The determination of the irreps of space groups was begun by Seitz (1936) and Bouckaert, Smoluchowski, and Wigner (1936). Thanks to the efforts of many scientists, tables of the irreps of the 230 space groups have now been published [Kovalev, 1961; Faddeev, 1961; Hurley, 1966; Miller and Love, 1967 (reprinted in Cracknell *et al.*, 1979); Zak *et al.*, 1969; Bradley and Cracknell, 1972]. Programs for computing the irreps of any little group $\mathbf{G}(\mathbf{k})$ have been prepared (e.g., Worlton, 1973; Neto, 1975). Extensive review papers and excellent books on space-group reps are available, such as those of Koster (1957), Johnston (1960), Slater (1962,1965), Altmann (1963), Bradley and Cracknell (1972), Maradudin and Vosko (1968), Birman (1974), and Cracknell (1975). Reviews of computational group theory in crystal systems are given by Davies (1982) and Neubüser (1982).

Therefore, it may seem that work on the determination of the irreps of space groups is finished. However, this is not true. For many purposes, e.g., for investigating symmetry change or symmetry breaking in continuous phase transitions (Birman, 1982; Deonarine and Birman, 1983a, 1983b; Tao, 1983), or for studying the compatibility relations for space groups (Bouckaert *et al.*, 1936; Cornwell, 1969; Dirl, 1977), we need to use an IRB and irreps adapted to a given group chain $\mathbf{G}(\mathbf{k})\supset\mathbf{G}(s)\supset\mathbf{T}$, where $\mathbf{G}(s)$ is a subgroup (or a subgroup chain) of the little group $\mathbf{G}(\mathbf{k})$, and $\mathbf{T}$ is the translation group. Unfortunately, this requirement is usually not met by the existing tables or programs for the irreps of space groups, and we have to construct the irreps anew in the given $\mathbf{G}(\mathbf{k})\supset\mathbf{G}(s)\supset\mathbf{T}$ classification.

Besides, the conventional approach to the space-group rep is not totally satisfactory. First, the theory itself is rather complicated and evasive for a person who has only a general knowledge of finite group representation. Second, the practical methods for constructing irreps of the little group are mainly Herring's little group method and the projective- (or ray) rep method (Herring, 1942; Döring, 1959; Bradley and Cracknell, 1972; Birman, 1974) or the variation of the projective-rep method (Lyubarskii, 1957; Kovalev and Lyubarskii, 1958). The former two methods require constructions of reps for groups with high order. For example, for the projective-rep method, the order can be as high as 192. In the Lyubarskii and Kovalev method, a set of matrix equations is set up for a few generators of the little co-group $\mathbf{G}_0(\mathbf{k})$ on a case by case basis. The projective-rep matrices for these generators are first found one by one from the matrix equations, and the whole projective rep results from matrix multiplication. The method used by Zak (1960), Klauder and Gay (1968), and Neto (1973) is based on the reduction of the reps of the little group $\mathbf{G}(\mathbf{k})$ induced from the irreps of its invariant subgroups of index two or three.

Recently, there have been many papers devoted to the Clebsch-Gordon (CG) coefficients for the permutation groups (Schindler and Mirman, 1977a,1977b; Chen and Gao, 1981; Gao and Chen, 1985; Chen, Gao, Shi, Vallieres, and Feng, 1984; Saharasbudhe *et al.*, 1981), for point groups (Van den Broek, 1979; Butler, 1981; Kotzev and Aroyo, 1980,1981), and for space groups (Litvin and Zak, 1968; Saulevich *et al.*, 1970; Gard, 1973; Sakata, 1974; Berenson and Birman, 1975; Berenson *et al.*, 1975; Rudra and Sikdar, 1976; Dirl, 1979,1980; Suffczynski and Kunert, 1982; Chen, Gao, and Ma, 1983). A program in ALGOL has been written for calculating the principle block CG coefficient of the space group (Birman, 1974) by Kowalczyk *et al.* (1980). Systematic tables of CG coefficients for permutation groups (Schindler and Mirman, 1977b; Chen and Gao, 1981; Gao and Chen, 1985), point groups (Koster *et al.*, 1963; Butler, 1981), and magnetic point groups (Kotzev *et al.*, 1980—1982) are available. More recently, the work on computer-generated space-group CG coefficients has been reported (Davies and Dirl, 1983). However, their coefficients are not subgroup symmetry adapted. One of the major aims of the present paper is to set up a simple algorithm for computing space-group CG coefficients adapted to any given subgroup chain.

B. A new approach to group representation theory

From the physical point of view, it is most desirable to have a group rep theory in accordance with the concepts and methods of quantum mechanics. The commuting-operator approach to the rep theory of semisimple Lie groups has met this requirement to a certain extent, due to the efforts of Racah (1951), Biedenharn (1963a,1963b), and Baird and Biedenharn (1963). Gamba (1969) and Killingbeck (1970,1973) expressed their desire to reform the rep theory for finite groups by suggesting a Lie-like approach and commuting-operator approach to the theory, but they have not pursued the subject far enough. Therefore, rep theory for finite groups remains basically the traditional one.

As pointed out by McVoy (1965), the theory of Lie groups, used properly with all the most powerful theorems, is both difficult and time consuming. However, the key theorems are perfectly understandable without a detailed knowledge of the trickery involved in their proof. In this regard, the rotation group SO_3 provides an excellent example. The main results for SO_3 rep theory can be summarized as follows (Chen, Wang, and Gao, 1975,1983).

The Casimir operator J^2 of SO_3 is called the first kind of complete set of commuting operators (CSCO-I) of SO_3. In the class parameter space,

$$J^2=-\frac{1}{\sin^2(\varphi/2)}\frac{d}{d\varphi}\left[\sin^2(\varphi/2)\frac{d}{d\varphi}\right], \tag{1.3}$$

and its eigenfunction gives the character of SO_3

$$J^2\chi^j(\varphi)=j(j+1)\chi^j(\varphi), \tag{1.4a}$$

$$\chi^j(\varphi)=\frac{\sin(j+\frac{1}{2})\varphi}{\sin(\varphi/2)}. \tag{1.4b}$$

The operator J^2 is a CSCO for the class parameter space.

Similarly, J_z is the CSCO-I of SO_2. (J^2,J_z) is called the CSCO-II of SO_3, and its eigenfunction gives the IRB adapted to the canonical subgroup chain $SO_3\supset SO_2$,

$$\begin{bmatrix}J^2\\J_z\end{bmatrix}\psi^j_m=\begin{bmatrix}j(j+1)\\m\end{bmatrix}\psi^j_m. \tag{1.5}$$

(J^2,J_z) is a CSCO for each irreducible space of SO_3.

Let $\bar{J}_x$, $\bar{J}_y$, and $\bar{J}_z$ be the components of angular momentum in the intrinsic frame of a rotating system. They are the generators for rotations around the intrinsic axes x, y, and z. The rotation group with $\bar{J}_x$, $\bar{J}_y$, and $\bar{J}_z$ as infinitesimal generators is called the intrinsic rotation group and denoted by $\overline{SO}_3$. It is well known that (Bohr and Mottelson, 1969)

$$[J_i,\bar{J}_k]=0,\quad i,k=x,y,z, \tag{1.6a}$$

$$[J_x,J_y]=iJ_z,\quad [\bar{J}_x,\bar{J}_y]=-i\bar{J}_z,\quad x,y,z \text{ in cyclic} \tag{1.6b}$$

$$J_x^2+J_y^2+J_z^2=\bar{J}_x^2+\bar{J}_y^2+\bar{J}_z^2. \tag{1.6c}$$

Therefore, the group SO_3 and its intrinsic group $\overline{SO}_3$ are commutative and anti-isomorphic.

$(J^2,J_z,\bar{J}_z)$ is called the CSCO-III of SO_3, and its eigenfunction in the group parameter space gives the complex conjugate of the irreducible matrix element.

$$\begin{bmatrix}J^2\\J_z\\\bar{J}_z\end{bmatrix}D^{(j)}_{mk}(\alpha\beta\gamma)^*=\begin{bmatrix}j(j+1)\\m\\k\end{bmatrix}D^{(j)}_{mk}(\alpha\beta\gamma)^*,$$

$$m,k=-j,-j+1,\ldots,j. \tag{1.7}$$

$(J^2,J_z,\bar{J}_z)$ is a CSCO for the group parameter space of SO_3. k is called the intrinsic quantum number and is used to distinguish between equivalent irreps (j) of SO_3.

It is thus seen that the characters, IRB, and irreducible matrix elements can be obtained by solving the eigenequations of the CSCO-I, -II, and -III, respectively.

Stimulated by the above simple results for the group SO_3, Chen and co-workers (Chen, Wang, and Gao, 1977a,1977b,1977c,1978a,1983; Chen *et al.*, 1979) developed a new approach to group rep theory. For any non-Abelian group G, a so-called intrinsic group $\overline{\mathbf{G}}$ was introduced, and three kinds of CSCO, CSCO-I, -II, and -III, were defined. The key theorems, like those presented above for the group SO_3, are first established easily for finite groups and then extended to compact Lie groups. Thus a unified approach for both finite and Lie groups is established.

For a finite group G, the CSCO-I is just the analogy of the set of l Casimir operators of a Lie group with rank equal to l [McVoy (1965) referred to it as the complete set of commuting observables of a Lie group]; the CSCO-II is, roughly speaking, a set of operators consisting of the CSCO-I of all the subgroups contained in a canonical subgroup chain, while the CSCO-III is a CSCO in the group space. The new approach distinguishes itself by its simplicity in concept and wide applicability in practice. It is also constructive in nature, leading to a new method, the so-called eigenfunction method (EFM), for determining group irreps. The problems of determining (1) the characters and isoscalar factors, (2) the IRB and Clebsch-Gordon coefficients (CGC), and (3) the irreducible matrices adapted to any subgroup chain are all reduced to a single recipe—seeking the eigenvectors of the CSCO-I, -II, and -III, respectively. The EFM proves to be very powerful and versatile in treating the point groups (Chen, Wang, and Gao, 1978c; Chen, Gao, Wang, and Yu, 1979; Chen, Wang, Gao, and Yu, 1980), permutation groups (Chen, Wang, and Gao 1977a; Chen, 1981; Chen and Gao, 1981,1982; Chen, Collinson, and Gao, 1983; Zhu and Chen, 1984), unitary groups (Chen, Wang, and Gao, 1977b,1978a,1978b; Chen, 1981; Chen, Shi, Feng, and Vallieres, 1983; Chen, Gao, Shi, Vallieres, and Feng, 1984), graded unitary groups (Chen, Chen, and Gao, 1983a,1983b,1984; Chen and Chen, 1983; Chen, Gao, and Chen, 1984a,1984b), and space groups (Chen, Gao, and Ma, 1983). For a systematic and extensive review of the new approach the reader is referred to the monograph by Chen (1984).

The EFM for the irreducible characters, IRB, irreducible matrices, and CGC of a finite group is much simpler than the conventional methods and is flexible enough to obtain the irreducible basis adapted to any given group chain $\mathbf{G}\supset\mathbf{G}(s)$ without need of any knowledge of the irreducible matrix, or conversely, to obtain all the irreducible matrices in any given subgroup chain $\mathbf{G}\supset\mathbf{G}(s)$ classification without any knowledge of the irreducible basis. Furthermore, since the ultimate step of the method is the diagonalization of the representative matrices of a certain kind of CSCO, the procedure can be easily translated into a computer program. Several codes are already available; these include one for the CGC and one for the outer-product reduction coefficients of the permutation group (Chen and Gao, 1981, in ALGOL-60), one for the transformation coefficients from the standard (i.e., the Yamanouchi) basis to the nonstandard basis of permutation groups (Chen, Collinson, and Gao, 1984, in FORTRAN IV), and one for the $SU(mn)\supset SU(m)\times SU(n)$ isoscalar factors for arbitrary m and n (Chen, Gao, Shi, Vallieres, and Feng, 1984, in FORTRAN IV).

C. The representation group

Suppose that $\hat{\mathbf{G}}$ is an abstract group with elements $\hat{R}_s$,

$$\hat{\mathbf{G}}=\{\hat{R}_s:s=1,2,\ldots,|\hat{\mathbf{G}}|\}. \tag{1.8}$$

Let R_s be the corresponding operators, or matrices, of $\hat{R}_s$ in a certain rep space L. Suppose that, of the $|\hat{\mathbf{G}}|$ operators (or matrices), only $|\mathbf{G}|$ ones are distinct and they form a group $\mathbf{G}$. With proper ordering, $\mathbf{G}$ can be expressed as

$$\mathbf{G}=\{R_s:s=1,2,\ldots,|\mathbf{G}|\}\ . \tag{1.9}$$

Obviously $\mathbf{G}$ is a subgroup of $\hat{\mathbf{G}}$ and forms a rep of $\hat{\mathbf{G}}$. According to the Lagrange theorem (Hamermesh, 1962),

$$|\hat{\mathbf{G}}|=\mathcal{N}|\mathbf{G}|\ , \tag{1.10}$$

$\mathcal{N}$ being an integer. If $\mathcal{N}=1$, $\mathbf{G}$ is a faithful rep of $\hat{\mathbf{G}}$. The $\mathcal{N}>1$ case is trivial, since the order of the abstract group $\hat{\mathbf{G}}$ can be restricted to be equal to $|\mathbf{G}|$ by imposing cyclic boundary conditions. Hence in the following we assume that $|\hat{\mathbf{G}}|=|\mathbf{G}|$.

These $|\mathbf{G}|$ operators, though distinct, may not be linearly independent. Suppose that there are only $|\mathbf{g}|=|\mathbf{G}|/m$ linearly independent operators R_i, where $m\geq 1$ is an integer, and the remaining operators are simply related to these $|\mathbf{g}|$ operators as

$$R_i^{(l)}=\varepsilon(i,l)R_i\ ,\quad i=1,2,\ldots,|\mathbf{g}|,\ l=0,1,\ldots,m-1\ , \tag{1.11a}$$

$$R_i^{(0)}=R_i\ ,\quad R_1=e\,(\text{identity}),\quad |\varepsilon(i,l)|=1\ ,$$

where $\varepsilon(i,l)$ are complex numbers. Then the group

$$\mathbf{G}=\{R_i^{(l)}:i=1,2,\ldots,|\mathbf{g}|,\ l=0,1,\ldots,m-1\} \tag{1.11b}$$

is called a representation (rep) group. The $|\mathbf{g}|$ operators R_i are called the active elements of $\mathbf{G}$ and constitute the fundamental set F of $\mathbf{G}$,

$$F=\{R_i:i=1,2,\ldots,|\mathbf{g}|\}\ . \tag{1.11c}$$

For simplicity, the rep group $\mathbf{G}$ of Eq. (1.11b) will be denoted as

$$\mathbf{G}=\{R_i:i=1,2,\ldots,|\mathbf{g}|\}_m\ . \tag{1.11d}$$

According to Eq. (1.11a), the multiplication relation of the rep group is fully determined by that of $|\mathbf{g}|$ active elements which can be written as

$$R_iR_j=\eta(i,j)R_{ij}\ , \tag{1.12}$$

where R_{ij} is one of the active elements and $\eta(i,j)$ are complex numbers with absolute value equal to one. The multiplication table of these $|\mathbf{g}|$ active elements will be referred to as the group table of the rep group $\mathbf{G}$.

If there is a group $\mathbf{g}$ with order $|\mathbf{g}|$ and elements γ_i,

$$\mathbf{g}=\{\gamma_i:i=1,2,\ldots,|\mathbf{g}|\}\ , \tag{1.13}$$

and if $\mathbf{g}$ has the multiplication relation

$$\gamma_i\gamma_j=\gamma_{ij}\ , \tag{1.14}$$

then the rep group $\mathbf{G}$ is an m-fold covering group of $\mathbf{g}$, and under the mapping $R_i\leftrightarrow\gamma_i$, the fundamental set F of the rep group $\mathbf{G}$ is said to be a projective (or ray, or multiplier) rep of the group $\mathbf{g}$, and $\eta(i,j)$ form what is called a factor system (Birman, 1974; Bradley and Cracknell, 1972; Altmann, 1977; Dirl, 1977). If $\eta(i,j)\equiv 1$, then F is an ordinary, or vector, rep of $\mathbf{g}$.

Thanks to Eq. (1.11a), to specify an irrep ν of the rep group $\mathbf{G}$, we need only give explicitly the irreducible matrices for the $|\mathbf{g}|$ active elements. Hence for simplicity we shall just say that

$$D^{(\nu)}(\mathbf{G})=\{D^{(\nu)}(R_i):i=1,2,\ldots,|\mathbf{g}|\} \tag{1.15}$$

is an irrep of the rep group $\mathbf{G}$. With this convention, $D^{(\nu)}(\mathbf{G})$ is clearly a projective irrep of the group $\mathbf{g}$ under the mapping $R_i\leftrightarrow\gamma_i$. Henceforth we shall simply say that each irrep of the rep group $\mathbf{G}$ gives a projective irrep of $\mathbf{g}$. Therefore, the construction of projective irreps of the group $\mathbf{g}$ for the factor system η (Kovalev and Lyubarskii, 1958; Mackey, 1958,1968; Dirl, 1977) can be replaced by the construction of vector irreps of the rep group $\mathbf{G}$, which is, as will be shown later, as easy as that for the finite group $\mathbf{g}$ with order $|\mathbf{g}|=|\mathbf{G}|/m$ ($|\mathbf{g}|$ can be called the "effective group order" of the rep group). Dirl (1977) used the induction procedure to obtain projective irreps of $\mathbf{g}$ adapted to a certain subgroup chain, starting from a given projective irrep of an invariant subgroup of $\mathbf{g}$. The procedure is far from simple and applicable only to the invariant subgroups of $\mathbf{g}$.

On the other hand, the IRB of the abstract group $\hat{\mathbf{G}}$ in the rep space L is obviously identical to the IRB of the rep group $\mathbf{G}$, and thus the former task can be replaced by the latter one. It is much easier to work with the rep group $\mathbf{G}$ than with the abstract group $\hat{\mathbf{G}}$, since the "effective" group order of $\mathbf{G}$ is only one mth of the order of $\mathbf{G}$.

In the case of $m=1$, all the $|\mathbf{G}|$ elements of $\mathbf{G}$ are linearly independent and the rep group $\mathbf{G}$ is identical, from the group-theoretical point of view, to the abstract group $\hat{\mathbf{G}}$. Therefore, the abstract group $\hat{\mathbf{G}}$ can be regarded as a special case of the rep group corresponding to $m=1$.

D. About this review

In the first part of this review (Secs. II–VIII), we extend the new approach for the rep theory of the abstract group to the rep-group case. The approach is entirely based on Dirac's CSCO theory, which is very familiar to physicists. All the theorems are proved in a "physical way," and abstract mathematical proofs are avoided as much as possible. The treatment is self-contained, and only a minimal knowledge of group theory is required, covering such topics as the Schur lemmas, the definition of class, cosets, representations, inductions, subductions, etc.

In Sec. II we begin with a brief review of some definitions and theorems for group reps. In Sec. III, the CSCO (or CSCO-I) is introduced for the rep group $\mathbf{G}$, which is analogous to the set of Casimir operators for Lie groups. In Sec. IV the intrinsic group $\overline{\mathbf{G}}$ is defined which is anti-isomorphic to and commuting with the group $\mathbf{G}$. The introduction of the intrinsic group $\mathbf{G}$ is crucial for distinguishing between the equivalent irreps. Sections V and VI

are the heart of the new approach to the projective irreps of a group **g**. Section VII is a summary of the eigenfunction method for constructing the irreducible basis, matrices, characters, and CGC, while Sec. VIII is an example of the application of the general theory for a rep group to a particular abstract group, i.e., the construction of the irreps and CGC of the point group C_{4v} adapted to two different subgroup chains.

In the second part of this review (Secs. IX–XX) the general theory developed in Secs. II–VII is applied to the space group, and a simple rep theory for the space group is established. Sections IX and X give the basic definitions required for dealing with space groups in the subsequent sections. In Sec. XI the representation groups $\mathbf{G}_\mathbf{k}$ and $\mathbf{G}'_\mathbf{k}$, related by a gauge transformation, are introduced and the relation between the irreps of the rep group $\mathbf{G}_\mathbf{k}$ or $\mathbf{G}'_\mathbf{k}$ and the small reps of the little group $\mathbf{G}(\mathbf{k})$ is established. Sections XII and XIII specify some details for applying rep-group theory to the representation group $\mathbf{G}'_\mathbf{k}$. Section XIV is devoted to the working out of several examples to show the ease with which irreducible characters and matrices of the little group $\mathbf{G}(\mathbf{k})$ can be obtained by the EFM. In Sec. XV a simple algorithm for obtaining the full rep matrices of the space group in terms of the small reps of the little group is given, in which all we need is the point-group multiplication instead of the much more complicated space-group multiplication. In Sec. XVI the regular rep of a space group **G** is totally decomposed to $|\mathbf{G}|$ one-dimensional spaces, each corresponding to an irreducible basis vector of **G**. In Sec. XVII, the intrinsic group $\overline{\mathbf{G}}$ and the CSCO-III of the space group **G** are introduced, and it is shown that the irreducible basis vectors resulting from the decomposition of the regular rep of **G** are the eigenvectors of the CSCO-III of **G**. Section XVIII is devoted to setting up an algorithm for the space group CG coefficients while Sec. XIX gives two examples of the construction of full rep matrices and the CGC of the space group O_h^7 for the **k** stars X and W. Various methods for calculating the space-group CGC are reviewed in Sec. XX, and a summary of the whole paper is given in Sec. XXI.

Since the abstract group $\hat{\mathbf{G}}$ is a special case of the rep group **G**, the theory for rep groups also contains that for abstract groups as a special case of $m=1$. In the following, for most cases we deal only with the rep group, and for simplicity we shall just say "the group **G**" instead of "the rep group **G**" when no confusion will arise. Besides, since every rep of a finite group is equivalent to a unitary rep, without loss of generality we assume that all reps discussed here are unitary. It should also be mentioned that the term "a vector space" throughout the paper means "a linear complex vector space."

We restrict ourselves to the single-valued reps of the unitary group. Extension to the double-valued reps is straightforward.

II. PRELIMINARY KNOWLEDGE

In this section we cite some definitions and theorems. The proofs of these theorems are omitted, since they can be found in any textbook on group theory, except for Theorems 2.1, 2.3, and 2.6, which may not be available in textbooks, at least not in the form we use.

A. A complete set of commuting operators

Definition 2.1. Suppose that there is an operator C defined in a linear vector space $\mathscr{L}$; the subspace $\mathscr{L}_v$ generated by all the eigenvectors **v** of C which belong to the same eigenvalue v of C is called an eigenspace of C,

$$\mathscr{L}_v=\{\mathbf{v}\in\mathscr{L}:C\mathbf{v}=v\mathbf{v}\}\ . \tag{2.1a}$$

Symbolically we write

$$C\mathscr{L}_v=v\mathscr{L}_v\ . \tag{2.1b}$$

Definition 2.2. A set of commuting operators $C=(C_1,C_2,\ldots,C_l)$ is said to be a complete set of commuting operators (CSCO) of the space $\mathscr{L}$ if in $\mathscr{L}$ all the eigenvalues of C are nondegenerate (or, equivalently, if the eigenspaces of C are all one dimensional).

A CSCO is said to be self-adjoint if it consists entirely of self-adjoint operators.

Theorem 2.1. A CSCO for a vector space $\mathscr{L}$ of finite dimensionality can always be chosen to consist of only a single operator.

Proof. The basis vectors $|\varphi_\lambda\rangle$ for an n-dimensional vector space $\mathscr{L}$ can always be labeled uniquely by a single discrete parameter λ, $\lambda=1,2,\ldots,n$. Without loss of generality, $|\varphi_\lambda\rangle$ can be assumed to be orthonormal.

Let us construct a linear operator C by

$$C=\sum_{\lambda=1}^{n}\lambda\,|\varphi_\lambda\rangle\langle\varphi_\lambda|\ . \tag{2.2a}$$

Obviously we have

$$C\,|\varphi_\lambda\rangle=\lambda\,|\varphi_\lambda\rangle\ . \tag{2.2b}$$

Thus each basis vector $|\varphi_\lambda\rangle$ is an eigenvector of the operator C with the parameter λ as the eigenvalue. According to the hypothesis of the uniqueness of the label λ, the single operator C is evidently a CSCO of the space $\mathscr{L}$.

Theorem 2.2. A linear operator which commutes with each operator of a CSCO is a function of the CSCO (see Dirac, 1958, Sec. 19).

B. Group representations

Definition 2.3. An invariant subspace of a group **G** is called a rep space of **G**.

Definition 2.4. A minimum invariant subspace of a group **G** is called an irreducible space of **G**.

For groups commonly used in physics, the group operators are unitary. In the following, this is always assumed to be true.

Theorem 2.3. The subspace $\mathscr{L}_v$ of a rep space of **G**, which is an eigenspace of an operator C commuting with the group **G**, is necessarily also a rep space of **G**.

Proof. From the hypothesis we have

$$C\mathscr{L}_\nu=\nu\mathscr{L}_\nu,\quad [C,R]=0\ \text{ for } R\in\mathbf{G}\ ; \tag{2.3}$$

it follows that

$$C(R\mathscr{L}_\nu)=RC\mathscr{L}_\nu=\nu(R\mathscr{L}_\nu)\ \text{ for } R\in\mathbf{G}\ .$$

Hence $R\mathscr{L}_\nu\in\mathscr{L}_\nu$, that is, the eigenspace $\mathscr{L}_\nu$ is invariant under the group. Therefore, $\mathscr{L}_\nu$ is a rep space of **G**.

The significance of this theorem is that a rep of **G** generated by the space $\mathscr{L}$ can be reduced by decomposing the space $\mathscr{L}$ into eigenspaces of an operator which commutes with the group **G**. This is the starting point of the new approach to group rep theory.

Theorem 2.4 (Schur lemma). Let $D^{(\nu)}(\mathbf{G})$ be an h_ν-dimensional rep of a group **G** and A be an $h_\nu\times h_\nu$ matrix; then the rep $D^{(\nu)}(\mathbf{G})$ is irreducible if and only if the only matrix A which satisfies

$$D^{(\nu)}(R)A=AD^{(\nu)}(R) \tag{2.4a}$$

for all $R\in\mathbf{G}$ is

$$A=\lambda\mathbf{I}\ , \tag{2.4b}$$

where **I** is an $h_\nu\times h_\nu$ unit matrix (see Miller, 1972, p. 70).

Theorem 2.4 is extremely useful because it gives a simple criterion for irreducibility of a rep.

Corollary 2.1. If C is an operator commuting with a group **G**, and if L is an invariant space of C and an irreducible space of **G**, then L is necessarily an eigenspace of C.

Definition 2.5. The $|\mathbf{g}|$-dimensional vector space L_g formed by the $|\mathbf{g}|$ linearly independent operators R_i is referred to as the group space of **G**,

$$L_g=\{R_i : i=1,2,\ldots,|\mathbf{g}|\}\ . \tag{2.5}$$

The metric tensor for the group space can be chosen as

$$g_{ij}=\langle R_i\,|\,R_j\rangle=\delta_{ij},\quad i,j=1,2,\ldots,|\mathbf{g}|\ . \tag{2.6}$$

Any vector in the group space L_g can be expressed as

$$P=\sum_{i=1}^{|\mathbf{g}|}u(R_i)R_i\ , \tag{2.7}$$

where $u(R_i)\equiv u_i$ are complex numbers. According to Eq. (2.6), the scalar product of two vectors in L_g is

$$\langle P^{(\nu)}\,|\,P^{(\mu)}\rangle=\sum_{i=1}^{|\mathbf{g}|}u^{(\nu)}(R_i)^*u^{(\mu)}(R_i)\ . \tag{2.8}$$

Apart from the scalar product (2.8), we can also define the group product of two vectors according to the rep-group multiplication rule (1.12),

$$P^{(\nu)}P^{(\mu)}=\sum_{i,j}{}_1^{|\mathbf{g}|}\,u^{(\nu)}(R_i)u^{(\mu)}(R_j)\eta(i,j)R_{ij}\ . \tag{2.9}$$

Obviously, the product $P^{(\nu)}P^{(\mu)}$ still belongs to the space L_g. Thus L_g is closed under the group multiplication rule and forms an algebra, called the rep-group algebra or the projective group algebra (Dirl, 1977). When $\eta(i,j)\equiv 1$, it reduces to ordinary (or vector) group algebra (Hamermesh, 1962; Littlewood, 1958; Löwdin, 1967; Miller, 1972).

Theorem 2.5. The space spanned by the inverse operators of R_i, $i=1,2,\ldots,|\mathbf{g}|$, coincides with the group space L_g, i.e.,

$$L_g=\{R_i^{-1} : i=1,2,\ldots,|\mathbf{g}|\}\ . \tag{2.10}$$

Proof. Since there are only $|\mathbf{g}|$ linearly independent vectors in L_g and any $|\mathbf{g}|$ linearly independent vectors in L_g span the same space L_g, we need only show that the $|\mathbf{g}|$ operators R_i^{-1} are linearly independent. If they are not, then one can write

$$R_i^{-1}=\sum_{j\neq i}{}_1^{|\mathbf{g}|}\,u_jR_j^{-1}\ . \tag{2.11a}$$

The unitarity of the operators R_i implies that

$$R_i^\dagger=\sum_{j\neq i}{}_1^{|\mathbf{g}|}\,u_jR_j^\dagger\ \text{ or }\ R_i=\sum_{j\neq i}{}_1^{|\mathbf{g}|}\,u_j^*R_j\ , \tag{2.11b}$$

in contradiction with the hypothesis that the $|\mathbf{g}|$ operators R_i are linearly independent. Hence the $|\mathbf{g}|$ operators $R_1^{-1},\ldots,R_g^{-1}$ are also linearly independent.

Definition 2.6. The rep $D(\mathbf{G})$ generated by the group space L_g is called the regular rep of **G**, namely,

$$\begin{aligned}&R_jR_k=\sum_{i=1}^{|\mathbf{g}|}D_{ik}(R_j)R_i,\quad j,k=1,2,\ldots,|\mathbf{g}|\ ,\\ &D_{ik}(R_j)=\langle R_i\,|\,R_j\,|\,R_k\rangle\equiv\langle i\,|\,R_j\,|\,k\rangle=\eta(j,k)\delta_{i,jk}\ .\end{aligned} \tag{2.12}$$

Notice that to determine a rep for the group **G**, we need only to give the rep matrices for the elements in the set F, since the rep matrices for other elements of **G** are given by

$$D(R_i^{(l)})=\varepsilon(i,l)D(R_i)\ . \tag{2.13}$$

Again Eq. (2.12) is a generalization of the usual regular rep for an abstract group $\hat{\mathbf{G}}$.

C. The class algebra

Suppose that the rep group **G** has N classes (N is also the number of classes of the abstract group $\hat{\mathbf{G}}$). The $m\,|\mathbf{g}|$ operators $R_i^{(l)}$ of **G** can be regrouped into N classes. Let $R_{(i,\kappa)}$ be the κth element of the ith class.

Definition 2.7. The algebraic sum of all the operators of **G** belonging to the same class is called the class operator,

$$C_i=\sum_{\kappa=1}^{g_i}R_{(i,\kappa)},\quad i=1,2,\ldots,N\ , \tag{2.14}$$

where g_i is the number of operators in the class i.

Furthermore, we use the notation

$$C_{i'}=\sum_{\kappa=1}^{g_i}R_{(i,\kappa)}^{-1} \tag{2.15}$$

to denote the class operator consisting of the inverse operators of $R_{(i,\kappa)}$.

Definition 2.8. The class i is said to be ambivalent if C_i

is equal to $C_{i'}$; otherwise it is said to be nonambivalent (Hamermesh, 1962).

Since the operators $R_i^{(l)}$ or $R_{(i,\kappa)}$ of the rep group **G** are not linearly independent, neither are the N class operators. Some of the class operators may be null operators, or some may differ by only a phase factor, $C_i=\xi_{ij}C_j$ with $|\xi_{ij}|=1$. Let $C_1(=e),C_2,\ldots,C_n$ be the linearly independent class operators of **G**, $n\leq N$ (the equality holds only when $m=1$).

Definition 2.9. The vector space spanned by the n linearly independent class operators $C_1,C_2,\ldots,C_n$ is called the class space of **G**, denoted as

$$L_n=\{C_i:i=1,2,\ldots,n\}\ . \tag{2.16}$$

The class space L_n is a subspace of the group space L_g. The metric tensor in the class space is decided by Eq. (2.6), i.e.,

$$\langle C_i\,|\,C_j\rangle=g_i\delta_{ij},\quad i,j=1,2,\ldots,n\ . \tag{2.17}$$

The class operators have the following important properties (Hamermesh, 1962).

(1) They commute with any element of **G**,

$$[C_i,R]=0\ \text{ for all } R\in\mathbf{G}\ . \tag{2.18a}$$

(2) They commute with one another,

$$[C_i,C_j]=0\ . \tag{2.18b}$$

(3) They are closed under group multiplication,

$$C_iC_j=\sum_{k=1}^{n}C_{ij}^kC_k,\quad i,j=1,2,\ldots,n\ . \tag{2.18c}$$

The coefficients C_{ij}^k are called the structure constants of the rep group. Note that they can be imaginary [for example, see Eqs. (14.6)], in contrast to the case of an abstract group whose structure constants are non-negative integers.

Any vector in the class space can be written as

$$Q=\sum_{i=1}^{n}q_iC_i\ , \tag{2.19}$$

where q_i are complex numbers.

The scalar product of two vectors in the class space is

$$\langle Q^{(1)}\,|\,Q^{(2)}\rangle=\sum_{i=1}^{n}g_iq_i^{(1)*}q_i^{(2)}\ . \tag{2.20}$$

Because of Eq. (2.18c), the class space is closed under group multiplication and therefore it forms an algebra—the class algebra. It is clear that the class algebra is a subalgebra of the rep-group algebra.

Theorem 2.6. Any operator constructed out of group operators and commuting with the group is necessarily a class operator or a linear combination of the class operators of the group (Wu, 1984).

Proof. Assume that the operator

$$A=\sum_{s=1}^{|\mathbf{G}|}y_sR_s=\sum_{i=1}^{|\mathbf{g}|}x_iR_i \tag{2.21}$$

commutes with the rep group **G**, where y_s and x_i are complex numbers. This means that

$$A=R_sAR_s^{-1},\quad s=1,2,\ldots,|\mathbf{G}|\ . \tag{2.22a}$$

Therefore,

$$A=\frac{1}{|\mathbf{G}|}\sum_{s=1}^{|\mathbf{G}|}R_sAR_s^{-1}=\sum_{i=1}^{|\mathbf{g}|}x_i\left[\frac{1}{|\mathbf{G}|}\sum_{s=1}^{|\mathbf{G}|}R_sR_iR_s^{-1}\right]$$
$$=\sum_{i=1}^{|\mathbf{g}|}\frac{x_i}{g_i}C_i\ , \tag{2.22b}$$

where

$$C_i=\frac{g_i}{|\mathbf{G}|}\sum_{s=1}^{|\mathbf{G}|}R_sR_iR_s^{-1}$$

is the class operator associated with the element R_i.

III. THE CSCO-I OF A GROUP G

A. The CSCO in the class space

Definition 3.1. A set of l operators $C_1,C_2,\ldots,C_l$, or a linear combination of them, selected out of the n linearly independent class operators of a group **G**, is called a CSCO-I of **G**, or simply a CSCO of **G**, if the set is a complete set of commuting operators in the class space of **G**, denoted as[1]

$$C=(C_1,C_2,\ldots,C_l)\ , \tag{3.1a}$$

or

$$C=\sum_{i=1}^{l}k_iC_i\ . \tag{3.1b}$$

Let $Q^{(\nu)}$ be an eigenvector of the CSCO of **G** in the class space

$$CQ^{(\nu)}=\nu Q^{(\nu)}\ . \tag{3.2a}$$

If C is given by Eq. (3.1a), then (3.2a) actually denotes a set of simultaneous eigenequations

$$C_iQ^{(\nu)}=\lambda_i^{(\nu)}Q^{(\nu)},\quad i=1,2,\ldots,l\ , \tag{3.2b}$$

and ν stands collectively for the set of eigenvalues

$$\nu=(\lambda_1^{(\nu)},\lambda_2^{(\nu)},\ldots,\lambda_l^{(\nu)})\ . \tag{3.3}$$

It follows from Definitions 2.2 and 3.1 that, for a rep group with n linearly independent class operators, C must have n distinct sets of eigenvalues ν. In the following, ν is also used as the index enumerating the sets of eigenvalues. Therefore, we can write $\nu=1,2,\ldots,n$.

From Theorem 2.2, we immediately have Theorem 3.1.

Theorem 3.1. Any class operator C_i of a group **G** is a function of the CSCO of **G**,

[1] C_1 does not necessarily mean the identity operator.

$$C_i = F_i(C), \quad i = 1,2,\ldots,n \ , \tag{3.4}$$

and in turn we also have Theorem 3.2.

Theorem 3.2. Any eigenvector of the CSCO of **G** is necessarily a simultaneous eigenvector of all the n class operators of **G**,

$$C_i Q^{(\nu)} = \lambda_i^{(\nu)} Q^{(\nu)}, \quad i = 1,2,\ldots,n \ . \tag{3.5}$$

The choice of the CSCO of **G** is not unique; however, different CSCO of **G** are all equivalent in the sense that they have, according to Theorem 3.2, identical eigenvectors $Q^{(\nu)}$, $\nu = 1,2,\ldots,n$. Thus we have Theorem 3.3.

Theorem 3.3. Different CSCO's of **G** are equivalent.

B. Irreps of the class algebra

Equation (2.18c) shows that the n basis vectors $C_1,\ldots,C_n$ of the class space L_n carry a rep of the class algebra,

$$C_i C_j = \sum_{k=1}^{n} \mathscr{D}_{kj}(C_i) C_k, \quad i,j = 1,2,\ldots,n \ . \tag{3.6}$$

The rep $\mathscr{D}(C_i)$ is called the natural rep of the class operator C_i with matrix elements

$$\mathscr{D}_{kj}(C_i) = C_{ij}^{k} \ . \tag{3.7}$$

With the eigenvectors $Q^{(\nu)}$ of the CSCO of **G** as basis vectors, the representation matrices of the n class operators all become diagonal,

$$\mathscr{D}(C_i) = \begin{bmatrix} C_{i1}^1 & C_{i2}^1 & \cdots & C_{in}^1 \\ \vdots & \vdots & & \vdots \\ C_{i1}^n & C_{i2}^n & \cdots & C_{in}^n \end{bmatrix} \rightarrow D(C_i)$$

$$= \begin{bmatrix} \lambda_i^{(\nu_1)} & & & 0 \\ & \lambda_i^{(\nu_2)} & & \\ & & \ddots & \\ 0 & & & \lambda_i^{(\nu_n)} \end{bmatrix} . \tag{3.8}$$

Hence we see that the natural rep of the class algebra is reducible, i.e., it can be reduced into n one-dimensional irreps of the class algebra.

Theorem 3.4. The set formed by all the n class operators $C_1,\ldots,C_n$ of a group **G** is necessarily a CSCO of **G**.

Proof. To prove the theorem, we need only show that, in the class space, the set of operators $(C_1,\ldots,C_n)$ has n distinct sets of eigenvalues. Let us regard the diagonal matrix elements of $D(C_i)$ in Eq. (3.8), $(\lambda_i^{(\nu_1)}, \lambda_i^{(\nu_2)},\ldots,\lambda_i^{(\nu_n)})$, as a column vector and put n such vectors together to form a matrix M,

$$M = \begin{bmatrix} \lambda_1^{(\nu_1)} & \lambda_2^{(\nu_1)} & \cdots & \lambda_n^{(\nu_1)} \\ \lambda_1^{(\nu_2)} & \lambda_2^{(\nu_2)} & \cdots & \lambda_n^{(\nu_2)} \\ \vdots & \vdots & & \vdots \\ \lambda_1^{(\nu_n)} & \lambda_2^{(\nu_n)} & \cdots & \lambda_n^{(\nu_n)} \end{bmatrix} . \tag{3.9}$$

The ith column vector $(\lambda_i^{(\nu_1)}, \lambda_i^{(\nu_2)},\ldots,\lambda_i^{(\nu_n)})$ is a representative of the class operator C_i. Since the n class operators are linearly independent, the n column vectors in the matrix M are necessarily also linearly independent. Therefore, the rank of the matrix M is equal to n, which in turn implies that the n row vectors $(\lambda_1^{(\nu_i)}, \lambda_2^{(\nu_i)},\ldots,\lambda_n^{(\nu_i)})$, $i = 1,2,\ldots,n$, are also linearly independent. Consequently, no two row vectors can be identical. Otherwise stated, the set of operators $(C_1,\ldots,C_n)$ has n distinct sets of eigenvalues.

Theorem 3.5. Any CSCO of **G** is equivalent to a self-adjoint CSCO of **G**.

Suppose that among the n class operators, n_1 are ambivalent and $2n_2$ are nonambivalent. Using the unitarity of the group operators and Eq. (2.15), it is easy to show that the ambivalent class operators are self-adjoint, while the nonambivalent class operators are not, i.e.,

$$C_i^{\dagger} = C_i, \quad i = 1,2,\ldots,n_1 \ , \tag{3.10a}$$

$$C_j^{\dagger} = C_{j'}, \quad j = n_1+1,\ldots,n_1+n_2 \ . \tag{3.10b}$$

However, out of the $2n_2$ non-self-adjoint operators $(C_j, C_{j'})$ we can construct another $2n_2$ self-adjoint operators,

$$K_l = C_j + C_{j'}, \quad K_l' = i(C_j - C_{j'}) \ , \quad l = j - n_1 = 1,2,\ldots,n_2 \ . \tag{3.11}$$

Thus we have a set of n self-adjoint operators

$$C' = (C_1,\ldots C_{n_1}, K_1,\ldots,K_{n_2}, K_1',\ldots,K_{n_2}') \ . \tag{3.12}$$

Repeating the proof of Theorem 3.4, C' must be a CSCO of **G**, while, according to Theorem 3.3, any CSCO of **G** is necessarily equivalent to C'.

The significance of Theorem 3.5 is that from now on in proving theorems we can always assume that the CSCO of **G** is self-adjoint and utilize all the results obtained in quantum mechanics related to the self-adjoint CSCO.

C. The finding of the CSCO of G

If all the primitive characters of **G** are known, it is trivial to find the CSCO of **G** (see Sec. VII.C). If the characters are unknown, we can use the following steps to find the CSCO of **G**.

First, we pick-out one class operator, say C_i, from the n class operators and seek its eigenvector,

$$Q = \sum_{j=1}^{n} q_j C_j \ , \tag{3.13a}$$

$$C_i Q = \lambda_i Q \ . \tag{3.13b}$$

This amounts to diagonalizing the matrix $\mathscr{D}(C_i)$,

$$\sum_{j=1}^{n}(C_{ij}^{k}-\lambda_i\delta_{jk})q_j=0,\quad k=1,2,\ldots,n\ . \tag{3.14}$$

The characteristic equation is

$$\det||C_{ij}^{k}-\lambda_i\delta_{jk}||=\prod_{\alpha}(\lambda_i-\lambda_i^{(\alpha)})^{m_\alpha}\ , \tag{3.15}$$

where the integer m_α is the degeneracy of the eigenvalue $\lambda_i^{(\alpha)}$. If all the degeneracies m_α are equal to one, i.e., if C_i has n distinct eigenvalues, then the single operator C_i is a CSCO of $\mathbf{G}$. Conversely, if for a certain eigenvalue $\lambda_i^{(\beta)}$ the degeneracy $m_\beta>1$, then C_i is not a CSCO of $\mathbf{G}$. From Eq. (3.14) we can obtain m_β linearly independent eigenvectors $Q_1,\ldots,Q_{m_\beta}$ belonging to the eigenvalue $\lambda_i^{(\beta)}$. They span a m_β-dimensional eigenspace L_β of C_i. In such a case, we have to pick another class operator, say C_j, and make linear combinations of $Q_1,\ldots,Q_{m_\beta}$, so that they become eigenvectors of C_j as well. If in the space L_β the eigenvalues of C_j are all nondegenerate, then (C_i,C_j) will be the CSCO of $\mathbf{G}$; otherwise we have to add more operators, until we find a set of operators, $C=(C_1,\ldots,C_l)$, whose eigenvalues have no degeneracy, in which case C is the CSCO of $\mathbf{G}$.

The CSCO for all point groups and for permutation groups S_n with n up to 14 are listed by Chen *et al.* (1977a,1977c). It is found that the number l of the class operators contained in the CSCO for the above groups is equal to one, two, or at most three. Hence l is much smaller than the number of classes, $l\ll N$. This fact has great practical significance for the eigenfunction method.

Suppose that $C=(C_1,\ldots,C_l)$ is a CSCO of $\mathbf{G}$. With known eigenvalues $\lambda_i^{(\nu)}$ of C_i, it is easy to find a single operator

$$C=\sum_{i=1}^{l}k_iC_i\ , \tag{3.16a}$$

k_i being coefficients properly chosen, such that C has n distinct eigenvalues

$$\lambda^{(\nu)}=\sum_{i=1}^{l}k_i\lambda_i^{(\nu)} \tag{3.16b}$$

Consequently we can choose this single operator C as the CSCO of $\mathbf{G}$. The advantage of choosing a single operator as the CSCO of $\mathbf{G}$ is obvious when a computer is used in practical calculation.

In the following, the CSCO of $\mathbf{G}$ can be understood either as Eq. (3.1a) or as the single operator (3.1b).

The n eigenvectors of C,

$$Q^{(\nu)}=\sum_{i=1}^{n}q_i^{(\nu)}C_i,\quad \nu=1,2,\ldots,n\ , \tag{3.17}$$

form an orthonormal and complete set in the class space. By the definition of the scalar product [Eq. (2.20)], the orthonormal and completeness conditions are

$$\sum_{i=1}^{n}g_iq_i^{(\nu)*}q_i^{(\mu)}=\delta_{\nu\mu}\ , \tag{3.18a}$$

$$\sum_{\nu=1}^{n}g_iq_i^{(\nu)*}q_j^{(\nu)}=\delta_{ij}\ . \tag{3.18b}$$

As mentioned before, the abstract group is a special case of the rep group. The above theorems and equations also hold for abstract groups by letting $m=1$, $|\mathbf{g}|=|\mathbf{G}|$, $n=N$. In order to illustrate this, in the following example we consider only the $m=1$ case, leaving the $m>1$ case to Sec. XIV.A.

D. Example: The CSCO of the point group C_{4v}

The point group C_{4v} has eight elements, $(C_{4z})^j$, $j=1,\ldots,4$, σ_x, σ_y, σ_{da}, and σ_{db}. Here we use the notations of Bradley and Cracknell (1972). For example, σ_x stands for a reflection plane with its normal in the x direction, and σ_{da} for one with a normal midway (45°) between the x and y axes. The group C_{4v} has five classes, and its class operators are

$$\begin{aligned}&C_1=e,\quad C_2=C_{2z},\quad C_3=C_{4z}^{+}+C_{4z}^{-}\ ,\\ &C_4=\sigma_x+\sigma_y,\quad C_5=\sigma_{da}+\sigma_{db}\ .\end{aligned} \tag{3.19}$$

From the group table of C_{4v} (see Table IV below), the class multiplication table can easily be constructed, as shown in Table II.

From Eq. (3.6) and Table II, we can construct the natural rep of the class algebra. For instance,

$$\mathscr{D}(C_4)=\begin{bmatrix}0&0&0&2&0\\0&0&0&2&0\\0&0&0&0&2\\1&1&0&0&0\\0&0&2&0&0\end{bmatrix},\qquad \mathscr{D}(C_5)=\begin{bmatrix}0&0&0&0&2\\0&0&0&0&2\\0&0&0&2&0\\0&0&2&0&0\\1&1&0&0&0\end{bmatrix}. \tag{3.20}$$

Clearly, we should choose as the members of a CSCO class operators having as many as possible distinct eigenvalues. C_1 has only one distinct eigenvalue, 1, while C_2 has two distinct eigenvalues, ±1, so they are not good candidates. Let us try to choose C_4 (in fact C_3 or C_5 would be equally good). By diagonalizing $\mathscr{D}(C_4)$, we find the following eigenvalues and eigenvectors:

TABLE II. The class multiplication table of C_{4v}.

C_1	C_2	C_3	C_4	C_5
C_2	C_1	C_3	C_4	C_5
C_3	C_3	$2C_1+2C_2$	$2C_5$	$2C_4$
C_4	C_4	$2C_5$	$2C_1+2C_2$	$2C_3$
C_5	C_5	$2C_4$	$2C_3$	$2C_1+2C_2$

$\lambda_4=2$, double degeneracy, $Q_1^{(2)}=C_1+C_2+C_4$,

$$Q_2^{(2)}=C_3+C_5 . \quad (3.21a)$$

$\lambda_4=-2$, double degeneracy, $Q_1^{(-2)}=C_1+C_2-C_4$,

$$Q_2^{(-2)}=C_3-C_5 . \quad (3.21b)$$

$\lambda_4=0$, no degeneracy, $Q^{(0)}=C_1-C_2$. (3.21c)

Due to the twofold degeneracy for $\lambda_4=\pm 2$, C_4 is not a CSCO of C_{4v}. We have to pick another class operator, say C_5, and recombine $Q_1^{(2)}$ and $Q_2^{(2)}$, as well as $Q_1^{(-2)}$ and $Q_2^{(-2)}$, so that they are eigenvectors of C_5. As can be checked, the eigenvector $Q^{(0)}$ for the single root of C_4 is already an eigenvector of C_5 with eigenvalue 0. Using Table II, we can get the simultaneous eigenvectors of (C_4,C_5), as listed in Table III.

In Table III, $\mathcal{N}$ is the norm decided by Eq. (3.18a). Now all the degeneracies have been lifted, and thus (C_4,C_5) is a CSCO of C_{4v}. We may as well choose

$$C=2C_4+C_5 \quad (3.22)$$

as the CSCO of C_{4v}, since it has five distinct eigenvalues, 6, 2, -6, -2, and 0. In Sec. VI.G, we shall see that the eigenvalues of the CSCO of G can be used to label inequivalent irreps of G.

E. The projection operator

From Eqs. (2.18b), (3.17), and (3.2a) we have

$$CQ^{(\nu)}Q^{(\mu)}=\nu Q^{(\nu)}Q^{(\mu)}=\mu Q^{(\nu)}Q^{(\mu)} . \quad (3.23)$$

Equation (3.23) shows that the product $Q^{(\nu)}Q^{(\mu)}$ is an eigenvector of C with the eigenvalue ν or μ. Since the eigenvalues of C are all nondegenerate, we must have

$$Q^{(\nu)}Q^{(\mu)}=\delta_{\nu\mu}\eta_\nu Q^{(\nu)} , \quad (3.24)$$

where η_ν is a constant depending only on ν. When we let

$$P^{(\nu)}=\eta_\nu^{-1}Q^{(\nu)} , \quad (3.25)$$

we have

$$P^{(\nu)}P^{(\mu)}=\delta_{\nu\mu}P^{(\nu)} . \quad (3.26)$$

Hence $P^{(\nu)}$ are idempotents.

From Eq. (3.18b), we get the inverse expansion of (3.17),

$$C_i=\sum_{\nu=1}^{n} g_i q_i^{(\nu)*}Q^{(\nu)} . \quad (3.27)$$

Multiplying Eq. (3.27) from the right with $Q^{(\mu)}$, and using (3.2b) and (3.24), we obtain

$$\lambda_i^{(\nu)}=\eta_\nu g_i q_i^{(\nu)*} . \quad (3.28a)$$

Letting i be the identity class and noting $\lambda_e^{(\nu)}=g_e=1$, we then have

$$\eta_\nu^{-1}=q_e^{(\nu)*} . \quad (3.28b)$$

We combine Eqs. (3.25), (3.27), and (3.28a),

$$C_i=\sum_{\nu=1}^{n}\lambda_i^{(\nu)}P^{(\nu)} . \quad (3.29)$$

With $C_i=e$, we obtain

$$e=\sum_{\nu=1}^{n}P^{(\nu)} . \quad (3.30)$$

Equation (3.30) is the decomposition formula for the identity operator of the rep group G. Notice that the rep group is defined in the representation space L of the abstract group $\hat{\mathbf{G}}$ and Eq. (3.30) is valid only in the space L.

Suppose that $\mathscr{L}$ is an arbitrary rep space, which is a subspace of L; then the subspace

$$\mathscr{L}_\nu=P^{(\nu)}\mathscr{L},\quad \mathscr{L}\subseteq L , \quad (3.31a)$$

either vanishes or is necessarily an eigenspace of the CSCO of G,

$$C\mathscr{L}_\nu=\nu\mathscr{L}_\nu . \quad (3.31b)$$

Since C is assumed to be self-adjoint, the different eigenspaces are mutually orthogonal,

$$\langle \mathscr{L}_\nu | \mathscr{L}_{\nu'}\rangle=0 \text{ if } \nu\neq\nu' . \quad (3.32)$$

Combining Eqs. (3.26), (3.30), and (3.31), we arrive at the following theorem.

Theorem 3.6. The eigenvectors $P^{(\nu)}$ are projection operators onto the eigenspaces of the CSCO of G.

Theorem 3.7. In any rep space $\mathscr{L}\subseteq L$, the possible eigenvalues of the CSCO of G cannot go beyond the n sets determined in the class space of G.

Proof. According to Eq. (3.30), for any rep space $\mathscr{L}\subseteq L$, we have

$$\mathscr{L}=e\mathscr{L}=\sum_{\nu=1}^{n}P^{(\nu)}\mathscr{L}=\sum_{\nu=1}^{n}\oplus\mathscr{L}_\nu . \quad (3.33)$$

If $\mathscr{L}_\mu$ is an eigenspace of C belonging to an eigenvalue μ other than those determined in the class space of G, i.e., if

TABLE III. The eigenvectors of the CSCO of C_{4v}. The first column is the Mulliken notation for irreducible representations of point groups.

	λ_4,λ_5	$\mathcal{N}$	C_1	C_2	C_3	C_4	C_5
A_1	2,2	$\sqrt{1/8}$	1	1	1	1	1
B_1	2,−2	$\sqrt{1/8}$	1	1	−1	1	−1
A_2	−2,−2	$\sqrt{1/8}$	1	1	1	−1	−1
B_2	−2,2	$\sqrt{1/8}$	1	1	−1	−1	1
E	0,0	$\sqrt{1/8}$	2	−2	0	0	0

$$C\mathscr{L}_\mu=\mu\mathscr{L}_\mu,\quad \mu\notin\{\nu=1,2,\ldots,n\}\,, \tag{3.34}$$

then we must have

$$\langle\mathscr{L}_\nu|\,\mathscr{L}_\mu\rangle=0\quad\text{for }\nu=1,2,\ldots,n\,, \tag{3.35}$$

due to Eq. (3.32). By virtue of Eq. (3.33), this implies that

$$\langle\mathscr{L}\,|\,\mathscr{L}_\mu\rangle=0\,. \tag{3.36}$$

Since $\mathscr{L}$ is an arbitrary subspace in L, $\mathscr{L}_\mu$ is necessarily a null space in L.

Theorem 3.8. In the group space of **G**, the CSCO of **G** has, and only has, the n distinct sets of eigenvalues $(\lambda_1^{(\nu)},\lambda_2^{(\nu)},\ldots,\lambda_l^{(\nu)})$, $\nu=1,2,\ldots,n$, determined from the class space of **G**.

Proof. Here "has" is trivial, since the group space contains the class space as its subspace, while "only has" follows from Theorem 3.7.

Theorem 3.9. The rep spaces $\mathscr{L}_\nu$ which are eigenspaces of the CSCO of **G** belonging to different eigenvalues are inequivalent.

Proof. For succinctness in exposition, the CSCO of **G** is assumed to consist of only a single operator C, as given by Eq. (3.16a). If the two rep spaces $\mathscr{L}_\nu$ and $\mathscr{L}_{\nu'}$ with different eigenvalues $\nu\neq\nu'$, were equivalent, then the matrices of the CSCO of **G** in the two rep spaces must relate to each other as

$$D^{(\nu)}(C)=TD^{(\nu')}(C)T^{-1}\,, \tag{3.37}$$

where T is a matrix. On the other hand, since $\mathscr{L}_\nu$ and $\mathscr{L}_{\nu'}$ are eigenspaces of C, the representative matrices of C in $\mathscr{L}_\nu$ ($\mathscr{L}_{\nu'}$) must be equal to the unit matrix multiplied by the eigenvalue ν (ν'):

$$D^{(\nu)}(C)=\nu\cdot\mathbf{I},\quad D^{(\nu')}(C)=\nu'\cdot\mathbf{I}\,. \tag{3.38}$$

Substituting Eq. (3.38) into (3.37), we get $\nu=\nu'$, in contradiction with the hypothesis. Thus the theorem is proved. Combining the above discussions, we have Theorem 3.10.

Theorem 3.10. The group space L_g of **G** can be decomposed into n rep spaces, orthogonal and inequivalent to each other:

$$L_g=\sum_{\nu=1}^{n}\oplus L_\nu,\quad L_\nu=P^{(\nu)}L_g\,. \tag{3.39}$$

In order to make clear the difference and connection between the abstract group $\hat{\mathbf{G}}$ and its rep group **G** defined in the space L, let us reinterpret the above results in terms of the abstract group $\hat{\mathbf{G}}$.

The group space of $\hat{G}$ is designated as

$$L_G=\{\hat{R}_s:s=1,2,\ldots,|\,\mathbf{G}\,|\} \tag{3.40}$$

with the metric tensor

$$\langle\hat{R}_s\,|\,\hat{R}_t\rangle=\delta_{st}\,. \tag{3.41}$$

The abstract group $\hat{\mathbf{G}}$ has N linearly independent class operators, $\hat{C}_j$, $j=1,2,\ldots,N$, which span the class space L_N of $\hat{\mathbf{G}}$.

Suppose that $\hat{\mathscr{C}}$ is a CSCO of $\hat{\mathbf{G}}$, and its eigenvectors in L_N are $\hat{P}^{(\mu_i)}$,

$$\hat{\mathscr{C}}\hat{P}^{(\mu_i)}=\mu_i\hat{P}^{(\mu_i)},\quad i=1,2,\ldots,N\,. \tag{3.42}$$

Then parallel to Eq. (3.30) we have the decomposition

$$e=\sum_{i=1}^{N}\hat{P}^{(\mu_i)}\,, \tag{3.43}$$

and corresponding to Theorem 3.7 we have Theorem 3.7′.

Theorem 3.7′. In any rep space, the possible eigenvalues of the CSCO of $\hat{\mathbf{G}}$ cannot go beyond the N sets, $\mu_1,\mu_2,\ldots,\mu_N$, determined from the class space L_N of $\hat{\mathbf{G}}$.

Let C_j, $\mathscr{C}$, and $P^{(\mu_i)}$ be the corresponding operators of $\hat{C}_j$, $\hat{\mathscr{C}}$, and $\hat{P}^{(\mu_i)}$, respectively, in the rep space L. Among the N class operators $C_1,\ldots,C_N$, now only n are linearly independent, and these can be chosen to be identical to those in (2.16). In the space L, Eq. (3.42) becomes

$$\mathscr{C}P^{(\mu_i)}=\mu_iP^{(\mu_i)},\quad i=1,2,\ldots,N\,, \tag{3.44}$$

where $P^{(\mu_i)}$ are linear combinations of n linearly independent class operators $C_1,\ldots,C_n$. According to Eq. (3.44) and Theorem 3.7′ the set $\{P^{(\mu_1)},\ldots,P^{(\mu_N)}\}$ exhausts all the eigenvectors of $\mathscr{C}$ in L_n, and since L_n is n dimensional, there are n and only n linearly independent eigenvectors of $\mathscr{C}$, say

$$P^{(\mu_i)},\quad i=1,2,\ldots,n\,, \tag{3.45}$$

where $\mu_1,\ldots,\mu_n$ are n distinct eigenvalues of $\mathscr{C}$. Therefore, $\mathscr{C}$ is a CSCO of the rep group **G**. (However, the reverse is not true, i.e., if C is a CSCO of the rep group **G**, then the corresponding operator $\hat{C}$ is not necessarily a CSCO of the abstract group $\hat{\mathbf{G}}$.) In a manner similar to the proof of Theorem 3.7, it can be shown that

$$P^{(\mu_j)}=0\quad\text{for }j=n+1,\ldots,N\,, \tag{3.46}$$

that is, for those μ_j which are not eigenvalues of the CSCO of the rep group **G**, the operators $P^{(\mu_j)}$ are identically null operators. It is seen that Eqs. (3.30), (3.43), and (3.46) are self-consistent.

In summary we have

$$\hat{P}^{(\mu_i)}L=P^{(\mu_i)}L\quad\text{for }i=1,2,\ldots,n\,, \tag{3.47a}$$

$$\hat{P}^{(\mu_j)}L=P^{(\mu_j)}L=0\quad\text{for }j=n+1,\ldots,N\,, \tag{3.47b}$$

where $\mu_1,\ldots,\mu_n$ are eigenvalues of the CSCO of the rep group **G**. Later we shall show that $\hat{P}^{(\mu_i)}$ are the projection operators onto the irreps μ_i of $\hat{\mathbf{G}}$. Therefore, Eqs. (3.47) tell us that in the rep space L, only the irreps $\mu_1,\ldots,\mu_n$ of $\hat{\mathbf{G}}$ are acceptable.

IV. THE INTRINSIC GROUP

A. The intrinsic group of an abstract group

The rep space L_v of $\mathbf{G}$ defined by Eq. (3.39) is in general reducible. According to Theorem 2.3, if we can find extra operators which commute with $\mathbf{G}$, then the rep generated by L_v can be further reduced by decomposing L_v into eigenspaces of these operators. Theorems 2.6 and 3.1 tell us that it is impossible to find such extra operators from the group $\mathbf{G}$ itself. In Sec. I.B we see that for the rotation group SO_3, there is an intrinsic rotation group $\overline{SO}_3$ commuting with and anti-isomorphic to the group SO_3. Although the CSCO-I of $\overline{SO}_3$ is equal to that of SO_3 and thus does not provide new operators, the CSCO-I $\bar{J}_z$ of the subgroup $\overline{SO}_2$ of the intrinsic group $\overline{SO}_3$ does provide a new operator. In parallel to this, Chen, Wang, and Gao (1977a) have introduced a so-called intrinsic group $\overline{\mathbf{G}}$ for any non-Abelian group $\mathbf{G}$, using the CSCO-I of the subgroups of $\overline{G}$, which play the same role as $\bar{J}_z$ for SO_3, to decompose the rep space L_v.

We begin with the introduction of the intrinsic group for an abstract group, or equivalently for a rep group with $m=1$. To simplify notation, we temporarily use $R,S,T,U,\ldots$ to denote the elements of a group $\mathbf{G}$ which span the $|\mathbf{G}|$-dimensional group space L_G.

Definition 4.1. For each element R of a group $\mathbf{G}$, we can define a corresponding operator $\bar{R}$ in the group space L_G through the following equation:

$$\bar{R}S=SR \quad \text{for all } S\in\mathbf{G} . \tag{4.1}$$

The group $\overline{G}$ formed by the totality of the operators $\bar{R}$ is called the intrinsic group of $\mathbf{G}$, or simply the intrinsic group $\overline{G}$ if no confusion will arise.

Let us first show that the operators $\bar{R}$ do form a group. According to Eq. (4.1), the operation of $\bar{R}$ on a vector S in L_G is to change it into another vector SR. It should be emphasized that (4.1) is the defining equation for the operator $\bar{R}$ rather than an identity relation. Hence it is not permissible to multiply Eq. (4.1) from the right by another vector T of L_G, i.e.,

$$\bar{R}ST\neq SRT . \tag{4.2}$$

Instead, we should regard ST as a new vector in L_G, and then use Eq. (4.1) to get

$$\bar{R}ST=\bar{R}(ST)=STR . \tag{4.3}$$

Suppose the multiplication relation for the group $\mathbf{G}$ is

$$RS=U . \tag{4.4a}$$

From (4.1) and (4.3) we have

$$\bar{S}\bar{R}T=\bar{S}TR=TRS=TU=\bar{U}T . \tag{4.5}$$

Since T is an arbitrary vector in L_G, one has

$$\bar{S}\bar{R}=\bar{U} . \tag{4.4b}$$

Therefore, there is a one-to-one correspondence between the elements $\bar{R}$ and R, and Eq. (4.4) shows that the totality of $\bar{R}$ form a group $\overline{\mathbf{G}}$ which is anti-isomorphic to the group $\mathbf{G}$.

Besides the property of being anti-isomorphic to $\mathbf{G}$, the intrinsic group $\overline{\mathbf{G}}$ has another important property, namely, that it commutes with the group $\mathbf{G}$. From Eq. (4.1) one has

$$S\bar{R}T=STR \quad \text{for all } T\in L_G . \tag{4.6}$$

Comparing Eq. (4.3) with (4.6), and noting that T is an arbitrary vector in L_G, one has

$$\bar{R}S=S\bar{R} , \tag{4.7a}$$

or

$$[\bar{R},S]=0 . \tag{4.7b}$$

Therefore, $\overline{\mathbf{G}}$ commutes with $\mathbf{G}$.

Note the essential difference between Eqs. (4.1) and (4.7a). The latter is an identity, while the former is not. The difference comes from the fact that in (4.1), S is regarded as a vector in L_G, while in (4.7a), S is an operator in L_G. The rule for determining whether a group element S is to be regarded as a basis vector or as an operator is very simple. If S is the last element behind an intrinsic group operator, then S should be looked upon as a basis vector; if S is followed by other group elements of $\mathbf{G}$, then S should be regarded as an operator.

We know that if $\overline{\mathbf{G}}$ is anti-isomorphic to $\mathbf{G}=\{R,S,T,\ldots\}$, then $\overline{\mathbf{G}}$ is isomorphic to the group $\mathbf{G}'=\{R^{-1},S^{-1},T^{-1},\ldots\}$. The difference between the groups $\mathbf{G}$ and $\mathbf{G}'$ is merely a matter of nomenclature for the elements. Hence we see that the intrinsic group $\overline{\mathbf{G}}$ is "essentially" isomorphic to $\mathbf{G}$. Consequently, all conclusions regarding the group $\mathbf{G}$ also apply to the intrinsic group $\overline{\mathbf{G}}$. For example, if C_i is a class operator of $\mathbf{G}$, then by replacing all the elements R in C_i by $\bar{R}$, we obtain the class operator $\bar{C}_i$ of $\overline{\mathbf{G}}$; if $C=\sum_i k_i C_i$ is the CSCO of $\mathbf{G}$, then $\bar{C}=\sum_i k_i\bar{C}_i$ is the CSCO of $\overline{\mathbf{G}}$; if $\mathbf{G}$ has a subgroup chain $\mathbf{G}\supset\mathbf{G}(1)\supset\mathbf{G}(2)\supset\cdots$, then $\overline{\mathbf{G}}$ has a subgroup chain $\overline{\mathbf{G}}\supset\overline{\mathbf{G}}(1)\supset\overline{\mathbf{G}}(2)\supset\cdots$; and if $C(i)$ is the CSCO of the subgroup $\mathbf{G}(i)$, then $\bar{C}(i)$ will be the CSCO of $\overline{\mathbf{G}}(i)$, etc.

Theorem 4.1. The CSCO of $\overline{\mathbf{G}}$ and $\mathbf{G}$ are equal.

Proof. To prove the theorem, one need only show that the class operators of $\overline{\mathbf{G}}$ and $\mathbf{G}$ are equal. From Eq. (4.1) one has

$$\bar{C}_i R=\sum_{\kappa=1}^{g_i}\bar{R}_{(i,\kappa)}R=R\sum_{\kappa=1}^{g_i}R_{(i,\kappa)}=RC_i , \tag{4.8}$$

and from Eq. (2.18a) one has

$$C_i R=RC_i . \tag{4.9}$$

Because R is an arbitrary basis vector in L_G, from Eqs. (4.8) and (4.9) we have

$$\bar{C}_i=C_i, \quad i=1,2,\ldots,N . \tag{4.10a}$$

Therefore,

$$\bar{C}=C . \tag{4.10b}$$

Equation (4.10b) is a generalization of (1.6c) for SO_3.

It must be emphasized that although the class operators of $\mathbf{G}$ and $\overline{\mathbf{G}}$ are equal, the class operators of the subgroup $\mathbf{G}(i)$ and $\overline{\mathbf{G}}(i)$ are not equal, since the former commute only with the subgroup $\mathbf{G}(i)$, whereas the latter commute with the whole group $\mathbf{G}$.

B. The intrinsic group of a representation group

Now consider the intrinsic group $\overline{\mathbf{G}}$ of a rep group $\mathbf{G}$ with $m>1$. We first define $|\mathbf{g}|$ operators $\overline{R}_j$ in the $|\mathbf{g}|$-dimensional group space L_g of $\mathbf{G}$ by

$$\overline{R}_j R_k = R_k R_j = \eta(k,j) R_{kj}, \quad j,k = 1,2,\ldots,|\mathbf{g}| , \tag{4.11a}$$

and define

$$\overline{R}_j^{(l)} = \varepsilon(j,l)\overline{R}_j, \quad j = 1,2,\ldots,|\mathbf{g}| , \quad l = 0,1,\ldots,m-1 . \tag{4.11b}$$

Then

$$\overline{\mathbf{G}} = \{\overline{R}_j^{(l)} : j = 1,2,\ldots,|\mathbf{g}|, \; l = 0,1,\ldots,m-1\} \tag{4.12}$$

form the intrinsic group $\overline{\mathbf{G}}$ of the rep group $\mathbf{G}$. All the discussions in Sec. IV.A remain valid for the intrinsic group $\overline{\mathbf{G}}$ of Eq. (4.12), with the single exception that now only $|\mathbf{g}|$ intrinsic group operators are linearly independent.

From Theorem 4.1 we know that the eigenvector $P^{(\nu)}$ of the CSCO of $\mathbf{G}$ is also the eigenvector of the CSCO of $\overline{\mathbf{G}}$.

Equation (4.11a) shows that the group space L_g also forms a rep space for the intrinsic group $\overline{\mathbf{G}}$,

$$\overline{R}_j R_k = \sum_{i=1}^{|\mathbf{g}|} D_{ik}(\overline{R}_j) R_i, \quad j,k = 1,2,\ldots,|\mathbf{g}| , \tag{4.13}$$

$$D_{ik}(\overline{R}_j) = \langle i \mid \overline{R}_j \mid k \rangle = \eta(k,j)\delta_{i,kj} .$$

The rep $D(\overline{\mathbf{G}})$ will be called the regular rep of the intrinsic group $\overline{\mathbf{G}}$.

For the case of $m=1$, the rep $D(\overline{\mathbf{G}})$ is referred to as the inverted rep of the group $\mathbf{G}$ by Boerner (1963), since $D(\overline{\mathbf{G}})$ is anti-isomorphic to $\mathbf{G}$. $D(\overline{\mathbf{G}})$ is also anti-isomorphic to the right regular rep of $\mathbf{G}$ (Miller, 1972).

Suppose A is an element of the group algebra and $\overline{A}$ is its intrinsic element,

$$A = \sum_{i=1}^{|\mathbf{g}|} x_i R_i, \quad \overline{A} = \sum_{i=1}^{|\mathbf{g}|} x_i \overline{R}_i . \tag{4.14a}$$

Let $D(A)$ and $D(\overline{A})$ be the representative matrices of A and $\overline{A}$ in L_g; then we have Theorem 4.2.

Theorem 4.2. The matrices $\widetilde{D}(A)$ and $D(\overline{A})$ are related by a similarity transformation, $\widetilde{D}(A)$ being the transpose of $D(A)$.

Proof. The matrix elements of $D(A)$ and $D(\overline{A})$ are denoted by

$$D_{ij}(A) = \langle i \mid A \mid j \rangle, \quad D_{ij}(\overline{A}) = \langle i \mid \overline{A} \mid j \rangle , \tag{4.14b}$$

and are decided by the following equations:

$$A R_j = \sum_i \langle i \mid A \mid j \rangle R_i , \tag{4.15a}$$

$$\overline{A} R_j = R_j A = \sum_i \langle i \mid \overline{A} \mid j \rangle R_i . \tag{4.15b}$$

Taking the Hermitian conjugate of (4.15a), letting $A \leftrightarrow A^{\dagger}$, and using the unitarity of the group operators,

$$R_j^{-1} A = \sum_i \langle j \mid A \mid i \rangle R_i^{-1} . \tag{4.15c}$$

Comparing Eq. (4.15b) with (4.15c), we obtain

$$\langle i \mid \overline{A} \mid j \rangle = \langle j^{-1} \mid A \mid i^{-1} \rangle , \tag{4.16}$$

where

$$\langle j^{-1} \mid A \mid i^{-1} \rangle = \langle R_j^{-1} \mid A \mid R_i^{-1} \rangle .$$

According to Theorem 2.5, R_i^{-1} and R_j^{-1} are still vectors of the group space L_g; therefore the matrices $||\langle j^{-1} \mid A \mid i^{-1} \rangle||$ and $||\langle j \mid A \mid i \rangle||$ are similar. Thus Eq. (4.16) shows that $D(\overline{A})$ and $\widetilde{D}(A)$ are similar matrices, i.e.,

$$D(\overline{A}) = T \widetilde{D}(A) T^{-1} . \tag{4.17}$$

C. Some remarks

The following points are worth noting.

(1) From Eq. (4.1) it is seen that, for an Abelian group, the intrinsic group $\overline{\mathbf{G}}$ coincides with the group $\mathbf{G}$ itself.

(2) The intrinsic group element $\overline{R}$ defined by Eq. (4.1) is not a conjugate element of the group element R. From (4.1), a formal relation between $\overline{R}$ and R can be written as

$$\overline{R} = S R S^{-1} \tag{4.18}$$

when $\overline{R}$ acts on S. It should be stressed that Eq. (4.18) is also not an identity. It only shows that when acting on S, $\overline{R}$ is equivalent to the operator SRS^{-1}, and that while acting on another vector T, $\overline{R}$ will be equivalent to TRT^{-1}. In other words, the element S in Eq. (4.18) is not fixed. It changes according to which vector the operator $\overline{R}$ is acting upon. This is the most important point, albeit a little tricky, for the understanding of the intrinsic group.

In contrast, a conjugate element T of the group element R is

$$T = S_0 R S_0^{-1} , \tag{4.19}$$

where S_0 is a fixed element of $\mathbf{G}$. Equation (4.19) is an identity relation, and T is an element of $\mathbf{G}$.

(3) It is important to distinguish between the subgroup $\overline{\mathbf{G}}(1)$ of the intrinsic group $\overline{\mathbf{G}}$ of $\mathbf{G}$, and the intrinsic group $\overline{\mathbf{G}}'(1)$ of the subgroup $\mathbf{G}(1)$ of $\mathbf{G}$. $\overline{\mathbf{G}}(1)$ is defined in the whole group space of $\mathbf{G}$, while $\overline{\mathbf{G}}'(1)$ is defined in the group space of $\mathbf{G}(1)$. Let R, $R(1)$, $\overline{R}(1)$, and $\overline{R}'(1)$ be the group elements of the groups $\mathbf{G}$, $\mathbf{G}(1)$, $\overline{\mathbf{G}}(1)$, and

$\bar{\mathbf{G}}'(1)$, respectively. The definitions for the groups $\bar{\mathbf{G}}(1)$ and $\bar{\mathbf{G}}'(1)$ are, respectively,

$$\bar{R}(1)R = RR(1) \quad \text{for all } R \in \mathbf{G} , \tag{4.20a}$$

$$\bar{R}'(1)S(1) = S(1)R(1) \quad \text{for all } S(1) \in \mathbf{G}(1) . \tag{4.20b}$$

Obviously, $\bar{\mathbf{G}}(1)$ commutes with the whole group $\mathbf{G}$, while $\bar{\mathbf{G}}'(1)$ commutes only with the subgroup $\mathbf{G}(1)$,

$$\begin{aligned} &[\bar{\mathbf{G}}(1),\mathbf{G}] = 0 , \\ &[\bar{\mathbf{G}}'(1),\mathbf{G}] \neq 0 , \\ &[\bar{\mathbf{G}}'(1),\mathbf{G}(1)] = 0 . \end{aligned} \tag{4.21}$$

The CSCO of $\bar{\mathbf{G}}(1)$ and $\mathbf{G}(1)$ are commutative but not equal, while the CSCO of $\bar{\mathbf{G}}'(1)$ and $\mathbf{G}(1)$ are equal.

(4) For a Lie group $\mathbf{G}$, Eq. (4.1) defines an intrinsic Lie group $\bar{G}$. Chen, Wang, and Gao (1983) showed that the intrinsic rotation group $\overline{\mathrm{SO}}_3$ is just the group describing rotations around the intrinsic coordinate axes of a rotating system, and in the group parameter space, the group $\mathbf{G}$ and its intrinsic group $\bar{\mathbf{G}}$ are precisely the first and second parameter groups discussed in great detail by Eisenhart (1933) and Racah (1951).

V. THE CSCO-II AND CSCO-III OF A GROUP G

A. For a canonical subgroup chain

Now let us seek the eigenvectors $P_l^{(\nu)}$ of the CSCO of $\mathbf{G}$ in the group space L_g:

$$CP_l^{(\nu)} = \nu P_l^{(\nu)}, \quad \nu = 1,2,\ldots,n, \quad l = 1,2,\ldots,m_\nu , \tag{5.1}$$

$$P_l^{(\nu)} = \sum_{i=1}^{|\mathbf{g}|} u_{\nu l,i} R_i , \tag{5.2}$$

where $u_{\nu l,i}$ are complex numbers; as specified in Theorem 3.8, the n distinct eigenvalues ν of C in L_g are the same as those obtained in the class space L_n. C is a CSCO for L_n but is in general no longer a CSCO for the $|\mathbf{g}|$-dimensional group space L_g. Therefore, the eigenvalues ν are in general degenerate in L_g. The degeneracy of ν is denoted by m_ν in Eq. (5.1). For a given ν, from (5.1) we can obtain m_ν linearly independent eigenvectors $P_l^{(\nu)}$, which can be chosen arbitrarily subject to the orthonormality condition. The m_ν eigenvectors form the eigenspace L_ν of C,

$$L_\nu = \{P_l^{(\nu)} : l = 0,1,\ldots,m_\nu\} , \tag{5.3}$$

and the group space L_g is decomposed into the direct sum of the n eigenspaces L_ν as indicated in Eq. (3.39). Dimension conservation requires that

$$\sum_{\nu=1}^{n} m_\nu = |\mathbf{g}| . \tag{5.4}$$

With $P_l^{(\nu)}$ as the new basis for L_g, the matrices of the operators $\bar{A}$ and A (or their transpose $\tilde{A}$) of Eq. (4.14a) now become quasidiagonal,

$$D'(\bar{A}) = UD(\bar{A})U^{-1} = \sum_{\nu=1}^{n} \oplus D_{(\nu)}(\bar{A}) , \tag{5.5a}$$

$$D'(\tilde{A}) = UD(\tilde{A})U^{-1} = \sum_{\nu=1}^{n} \oplus D_{(\nu)}(\tilde{A}) , \tag{5.5b}$$

where the matrix elements $U_{\nu l,i} = u^*_{\nu l,i}$, $D_{(\nu)}(\bar{A})$, and $D_{(\nu)}(\tilde{A})$ are the representative matrices of $\bar{A}$ and $\tilde{A}$ in the eigenspace L_ν.

From Eqs. (4.17) and (5.5), with $\tilde{D}(A) = D(\tilde{A})$, we have

$$D'(\bar{A}) = T'\tilde{D}'(A)T'^{-1}, \quad T' = UTU^{-1} , \tag{5.6a}$$

i.e.,

$$\sum_{\nu=1}^{n} \oplus D_{(\nu)}(\bar{A}) = T' \sum_{\nu=1}^{n} \oplus \tilde{D}_{(\nu)}(A) T'^{-1} . \tag{5.6b}$$

Since (5.6b) holds for any element A of the group algebra, T' has to be also quasidiagonal,

$$T' = \sum_{\nu=1}^{n} \oplus T'_{(\nu)} . \tag{5.6c}$$

From Eqs. (5.6b) and (5.6c) we immediately have

$$D_{(\nu)}(\bar{A}) = T'_{(\nu)} \tilde{D}_{(\nu)}(A) T'^{-1}_{(\nu)} \quad \text{for } \nu = 1,2,\ldots,n . \tag{5.7}$$

This shows that, as in L_g, the representative matrices of $\bar{A}$ and A in the eigenspaces L_ν are still related by similarity transformations. Since the determinant of a matrix is invariant under matrix transposition, this in turn means that in L_ν the operators $\bar{A}$, $\tilde{A}$, and A have the same characteristic equations and therefore have the same eigenvalues. This leads to Theorem 5.1.

Theorem 5.1. In the eigenspace L_ν of C, the eigenvalues of an operator A defined in L_g and its intrinsic operator $\bar{A}$ are exactly the same.

To lift the degeneracy of ν entirely, or to fix $P_l^{(\nu)}$ unambiguously, we have to add extra operators to the operator set C, so that it becomes a CSCO of the $|\mathbf{g}|$-dimensional group space L_g. These extra operators must commute with C and with one another. By virtue of Theorem 3.1, the other class operators of $\mathbf{G}$ that are not included in C are useless for lifting the degeneracy. The possible candidates for these extra operators are the CSCO of subgroups of $\mathbf{G}$. Suppose that $\mathbf{G}$ has a subgroup chain

$$\mathbf{G} \supset \mathbf{G}(s), \quad \mathbf{G}(s) \equiv \mathbf{G}(1) \supset \mathbf{G}(2) \supset \cdots . \tag{5.8a}$$

We use $C(i)$ to designate the CSCO of the subgroup $\mathbf{G}(i)$ and $C(s)$ the set of operators $(C(1),C(2),\ldots)$. $C(s)$ will be called the CSCO of the subgroup chain $\mathbf{G}(s)$. Obviously, the operators $C(i)$ commute with C as well as with one another.

Due to the anti-isomorphism between $\mathbf{G}$ and $\bar{\mathbf{G}}$, corresponding to (5.8a), we have the intrinsic subgroup chain

$$\bar{G} \supset \bar{G}(s), \quad \bar{G}(s) \equiv \bar{G}(1) \supset \bar{G}(2) \supset \cdots \tag{5.8b}$$

and the CSCO $\bar{C}(s) = (\bar{C}(1),\bar{C}(2),\ldots)$. $\bar{C}(s)$ commutes with both C and $C(s)$,

$$[\bar{C}(s),C] = 0, \quad [\bar{C}(s),C(s)] = 0 . \tag{5.9}$$

Since $\bar{C}=C$ [see Eq. (4.10b)], $\bar{C}$ does not provide any new operators. However, $\bar{C}(s)\neq C(s)$; therefore the operators $\bar{C}(s)$ are also candidates for these extra operators to be added to the CSCO of **G**.

Definition 5.1. If, starting from the group **G**, we can find a group chain (5.8a) and the corresponding operator set K,

$$K=(C,C(s),\bar{C}(s)) , \tag{5.10a}$$

$$C(s)=(C(1),C(2),\ldots) ,$$
$$\bar{C}(s)=(\bar{C}(1),\bar{C}(2),\ldots) , \tag{5.10b}$$

such that K is a CSCO for the $|\mathbf{g}|$-dimensional group space L_g, then K is called a CSCO-III of **G**, while

$$M=(C,C(s)) \tag{5.10c}$$

is called a CSCO-II of **G**, and $\mathbf{G}\supset\mathbf{G}(s)$ is said to be a canonical subgroup chain.

As will be seen later, the meaning of the canonical subgroup chain is identical to the usual one (e.g., see Butler and Wybourne, 1976a).

It is clear that the operator set K in (5.10a) is a generalization of $(J^2,J_z,\bar{J}_z)$ for SO_3.

In many cases, the operator set K in (5.10a) is overdetermined in the sense that the following K may already be a CSCO in L_g,

$$K=(C',C'(s),\bar{C}'(s)) , \tag{5.11a}$$

$$C'(s)=(C'(1),C'(2),\ldots) ,$$
$$\bar{C}'(s)=(\bar{C}'(1),\bar{C}'(2),\ldots) , \tag{5.11b}$$

where C' and $C'(i)$ involve only some of the class operators contained in the CSCO of G and $G(i)$, and thus are not the CSCO of **G** and **G**(i), respectively. For examples, see Sec. VIII.

Furthermore, in analogy with Eq. (3.16a), each operator set $C'(i)$ can be assumed to consist of only a single operator, and we can use a single operator

$$A=\sum_i d_i C'(i) \tag{5.12a}$$

and

$$\bar{A}=\sum_i d_i \bar{C}'(i) \tag{5.12b}$$

to replace $C'(s)$ and $\bar{C}'(s)$, where the coefficients d_i are properly chosen so that

$$K=(C',A,\bar{A}) \tag{5.12c}$$

is a CSCO of L_g.

The above consideration leads to a more general definition for the CSCO-II and -III of **G**.

Definition 5.1'. A set of commuting operators $K=(C',A,\bar{A})$, with C' being commutative with **G**, and A an operator set or an operator in L_g, is called a CSCO-III of **G** if K is a CSCO of L_g and

$$M=(C',A) \tag{5.12d}$$

is called a CSCO-II of **G**.

Therefore, each of the operator sets K of Eqs. (5.10a), (5.11a), and (5.12c) is a possible form of the CSCO-III of **G**. In the following, we still use $K=(C,C(s),\bar{C}(s))$ to denote a CSCO-III of **G**, keeping in mind that actually K could take other forms as well.

B. For a noncanonical subgroup chain

In the above discussion, $\mathbf{G}\supset\mathbf{G}(s)$ is assumed to be a canonical subgroup chain. Now let us pass on to the general case where $\mathbf{G}\supset\mathbf{G}(s)$ is not a canonical subgroup chain. In such a case, $(C,C(s),\bar{C}(s))$ is not a CSCO in L_g and thus is not a CSCO-III of **G**.

According to Dirac (1958, Sec. 14), any set of commuting operators can be made into a complete set of commuting operators by adding certain operators to it. Let us first add one operator, say ξ, which can always be written as a linear combination of $|\mathbf{g}|$ elements in the fundamental set F, $\xi=\sum_i \xi_i R_i$, ξ_i being complex numbers, since we are working in the group space L_g. Corresponding to ξ, there is the intrinsic operator $\bar{\xi}=\sum_i \xi_i \bar{R}_i$. Thus the additional operators always occur pairwise. If $(C,C(s),\xi,\bar{C}(s),\bar{\xi})$ is not yet a CSCO of L_g, we add another pair of operators η and $\bar{\eta}$, etc., until

$$(C,C''(s),\bar{C}''(s)) \tag{5.13a}$$

is a CSCO of L_g, where

$$C''(s)=(C(s),\xi,\eta,\ldots) ,$$
$$\bar{C}''(s)=(\bar{C}(s),\bar{\xi},\bar{\eta},\ldots) . \tag{5.13b}$$

Hence we can always find a CSCO-III of **G** regardless of whether $\mathbf{G}\supset\mathbf{G}(s)$ is a canonical subgroup chain. To be specific, in the following, we shall assume that $\mathbf{G}\supset\mathbf{G}(s)$ is a canonical subgroup chain unless otherwise stated. For the noncanonical case, all we need to do is to reinterpret the meaning of $C(s)$ and $\bar{C}(s)$ in accordance with Eq. (5.13).

In analogy with Eq. (3.16a), we can choose a single operator

$$K=C+\sum_i [\alpha_i C(i)+\beta_i \bar{C}(i)] \tag{5.14}$$

as a CSCO-III of **G**, where the coefficients α_i and β_i are properly chosen so that K has $|\mathbf{g}|$ distinct eigenvalues.

The CSCO-II for point groups is given by Chen, Wang, and Gao (1977a).

VI. FULL REDUCTION OF THE REGULAR REPRESENTATION

A. The eigenvectors of the CSCO-III

Let $P_a^{(\nu)b}$ be the eigenvectors of the CSCO-III of **G** in the group space L_g,

$$\begin{bmatrix} C \\ C(s) \\ \bar{C}(s) \end{bmatrix} P_a^{(\nu)b} = \begin{bmatrix} \nu \\ a \\ b \end{bmatrix} P_a^{(\nu)b} . \tag{6.1a}$$

Using Eq. (4.1), we can rewrite the third equation in (6.1a) as

$$\bar{C}(s)P_a^{(\nu)b} = P_a^{(\nu)b}C(s) = bP_a^{(\nu)b} , \tag{6.1b}$$

where a (b) denotes a set of eigenvalues

$$a = (\lambda_1, \lambda_2, \ldots), \quad b = (\bar{\lambda}_1, \bar{\lambda}_2, \ldots) , \tag{6.1c}$$

λ_i $(\bar{\lambda}_i)$ being the eigenvalue of $C(i)$ $[\bar{C}(i)]$, if $C(s)$ $[\bar{C}(s)]$ is interpreted as in Eq. (5.10b); if $C(s)$ $[\bar{C}(s)]$ is interpreted as in Eq. (5.12), then a (b) denotes the eigenvalue of A $(\bar{A})$.

According to Theorem 5.1, in the eigenspace L_ν of C, $C(s)$ and $\bar{C}(s)$ have exactly the same, say h_ν, distinct eigenvalues,

$$a,b = a_1, a_2, \ldots, a_{h_\nu} , \tag{6.1d}$$

where h_ν is an integer to be decided below. In the following, $a(b)$ is also used as an index enumerating the eigenvalues, and thus we can write $a,b = 1,2,\ldots,h_\nu$.

According to the hypothesis that $(C,C(s),\bar{C}(s))$ is a CSCO of L_g, it is necessary that $(C(s),\bar{C}(s))$ be a CSCO in each of the eigenspaces L_ν, $\nu = 1,2,\ldots,n$. Thus the total number of distinct eigenvalues (a,b) of $(C(s),\bar{C}(s))$ in L_ν has to be equal to the dimension of L_ν,

$$h_\nu^2 = m_\nu . \tag{6.2}$$

This leads to Theorem 6.1.

Theorem 6.1. The dimension of the eigenspace L_ν of C is necessarily a square of an integer.

From Eqs. (5.4) and (6.2) we get

$$\sum_{\nu=1}^{n} h_\nu^2 = |\mathbf{g}| . \tag{6.3}$$

The eigenvectors $P_a^{(\nu)b}$ can be expressed in terms of the basis vectors of L_g,

$$P_a^{(\nu)b} = \sum_{i=1}^{|\mathbf{g}|} u_{\nu ab,i} R_i . \tag{6.4}$$

The eigenequation (6.1a) can be written in matrix form,

$$\sum_{j=1}^{|\mathbf{g}|} \left[\left\langle i \left| \begin{matrix} C \\ C(s) \\ \bar{C}(s) \end{matrix} \right| j \right\rangle - \begin{bmatrix} \nu \\ a \\ b \end{bmatrix} \delta_{ij} \right] u_{\nu ab,j} = 0 . \tag{6.5}$$

The h_ν eigenvectors $P_1^{(\nu)b}, P_2^{(\nu)b}, \ldots, P_{h_\nu}^{(\nu)b}$, with the same ν and b, span an eigenspace $L_{(\nu)b}$ of $(C,\bar{C}(s))$. According to Theorem 2.3 and the fact that $(C,\bar{C}(s))$ commutes with $\mathbf{G}$, $L_{(\nu)b}$ is necessarily a rep space of $\mathbf{G}$. Consequently, the eigenspace L_ν of C is further decomposed into h_ν rep spaces of $\mathbf{G}$,

$$L_\nu = \sum_{b=1}^{h_\nu} \oplus L_{(\nu)b}, \quad L_{(\nu)b} = \{P_a^{(\nu)b} : a = 1,2,\ldots,h_\nu\} . \tag{6.6}$$

Analogously, the eigenspace of $(C,C(s))$,

$$\bar{L}_{(\nu)a} = \{P_a^{(\nu)b} : b = 1,2,\ldots,h_\nu\} , \tag{6.7a}$$

is a rep space of the intrinsic group $\bar{\mathbf{G}}$, since $(C,C(s))$ commutes with $\bar{\mathbf{G}}$. Hence the space L_ν can also be decomposed into h_ν rep spaces $\bar{L}_{(\nu)a}$ of $\bar{\mathbf{G}}$,

$$L_\nu = \sum_{a=1}^{h_\nu} \oplus \bar{L}_{(\nu)a} . \tag{6.7b}$$

The eigenvectors of the CSCO-III form an orthonormal and complete set in the group space L_g,

$$\langle P_a^{(\nu)b} | P_{a'}^{(\nu')b'} \rangle = \delta_{\nu\nu'}\delta_{aa'}\delta_{bb'} , \tag{6.8a}$$

$$\sum_{\nu=1}^{n} \sum_{a=1}^{h_\nu} \sum_{b=1}^{h_\nu} |P_a^{(\nu)b}\rangle\langle P_a^{(\nu)b}| = 1 . \tag{6.8b}$$

Using Eq. (6.4), (6.8) becomes

$$\sum_{i=1}^{|\mathbf{g}|} u^*_{\nu ab,i} u_{\nu' a'b',i} = \delta_{\nu\nu'}\delta_{aa'}\delta_{bb'} , \tag{6.9a}$$

$$\sum_{\nu=1}^{n} \sum_{a=1}^{h_\nu} \sum_{b=1}^{h_\nu} u^*_{\nu ab,i} u_{\nu ab,j} = \delta_{ij} . \tag{6.9b}$$

With the help of Eq. (6.9b), the inverse expansion of Eq. (6.4) is

$$R_i = \sum_{\mu=1}^{n} \sum_{c=1}^{h_\nu} \sum_{d=1}^{h_\nu} u^*_{\mu cd,i} P_c^{(\mu)d}, \quad i = 1,2,\ldots,|\mathbf{g}| . \tag{6.10}$$

B. The representations $D^{(\nu)b}(\mathbf{G})$ and $D^{(\nu)a}(\bar{\mathbf{G}})$

Since C commutes with the group elements and in turn with $P_c^{(\mu)d}$,

$$CP_c^{(\mu)d}P_a^{(\nu)b} = \mu P_c^{(\mu)d}P_a^{(\nu)b} = \nu P_c^{(\mu)d}P_a^{(\nu)b} . \tag{6.11}$$

Therefore,

$$(\mu - \nu)P_c^{(\mu)d}P_a^{(\nu)b} = 0 . \tag{6.12a}$$

From Eq. (6.1a), it follows that

$$C(s)(P_c^{(\mu)d}P_a^{(\nu)b}) = c(P_c^{(\mu)d}P_a^{(\nu)b}) , \tag{6.12b}$$

$$\bar{C}(s)(P_c^{(\mu)d}P_a^{(\nu)b}) = P_c^{(\mu)d}\bar{C}(s)P_a^{(\nu)b} = b(P_c^{(\mu)d}P_a^{(\nu)b}) . \tag{6.12c}$$

Furthermore,

$$P_c^{(\mu)d}(C(s)P_a^{(\nu)b}) = aP_c^{(\mu)d}P_a^{(\nu)b} = (P_c^{(\mu)d}C(s))P_a^{(\nu)b} = dP_c^{(\mu)d}P_a^{(\nu)b} .$$

Thus

$$(a - d)P_c^{(\mu)d}P_a^{(\nu)b} = 0 . \tag{6.12d}$$

Due to the nondegeneracy of the eigenvalues of the CSCO-III, Eq. (6.12) implies that

$$P_c^{(\mu)d}P_a^{(\nu)b} = \delta_{\mu\nu}\delta_{ad}\xi^{(\nu)}_{abc}P_c^{(\nu)b} , \tag{6.13}$$

where $\xi^{(\nu)}_{abc}$ is a constant to be decided.

Applying R_i of Eq. (6.10) to $P^{(\nu)b}_a$, and using Eq. (6.13), one gets

$$R_i P^{(\nu)b}_a = \sum_{c=1}^{h_\nu} D^{(\nu)b}_{ca}(R_i) P^{(\nu)b}_c \ , \tag{6.14a}$$

with

$$D^{(\nu)b}_{ca}(R_i) = \xi^{(\nu)}_{abc} u^*_{vca,i} \ . \tag{6.14b}$$

On the other hand, from Eqs. (6.14a) and (6.8a),

$$D^{(\nu)b}_{ca}(R_i) = \langle P^{(\nu)b}_c \mid R_i \mid P^{(\nu)b}_a \rangle \ . \tag{6.14c}$$

From Eqs. (1.12), (6.14c), and (6.8), we have

$$D^{(\nu)b}(R_i) D^{(\nu)b}(R_j) = \eta(i,j) D^{(\nu)b}(R_{ij}) \ . \tag{6.14d}$$

Equation (6.14) shows that the eigenvectors $P^{(\nu)b}_a$ ($a=1,2,\ldots,h_\nu$) form the basis for the bth rep (ν) of the rep group $\mathbf{G}$ with the rep matrices $D^{(\nu)b}(R_i)$, $b=1,2,\ldots,h_\nu$.

Similarly for the group $\bar{\mathbf{G}}$ one has

$$\bar{R}_i P^{(\nu)b}_a = \sum_{d=1}^{h_\nu} D^{(a)}_{db}(\bar{R}_i) P^{(\nu)d}_a \ , \tag{6.15a}$$

$$D^{(\nu)a}_{db}(\bar{R}_i) = \xi^{(\nu)}_{bda} u^*_{vbd,i} \tag{6.15b}$$

$$= \langle P^{(\nu)d}_a \mid \bar{R}_i \mid P^{(\nu)b}_a \rangle \ , \tag{6.15c}$$

$$D^{(\nu)a}(\bar{R}_i) D^{(\nu)a}(\bar{R}_j) = \eta(j,i) D^{(\nu)a}(\bar{R}_{ji}) \ . \tag{6.15d}$$

Equation (6.15) shows that the eigenvectors $P^{(\nu)b}_a$ ($b=1,2,\ldots,h_\nu$) form the basis of the ath rep (ν) of the intrinsic rep group $\bar{\mathbf{G}}$ with the rep matrices $D^{(\nu)a}(\bar{R}_i)$, $a=1,2,\ldots,h_\nu$.

C. The standard phase choice for $P^{(\nu)b}_a$

The eigenvector $P^{(\nu)b}_a$ in Eq. (6.1a) can be determined only up to a phase factor. Until now the phase has been assumed to be chosen arbitrarily. From Eq. (6.13) it is seen that the constant $\xi^{(\nu)}_{abc}$ depends on the phase choice of $P^{(\nu)b}_a$. Let us make the ansatz

$$P^{(\nu)a}_c P^{(\nu)b}_a = \xi^{(\nu)} P^{(\nu)b}_c \ , \tag{6.16}$$

where $\xi^{(\nu)}$ depends only on ν, and later we shall show how this can be achieved by a suitable phase choice.

With Eq. (6.16), (6.14b) now becomes

$$D^{(\nu)}_{ca}(R_i) = \xi^{(\nu)} u^*_{vca,i} \ . \tag{6.17}$$

From Eqs. (6.9a) and (6.17)

$$\sum_{i=1}^{|\mathbf{g}|} | D^{(\nu)}_{ca}(R_i) |^2 = | \xi^{(\nu)} |^2 \ . \tag{6.18}$$

Summing Eq. (6.18) over the index a from 1 to h_ν and using the unitarity of the rep $D^{(\nu)}$, we obtain

$$| \xi^{(\nu)} |^2 = | \mathbf{g} | / h_\nu \ .$$

Choosing $\xi^{(\nu)}$ to be real positive, we have

$$\xi^{(\nu)} = (| \mathbf{g} | / h_\nu)^{1/2} \ . \tag{6.19}$$

Hence Eq. (6.13) becomes

$$P^{(\mu)d}_c P^{(\nu)b}_a = \delta_{\mu\nu} \delta_{ad} (| \mathbf{g} | / h_\nu)^{1/2} P^{(\nu)b}_c \ . \tag{6.20}$$

From (6.20) it is seen that the real positive choice for $\xi^{(\nu)}$ corresponds to the requirement that the coefficient $u_{vaa,e}$ in front of the identity e in $P^{(\nu)a}_a$ be always real positive,

$$u_{vaa,e} > 0, \quad a = 1,2,\ldots,h_\nu \ . \tag{6.21}$$

Equations (6.14), (6.15), (6.4), and (6.10) reduce to

$$R_i P^{(\nu)b}_a = \sum_{a'=1}^{h_\nu} D^{(\nu)}_{a'a}(R_i) P^{(\nu)b}_{a'}, \quad a,b = 1,2,\ldots,h_\nu \ , \tag{6.22a}$$

$$\bar{R}_i P^{(\nu)b}_a = P^{(\nu)b}_a R_i = \sum_{b'=1}^{h_\nu} D^{(\nu)}_{b'b}(\bar{R}_i) P^{(\nu)b'}_a \ , \quad a,b = 1,2,\ldots,h_\nu \ , \tag{6.22b}$$

$$D^{(\nu)}_{ab}(R_i) = D^{(\nu)}_{ba}(\bar{R}_i) = (| \mathbf{g} | / h_\nu)^{1/2} u^*_{vab,i} \ , \tag{6.23}$$

$$D^{(\nu)}(R_i) D^{(\nu)}(R_j) = \eta(i,j) D^{(\nu)}(R_{ij}) \ , \tag{6.24a}$$

$$D^{(\nu)}(\bar{R}_i) D^{(\nu)}(\bar{R}_j) = \eta(j,i) D^{(\nu)}(\bar{R}_{ji}) \ , \tag{6.24b}$$

$$P^{(\nu)b}_a = (h_\nu / | \mathbf{g} |)^{1/2} \sum_{i=1}^{|\mathbf{g}|} D^{(\nu)}_{ab}(R_i)^* R_i \ , \tag{6.25a}$$

$$R_i = \sum_{\nu=1}^{n} \sum_{a=1}^{h_\nu} \sum_{b=1}^{h_\nu} (h_\nu / | \mathbf{g} |)^{1/2} D^{(\nu)}_{ab}(R_i) P^{(\nu)b}_a \ , \tag{6.25b}$$

while Eq. (6.9) becomes

$$(h_\nu / | \mathbf{g} |) \sum_{i=1}^{|\mathbf{g}|} D^{(\nu)}_{ab}(R_i)^* D^{(\mu)}_{cd}(R_i) = \delta_{\nu\mu} \delta_{ac} \delta_{bd} \ , \tag{6.26a}$$

$$\sum_{\nu=1}^{n} \sum_{a=1}^{h_\nu} \sum_{b=1}^{h_\nu} (h_\nu / | \mathbf{g} |) D^{(\nu)}_{ab}(R_i)^* D^{(\nu)}_{ab}(R_j) = \delta_{ij} \ . \tag{6.26b}$$

The phase choice of Eqs. (6.16) and (6.19) which leads to Eqs. (6.22)–(6.26) is referred to as the standard phase choice. From (6.21) and (6.23) we know that the steps for reaching the standard phase choices are as follows.

(1) The coefficient in front of the identity element e in the eigenvector $P^{(\nu)a}_a$ should be real positive.

(2) Among the h_ν reps of $\mathbf{G}$, the phases of the basis vectors of one rep, say the first one, $P^{(\nu)b=1}_a$, $a=2,3,\ldots,h_\nu$, can be chosen arbitrarily.

(3) The phase of the eigenvector $P^{(\nu)b}_a$ for $b \neq 1$ can be fixed by requiring that the coefficient $u_{vab,i}$ in front of a certain element R_i be equal to

$$(h_\nu / | \mathbf{g} |)^{1/2} \langle P^{(\nu)1}_a \mid R_i \mid P^{(\nu)1}_b \rangle^* \ , \tag{6.27}$$

where the element R_i can be chosen arbitrarily so long as $u_{vab,i} \neq 0$.

Finally we need to show that the system of eigenvectors $P^{(\nu)b}_a$ of Eq. (6.25a) satisfies the ansatz (6.16). Using Eqs. (6.25a), (6.22a), and (6.26a), we may soon verify that (6.16) is satisfied.

From Eqs. (6.22) and (6.23) it is seen that, under the standard phase choice, the h_ν reps $D^{(\nu)b}(\mathbf{G})$, $b=1,2,\ldots,h_\nu$, become identical; the h_ν reps $D^{(\nu)a}(\bar{\mathbf{G}})$,

$a=1,2,\ldots,h_\nu$, also become identical, and $D^{(\nu)}(\overline{\mathbf{G}})$ is identical to $\tilde{D}^{(\nu)}(\mathbf{G})$. Therefore, we have Theorem 6.2.

Theorem 6.2. The reps $D^{(\nu)b}(\mathbf{G})$ $[D^{(\nu)a}(\overline{\mathbf{G}})]$ with the same eigenvalue ν of the CSCO of $\mathbf{G}$ are equivalent and can be made to be identical to one another by using the standard phase choice.

D. The irreducibility of $D^{(\nu)}(\mathbf{G})$

Theorem 6.3. The n inequivalent reps $D^{(\nu)}(\mathbf{G})$ resulting from the decomposition of the group space L_g of $\mathbf{G}$ are irreducible.

Proof. Suppose that an $h_\nu\times h_\nu$ matrix A satisfies

$$AD^{(\nu)}(R_i)=D^{(\nu)}(R_i)A,\quad i=1,2,\ldots,|\mathbf{g}| \tag{6.28a}$$

or

$$\sum_{b'}A_{ab'}D^{(\nu)}_{b'c}(R_i)=\sum_{b'}D^{(\nu)}_{ab'}(R_i)A_{b'c}\ . \tag{6.28b}$$

Multiplying both sides of Eq. (6.28b) by $(h_\nu/|\mathbf{g}|)D^{(\nu)}_{bc}(R_i)^*$, and summing over i, from (6.26a) we obtain

$$A_{ab}=\delta_{ab}A_{cc}\ . \tag{6.29}$$

This shows that the only matrix which commutes with all the matrices of the rep $D^{(\nu)}$ is a multiple of the unit matrix. According to Theorem 2.4 (the Schur lemma), $D^{(\nu)}(\mathbf{G})$ is irreducible.

Similarly, the reps $D^{(\nu)}(\overline{\mathbf{G}})$ for the intrinsic group are also irreducible.

From Eq. (6.3) we have Theorem 6.4.

Theorem 6.4. The regular rep of $\mathbf{G}$ contains n inequivalent irreps $D^{(\nu)}$, n being the number of linearly independent class operators of $\mathbf{G}$; the number of ti es each irrep ν occurs is equal to its dimension.

This is an extension of the Burnside theore for an abstract group $\hat{\mathbf{G}}$.

E. The generalized projection operator

Let us define the operator $P^{(\nu)}_{ab}$

$$P^{(\nu)}_{ab}=\left[\frac{h_\nu}{|\mathbf{g}|}\right]^{1/2}P^{(\nu)b}_a$$

$$=\frac{h_\nu}{|\mathbf{g}|}\sum_{i=1}^{|\mathbf{g}|}D^{(\nu)}_{ab}(R_i)^*R_i\ . \tag{6.30}$$

From Eq. (6.20),

$$P^{(\nu)}_{ab}P^{(\mu)}_{cd}=\delta_{\nu\mu}\delta_{bc}P^{(\nu)}_{ad}\ . \tag{6.31a}$$

It can be easily verified that

$$(P^{(\nu)}_{ab})^\dagger=P^{(\nu)}_{ba}\ . \tag{6.31b}$$

If $\{\psi^{(\mu)\tau}_a:a=1,\ldots h_\mu\}$ is the basis for the τth irrep μ of $\mathbf{G}$, it is easy to show that

$$\psi^{(\nu)\tau}_a=\delta_{\nu\mu}\delta_{bc}P^{(\nu)}_{ab}\psi^{(\mu)\tau}_c\ . \tag{6.31c}$$

There are many names for the operator $P^{(\nu)}_{ab}$, such as the normal unit (Rutherford, 1948), unit (Dirl, 1977), shift operator (Bohr and Mottelson, 1969), irreducible symmetry operator (Folland, 1977), etc. We prefer to call it the generalized projection operator (Elliott and Dawber, 1979), and call $P^{(\nu)b}_a$ the normalized generalized projection operator.

From Eq. (6.30), we can obtain the generalized projection operator for an abstract group $\hat{\mathbf{G}}$ with order $m|\mathbf{g}|$,

$$\hat{P}^{(\nu)}_{ab}=\frac{h_\nu}{m|\mathbf{g}|}\sum_{i=1}^{|\mathbf{g}|}\sum_{l=0}^{m-1}D^{(\nu)}_{ab}(\hat{R}^{(l)}_i)^*\hat{R}^{(l)}_i\ ,$$

$$\nu=1,2,\ldots,N\ . \tag{6.32}$$

In the rep space L, due to Eqs. (1.11a), (2.13), and (3.36), the operator becomes

$$P^{(\nu)}_{ab}=\begin{cases}\dfrac{h_\nu}{|\mathbf{g}|}\displaystyle\sum_{i=1}^{|\mathbf{g}|}D^{(\nu)}_{ab}(R_i)^*R_i, & \nu=1,2,\ldots,n\\ 0, & \nu=n+1,\ldots,N\ ,\end{cases} \tag{6.33}$$

which leads to Theorem 6.5.

Theorem 6.5. In the rep space L, the acceptable or allowable irreps of $\hat{\mathbf{G}}$ are just the n irreps of the rep group $\mathbf{G}$ defined in the space L.

To find the irreducible basis in the space L, one might first decompose the regular rep of the abstract group $\hat{\mathbf{G}}$ and construct the generalized projection operator $\hat{P}^{(\nu)}_{ab}$, and then apply it to the vectors in L (Bradley and Cracknell, 1972). Since the dimension for the regular rep of the abstract group $\hat{\mathbf{G}}$ is $m|\mathbf{g}|$, whereas that for the rep group $\mathbf{G}$ is only $|\mathbf{g}|$, it is much easier to decompose the regular rep of $\mathbf{G}$, construct the generalized projection operator $P^{(\nu)}_{ab}$ of Eq. (6.33), and then apply it to the vectors in L.

Melvin (1956) suggested a factored form for the generalized projection operator. He considered all operations h in the group $\mathbf{G}$ whose rep matrices in the irrep (ν) have a lone nonvanishing diagonal element equal to one in the given ath row. The set of operators forms a subgroup $\mathbf{H}=\{h\}^{(\nu)}_a$. The group $\mathbf{G}$ can be expanded in left cosets of $\mathbf{H}$,

$$\mathbf{G}=S\mathbf{H}\ , \tag{6.34}$$

where $S=\{e=s_1,s_2,\ldots,s_q\}$ is a set of q coset representatives (or generators). Then it is easy to show that

$$P^{(\nu)}_{aa}=\frac{h_\nu}{|\mathbf{g}|}\sum_{\sigma=1}^{q}D^{(\nu)}_{aa}(s_\sigma)^*\sum_{h\in\mathbf{H}}h\ . \tag{6.35}$$

Melvin worked out the factored projection operator $P^{(\nu)}_{aa}$ for all the point groups except the icosahedral groups I and I_h.

Folland (1977,1979) extended Melvin's technique. He let

$$P^{(\nu)}_{ab}=\frac{h_\nu}{|\mathbf{H}|}\sum_h D^{(\nu)}_{ab}(h)^*h \tag{6.36}$$

be the generalized projection operator for the subgroup $\mathbf{H}$,

h_ν being the dimension of the irrep (ν). The symmetry operator for the induced rep $(\nu\uparrow\mathbf{G})$ of dimension qh_ν was shown to be

$$P^{(\nu\uparrow G)}_{\sigma a,\tau b}=s_\sigma P^{(\nu)}_{ab} s_\tau^{-1} , \tag{6.37}$$

where the double index σa or τb is used to label rows or columns of the induced rep $(\nu\uparrow\mathbf{G})$. If the induced rep $(\nu\uparrow\mathbf{G})$ is irreducible, then Eq. (6.37) gives the generalized projection operator of $\mathbf{G}$ in terms of its subgroup $\mathbf{H}$.

F. The character

In traditional group theory, the character plays a predominant role; however, in our new approach, its importance is greatly reduced. In fact, up to now, we have not explicitly used the character. In this section, we shall establish a simple relation between the character vector and the eigenvector of C in the class space.

From Eqs. (6.25b) and (6.30), we get the decomposition of the identity,

$$e=\sum_{\nu=1}^{n}\sum_{a=1}^{h_\nu} P^{(\nu)}_{aa} . \tag{6.38}$$

From Eqs. (6.31) it is seen that $P^{(\nu)}_{aa}$ is self-adjoint and also is an idempotent, the so-called primitive idempotent.

Define

$$P^{(\nu)}=\sum_{a=1}^{h_\nu} P^{(\nu)}_{aa} . \tag{6.39a}$$

From Eq. (6.31a) it is easy to show that

$$P^{(\nu)}P^{(\mu)}=\delta_{\nu\mu}P^{(\nu)} . \tag{6.39b}$$

According to Eqs. (6.39a) and (6.30),

$$P^{(\nu)}=\frac{h_\nu}{|\mathbf{g}|}\sum_{i=1}^{n}\chi_i^{(\nu)*}C_i , \tag{6.40a}$$

$$\chi_i^{(\nu)}=\mathrm{Tr}D^{(\nu)}(R) \quad \text{for } R\in \text{class } i , \tag{6.40b}$$

where $\chi_i^{(\nu)}$ is the character, or primitive character, of the class i in the irrep (ν).

Obviously, $P^{(\nu)}$ is an eigenvector of C with eigenvalue ν. Moreover, Eq. (6.39b) is precisely Eq. (3.26). Hence the operator $P^{(\nu)}$ in (6.39a) resulting from a contraction of the eigenvectors $P^{(\nu)}_{aa}$ of the CSCO-III in L_g is identical with $P^{(\nu)}$ in Eq. (3.25). Comparing (6.40a) with (3.25), one has

$$\frac{h_\nu}{|\mathbf{g}|}\chi_i^{(\nu)*}=\frac{1}{\eta_\nu}q_i^{(\nu)} . \tag{6.41a}$$

Letting i be the identity class and using Eq. (3.28b),

$$|\eta_\nu|^{-2}=\frac{h_\nu^2}{|\mathbf{g}|} . \tag{6.41b}$$

We choose the phase of η_ν so that it is real positive,

$$\eta_\nu^{-1}=\frac{h_\nu}{|\mathbf{g}|^{1/2}} . \tag{6.42}$$

Substituting Eq. (6.42) into (6.41a), we get a simple relation between $q_i^{(\nu)}$ and $\chi_i^{(\nu)}$,

$$\chi_i^{(\nu)}=|\mathbf{g}|^{1/2}q_i^{(\nu)*} . \tag{6.43}$$

Therefore, the orthonormality and completeness conditions, (3.18a) and (3.18b), for the eigenvectors of the CSCO-I are just the two orthogonal theorems for the character,

$$\sum_{i=1}^{n}\frac{g_i}{|\mathbf{g}|}\chi_i^{(\nu)*}\chi_i^{(\nu')}=\delta_{\nu\nu'} , \tag{6.44a}$$

$$\frac{g_i}{|\mathbf{g}|}\sum_{\nu=1}^{n}\chi_i^{(\nu)*}\chi_j^{(\nu)}=\delta_{ij} . \tag{6.44b}$$

Either (6.44a) or (6.44b) can be used as a criterion for the irreducibility of a rep.

From Eq. (6.44) we can easily reestablish the theorems involving the primitive characters. They are discussed elsewhere and hence will be omitted here.

From Eq. (3.4) we know that the eigenvalue of a class operator C_i is a function of the eigenvalue of C,

$$\lambda_i^{(\nu)}=F_i(\nu) . \tag{6.45}$$

By taking the trace of

$$D^{(\nu)}(C_i)=\sum_{\kappa=1}^{g_i}D^{(\nu)}(R_{(i,\kappa)}) , \tag{6.46}$$

we get

$$\chi_i^{(\nu)}=\frac{h_\nu}{g_i}\lambda_i^{(\nu)} . \tag{6.47}$$

From Eqs. (6.45) and (6.47) we obtain

$$\chi_i^{(\nu)}=\frac{h_\nu}{g_i}F_i(\nu) . \tag{6.48}$$

This shows that the characters of the n classes are functionally dependent and uniquely decided by the eigenvalue ν. Since the equality of the characters is the necessary and sufficient condition for two irreps to be equivalent, Theorem 6.6 follows.

Theorem 6.6. The equality of the eigenvalues ν of the CSCO of $\mathbf{G}$ is the necessary and sufficient condition for two irreps to be equivalent.

G. Summary and discussion

Representation group theory includes the theory for abstract groups as a special case of $m=1$. Therefore, all the important theorems for the finite abstract group have been reestablished through a quite different route from the usual one. The traditional approach relies heavily on the character theory, whereas the new approach is based on decomposition of the regular rep space by a set of commuting operators. The former approach may seem to be more elegant from a mathematical point of view. However, it has the fatal drawback that it does not provide us any practical method for reducing the regular rep. The new approach, though a bit lengthy in proving some

theorems, is very instructive in nature. It not only offers more insights into group structure, revealing the duality between the group $\mathbf{G}$ and its intrinsic group $\overline{\mathbf{G}}$, but also gives a simple and universal method for decomposing the regular rep into irreps subducted according to any given subgroup chain $\mathbf{G}\supset\mathbf{G}(s)$. Furthermore, this can be done without any knowledge of the characters. Consequently, the main advantages of the new approach are its practicality and flexibility.

On the other hand, representation group theory gives the theory for projective irreps of the group $\mathbf{g}$. The set of matrices

$$\{D^{(\nu)}(\gamma_i):i=1,2,\ldots,|\mathbf{g}|\},\quad D^{(\nu)}(\gamma_i)\equiv D^{(\nu)}(R_i) \tag{6.49}$$

gives what is called the projective irrep of the group $\mathbf{g}$. Equations (6.22a), (6.23), (6.24a), (6.25), and (6.26) are just the key equations for the projective irreps of the group $\mathbf{g}$ for a given factor system η (Altmann, 1977; Dirl, 1977; Mackey, 1968; Coleman, 1968; Jansen and Boon, 1967). Several methods have been proposed for constructing projective irreps of a finite group $\mathbf{G}$ for a given factor system. Dirl (1977) proposed a new method based on the induction from the projective irreps of an invariant subgroup $\mathbf{N}$ of $\mathbf{G}$; by this method he determined complete sets of projective irreps for all little co-groups of the nonsymmorphic space group O_h^2.

Some of the new features of the present approach are as follows.

(1) The inequivalent irreps are labeled by the eigenvalue ν of the CSCO of $\mathbf{G}$, just as the irreps of a compact Lie group are labeled by the eigenvalues of the Casimir invariants of the Lie group.

(2) The subgroup chain is introduced for classifying irreducible basis and irreps. If $C(s)$ and $\overline{C}(s)$ in Eq. (6.1a) are to be understood as in Eq. (5.10b) with their eigenvalues a and b denoted by Eq. (6.1c), then by solving (6.1a) we can obtain the $\mathbf{G}\supset\mathbf{G}(s)$ and $\overline{\mathbf{G}}\supset\overline{\mathbf{G}}(s)$ irreducible basis

$$P_a^{(\nu)b}\equiv P_{\lambda_1,\lambda_2,\ldots}^{(\nu)\bar{\lambda}_1,\bar{\lambda}_2,\ldots}, \tag{6.50}$$

which belongs to the irreps $\nu,\lambda_1,\lambda_2,\ldots$ of the groups $\mathbf{G}\supset\mathbf{G}(1)\supset\mathbf{G}(2)\supset\cdots$ as well as to the irreps $\nu,\bar{\lambda}_1,\bar{\lambda}_2,\ldots$ of the groups $\overline{\mathbf{G}}\supset\overline{\mathbf{G}}(1)\supset\overline{\mathbf{G}}(2)\supset\cdots$, respectively. If $\mathbf{G}\supset\mathbf{G}(s)$ is a canonical subgroup chain, then in subduction from $\mathbf{G}(i)$ to its nearest subgroup $\mathbf{G}(i+1)$, the irreps λ_{i+1} of $\mathbf{G}(i+1)$ can occur at most once in a given irrep λ_i of $\mathbf{G}(i)$ [otherwise there would be degeneracy for some eigenvalues λ_{i+1} in contradiction with the definition of the canonical subgroup chain for which $(C,C(s),\overline{C}(s))$ is a CSCO in L_g].

For a system with $\mathbf{G}$ as its symmetry group, the eigenvalues ν and a are good quantum numbers.

(3) Using Eq. (6.23), we can obtain all the irreducible matrices $D^{(\nu)}(R)$ in the $\mathbf{G}\supset\mathbf{G}(s)$ classification, which have the useful property of decomposing immediately into direct sums of irreps of the corresponding subgroups contained in $\mathbf{G}(s)$, if the subduction is carried out.

(4) The intrinsic group $\overline{\mathbf{G}}$ provides a new quantum number, the intrinsic quantum number b, for distinguishing the h_ν equivalent irreps $D^{(\nu)b}$ of $\mathbf{G}$ with the basis $\{P_a^{(\nu)b}:a=1,2,\ldots,h_\nu\}$. Equation (6.14a) shows that, under the group $\mathbf{G}$, the basis vector $P_a^{(\nu)b}$ only changes its external quantum number a.

(5) Analogously, in the group space, the irrep (ν) of the intrinsic group $\overline{\mathbf{G}}$ also occurs h_ν times. The h_ν equivalent irreps $D^{(\nu)a}$ with the basis $\{P_a^{(\nu)b}:b=1,2,\ldots,h_\nu\}$ are distinguished by the external quantum number a. Equation (6.15a) shows that under the group $\overline{\mathbf{G}}$, the basis vector $P_a^{(\nu)b}$ only changes its intrinsic quantum number b.

For a given ν, the external and intrinsic quantum numbers a and b have exactly the same h_ν distinct values.

(6) Under the standard phase choice for the eigenvectors $P_a^{(\nu)b}$, we have

$$\begin{aligned} &D^{(\nu)b}(\mathbf{G})=D^{(\nu)}(\mathbf{G}),\\ &D^{(\nu)a}(\overline{\mathbf{G}})=D^{(\nu)}(\overline{\mathbf{G}}),\\ &D^{(\nu)}(\overline{\mathbf{G}})=\widetilde{D}^{(\nu)}(\mathbf{G}). \end{aligned} \tag{6.51}$$

(7) The two orthogonal theorems for the characters [Eq. (6.44)] and those for the irreducible matrix elements [Eq. (6.26)], now can be interpreted as the orthonormality and completeness conditions for the eigenvectors of the CSCO-I and -III, respectively.

(8) Thus far, for all the irreps of $\mathbf{G}$, we have adopted the same $\mathbf{G}\supset\mathbf{G}(s)$ basis. In fact, for different irreps (ν) we can choose different classification schemes. Otherwise stated, the choice of the subgroup chain $\mathbf{G}(s)$, and therefore of the operator set $C(s)$, may depend on ν. Equation (6.1a) can thus be generalized to

$$\begin{bmatrix} C\\ C^{(\nu)}(s)\\ \overline{C}^{(\nu)}(s)\end{bmatrix}P_a^{(\nu)b}=\begin{bmatrix}\nu\\ a\\ b\end{bmatrix}P_a^{(\nu)b}, \tag{6.52}$$

where $C^{(\nu)}(s)$ is the CSCO of the subgroup chain $\mathbf{G}(s)$ chosen for classifying basis vectors of the irrep (ν).

Flodmark and Blokker (1972) have proposed a scheme for constructing irreps of finite groups. They first decompose the regular rep space of a group $\mathbf{G}$ into subspaces L_ν by using the projection operator $P^{(\nu)}$ [see Eq. (3.39)], and then use a systematic but rather complicated procedure to decompose L_ν into h_ν irreducible spaces. This procedure has been programmed by Flodmark and Jannson (1982). The irreps constructed by this scheme still suffer from the drawback that they are not adapted to a definite subgroup chain.

VII. THE EIGENFUNCTION METHOD (EFM)

A. EFM for the irreducible basis

Theorem 7.1. A necessary and sufficient condition for a function $\psi^{(\nu)}$ to belong to the irrep (ν) of a group $\mathbf{G}$ is that $\psi^{(\nu)}$ be an eigenfunction of the CSCO of $\mathbf{G}$,

$$C\psi^{(\nu)}=\nu\psi^{(\nu)} . \tag{7.1}$$

Proof. The "necessary" follows from the following consideration. Suppose $\psi^{(\nu)}$ is a vector of an irreducible space L of $\mathbf{G}$. Obviously L is a representation space for any class operator of $\mathbf{G}$ and thus is an invariant subspace of C. According to Corollary 2.1, $\psi^{(\nu)}$ is necessarily an eigenfunction of C.

Next we prove that (7.1) is a sufficient condition.

If Eq. (7.1) is true, then $\psi^{(\nu)}$ must belong to the eigenspace $\mathscr{L}_\nu$ of C with the eigenvalue ν. The space $\mathscr{L}_\nu$ may be decomposed into several irreducible spaces $\mathscr{L}_{(\nu)\tau}$, $\tau=1,2,\ldots,$ each generating an irrep. All these irreps are labeled by the same eigenvalue ν of C and thus are equivalent to one another on account of Theorem 6.6. Therefore, the function $\psi^{(\nu)}$ is necessarily a basis vector for one of those equivalent irreps, or a linear combination of their basis vectors. This is exactly what it means for a function to belong to the irrep (ν).

Note that if both $\psi_1^{(\nu)}$ and $\psi_2^{(\nu)}$ belong to the irrep (ν) of $\mathbf{G}$, it does not necessarily mean that they are two components (or partners) of an irrep, since it may be that $\psi_1^{(\nu)}$ is a basis vector of the first irrep (ν), whereas $\psi_2^{(\nu)}$ is a basis vector of the second irrep (ν).

A natural extension of Theorem 7.1 is Theorem 7.2.

Theorem 7.2. A necessary and sufficient condition for $\psi^{(\nu)}_{\lambda_1\lambda_2}\ldots$ to belong to the irrep $\nu,\lambda_1,\lambda_2,\ldots$ of a subgroup chain $G\supset G(1)\supset G(2)\supset\cdots$, is that it satisfy the following eigenequations:

$$\begin{bmatrix} C \\ C(1) \\ C(2) \\ \vdots \end{bmatrix}\psi^{(\nu)}_{\lambda_1\lambda_2}\ldots=\begin{bmatrix} \nu \\ \lambda_1 \\ \lambda_2 \\ \vdots \end{bmatrix}\psi^{(\nu)}_{\lambda_1\lambda_2}\ldots . \tag{7.2}$$

Equation (7.2) offers a method, the eigenfunction method (EFM), for finding the IRB of a group $\mathbf{G}$ in any chosen $\mathbf{G}\supset\mathbf{G}(s)$ classification without need of any knowledge of the characters or irreducible matrices.

Suppose that there are $\mathscr{N}$ orthonormal wave functions

$$\varphi_j(X),\quad j=1,2,\ldots,\mathscr{N} , \tag{7.3}$$

which carry a reducible rep of the group $\mathbf{G}$, and we need to find the $\mathbf{G}\supset\mathbf{G}(s)$ IRB $\psi_a^{(\nu)}$, which can be expressed as

$$\psi_a^{(\nu)}=\sum_j u_{\nu a,j}\varphi_j . \tag{7.4}$$

The set of eigenequations (7.2) can be rewritten in a more compact form as

$$\begin{bmatrix} C \\ C(s) \end{bmatrix}\psi_a^{(\nu)}=\begin{bmatrix} \nu \\ a \end{bmatrix}\psi_a^{(\nu)} , \tag{7.5a}$$

which is a generalization of Eq. (1.5) for the $SO_3\supset SO_2$ IRB.

From Eqs. (7.4) and (7.5a) we obtain

$$\sum_{l=1}^{\mathscr{N}}\left[\left\langle\varphi_j\left|\begin{matrix} C \\ C(s)\end{matrix}\right|\varphi_l\right\rangle-\begin{bmatrix}\nu \\ a\end{bmatrix}\delta_{jl}\right]u_{\nu a,l}=0 . \tag{7.5b}$$

If the eigenvalue (ν,a) is a single root, it means that the irrep ν occurs only once, and corresponding to each (ν,a), $a=a_1,a_2,\ldots,a_{h_\nu}$, there is only one eigenvector. These h_ν eigenvectors $\psi_a^{(\nu)}$ carry the irrep ν of $\mathbf{G}$.

In the foregoing procedure, a knowledge of the irreducible matrices is unnecessary. However, in some cases, certain conventional or standard irreducible matrices in the $\mathbf{G}\supset\mathbf{G}(s)$ scheme are given. In order that the IRB found from the EFM be consistent (including the phase) with the standard matrices, we can use the following technique.

We need only find one component, say $\psi_a^{(\nu)}$, for each possible ν from Eq. (7.5). Using the known matrix elements, we can construct an operator $F^{(\nu)}_{a'a}(R)$, a suitable linear combination of the group elements, by means of which the other a'th component can be derived from the known component a successively,

$$\psi_{a'}^{(\nu)}=F^{(\nu)}_{a'a}(R)\psi_a^{(\nu)} . \tag{7.6a}$$

The form of the operator $F^{(\nu)}_{a'a}(R)$ is very simple for the commonly used finite groups and can be easily found. For example, suppose that $R_i\psi_a^{(\nu)}=c_1\psi_a^{(\nu)}+c_2\psi_{a'}^{(\nu)}$, then

$$F^{(\nu)}_{a'a}(R)=(R_i-c_1)/c_2 . \tag{7.6b}$$

Suppose that the eigenvalue (ν,a) is a τ_ν-fold root; then it indicates that the irrep ν occurs τ_ν times, and for given (ν,a) there are τ_ν linearly independent solutions to Eq. (7.5),

$$\psi_a^{(\nu)\tau},\quad \tau=1,2,\ldots,\tau_\nu . \tag{7.7}$$

The eigenvectors $\psi_a^{(\nu)\tau}$ can be chosen to be orthogonal in the multiplicity label τ. However, it should be stressed that the eigenvectors $\psi_a^{(\nu)\tau}$, $a=1,2,\ldots,h_\nu$, thus chosen arbitrarily except for the requirement of orthogonality with respect to τ, in general do not generate an irrep of $\mathbf{G}$. To obtain the IRB we can use either one of the following two methods.

(1) We can use the intrinsic quantum number β_i to distinguish the τ_ν sets of eigenvectors $\{\psi_a^{(\nu)\beta_i}\}$, $i=1,2,\ldots,\tau_\nu$. For details see Chen and Gao (1982).

(2) For a given eigenvalue (ν,a), we can get from Eq. (7.5) τ_ν linearly independent solutions. After Schmidt's orthogonalization, they become $\psi_a^{(\nu)\tau}$, $\tau=1,2,\ldots,\tau_\nu$. The other components $\psi_{a'}^{(\nu)\tau}$ can be obtained through

$$\psi_{a'}^{(\nu)\tau}=F^{(\nu)}_{a'a}(R)\psi_a^{(\nu)\tau},\quad \tau=1,2,\ldots,\tau_\nu . \tag{7.8}$$

The functions $\psi_1^{(\nu)\tau},\ldots,\psi_{h_\nu}^{(\nu)\tau}$ carry the τth irrep ν. Now the index τ is an additional label rather than the intrinsic quantum number.

The conventional method for constructing an IRB is the projection-operator method. From Theorem 7.2, we know that, acting on a normalized function $\Phi_0(X)$ without any symmetry under the group $\mathbf{G}$, the normalized generalized projection operator $P_a^{(\nu)b}$ yields the $\mathbf{G}\supset\mathbf{G}(s)$ and $\bar{\mathbf{G}}\supset\bar{\mathbf{G}}(s)$ IRB

$$\psi_a^{(\nu)b}=P_a^{(\nu)b}\Phi_0(X) . \tag{7.9}$$

While acting on a wave function $\Phi(X)$ that has partial symmetry with respect to the group $\mathbf{G}$, it yields the unnormalized $\mathbf{G}\supset\mathbf{G}(s)$ IRB

$$\psi_a^{(\nu)}=\text{const}\times P_a^{(\nu)b}\Phi(X)\ . \tag{7.10}$$

However, Eq. (7.10) is in general no longer the IRB of $\overline{\mathbf{G}}\supset\overline{\mathbf{G}}(s)$ (Chen and Gao, 1982).

The projection-operator method epitomized in Eq. (7.10), though simple in principle, may well be very laborious, and is not convenient for groups of large order. The eigenfunction method is simpler and especially suitable for computer calculation.

B. EFM for irreducible matrices

Let us define the column vector

$$\mathbf{D}_{ab}^{(\nu)}=\text{col}(D_{ab}^{(\nu)}(R_1),\ldots,D_{ab}^{(\nu)}(R_{|\mathbf{g}|})) \tag{7.11a}$$

as the irreducible-matrix-element vector. Then according to Eqs. (6.5) and (6.23) we have Theorem 7.3.

Theorem 7.3. In the group space, the eigenvectors of the CSCO-III of $\mathbf{G}$ are proportional to the complex conjugate of the irreducible-matrix-element vectors,

$$\sum_{j=1}^{|\mathbf{g}|}\left[\left\langle R_i\left|\begin{matrix}C\\C(s)\\\overline{C}(s)\end{matrix}\right|R_j\right\rangle-\begin{bmatrix}\nu\\a\\b\end{bmatrix}\delta_{ij}\right]D_{ab}^{(\nu)}(R_j)^*=0\ . \tag{7.11b}$$

From Eqs. (7.11b) and (6.26a), or equivalently from Eqs. (6.5) and (6.23), and using the standard phase choice in Sec. VI.C, we can determine all the matrices in the $\mathbf{G}\supset\mathbf{G}(s)$ classification.

Equation (7.11b) is a generalization of Eq. (1.7) for the $SO_3\supset SO_2$ irreducible matrix elements.

Sometimes we need the generalized shift operator from the $\mathbf{G}\supset\mathbf{G}(s)'$ IRB $\varphi_\kappa^{(\nu)}$ to the $\mathbf{G}\supset\mathbf{G}(s)$ IRB $\psi_a^{(\nu)}$, where $\mathbf{G}(s)'$ and $\mathbf{G}(s)$ are two different subgroup chains of $\mathbf{G}$. The generalized shift operator is given by

$$P_{a\kappa}^{(\nu)}=\frac{h_\nu}{|\mathbf{g}|}\sum_{i=1}^{|\mathbf{g}|}\mathscr{D}_{a\kappa}^{(\nu)}(R_i)^*R_i\ , \tag{7.12a}$$

where $\mathscr{D}_{a\kappa}^{(\nu)}(R_i)$ are the generalized matrix elements, or the skew matrix elements (Klein and Seligman, 1982),

$$\mathscr{D}_{a\kappa}^{(\nu)}(R_i)=\langle\psi_a^{(\nu)}\,|\,R_i\,|\,\varphi_\kappa^{(\nu)}\rangle\ . \tag{7.12b}$$

As in Eq. (7.11b), $\mathscr{D}_{a\kappa}^{(\nu)}(R_i)$ satisfy the eigenequations

$$\sum_{j=1}^{|\mathbf{g}|}\left[\left\langle R_i\left|\begin{matrix}C\\C(s)\\\overline{C}(s)'\end{matrix}\right|R_j\right\rangle-\begin{bmatrix}\nu\\a\\\kappa\end{bmatrix}\delta_{ij}\right]\mathscr{D}_{a\kappa}^{(\nu)}(R_j)^*=0\ , \tag{7.13}$$

where $\overline{C}(s)'$ is the intrinsic operator set corresponding to the CSCO $C(s)'$ of the subgroup chain $\mathbf{G}(s)'$. From Eq. (7.13) and a normalization condition similar to (6.26a) with D replaced by $\mathscr{D}$, we can evaluate the generalized matrix elements.

It is thus seen that the flexibility of the EFM makes possible the construction of both the IRB and the irreducible matrix in any given group chain, and the puzzle of solving two interdependent problems in the traditional theory is solved satisfactorily.

C. EFM and conventional methods for irreducible characters

From Eqs. (3.14) and (6.43) we have Theorem 7.4.

Theorem 7.4. The eigenvectors of the CSCO-I of $\mathbf{G}$ in the class space are proportional to the complex conjugate of the irreducible character vectors,

$$\mathscr{D}(C)\boldsymbol{\chi}^{(\nu)*}=\nu\boldsymbol{\chi}^{(\nu)*}\ . \tag{7.14}$$

This is a generalization of Eq. (1.4a) for the SO_3 character.

It should be mentioned that Theorems 7.3 and 7.4 remain true for compact Lie groups if the group (class) space is replaced by the group (class) parameter space, and the eigenvectors by the eigenfunctions (Chen, Wang, and Gao, 1983).

The EFM for characters can be summarized as follows.

Using the structure constants C_{ij}^k of the group $\mathbf{G}$ to form the natural representative matrices $\mathscr{D}(C_i)$ for the classes contained in the CSCO of $\mathbf{G}$,

$$\mathscr{D}_{kj}(C_i)=C_{ij}^k,\quad i=1,2,\ldots,l\ . \tag{7.15a}$$

Let $\mathbf{q}=\text{col}(q_1,q_2,\ldots,q_n)$. Suppose that $\mathbf{q}^{(\nu)}$ are simultaneous eigenvectors of $\mathscr{D}(C_1),\ldots,\mathscr{D}(C_l)$, i.e.,

$$\mathscr{D}(C_i)\mathbf{q}^{(\nu)}=\lambda_i^{(\nu)}\mathbf{q}^{(\nu)},\quad i=1,2,\ldots,l\ , \tag{7.15b}$$

and that they obey the normalization condition

$$\sum_{i=1}^{n}g_i\,|\,q_i^{(\nu)}\,|^2=1\ , \tag{7.15c}$$

as well as the phase convention that all $q_e^{(\nu)}$ for the identity e are real positive. Then the primitive character of $\mathbf{G}$ is given by

$$\chi_i^{(\nu)}=\sqrt{|\mathbf{g}|}\,q_i^{(\nu)*}\ . \tag{7.16}$$

For example, Table III is precisely the character table of the point group C_{4v}, where $\sqrt{1/8}=|\mathbf{g}|^{-1/2}=|\mathbf{G}|^{-1/2}$.

Before the EFM was proposed, several conventional methods were available for determining the characters of an abstract group $\mathbf{G}$ with N classes. These include the following.

1. Jones's method (1975)

First find all the N^2 eigenvalues $\lambda_i^{(\nu)}$, $\nu,i=1,2,\ldots,N$ from the characteristic equations of the N matrices $\mathscr{D}(C_i)$, $i=1,2,\ldots,N$; next use the relation $\chi_i^{(\nu)}=(h_\nu/g_i)\lambda_i^{(\nu)}$ to get the N^2 characters $\chi_i^{(\nu)}$; and finally use the orthogonality of the characters to arrange the N^2 characters into the character table.

2. Boerner's method (1963)

From Eq. (2.18c) one obtains a set of equations for the eigenvalues of the N classes

$$\lambda_i^{(\nu)}\lambda_j^{(\nu)}=\sum_{k=1}^{N} C_{ij}^k\lambda_k^{(\nu)} . \tag{7.17a}$$

Multiplying both sides of Eq. (7.17a) by an indeterminate u_i and summing over i, one gets an eigenequation for $\boldsymbol{\lambda}^{(\nu)}=\mathrm{col}(\lambda_1^{(\nu)},\ldots,\lambda_N^{(\nu)})$,

$$L(u)\boldsymbol{\lambda}^{(\nu)}=\xi^{(\nu)}\boldsymbol{\lambda}^{(\nu)} , \tag{7.17b}$$

where $L(u)$ is a matrix with the matrix elements

$$L_{jk}(u)=\sum_{i=1}^{N} C_{ij}^k u_i , \tag{7.17c}$$

and

$$\xi^{(\nu)}=\sum_{i}^{N}{}_1\lambda_i^{(\nu)}u_i .$$

By decomposing the determinant of the matrix $(L(u)-u_0\mathbf{I})$ into linear factors,

$$\det(L(u)-u_0\mathbf{I})=\prod_{\nu=1}^{N}\left[u_0-\sum_{i=1}^{N}\lambda_i^{(\nu)}u_i\right]=0 , \tag{7.17d}$$

one can determine the N^2 eigenvalues $\lambda_i^{(\nu)}$, and then use Eq. (6.47) to obtain the N^2 characters. Boerner's method avoids the rearrangement of $\chi_i^{(\nu)}$; however the decomposition procedure (7.17d) is not easy for higher-order groups.

3. Bradley and Cracknell's method (1972)

From Eqs. (7.17a) and (6.47) one has

$$g_i g_j\chi_i^{(\nu)}\chi_j^{(\nu)}=h_\nu\sum_{k=1}^{N} C_{ij}^k g_k\chi_k^{(\nu)} . \tag{7.18}$$

From Eq. (7.18) along with (6.3) and (6.44a) (noting that here $|\mathbf{g}|$ and n should be replaced by $|\mathbf{G}|$ and N, respectively), one can determine the characters. The major difficulty of this method is that Eq. (7.18) is a nonlinear algebraic equation for $\chi_i^{(\nu)}$.

4. Burnside's method (1955)

Equation (7.17a) can be rewritten as

$$M_i\boldsymbol{\lambda}^{(\nu)}=\lambda_i^{(\nu)}\boldsymbol{\lambda}^{(\nu)} , \tag{7.19a}$$

where

$$M_i=\tilde{\mathscr{D}}(C_i),\quad (M_i)_{jk}=C_{ij}^k . \tag{7.19b}$$

Therefore, the N column vectors $\boldsymbol{\lambda}^{(\nu)}$ are common vectors of the N matrices M_i, $i=1,2,\ldots,N$. From Eq. (7.19a) we can find N eigenvectors $\boldsymbol{\lambda}^{(\nu)}$ normalized according to $\lambda_e^{(\nu)}\equiv 1$. The dimension h_ν is decided by

$$\sum_{i=1}^{N}|\lambda_i^{(\nu)}|^2/g_i=|\mathbf{G}|/h_\nu^2 , \tag{7.19c}$$

while the characters are obtained from Eq. (6.47). The main difficulty of this method is that it involves the calculation of the common eigenvectors of N matrices.

The common feature of these four methods is that the concept of the CSCO for the class space has not been introduced, and thus all the structure constants C_{ij}^k of the group are required. These methods are not easily applied to higher-order groups.

5. Dixon's method (1967)

Dixon (1967) improved upon Burnside's method by transposing the problem from the field of complex numbers into the field of integers modulo p for a suitable prime p. It is much easier to compute the modular characters in the latter field, and from these characters one can calculate the ordinary irreducible character. An efficient program has been written by Dixon.

In contrast, the equation for the EFM (7.14) is linear, and only the natural representation matrices of the l class operators contained in the CSCO of $\mathbf{G}$ are required. Usually l is much smaller than the class number N. The EFM is also suitable for high-order groups; for example, the characters of the permutation group S_{11} with $N=56$ have been calculated by diagonalizing only a single matrix, the natural representation of the two-cycle class operator (Gao *et al.*, 1976; Chen and Gao, 1982).

6. Seeking the CSCO of G from known characters

As mentioned before, in the new approach, the character recedes from its predominant role in the traditional theory. We can now carry out the reduction of a rep without any knowledge of the characters. However, if the primitive characters of a group $\mathbf{G}$ are known, use can be made of them to simplify the calculation.

The character has the following two major applications in the new approach.

(1) Finding the CSCO of $\mathbf{G}$. With the known character table and Eq. (6.47), we can get the following array for the n^2 eigenvalues $\lambda_i^{(\nu)}$:

$$\begin{bmatrix} \lambda_1^{(\nu_1)} & \lambda_2^{(\nu_1)} & \cdots & \lambda_n^{(\nu_1)} \\ \lambda_1^{(\nu_2)} & \lambda_2^{(\nu_2)} & \cdots & \lambda_n^{(\nu_2)} \\ \vdots & \vdots & & \vdots \\ \lambda_1^{(\nu_n)} & \lambda_2^{(\nu_n)} & \cdots & \lambda_n^{(\nu_n)} \end{bmatrix} . \tag{7.20}$$

If we can find a column, say column i, in the array which has n different eigenvalues $\lambda_i^{(\nu_1)},\lambda_i^{(\nu_2)},\ldots,\lambda_i^{(\nu_n)}$, then the class operator C_i is the CSCO of the rep group $\mathbf{G}$. Otherwise, we look for two columns, say i and j, and if the n pairs of eigenvalues $(\lambda_i^{(\nu_1)},\lambda_j^{(\nu_1)}),\ldots,(\lambda_i^{(\nu_n)},\lambda_j^{(\nu_n)})$ are all different, then (C_i,C_j) is a CSCO of the rep group, etc. Consequently, if the character table is known, it is trivial to find the CSCO of the group.

(2) Determining the number of times a given irrep ν occurs in a rep D. Let τ_ν be the number of times the irrep ν occurs in the decomposition of a reducible rep D with characters χ_i,

$$\chi_i=\sum_\nu \tau_\nu \chi_i^{(\nu)} . \tag{7.21}$$

From Eqs. (6.44a) and (7.21) we get the well-known expression for τ_ν,

$$\tau_\nu=\sum_{i=1}^{n}\frac{g_i}{|\mathbf{g}|}\chi_i\chi_i^{(\nu)*} . \tag{7.22}$$

D. EFM for Clebsch-Gordan coefficients

Suppose that $\mathbf{G}$ is an abstract group (for notational convenience, we omit the caret). Let

$$\{\psi_{a_\sigma}^{(\nu_\sigma)}:a_\sigma=1,2,\ldots,h_{\nu_\sigma}\},\quad \sigma=1,2 , \tag{7.23a}$$

be the $\mathbf{G}\supset\mathbf{G}(s_\sigma)$ basis for the projective irrep $D^{(\nu_\sigma)}$ of $\mathbf{G}$ with the factor system $\eta^{(\sigma)}$,

$$D^{(\nu_\sigma)}(R_s)D^{(\nu_\sigma)}(R_t)=\eta^{(\sigma)}(s,t)D^{(\nu_\sigma)}(R_sR_t) ,$$
$$\sigma=1,2,\ s,t=1,2,\ldots,|\mathbf{G}| . \tag{7.23b}$$

The $h_{\nu_1}h_{\nu_2}$ vectors

$$|a_1a_2\rangle\equiv\psi_{a_1}^{(\nu_1)}\psi_{a_2}^{(\nu_2)} \tag{7.23c}$$

carry the Kronecker product rep of $\mathbf{G}$ (or the uncoupled rep of $\mathbf{G}$)

$$D^{(\nu_1)\times(\nu_2)}=D^{(\nu_1)}\otimes D^{(\nu_2)} . \tag{7.23d}$$

It is easy to show that $D^{(\nu_1)\times(\nu_2)}$ is a projective rep of $\mathbf{G}$ for the factor system

$$\eta(s,t)=\eta^{(1)}(s,t)\eta^{(2)}(s,t) . \tag{7.23e}$$

The Kronecker product rep can be reduced into the projective irreps ν of $\mathbf{G}$ for the factor system η,

$$D^{(\nu_1)\times(\nu_2)}=\sum_\nu(\nu_1\nu_2\nu)D^{(\nu)} , \tag{7.24}$$

where $(\nu_1\nu_2\nu)$ is the number of times that the projective irrep ν occurs in the Kronecker product rep. Equation (7.24) is referred to as the CG series. To effect the reduction, the product basis vectors of (7.23a) need to be recombined into the $\mathbf{G}\supset\mathbf{G}(s)$ IRB

$$|\nu\tau a\rangle=\sum_{a_1a_2}(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)\,|a_1a_2\rangle ,$$
$$\tau=1,2,\ldots,(\nu_1\nu_2\nu) , \tag{7.25}$$

where τ is a multiplicity label and $(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)$ is called the Clebsch-Gordan coefficient (CGC) (or the Wigner coefficient or the coupling coefficient). Notice that the subgroup chains $\mathbf{G}(s_1)$, $\mathbf{G}(s_2)$, and $\mathbf{G}(s)$ may be different from one another or may be identical.

According to Eq. (7.5), the CGC satisfies the eigenequations

$$\sum_{a_1a_2}\left[\left\langle b_1b_2\left|\begin{matrix}C\\C(s)\end{matrix}\right|a_1a_2\right\rangle-\begin{bmatrix}\nu\\a\end{bmatrix}\delta_{a_1b_1}\delta_{a_2b_2}\right]$$
$$\times(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)=0 . \tag{7.26}$$

It shows that the CGC results from a diagonalization of the representative matrix of the CSCO-II of $\mathbf{G}$ in the product basis. The matrix elements of a class operator C_i are given by

$$\langle b_1b_2\,|\,C_i\,|\,a_1a_2\rangle=\sum_{\kappa=1}^{g_i}D_{b_1a_1}^{(\nu_1)}(R_{(i,\kappa)})D_{b_2a_2}^{(\nu_2)}(R_{(i,\kappa)}) . \tag{7.27}$$

Using Eq. (7.27) we can calculate the matrix elements of the CSCO-II of $\mathbf{G}$. From the characteristic equation of (7.26), we can obtain the eigenvalue (ν,a) along with its degeneracy, which gives the multiplicity $(\nu_1\nu_2\nu)$ in the CG series (7.24).

When $(\nu_1\nu_2\nu)>1$, for given (ν,a), there are $(\nu_1\nu_2\nu)$ sets of linearly independent solutions to Eq. (7.26). Subject to the orthogonality requirement with respect to the multiplicity label τ, i.e.,

$$\sum_{a_1a_2}(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)^*(\nu_1a_1\nu_2a_2\,|\,\nu\tau' a)=\delta_{\tau\tau'} , \tag{7.28}$$

the $(\nu_1\nu_2\nu)$ sets of solutions can be chosen arbitrarily.

If the solution for one component a is known, the other components b can be found with the help of Eq. (7.8),

$$|\nu\tau b\rangle=F_{ba}^{(\nu)}(R)\,|\nu\tau a\rangle,\quad \tau=1,2,\ldots,(\nu_1\nu_2\nu) . \tag{7.29}$$

Substituting Eq. (7.25) into (7.29) and multiplying (7.29) from the left by $\langle b_1b_2\,|$, we obtain

$$(\nu_1b_1\nu_2b_2\,|\,\nu\tau b)=\sum_{a_1a_2}\langle b_1b_2\,|\,F_{ba}^{(\nu)}(R)\,|\,a_1a_2\rangle$$
$$\times(\nu_1a_1\nu_2a_2\,|\,\nu\tau a) . \tag{7.30}$$

Following a procedure similar to that described after Eq. (7.7), for each possible ν we take only the CGC for a particular a from Eq. (7.26); the remaining CG coefficients of the projective irrep ν should be evaluated from Eq. (7.30).

When $\eta^\sigma(s,t)\equiv1$, for $\sigma=1,2$, $s,t,=1,2,\ldots,|\mathbf{G}|$, all the projective irreps of $\mathbf{G}$ become the vector irreps of $\mathbf{G}$, and Eqs. (7.24)—(7.30) continue to be valid.

It is to be noted that the multiplicity separation is arbitrary, and the following linear combination satisfies all our requirements for the CGC:

$$(\nu_1a_1\nu_2a_2\,|\,\nu\theta a)=\sum_\tau S_{\theta\tau}^{(\nu)}(\nu_1a_1\nu_2a_2\,|\,\nu\tau a) , \tag{7.31}$$

where $S^{(\nu)}$ is a $(\nu_1\nu_2\nu)\times(\nu_1\nu_2\nu)$ unitary matrix. Hence the CGC can be determined only up to a unitary transformation.

The advantage of the EFM for the CGC lies in the fact that here only the irreducible matrices of a few group elements are required, and these are contained in the CSCO-

II of G, while in the projection-operator method (see Sec. VII.E), the irreducible matrices of all the $|\mathbf{G}|$ group elements are required. Another feature of the EFM is that the CG series and CGC are obtained simultaneously.

The EFM is powerful for constructing the CGC or isoscalar factor (ISF) of compact groups. As early as in 1966, Bayman and Lande calculated the $SU_{2j+1} \supset SP_{2j+1} \supset SO_3$ ISF by diagonalizing the operator $C(SU_{2j+1}) + 0.11\,C(SP_{2j+1})$, where $C(SU_{2j+1})$ and $C(SP_{2j+1})$ are the Casimir operators of SU_{2j+1} and SP_{2j+1}, respectively. The EFM has been used for computing the CGC of the permutation groups S_2–S_6 (Chen and Gao, 1981; Gao and Chen, 1985), the unitary groups (Chen, Wang, and Gao, 1978a; Chen, Gao, Shi, Vallieres, and Feng, 1984; So and Strottman, 1979), and the graded unitary groups (Chen, Gao, and Chen, 1984a,1984b; Chen, Chen, and Gao, 1984).

It is seen that there is virtually no difference between the treatment of the CGC for projective irreps and that for vector irreps. Therefore, we shall discuss only the CGC of vector irreps from now on.

E. Various methods of obtaining Clebsch-Gordan coefficients

The conventional method for calculating the CGC is the projection-operator method. In contrast to the EFM, it requires a knowledge of the CG series. From Eqs. (7.22) and (7.23d), the multiplicity $(\nu_1\nu_2\nu)$ can be calculated by

$$(\nu_1\nu_2\nu)=\sum_{i=1}^{N}\frac{g_i}{|\mathbf{G}|}\chi_i^{(\nu)*}\chi_i^{(\nu_1)}\chi_i^{(\nu_2)} . \tag{7.32}$$

The projection-operator method in its primitive version works as follows (Tinkham, 1964). By successive application of the projection operator $P_{aa}^{(\nu)}$ and the shift operators $P_{ba}^{(\nu)}$ $(b\neq a)$ to the basis vectors of the Kronecker product rep, one can generate the irreducible basis vectors one by one, whose components give the CGC. The main disadvantage of this method is that one sometimes performs a good deal of work in vain if a vanishing result is obtained. In such a case, one must apply the projection operator to another basis vector. This procedure must be repeated until $(\nu_1\nu_2\nu)$ linearly independent IRB are obtained for a given irrep ν.

In the following we discuss several variations of the projection-operator method. The original derivation for them is rather lengthy. However, shortcuts are possible by using the key equation (7.33b) below.

1. Koster's method

In the Kronecker product space, the generalized projection operator

$$P_{ab}^{(\nu)}=\frac{h_\nu}{|\mathbf{G}|}\sum_R D_{ab}^{(\nu)}(R)^*R \tag{7.33a}$$

can be written as

$$P_{ab}^{(\nu)}=\sum_{\tau=1}^{(\nu_1\nu_2\nu)} |\,\nu\tau a\,\rangle\langle\,\nu\tau b\,| . \tag{7.33b}$$

Equation (7.33b) is easily justified by showing that it satisfies Eq. (6.31). Hence

$$\langle a_1a_2\,|\,P_{ab}^{(\nu)}\,|\,b_1b_2\,\rangle=\sum_{\tau=1}^{(\nu_1\nu_2\nu)}\langle a_1a_2\,|\,\nu\tau a\,\rangle\langle\,\nu\tau b\,|\,b_1b_2\,\rangle . \tag{7.34a}$$

Using Eq. (7.33a), we have

$$\frac{h_\nu}{|\mathbf{G}|}\sum_R D_{ab}^{(\nu)}(R)^*D_{a_1b_1}^{(\nu_1)}(R)D_{a_2b_2}^{(\nu_2)}(R) =\sum_{\tau=1}^{(\nu_1\nu_2\nu)}(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)(\nu_1b_1\nu_2b_2\,|\,\nu\tau b)^* . \tag{7.34b}$$

This is the formula proposed by Koster (1958) for obtaining the CGC. For the multiplicity-free case $[(\nu_1\nu_2\nu)=1]$, the CGC can be calculated from Eq. (7.34b) by holding a_1, a_2, and a fixed, letting b run from 1 to h_ν, and letting b_1b_2 run from 1 to $h_{\nu_1}h_{\nu_2}$. For the $(\nu_1\nu_2\nu)>1$ case, a systematic procedure for obtaining all $(\nu_1\nu_2\nu)$ sets of CGC is given by Koster (1958) and Birman (1974, p. 38). The disadvantage of this method is that it is rather tedious.

This method has been used for calculating the CGC of the point groups (Statz and Koster, 1959; Koster *et al.*, 1963), the permutation group S_5 (Hamermesh, 1962), and the space groups (Litvin and Zak, 1968; Berenson and Birman, 1975; Berenson *et al.*, 1975).

2. Schindler, Mirman, and Dirl's method

A significant improvement in the method of computing the CGC is due to Schindler and Mirman (1977a), who recognized the fact that the $(\nu_1\nu_2\nu)$ independent columns of the projection matrix yield, after being orthonormalized, the $(\nu_1\nu_2\nu)$ sets of CG coefficients.

From Eq. (7.33b) or (6.31c) we have

$$P_{aa}^{(\nu)}\,|\,\nu\tau a\,\rangle=|\,\nu\tau a\,\rangle , \tag{7.35a}$$

$$P_{ba}^{(\nu)}\,|\,\nu\tau a\,\rangle=|\,\nu\tau b\,\rangle . \tag{7.35b}$$

Written in matrix form, this is

$$\mathbf{P}_{aa}^{(\nu)}\mathbf{U}_a^{(\nu)\tau}=\mathbf{U}_a^{(\nu)\tau} , \tag{7.36a}$$

$$\mathbf{P}_{ba}^{(\nu)}\mathbf{U}_a^{(\nu)\tau}=\mathbf{U}_b^{(\nu)\tau} , \tag{7.36b}$$

where $\mathbf{P}_{ba}^{(\nu)}$ and $\mathbf{U}_a^{(\nu)\tau}$ are the representatives of $P_{ba}^{(\nu)}$ and $|\,\nu\tau a\,\rangle$ in the Kronecker product rep, respectively. The matrix elements of $\mathbf{P}_{ba}^{(\nu)}$ are given by

$$(\mathbf{P}_{ba}^{(\nu)})_{a_1a_2,b_1b_2}=\langle a_1a_2\,|\,P_{ba}^{(\nu)}\,|\,b_1b_2\,\rangle =\frac{h_\nu}{|\mathbf{G}|}\sum_R D_{ab}^{(\nu)}(R^{-1})D_{a_1b_1}^{(\nu_1)}(R)D_{a_2b_2}^{(\nu_2)}(R) . \tag{7.37}$$

$\mathbf{P}_{aa}^{(\nu)}$ is called the projection matrix. $\mathbf{U}_a^{(\nu)\tau}$ is called the CGC vector with components

$$(\mathbf{U}_a^{(\nu)\tau})_{a_1a_2}=(\nu_1 a_1 \nu_2 a_2 \mid \nu\tau a),\quad a_1a_2=1,2,\ldots,h_{\nu_1}h_{\nu_2}\ . \tag{7.38}$$

In Eq. (7.36a), the CGC vectors $\mathbf{U}_a^{(\nu)\tau}$, $\tau=1,2,\ldots,(\nu_1\nu_2\nu)$ can be regarded as the vectors that span the eigenspace of the projection matrix $\mathbf{P}_{aa}^{(\nu)}$ with eigenvalue equal to one. From Eqs. (7.34b) and (7.31) it can be easily shown that the matrix $\mathbf{P}_{aa}^{(\nu)}$ has $(\nu_1\nu_2\nu)$ and only $(\nu_1\nu_2\nu)$ linearly independent columns. Using the Schmidt process, we obtain $(\nu_1\nu_2\nu)$ orthonormal column vectors which are eigenvectors of $\mathbf{P}_{aa}^{(\nu)}$ with eigenvalues all equal to one, whose components are the required CGC $(\nu_1 a_1 \nu_2 a_2 \mid \nu\tau a)$, $\tau=1,2,\ldots,(\nu_1\nu_2\nu)$. The CG coefficients for the other components b are obtained either from Eq. (7.36b) or from Eq. (7.34b).

Dirl (1979a) went on to show how the multiplicity index of the CGC can be identified with the special column indices of the projection matrix and to give an explicit expression for the CGC in terms of the matrix elements of $\mathbf{P}_{ba}^{(\nu)}$. A simple derivation of Dirl's result is given below.

Applying the projection operator $P_{aa}^{(\nu)}$ to a vector $\mid b_1b_2\rangle$ in the Kronecker product space, if the result is nonvanishing we obtain an un-normalized basis vector for the irrep ν of G,

$$\mid \nu\theta=(b_1b_2)a\rangle = N_{b_1b_2}^{(\nu)a} P_{aa}^{(\nu)} \mid b_1b_2\rangle\ , \tag{7.39a}$$

where the multiplicity index θ is identified with the column index b_1b_2 of the Kronecker product, and $N_{b_1b_2}^{(\nu)a}$ is a norm that can be easily shown, upon using (6.31a), to be

$$N_{b_1b_2}^{(\nu)a} = \mid \langle b_1b_2 \mid P_{aa}^{(\nu)} \mid b_1b_2\rangle \mid^{-1/2}\ . \tag{7.39b}$$

From Eq. (7.39a) one immediately gets

$$(\nu_1 a_1 \nu_2 a_2 \mid \nu\theta=(b_1b_2)a)=N_{b_1b_2}^{(\nu)a}\langle a_1a_2 \mid P_{aa}^{(\nu)} \mid b_1b_2\rangle\ . \tag{7.40a}$$

The other components $\mid \nu\theta=(b_1b_2)b\rangle$ can be obtained from

$$\mid \nu\theta=(b_1b_2)b\rangle = P_{ba}^{(\nu)} \mid \nu\theta=(b_1b_2)a\rangle\ .$$

Using Eqs. (7.37) and (7.39), one obtains

$$\begin{aligned}(\nu_1 a_1 \nu_2 a_2 \mid \nu\theta=(b_1b_2)b) &= N_{b_1b_2}^{(\nu)a}\langle a_1a_2 \mid P_{ba}^{(\nu)} \mid b_1b_2\rangle \\ &= \left[\frac{h_\nu}{\mid \mathbf{G}\mid}\right]^{1/2} \sum_R D_{ab}^{(\nu)}(R^{-1}) D_{a_1b_1}^{(\nu_1)}(R) D_{a_2b_2}^{(\nu_2)}(R) \\ &\quad\times \left| \sum_R D_{aa}^{(\nu)}(R^{-1}) D_{b_1b_1}^{(\nu_1)}(R) D_{b_2b_2}^{(\nu_2)}(R) \right|^{-1/2},\quad b=1,\ldots,a,\ldots,h_\nu\ .\end{aligned} \tag{7.40b}$$

If by varying the column index b_1b_2 we can obtain $(\nu_1\nu_2\nu)$ orthogonal vectors

$$\mid \nu\theta=(b_1b_2)_\upsilon a\rangle,\quad \upsilon=1,2,\ldots,(\nu_1\nu_2\nu)\ ,$$

then the multiplicity index θ can be explained completely by the special value of the column indices of the projection matrix. On the other hand, if we can obtain only $n<(\nu_1\nu_2\nu)$ orthogonal column vectors in the matrix $\mathbf{P}_{aa}^{(\nu)}$, then we have to apply Schmidt's procedure to obtain the complete CGC.

Equation (7.40a) clearly shows that the columns of the projection matrix $\mathbf{P}_{aa}^{(\nu)}$ give the CGC vectors.

It is also interesting to note the connection between Eqs. (7.40a) and (7.34a), where the multiplicity τ is chosen arbitrarily. From these two equations one has

$$\begin{aligned}&(\nu_1 a_1 \nu_2 a_2 \mid \nu\theta=(b_1b_2)a) \\ &\quad = N_{b_1b_2}^{(\nu)a} \sum_\tau (\nu_1 a_1 \nu_2 a_2 \mid \nu\tau a)(\nu_1 b_1 \nu_2 b_2 \mid \nu\tau a)^*\ .\end{aligned} \tag{7.41a}$$

By identifying

$$S_{\theta\tau}^{(\nu)} = N_{b_1b_2}^{(\nu)a}(\nu_1 b_1 \nu_2 b_2 \mid \nu\tau a)^*\ , \tag{7.41b}$$

we see that Eq. (7.41a) is precisely Eq. (7.31), that is, the two sets of CG coefficients with multiplicity indices θ and τ are related by a unitary transformation.

van den Broek and Cornwell (1978) made a further improvement in the solution of the multiplicity problem of the CGC. After obtaining a CGC vector by using Eq. (7.39a), which is now denoted as

$$\mid \nu\tau=1,a\rangle = N_{b_1b_2}^{(\nu)a} P_{aa}^{(\nu)} \mid b_1b_2\rangle\ , \tag{7.42a}$$

they construct a new operator

$$P_{aa}'^{(\nu)} = P_{aa}^{(\nu)} - \mid \nu 1a\rangle\langle \nu 1a \mid\ . \tag{7.42b}$$

From Eqs. (7.33b) and (7.42b) one has

$$P_{aa}'^{(\nu)} = \sum_{\tau=2}^{(\nu_1\nu_2\nu)} \mid \nu\tau a\rangle\langle \nu\tau a \mid\ , \tag{7.42c}$$

where $\mid \nu\tau a\rangle$, $\tau=2,3,\ldots,(\nu_1\nu_2\nu)$ are the CGC vectors to be decided. Therefore, $P_{aa}'^{(\nu)}$ is again a projection operator, but it is for the $[(\nu_1\nu_2\nu)-1]$-dimensional space, and one can play the same game with $P_{aa}'^{(\nu)}$ to obtain another CGC vector

$$\mid \nu\tau=2,a\rangle = N_{b_1'b_2'}'^{(\nu)a} P_{aa}'^{(\nu)} \mid b_1'b_2'\rangle\ , \tag{7.42d}$$

where

$$N_{b_1'b_2'}'^{(\nu)a} = \mid \langle b_1'b_2' \mid P_{aa}'^{(\nu)} \mid b_1'b_2'\rangle \mid^{-1/2}\ . \tag{7.42e}$$

It is easily seen that the CGC vectors $|\nu\tau a\rangle$, $\tau=1,2$ are the eigenvectors of $P'^{(\nu)}_{aa}$ corresponding to the eigenvalues 0 and 1, respectively. Hence they are orthogonal. One may proceed in this way until the $(\nu_1\nu_2\nu)$ orthonormal CGC vectors are obtained.

This method in its original version was used for computing the CGC of the permutation group S_3–S_6 (Schindler and Mirman, 1977b,1978). Later the method was extended to treat the CGC for space groups (Dirl, 1979d; van den Broek, 1979a), for finite magnetic groups (van den Broek, 1979b), and for space magnetic groups (Dirl, 1980a,1980b).

3. Sakata's method

Suppose that A is a $h_{\nu_1}h_{\nu_2}\times h_\nu$ rectangular matrix. Multiplying both sides of Eq. (7.34b) by $(|\mathbf{G}|/h_\nu)A_{b_1b_2,b}$ and summing over b_1b_2 and b, we obtain an equation that can be put into the form

$$M(\xi)_{a_1a_2,a}=\sum_{\tau=1}^{(\nu_1\nu_2\nu)}\xi_\tau(\nu_1a_1\nu_2a_2\,|\,\nu\tau a)\,, \tag{7.43a}$$

where ξ is a vector

$$\xi=(\xi_1,\xi_2,\ldots,\xi_\varphi),\quad \varphi\equiv(\nu_1\nu_2\nu)\,, \tag{7.43b}$$

$$\xi_\tau=\frac{|\mathbf{G}|}{h_\nu}\sum_{b_1b_2b}A_{b_1b_2,b}(\nu_1b_1\nu_2b_2\,|\,\nu\tau b)^*\,, \tag{7.43c}$$

and $M(\xi)_{a_1a_2,a}$ is the matrix element of a $h_{\nu_1}h_{\nu_2}\times h_\nu$ matrix $M(\xi)$ containing $(\nu_1\nu_2\nu)$ parameters $\xi_1,\ldots,\xi_\varphi$,

$$M(\xi)=\sum_R[D^{(\nu_1)}(R)\otimes D^{(\nu_2)}(R)]AD^{(\nu)}(R)^\dagger\,. \tag{7.44}$$

In the case of $(\nu_1\nu_2\nu)=1$, Eq. (7.43a) shows that the CGC vectors $\mathbf{U}^{(\nu)}_a$ are obtained by normalizing the columns of the matrix $M(\xi=1)$. In the case of $(\nu_1\nu_2\nu)>1$, by taking $(\nu_1\nu_2\nu)$ linearly independent vectors ξ, such as $\xi^{(1)}=(1,0,\ldots,),\xi^{(2)}=(0,1,\ldots,0),\ldots,$ $\xi^{(\varphi)}=(0,0,\ldots,1)$, we get $(\nu_1\nu_2\nu)$ matrices $M(\xi^{(\theta)})$, $\theta=1,2,\ldots,(\nu_1\nu_2\nu)$. After normalizing each column vector of these matrices and using the Schmidt process, we obtain $(\nu_1\nu_2\nu)$ sets of CGC (Sakata, 1974).

If $\mathbf{H}$ is a subgroup of $\mathbf{G}$, and $(s_1=e,\ldots,s_q)$ is a set of coset representatives of $\mathbf{H}$ in $\mathbf{G}$ [see Eq. (6.34)], then the matrix $M(\xi)\equiv M(\mathbf{G})$ can be rewritten as

$$M(\mathbf{G})=M(\mathbf{H})+[D^{(\nu_1)}(s_2)\otimes D^{(\nu_2)}(s_2)]\times M(\mathbf{H})D^{(\nu)}(s_2)^\dagger+\cdots\,, \tag{7.45a}$$

$$M(\mathbf{H})=\sum_{h\in\mathbf{H}}[D^{(\nu_1)}(h)\otimes D^{(\nu_2)}(h)]AD^{(\nu)}(h)^\dagger\,. \tag{7.45b}$$

This method is suggested by Sakata (1974) and used to compute the CGC of the double point group $\bar{D}_3$ and the double space group $\bar{D}^{14}_{4h}$. The method is rather tedious and has an *ad hoc* nature.

A common feature of the above methods is that the irreducible matrices of all the $|\mathbf{G}|$ elements are required. The total number of irreducible matrix elements is equal to $|\mathbf{G}|^2$, which is quite large for a high-order group. This is the main difficulty in applying the projection-operator method.

4. Butler and Wybourne's method

Butler and Wybourne (1976a,1976b) adopted a quite different approach to the CGC problem for compact groups. According to Racah's factorization lemma (1951), the calculation of the CGC for the subgroup chain $\mathbf{G}\supset\mathbf{G}(1)\supset\mathbf{G}(2)\supset\cdots$ is reduced to the calculation of the isoscalar factors for $\mathbf{G}\supset\mathbf{G}(1),\mathbf{G}(1)\supset\mathbf{G}(2),\ldots$. The Butler-Wybourne method is for computing the $6j$ symbols and $3jm$ factors of $\mathbf{G}$, the latter being the symmetrized isoscalar factors. The distinguishing feature of this method is that it requires only a knowledge of character theory, chiefly the product and branching rules. It is particularly useful for groups with irreps of large dimensions.

This method has been used to compute the CGC for point groups (Butler and Wybourne, 1976b; Butler, 1981) and the $3jm$ factors for $SU(3)\supset SU(2)$ and $SU(6)\supset SU(3)\times SU(2)$ (Bickerstaff *et al.*, 1982).

VIII. EXAMPLE: THE IRREPS AND CLEBSCH-GORDAN COEFFICIENTS OF THE GROUP C_{4v}

We now take the group C_{4v} as an example to illustrate the application of the EFM for obtaining irreps and CG coefficients. Again we consider only the $m=1$ case and leave the $m>1$ case to Secs. XIV.C and XIX.

A. Construction of irreducible matrices

The group elements of C_{4v} are given in Sec. III.D. The group table of C_{4v} is given in Table IV.

According to Eqs. (2.12) and (4.13), as well as Table IV, it is easy to find the regular reps of the groups C_{4v} and $\bar{C}_{4v}$. In fact, the nth row of Table IV gives the rep of the nth element R_n of C_{4v}, e.g.,

$$\begin{aligned}&D(R_5)=D(\sigma_x)=(58671342)\,,\\&D(R_6)=D(\sigma_y)=(67583124)\,,\\&D(R_7)=D(\sigma_{da})=(75862413)\,,\\&D(R_8)=D(\sigma_{db})=(86754231)\,,\end{aligned} \tag{8.1}$$

and the nth column of Table IV gives the rep of the intrinsic group element $\bar{R}_n$, e.g.,

$$D(\bar{R}_5)=D(\bar{\sigma}_x)=(57681324)\,, \tag{8.2}$$

where $(ijkl\ldots)$ denotes a matrix with the matrix elements all equal to one at the entries $(a,b)=(i,1),(j,2),(k,3),(l,4),\ldots$, and equal to zero elsewhere, and where a (b) is the row (column) number.

TABLE IV. Group table of C_{4v}.

e	C_{4z}^{+}	C_{2z}	C_{4z}^{-}	σ_x	σ_y	σ_{da}	σ_{db}
1	2	3	4	5	6	7	8
2	3	4	1	7	8	6	5
3	4	1	2	6	5	8	7
4	1	2	3	8	7	5	6
5	8	6	7	1	3	4	2
6	7	5	8	3	1	2	4
7	5	8	6	2	4	1	3
8	6	7	5	4	2	3	1

We can use the complete set of commuting operators (C_4, C_5) of C_{4v}, found from the class space of C_{4v} in Sec. III.D, to decompose the regular rep. However, we can also find a CSCO of C_{4v} directly from the group space by looking for an operator $C=\sum_i k_i C_i$ that has $N=5$ distinct eigenvalues. Let us try $C=2C_4+C_5$. The rep matrix of C in the group space is given by

$$D(C)=2[D(\sigma_x)+D(\sigma_y)]+D(\sigma_{da})+D(\sigma_{db}) . \quad (8.3)$$

A diagonalization of $D(C)$ gives

four single roots, $\nu=6,2,-2,-6$; $m_\nu=1$,
one fourfold root, $\nu=0$; $m_\nu=4$.

The fact that $m_\nu=h_\nu^2$ implies that $\nu=6,2,-2,-6$ corresponds to four one-dimensional irreps, while $\nu=0$ corresponds to a two-dimensional irrep that occurs twice. The operator C has five distinct eigenvalues, and thus it is a CSCO of C_{4v}.

For the four single roots, we can find four unique eigenvectors of $D(C)$ as listed in Table V below. They give the IRB for the one-dimensional irreps $\nu=6,2,-2,-6$, and are identical to the first four vectors listed in Table III except for a constant factor. For the fourfold root, from the eigenequation

$$D(C)\mathbf{u}=\nu\mathbf{u}=0, \quad \mathbf{u}=\mathrm{col}(u_1,u_2,\ldots,u_8) ,$$

we obtain the following equations for u_i:

$$\begin{aligned} &u_1+u_3=0, \quad u_2+u_4=0 , \\ &u_5+u_6=0, \quad u_7+u_8=0 . \end{aligned} \quad (8.4)$$

To lift the degeneracy, or to determine uniquely the solution to (8.4), we need to introduce the operator $C(s)$ and $\bar{C}(s)$. Obviously, for our problem here, any element of C_{4v} except the identity can serve as $C(s)$. Let us take $C(s)=\sigma_x$. It means that we choose the $C_{4v}\supset\mathscr{C}_s$ classification for the irreps with $\mathscr{C}_s=(e,\sigma_x)$. The solution to the eigenequations

$$D(\sigma_x)\mathbf{u}=a\mathbf{u}, \quad D(\bar{\sigma}_x)\mathbf{u}=b\mathbf{u} \quad (8.5)$$

can be read out from the fifth row and fifth column, respectively, of Table IV, i.e.,

$$\begin{aligned} &a=\pm1{:}u_1=\pm u_5,\ u_2=\pm u_8,\ u_3=\pm u_6,\ u_4=\pm u_7 , \\ &b=\pm1{:}u_1=\pm u_5,\ u_2=\pm u_7,\ u_3=\pm u_6,\ u_4=\pm u_8 . \end{aligned} \quad (8.6)$$

The four one-dimensional bases are of course the eigenfunctions of σ_x and $\bar{\sigma}_x$, as can be seen by comparing Table V with Eq. (8.6). By combining Eqs. (8.4) and (8.6), we determine another four eigenvectors $P_1^{(0)1}$, $P_{-1}^{(0)1}$, $P_1^{(0)-1}$, and $P_{-1}^{(0)-1}$ of $K=(C,\sigma_x,\bar{\sigma}_x)$ up to some phase factor. It is easily seen that K has eight distinct eigenvalues, as shown in the second column of Table V. Therefore, K is a CSCO-III of C_{4v}.

We now follow the three steps given in Sec. VI.C to

TABLE V. The irreps of C_{4v} in the $C_{4v}\supset\mathscr{C}_s$ classification. The parameters ν, ν', a, and b are the eigenvalues of C, C_5, σ_x, and $\bar{\sigma}_x$, respectively; $\mathscr{N}=\sqrt{h_\nu/|\mathbf{G}|}$.

$P_a^{(\nu)b}$	(ν,a,b)	(ν',a,b)	$\mathscr{N}$	e 1	C_{4z}^{+} 2	C_{2z} 3	C_{4z}^{-} 4	σ_x 5	σ_y 6	σ_{da} 7	σ_{db} 8	$D_{ab}^{(\nu)}$
$P_1^{(6)1}$	(6,1,1)	(2,1,1)	$\sqrt{1/8}$	1	1	1	1	1	1	1	1	D^{A_1}
$P_1^{(2)1}$	(2,1,1)	(−2,1,1)	$\sqrt{1/8}$	1	−1	1	−1	1	1	−1	−1	D^{B_1}
$P_{-1}^{(-6)-1}$	(−6,−1,−1)	(−2,−1,−1)	$\sqrt{1/8}$	1	1	1	1	−1	−1	−1	−1	D^{A_2}
$P_{-1}^{(-2)-1}$	(−2,−1,−1)	(2,−1,−1)	$\sqrt{1/8}$	1	−1	1	−1	−1	−1	1	1	D^{B_2}
$P_1^{(0)1}$	(0,1,1)	(0,1,1)	$\frac{1}{2}$	1	0	−1	0	1	−1	0	0	D_{11}^{E}
$P_{-1}^{(0)1}$	(0,−1,1)	(0,−1,1)	$\frac{1}{2}$	0	1	0	−1	0	0	1	−1	D_{21}^{E}
$P_1^{(0)-1}$	(0,1,−1)	(0,1,−1)	$\frac{1}{2}$	0	−1	0	1	0	0	1	−1	D_{12}^{E}
$P_{-1}^{(0)-1}$	(0,−1,−1)	(0,−1,−1)	$\frac{1}{2}$	1	0	−1	0	−1	1	0	0	D_{22}^{E}

determine the phases of $P_a^{(\nu)b}$. The phases of $P_1^{(0)1}$ and $P_{-1}^{(0)-1}$ are fixed by step (1). The phase of $P_{-1}^{(0)1}$ can be chosen arbitrarily according to the step (2). Suppose that it has been chosen as shown in Table V. To determine the phase of $P_1^{(0)-1}$, we need first to calculate a nonvanishing matrix element $D_{1-1}^{(0)}(R_i)$ from the known IRB $P_a^{(0)b=1}$. R_i can be chosen freely; for example, we might choose $R_i=R_2=C_{4z}^+$. From the fifth and sixth rows of Table V and using Table IV we can calculate

$$D_{1-1}^{(0)}(R_2)=\langle P_1^{(0)1}\,|\,R_2\,|\,P_{-1}^{(0)1}\rangle$$

$$=\tfrac{1}{4}\langle 1-3+5-6\,|\,R_2\,|\,2-4+7-8\rangle=-1\ ,$$

where the shorthand symbols for group elements have been used. The phase of $P_1^{(0)-1}$ is now determined by requiring that its coefficient u_2 be equal to $\sqrt{2/8}D_{1-1}^{(0)}(R_2)^*=-\frac{1}{2}$.

Having adjusted the phase, thanks to Eq. (6.23) we can read out from Table V all the irreps of C_{4v}. For instance,

$$D^{(0)}(R_2)=D^E(C_{4z}^+)=\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}. \tag{8.7}$$

If the phase of $P_1^{(0)-1}$ has not been appropriately chosen, say if it has been chosen as opposite to that given in Table V, and if we still use Eq. (6.23) to obtain matrix elements from $u_{vab,i}$, we will get

$$D^{(0)}(R_2)=D^E(C_{4z}^+)=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},$$

and $[D^E(C_{4z}^+)]^2$ will be equal to $\mathbf{I}$, in disagreement with $[D^E(C_{4z}^+)]^2=D^E(R_3)=-\mathbf{I}$.

In the above, we first solve the eigenequation of C and then those of $C(s)$ and $\bar{C}(s)$. In fact, a more convenient way is to use first the eigenequations of $C(s)$ and $\bar{C}(s)$ to eliminate the non-independent variables and thus to decrease the order of the eigenequation of C. Let us redo the above problem by this alternative procedure. From Eq. (8.6) we get

$$\begin{aligned}(a,b)&=(1,1):u_1=u_5,\ u_2=u_4=u_7=u_8,\ u_3=u_6\ ,\\ &=(-1,1):u_1=u_5=0,\ u_2=-u_4=u_7=-u_8,\ u_3=u_6=0\ ,\\ &=(1,-1):u_1=u_5=0,\ u_2=-u_4=-u_7=u_8,\ u_3=u_6=0\ ,\\ &=(-1,-1):u_1=-u_5,\ u_2=u_4=-u_7=-u_8,\ u_3=-u_6\ .\end{aligned} \tag{8.8}$$

The eigenvalues $(a,b)=(1,1)$ and $(-1,-1)$ have threefold degeneracy. For each of them we have three independent solutions,

$$\begin{aligned}(a,b)&=(1,1):\varphi_1=(1+5),\ \varphi_2=(2+4+7+8),\ \varphi_3=(3+6)\ ,\\ &=(-1,-1):\varphi_1'=(1-5),\ \varphi_2'=(2+4-7-8),\ \varphi_3'=(3-6)\ .\end{aligned} \tag{8.9}$$

To lift the degeneracy, we need the class operator of C_{4v}. Let us combine them into eigenvectors of the class operator $C_5=(7+8)$. The representative matrices $D(C_5)$ and $D'(C_5)$ in the un-normalized bases $\{\varphi_i\}$ and $\{\varphi_i'\}$, respectively, are equal to

$$D(C_5)=-D'(C_5)=\begin{bmatrix}0 & 2 & 0\\ 1 & 0 & 1\\ 0 & 2 & 0\end{bmatrix}. \tag{8.10}$$

A diagonalization of $D(C_5)$ gives the basis vectors $P_1^{(2)1}$,$P_1^{(-2)1}$,$P_1^{(0)1}$, and $P_{-1}^{(2)-1}$,$P_{-1}^{(-2)-1}$,$P_{-1}^{(0)-1}$. The result is identical with Table V.

The eigenvalues $(a,b)=(1,-1)$ and $(-1,1)$ have no degeneracy, and from Eqs. (8.8) we obtain unique solutions. It is easy to infer that these solutions belong to the two-dimensional irrep, and thus they are just $P_{-1}^{(0)1}$ and $P_1^{(0)-1}$ listed in Table V.

It is easily seen that the two-dimensional irrep given by Table V corresponds to the rep with $(y,-x)$ as the two basis vectors.

From this example, it is seen that $(C_5,\sigma_x,\bar{\sigma}_x)$ is a CSCO-III of C_{4v}, although C_5 is not a CSCO-I of C_{4v}. The CSCO-III $(C_4,C_5,\sigma_x,\bar{\sigma}_x)$, $(2C_4+C_5,\sigma_x,\bar{\sigma}_x)$, and $(C_5,\sigma_x,\bar{\sigma}_x)$ are all equivalent in the sense that they give identical irreps.

Furthermore, we can also choose

$$K=C_5+3\sigma_x+2\bar{\sigma}_x \tag{8.11}$$

as a CSCO-III of C_{4v}. From the third column of Table V we know that K has eight distinct eigenvalues,

$$\mu=\nu'+3a+2b=7,3,-7,-3,5,-1,1,-5\ , \tag{8.12a}$$

where ν' is the eigenvalue of C_5. Similarly we can choose

$$M=C_5+3\sigma_x \tag{8.12b}$$

as a CSCO-II of C_{4v}, which has $\sum_\nu h_\nu=6$ distinct eigenvalues, 5, 1, -5, -1, 3, and -3.

Suppose that we need the irreps of C_{4v} in the $C_{4v}\supset\mathscr{C}_4$ classification, where $\mathscr{C}_4$ is the cyclic group generated by C_{4z}^+; then $C(s)$ should be chosen as the CSCO of $\mathscr{C}_4$, i.e., $C(s)=C_{4z}^+$. The simultaneous eigenvectors of $(C,C_{4z}^+,\bar{C}_{4z}^+)$ are listed in Table VI, where $C=2C_4+C_5$. The one-dimensional irreducible bases are of course identical with those of Table V, but the two-dimensional IRB are changed. From Table VI we can read out the irreps in the $C_{4v}\supset\mathscr{C}_4$ classification. For example,

$$D^{(0)}(R_2)=D^E(C_{4z}^+)=\begin{bmatrix}i & 0\\ 0 & -i\end{bmatrix}. \tag{8.13}$$

TABLE VI. The irreps of C_{4v} in the $C_{4v}\supset\mathscr{C}_4$ classification. The parameter v,a,b are the eigenvalues of $C,C_{4z}^{+},\bar{C}_{4z}^{+}$, respectively.

(v,a,b)	$\sqrt{h_v/\lvert\mathbf{G}\rvert}$	e 1	C_{4z}^{+} 2	C_{2z} 3	C_{4z}^{-} 4	σ_x 5	σ_y 6	σ_{da} 7	σ_{db} 8	
(6,1,1)	$\sqrt{1/8}$	1	1	1	1	1	1	1	1	D^{A_1}
$(2,-1,-1)$	$\sqrt{1/8}$	1	−1	1	−1	1	1	−1	−1	D^{B_1}
$(-6,1,1)$	$\sqrt{1/8}$	1	1	1	1	−1	−1	−1	−1	D^{A_2}
$(-2,-1,-1)$	$\sqrt{1/8}$	1	−1	1	−1	−1	−1	1	1	D^{B_2}
$(0,i,i)$	$\frac{1}{2}$	1	$-i$	−1	i	0	0	0	0	$(D_{11}^{E})^{*}$
$(0,-i,i)$	$\frac{1}{2}$	0	0	0	0	−1	1	$-i$	i	$(D_{21}^{E})^{*}$
$(0,i,-i)$	$\frac{1}{2}$	0	0	0	0	−1	1	i	$-i$	$(D_{12}^{E})^{*}$
$(0,-i,-i)$	$\frac{1}{2}$	1	i	−1	$-i$	0	0	0	0	$(D_{22}^{E})^{*}$

It can be easily recognized that the two-dimensional irreps given by Table VI corresponds to the rep with $[\sqrt{1/2}(x-iy),\sqrt{1/2}(x+iy)]$ as basis vectors.

From the above example, we see clearly that the EFM has great flexibility in constructing the irreps of a group $\mathbf{G}$ in any $\mathbf{G}\supset\mathbf{G}(s)$ classification.

B. Construction of the CG coefficients

Let us construct the CGC for the Kronecker product $E\times E$ of C_{4v} in the $C_{4v}\supset\mathscr{C}_s$ classification. The CSCO-II is chosen to be $M=(C_5,\sigma_x)$. There are four vectors,

$$|a_1a_2\rangle=\psi_{a_1}^{E}\psi_{a_2}^{E},\quad a_1a_2=11,12,21,22\ , \tag{8.14}$$

in the Kronecker product space with $\psi_1^{E}=\psi_1^{(0)}$ and $\psi_2^{E}=\psi_{-1}^{(0)}$. A diagonalization of (C_5,σ_x) in the basis of Eq. (8.14) gives the CGC. The diagonalization of σ_x is trivial, since $|a_1a_2\rangle$ are already eigenvectors of σ_x:

$$\sigma_x=1:|11\rangle,\ |22\rangle\ , \tag{8.15a}$$

$$\sigma_x=-1:|12\rangle,\ |21\rangle\ . \tag{8.15b}$$

Therefore, it is only necessary to diagonalize C_5 in the subspaces $(|11\rangle,|22\rangle)$ and $(|12\rangle,|21\rangle)$. Equation (7.27) for the matrix elements of C_5 now reads

$$\begin{aligned}\langle a_1a_2|C_5|b_1b_2\rangle&=\sum_{i=da}^{db}D_{a_1b_1}^{E}(\sigma_i)D_{a_2b_2}^{E}(\sigma_i)\ ,\\ \langle a_1a_1|C_5|b_1b_1\rangle&=\langle a_1b_1|C_5|b_1a_1\rangle\\ &=\sum_{i=da}^{db}[D_{a_1b_1}^{E}(\sigma_i)]^2\ .\end{aligned} \tag{8.16}$$

Using Table V, we easily find the matrices of C_5 in the two subspaces,

$$\begin{aligned}\mathscr{D}(C_5)&=\begin{bmatrix}0&2\\2&0\end{bmatrix},\\ \mathscr{D}'(C_5)&=\begin{bmatrix}0&-2\\-2&0\end{bmatrix}.\end{aligned} \tag{8.17}$$

Diagonalizing $\mathscr{D}(C_5)$ and $\mathscr{D}'(C_5)$ gives four irreducible bases:

$$\begin{aligned}\Psi^{A_1}&=\Psi_1^{(2)}=\sqrt{1/2}(|11\rangle+|22\rangle)\ ,\\ \Psi^{B_1}&=\Psi_1^{(-2)}=\sqrt{1/2}(|11\rangle-|22\rangle)\ ,\\ \Psi^{A_2}&=\Psi_{-1}^{(-2)}=\sqrt{1/2}(|12\rangle+|21\rangle)\ ,\\ \Psi^{B_2}&=\Psi_{-1}^{(2)}=\sqrt{1/2}(|12\rangle-|21\rangle)\ .\end{aligned} \tag{8.18}$$

The identification of the eigenvalues of (C_5,σ_x) with the Mulliken notation is made on the basis of Tables III and V. Equation (8.18) gives the CGC for the product $E\times E$ of C_{4v} and shows that $E\times E=A_1+A_2+B_1+B_2$.

It is seen that (1) the CG coefficients are obtained without *a priori* knowledge of the CG series and (2) only the irreducible matrices of the elements σ_{da}, σ_{db}, and σ_x are required, which are contained in the CSCO-II of C_{4v}. In other words, here we need only $3\times4=12$ matrix elements, while for the projection-operator method we need $12^2=144$ matrix elements. The superiority of the EFM over the projection-operator method for finding the CGC is especially conspicuous for higher-order groups.

IX. BASIC KNOWLEDGE OF THE SPACE GROUP

Starting from this section, we shall apply the general theory for the rep group developed in the previous sections to the space group. We begin with a brief statement of some basic definitions and relations concerning the space group for the purpose of easier accessibility and establishing notation. Additional information can be found in review papers or books on space group reps, such as those of Bradley and Cracknell (1972), Birman (1974), and Koster (1957).

A. Symmorphic and nonsymmorphic space groups

A crystal is formed by arranging atoms, ions, molecules, complexes, etc., in a space lattice $L=\{\mathbf{R}_n\}$, called an empty lattice, defined by sets of points (the lattice points)

$$\mathbf{R}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3 , \tag{9.1a}$$

with integers n_i. The $\mathbf{t}_i$ are called the primitive or basic translations, and $\mathbf{R}_n$ the lattice vector.

All the rotations α which preserve $\mathbf{R}_n$ on the lattice L form a point group $\mathbf{P}$,

$$\mathbf{P} = \{\alpha : \alpha\mathbf{R}_n \in L\} , \tag{9.1b}$$

called the point group of the empty lattice or the holosymmetric point group of the lattice.

The symmetric group of an infinite crystal is called a space group $\mathbf{G}$. Its elements are denoted by the Seitz notation

$$\{\alpha \mid \mathbf{a}\} = \{\alpha \mid \mathbf{V}(\alpha) + \mathbf{R}_n\} , \tag{9.2a}$$

where α is a rotational (proper or improper) operator belonging to the so-called isogonal point group $\mathbf{G}_0$, or the point group of the space group $\mathbf{G}$. The vector $\mathbf{V}(\alpha)$ associated with α is called the nonprimitive, or fractional, translation. $\mathbf{V}(\alpha)$ is either zero or a translation which is less than a lattice vector. $\mathbf{V}(\alpha)$ has the general form

$$V(\alpha) = \frac{1}{m}(m_1\mathbf{t}_1 + m_2\mathbf{t}_2 + m_3\mathbf{t}_3) , \tag{9.2b}$$

where m takes only four possible values, $m = 2$, 3, 4, and 6, while $m_i = 0, 1, \ldots, m-1$. We always associate a primitive translation with the identity rotation ε, so that $V(\varepsilon) = 0$. A space group $\mathbf{G}$ is designated by

$$\mathbf{G} = \{\{\alpha_i \mid \mathbf{V}(\alpha_i) + \mathbf{R}_n\} : i = 1, 2, \ldots, \mid \mathbf{G}_0 \mid , \mathbf{R}_n \in L\} . \tag{9.3}$$

A space group is said to be symmorphic if its nonprimitive translations $\mathbf{V}(\alpha) = 0$ for all α. Clearly the point group $\mathbf{G}_0$ is a subgroup of the symmorphic space group. A space group is said to be nonsymmorphic if its $\mathbf{V}(\alpha)$ is not zero for at least one α. The point group $\mathbf{G}_0$ is not a subgroup of the nonsymmorphic space group $\mathbf{G}$. Among the 230 space groups, 73 are symmorphic and 157 are nonsymmorphic.

As mentioned before, a crystal is formed by arranging a collection of ions or complexes in an empty lattice. Both the arrangement and the ions or complexes have some symmetry of their own; therefore the symmetry of the point group $\mathbf{G}_0$ is lower than that of $\mathbf{P}$, unless the arrangement as well as the ions have a symmetry higher than or equal to that of the empty lattice. In other words, $\mathbf{G}_0$ is generally a subgroup of $\mathbf{P}$: $\mathbf{P} \supset \mathbf{G}_0$.

The operation of $\{\alpha \mid \mathbf{a}\}$ on a vector $\mathbf{x}$ is defined by

$$\{\alpha \mid \mathbf{a}\}\mathbf{x} = \alpha\mathbf{x} + \mathbf{a} , \tag{9.4}$$

i.e., a rotation on $\mathbf{x}$ followed by a translation $\mathbf{a}$. From Eq. (9.4) we obtain the multiplication rule,

$$\{\alpha \mid \mathbf{a}\}\{\beta \mid \mathbf{b}\} = \{\alpha\beta \mid \alpha\mathbf{b} + \mathbf{a}\} . \tag{9.5}$$

Setting $\{\alpha\beta \mid \alpha\mathbf{b} + \mathbf{a}\} = \{\varepsilon \mid 0\}$, we get the inverse element

$$\{\alpha \mid \mathbf{a}\}^{-1} = \{\alpha^{-1} \mid -\alpha^{-1}\mathbf{a}\} . \tag{9.6}$$

From Eq. (9.5) we have

$$\{\alpha \mid \mathbf{a}\} = \{\varepsilon \mid \mathbf{a}\}\{\alpha \mid 0\} = \{\alpha \mid 0\}\{\varepsilon \mid \alpha^{-1}\mathbf{a}\} . \tag{9.7}$$

Therefore, the translation and rotation do not commute, except when the translation $\mathbf{a}$ is parallel to the rotation axis or the reflection plane.

Following the multiplication rule

$$\{\alpha \mid \mathbf{V}(\alpha) + \mathbf{R}_n\}\{\beta \mid \mathbf{V}(\beta) + \mathbf{R}_m\} = \{\alpha\beta \mid \mathbf{V}(\alpha) + \alpha\mathbf{V}(\beta) + \alpha\mathbf{R}_m + \mathbf{R}_n\} , \tag{9.8}$$

one infers that the lattice vector and nonprimitive translation must satisfy the following conditions:

$$\alpha\mathbf{R}_m = \mathbf{R}_l , \tag{9.9}$$

$$\mathbf{V}(\alpha) + \alpha\mathbf{V}(\beta) = \mathbf{V}(\alpha\beta) + \mathbf{R}_{\alpha\beta} , \tag{9.10}$$

where $\mathbf{R}_l$ and $\mathbf{R}_{\alpha\beta}$ are lattice vectors.

The operation of $\{\alpha \mid \mathbf{a}\}$ on a function $\psi(\mathbf{x})$ is defined by

$$\{\alpha \mid \mathbf{a}\}\psi(\mathbf{x}) = \psi(\{\alpha \mid \mathbf{a}\}^{-1}\mathbf{x}) = \psi(\alpha^{-1}(\mathbf{x} - \mathbf{a})) . \tag{9.11}$$

With this definition, the multiplication rule for the function operator is identical with Eq. (9.5) for the operator in the coordinate space:

$$\begin{aligned}\{\alpha \mid \mathbf{a}\}\{\beta \mid \mathbf{b}\}\psi(\mathbf{x}) &= \{\alpha \mid \mathbf{a}\}\psi(\beta^{-1}\mathbf{x} - \beta^{-1}\mathbf{b}) \\ &= \psi(\beta^{-1}\{\alpha \mid \mathbf{a}\}^{-1}\mathbf{x} - \beta^{-1}\mathbf{b}) \\ &= \psi(\{\alpha\beta \mid \alpha\mathbf{b} + \mathbf{a}\}^{-1}\mathbf{x}) \\ &= \{\alpha\beta \mid \alpha\mathbf{b} + \mathbf{a}\}\psi(\mathbf{x}) .\end{aligned} \tag{9.12}$$

Hence for simplicity we do not distinguish between the coordinate transformation operator in Eq. (9.4) and the function operator in Eq. (9.11). However, it is worth mentioning that in applying a function operator one must be very careful to notice the following points:

$$\begin{aligned}&\{\varepsilon \mid \mathbf{a}\}\psi(\alpha^{-1}\mathbf{x}) = \psi(\alpha^{-1}(\mathbf{x} - \mathbf{a})) \neq \psi(\alpha^{-1}\mathbf{x} - \mathbf{a}) , \\ &\{\alpha \mid 0\}\psi(\mathbf{x} - \mathbf{b}) = \psi(\alpha^{-1}\mathbf{x} - \mathbf{b}) \neq \psi(\alpha^{-1}(\mathbf{x} - \mathbf{b})) , \\ &\{\alpha \mid 0\}\psi(\beta^{-1}\mathbf{x}) = \psi(\beta^{-1}\alpha^{-1}\mathbf{x}) \neq \psi(\alpha^{-1}\beta^{-1}\mathbf{x}) .\end{aligned} \tag{9.13}$$

It is convenient to use the coordinate system with $\mathbf{t}_i$ as basis vectors,

$$\mathbf{x} = \xi_1\mathbf{t}_1 + \xi_2\mathbf{t}_2 + \xi_3\mathbf{t}_3 . \tag{9.14}$$

The transformation of $\mathbf{x}$ under a rotation α is determined by that of $\mathbf{t}_i$:

$$\alpha\mathbf{t}_i = \sum_j D_{ji}(\alpha)\mathbf{t}_j . \tag{9.15}$$

By virtue of Eq. (9.9), $D_{ji}(\alpha)$ have to be integers ± 1 or 0 (see Table 3.2 in Bradley and Cracknell, 1972).

From Eq. (9.11), it is easily shown that, acting on $\psi(\mathbf{x})$, the translation operator

$$\{\varepsilon \mid \mathbf{a}\} = \exp(-\mathbf{a}\cdot\nabla) = \exp(-i\hat{\mathbf{k}}\cdot\mathbf{a}) , \tag{9.16a}$$

where $\hat{\mathbf{k}} = -i\nabla$, is the momentum operator (choosing the Planck constant $\hbar = 1$).

The space group is a discrete infinite group. However, to define a space group one need only specify the three primitive translations $\mathbf{t}_i$ and a finite number of elements $\{\alpha \mid \mathbf{v}(\alpha)\}$, or more economically, just few generators. The generators for the 230 space groups are listed in Table 3.7 of Bradley and Cracknell (1972).

B. Crystal systems and Bravais lattices

It can be shown that the allowable point groups **P** of the empty lattice are restricted to the following seven point groups:

$$\begin{array}{ccccccc} O_h & \supset & D_{4h} & \supset & D_{2h} & \supset & C_{2h} \supset \mathscr{C}_i \\ & & \cap & & \cap & & \\ & & D_{6h} & \supset & D_{3d} , & & \end{array} \tag{9.17}$$

where we have shown their genealogical relations.

Two empty lattices are said to belong to the same crystal system if they have the same holosymmetric point group **P**. Therefore, there are only seven possible crystal systems, namely the triclinic (C_i), monoclinic (C_{2h}), orthorhombic (D_{2h}), trigonal (D_{3d}), tetragonal (D_{4d}), hexagonal (D_{6h}), and cubic (O_h).

The seven crystal systems contain 14 different types of crystal structure, known as the Bravais lattices. For their names, symbols, and primitive translations, see Table 3.1 in Bradley and Cracknell (1972).

C. The translation group T and its irreps

The group

$$\mathbf{T}=\{\{\varepsilon \mid \mathbf{R}_m\}\}$$

is called the translation group. **T** is an invariant subgroup of the space group **G**, since

$$\{\alpha \mid \mathbf{a}\}\{\varepsilon \mid \mathbf{R}_n\}\{\alpha \mid \mathbf{a}\}^{-1}=\{\varepsilon \mid \alpha\mathbf{R}_n\}\in\mathbf{T} . \tag{9.18}$$

The basis vectors $\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3$ are in general not orthonormal; from these vectors we can introduce another set of dual basis vectors $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$, such that

$$\mathbf{b}_i\cdot\mathbf{t}_j=2\pi\delta_{ij} , \tag{9.19}$$

where the factor 2π is introduced for later convenience.

It is easily seen that the relation between $\mathbf{b}_i$ and $\mathbf{t}_i$ is

$$\mathbf{b}_i=2\pi\mathbf{t}_j\times\mathbf{t}_k/[\mathbf{t}_i\cdot(\mathbf{t}_j\times\mathbf{t}_k)],\quad i,j,k \text{ cyclic in } 1,2,3 .$$

$\mathbf{t}_i$ and $\mathbf{b}_i$ are the covariant and contravariant bases, respectively, while $\mathbf{b}_i\cdot\mathbf{t}_j=2\pi\delta_{ij}$ is an invariant.

The gradient operator ∇ can be written as

$$\nabla=\left[\frac{\partial}{\partial\xi_1}\mathbf{b}_1+\frac{\partial}{\partial\xi_2}\mathbf{b}_2+\frac{\partial}{\partial\xi_3}\mathbf{b}_3\right]\Big/2\pi . \tag{9.16b}$$

Let us define

$$\mathbf{K}_m=m_1\mathbf{b}_1+m_2\mathbf{b}_2+m_3\mathbf{b}_3 . \tag{9.20a}$$

$\mathbf{K}_m$ are called the reciprocal lattice vectors, and the lattice formed by all $\mathbf{K}_m$ is called the reciprocal lattice, denoted as

$$L^{-1}=\{\mathbf{K}_m\} .$$

Obviously we have

$$\mathbf{K}_m\cdot\mathbf{R}_n=2\pi\times \text{ integer} . \tag{9.20b}$$

It can readily be proved that the reciprocal lattice and the ordinary space lattice have the same symmetry group **P**, and thus belong to the same crystal system, but they do not necessarily have the same type of crystal structures. For the orthorhombic and cubic systems, the body-centered space lattice corresponds to the face-centered reciprocal lattice, and vice versa. However, for all other cases (including the simple or base-centered orthorhombic and simple cubic), the space lattice and its reciprocal lattice are of the same type.

The translation group **T** is Abelian. Therefore, its CSCO can be chosen simply as the group operator

$$\{\varepsilon \mid \mathbf{R}_n\}=\exp(-i\hat{\mathbf{k}}\cdot\mathbf{R}_n) . \tag{9.21a}$$

The irreducible basis of **T** can be found from the solution to the eigenequation

$$\{\varepsilon \mid \mathbf{R}_n\}u_{\mathbf{k}}(\mathbf{r})=e^{-i\mathbf{k}\cdot\mathbf{R}_n}u_{\mathbf{k}}(\mathbf{r}) . \tag{9.22}$$

The eigenvalue **k** of the operator $\hat{\mathbf{k}}$ is called the wave vector and is used to label irreps of **T**. Assuming

$$\mathbf{k}=p_1\mathbf{b}_1+p_2\mathbf{b}_2+p_3\mathbf{b}_3 , \tag{9.23}$$

one of the solutions of Eq. (9.22) is easily found to be

$$\begin{aligned} u_{\mathbf{k}}(r)&=\exp(i\mathbf{k}\cdot\mathbf{r}) \\ &=\exp[2\pi i(p_1\xi_1+p_2\xi_2+p_3\xi_3)] . \end{aligned} \tag{9.24}$$

Since $\exp(i\mathbf{K}_m\cdot\mathbf{R}_n)=1$ from Eq. (9.19), $u_{\mathbf{k}+\mathbf{K}_m}=\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot r]$ is also a solution to Eq. (9.22) with the same eigenvalue. Consequently the irreps **k** and $\mathbf{k}+\mathbf{K}_m$ of **T** are equivalent. **k** and $\mathbf{k}+\mathbf{K}_m$ are referred to as the equivalent wave vectors, denoted as

$$\mathbf{k}\doteq\mathbf{k}+\mathbf{K}_m . \tag{9.25}$$

The CSCO of the translation group **T**, $\{\varepsilon \mid \mathbf{R}_n\}$, can be replaced by the momentum operator

$$\hat{\mathbf{k}}=-i\nabla \tag{9.21b}$$

with eigenvalues **k** modulo $\mathbf{K}_m$.

The most general form of the basis belonging to the irrep **k** of **T** is the so-called Bloch function,

$$\varphi^{\mathbf{k}}(\mathbf{r})=\sum_{\mathbf{K}_m} v(\mathbf{k}+\mathbf{K}_m)\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] , \tag{9.26}$$

where $v(\mathbf{k}+\mathbf{K}_m)$ are coefficients.

The projection operator for the translation group is

$$P^{(\mathbf{k})}=\text{const}\times\sum_{\mathbf{R}_n}\exp[i(\mathbf{k}-\hat{\mathbf{k}})\cdot\mathbf{R}_n] . \tag{9.27}$$

D. The Brillouin zone

In order to visualize the region of space in which $\mathbf{k}$ must lie, let us introduce the so-called Wigner-Seitz unit cell, defined as the region around an origin 0 (which may be any one of the reciprocal lattice points) bounded by the planes bisecting perpendicularly the vectors joining the origin to all neighboring reciprocal lattice points. This region surrounding the origin is called the Brillouin zone or the first Brillouin zone.

According to Eq. (9.25), to obtain all the inequivalent irreps of the translation group, one need only let the wave vector $\mathbf{k}$ run over all the points in the Brillouin zone. Nice diagrams of the Brillouin zones for the 14 Bravais lattices are given by Bradley and Cracknell (1972, Figs. 3.2–3.15).

The points in a Brillouin zone are divided into two groups.

(1) General points. A wave vector $\mathbf{k}$ is called a general point if it does not have any symmetry, i.e., for any operator $\alpha \in \mathbf{G}_0$, $\alpha\mathbf{k}$ and $\mathbf{k}$ are not equivalent.

(2) Special points. A point with a certain kind of symmetry is called a special point, for example, the point that lies on a rotation axis or a reflection plane and therefore is invariant under the rotation or reflection, or the point $\mathbf{k}$ on a surface of the Brillouin zone which may be invariant or goes to its equivalent point $\mathbf{k}'=\mathbf{k}+\mathbf{K}_m$ under a rotation or reflection.

Special points are subdivided into (Bradley and Cracknell, 1972) two groups.

(a) Points of symmetry: $\mathbf{k}$ is called a point of symmetry if there exists a neighborhood of $\mathbf{k}$ in which $\mathbf{k}$ is the point with the highest symmetry.

(b) Lines or planes of symmetry: $\mathbf{k}$ is called a line (plane) of symmetry if in a sufficiently small neighborhood of $\mathbf{k}$ there is always a line (plane) passing through $\mathbf{k}$, all points of which have the same symmetry as that of $\mathbf{k}$.

The special points in a Brillouin zone are labeled by the standard solid-state physics symbols, e.g., Γ, X, M, etc. (see Bradley and Cracknell, 1972, pp. 96–118).

Of all the rotations in the point group $\mathbf{P}$, those which leave the wave vector $\mathbf{k}$ invariant modulo a reciprocal lattice vector form a subgroup of $\mathbf{P}$, designated as $\mathbf{P}(\mathbf{k})$:

$$\mathbf{P}(\mathbf{k})=\{\alpha\in\mathbf{P}:\alpha\mathbf{k}\doteq\mathbf{k}\} . \tag{9.28}$$

$\mathbf{P}(\mathbf{k})$ is referred to as the symmetric group of the wave vector $\mathbf{k}$.

The symmetry groups $\mathbf{P}(\mathbf{k})$ are listed by Bradley and Cracknell (1972) in their Table 3.6 for the wave vectors $\mathbf{k}$ that lie in the so-called basic domain of the Brillouin zone.

If a wave vector $\mathbf{k}_1$ lies outside the basic domain, but is related to a wave vector $\mathbf{k}$ that is in the basic domain by

$$\mathbf{k}_1=\alpha\mathbf{k},\quad \alpha\in\mathbf{P} , \tag{9.29a}$$

then the symmetry group $\mathbf{G}(\mathbf{k}_1)$ of the wave vector $\mathbf{k}_1$ is obtained from $\mathbf{P}(k)$ by conjugation,

$$P(\mathbf{k}_1)=\alpha P(\mathbf{k})\alpha^{-1} . \tag{9.29b}$$

X. THE LITTLE GROUP

A. Representation space of the space group

Since the translation group $\mathbf{T}$ is a subgroup of the space group $\mathbf{G}$, naturally we shall choose the group chain $\mathbf{G}\supset\mathbf{T}$ to classify the IRB of $\mathbf{G}$. From Eq. (9.25) we know that

$$\psi_{\mathbf{k}}=\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] \tag{10.1a}$$

carries the irrep $\mathbf{k}$ of $\mathbf{T}$, with $\mathbf{k}$ restricted to the Brillouin zone. The functions of Eq. (10.1a) with the same $\mathbf{k}$ but all possible $\mathbf{K}_m$ form an eigenspace $\mathscr{L}_{\mathbf{k}}$ of the translation operator $\{\varepsilon\,|\,\mathbf{R}_n\}$,

$$\mathscr{L}_{\mathbf{k}}=\{\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}]:K_m\in L^{-1}\} . \tag{10.1b}$$

Our primary task is to find linear combinations of (10.1a) with $\mathbf{k}$ and $\mathbf{K}_m$ such that the combinations form the irreducible bases of the space group $\mathbf{G}$. As a routine procedure, we apply all the group elements of $\mathbf{G}$ to the single function $\psi_{\mathbf{k}}$ and pick out the linearly independent functions that will carry a rep of $\mathbf{G}$, and then reduce this rep into irreps of $\mathbf{G}$. From Eqs. (9.11) and (10.1a),

$$\{\alpha\,|\,\mathbf{a}\}\psi_{\mathbf{k}}=\exp[-i\alpha(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{a}]\exp[i\alpha(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}] . \tag{10.2a}$$

It is seen that the translation part $\{\varepsilon\,|\,\mathbf{a}\}$ of the group element $\{\alpha\,|\,\mathbf{a}\}$ only affects the phase factor, whereas the rotation part α changes the wave vector $\mathbf{k}+\mathbf{K}_m$ into $\alpha(\mathbf{k}+\mathbf{K}_m)$. Therefore, $\{\alpha\,|\,\mathbf{a}\}\psi_{\mathbf{k}}$ belongs to the eigenspace $\mathscr{L}_{\alpha\mathbf{k}}$ of $\{\varepsilon\,|\,\mathbf{R}_n\}$. Equation (10.2a) shows that the functions $\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\}\psi_{\mathbf{k}}$ with the same α but different $\mathbf{R}_n$ are linearly dependent. Consequently, although the space group $\mathbf{G}$ has an infinite number of elements, it generates from $\psi_{\mathbf{k}}$ only $|\mathbf{G}_0|$ linearly independent functions, which can be chosen as

$$\begin{aligned}\psi_{\alpha_j\mathbf{k}}&=\{\alpha_j\,|\,\mathbf{V}(\alpha_j)\}\psi_{\mathbf{k}}\\&=\exp[i\alpha_j(\mathbf{k}+\mathbf{K}_m)\cdot(\mathbf{r}-\mathbf{V}(\alpha_j)] ,\\&\qquad j=1,2,\ldots,|\mathbf{G}_0| .\end{aligned} \tag{10.2b}$$

They form a rep space

$$\mathscr{L}(*\mathbf{k})=\{\psi_{\alpha_i\mathbf{k}}:i=1,2,\ldots,|\mathbf{G}_0|\} \tag{10.2c}$$

for the space group $\mathbf{G}$. In general $\mathscr{L}(*k)$ is a reducible space of $\mathbf{G}$.

Stated differently, in a rep space with Bloch functions as basis vectors, the space group $\mathbf{G}$ has only $|\mathbf{G}_0|$ linearly independent operators $\{\alpha_i\,|\,\mathbf{V}(\alpha_i)\}$, which form a rep space

$$L(*\mathbf{k})=\{\{\alpha_i\,|\,\mathbf{V}(\alpha_i)\}:i=1,2,\ldots,|\mathbf{G}_0|\} \tag{10.2d}$$

for the space group $\mathbf{G}$. The spaces $\mathscr{L}(*\mathbf{k})$ and $L(*\mathbf{k})$ are isomorphic.

B. The little co-group $G_0(k)$

The problem we face now is how to reduce this $|G_0|$-dimensional rep of G. According to the procedure introduced in Sec. VI, we need first to find the CSCO of the space group, and then to find the eigenvectors of the CSCO in the space $\mathscr{L}(*k)$. However, this procedure proves to be unsuitable, due to the fact that the class operator of the space group has a rather complicated structure. We have to resort to other strategy. We first sandwich a group H between the space group G and the translation group T; then we determine the $H \supset T$ IRB, and finally we get the $G \supset H \supset T$ IRB.

Of the $|G_0|$ rotations in the point group G_0, all the rotations γ which leave the wave vector k invariant modulo a reciprocal lattice vector, i.e.,

$$\gamma k = k + K_m \doteq k , \tag{10.3}$$

form a subgroup of G_0, which is designated as

$$G_0(k) = \{\gamma \in G_0 : \gamma k \doteq k\} \tag{10.4a}$$

and is called the little co-group (Bradley and Cracknell, 1972).

It is easily recognized that the little co-group $G_0(k)$ is the intersection of the symmetry group $P(k)$ of k and the isogonal point group G_0, i.e.,

$$G_0(k) = P(k) \cap G_0 . \tag{10.4b}$$

C. The little group G(k)

All the elements $\{\gamma \mid V(\gamma)+R_n\}$, for $\gamma \in G_0(k)$ and $R_n \in L$, form another space group designated as

$$G(k) = \{\{\gamma_i \mid V(\gamma_i)+R_n\} : i = 1,2,\ldots,|G_0(k)|, R_n \in L\} . \tag{10.5}$$

$G(k)$ is referred to as the little group, or the group of the wave vector k. $G(k)$ is a subgroup of G and contains T as its subgroup. Therefore, the group $G(k)$ is a candidate for the group H to be sandwiched between G and T. Another way of saying this is that for any subgroup H of the space group G, the point group of H must be the symmetry group of a certain wave vector k. Thus we can use the wave vector k to label this subgroup, that is, use $G(k)$ to denote H.

The order of $G_0(k)$ is a divisor of the order of G_0,

$$q = |G_0| / |G_0(k)| , \tag{10.6}$$

where q is an integer.

The $|G_0(k)|$ linearly independent functions

$$\psi_{\gamma_i k} = \{\gamma_i \mid V(\gamma_i)\}\psi_k \tag{10.7a}$$

form a space

$$\mathscr{L}(k) = \{\psi_{\gamma_i k} : i = 1,2,\ldots,|G_0(k)|\} . \tag{10.7b}$$

$\mathscr{L}(k)$ is a subspace of $\mathscr{L}_k$ as well as a subspace of $\mathscr{L}(*k)$, and is a $|G_0(k)|$-dimensional rep space of the little group $G(k)$. $\mathscr{L}(k)$ is in general reducible. By decomposing $\mathscr{L}(k)$, we can get the $G(k) \supset T$ IRB.

Since $\mathscr{L}(k)$ is an eigenspace of $\{\varepsilon \mid R_n\}$, in $\mathscr{L}(k)$ we have

$$\{\varepsilon \mid R_n\} = \exp(-ik\cdot R_n)\cdot I , \tag{10.8}$$

where I is a unit matrix. Therefore, in the space $\mathscr{L}(k)$, the translation operator $\{\varepsilon \mid R_n\}$ commutes with any operator of $G(k)$.

XI. THE REPRESENTATION GROUPS G_k AND G'_k

A. The rep group G_k

From

$$\{\gamma_j \mid V(\gamma_j)+R_n\} = \{\varepsilon \mid R_n\}\{\gamma_j \mid V(\gamma_j)\} \tag{11.1a}$$

and Eq. (10.8), we see that the group operators of $G(k)$ in the space $\mathscr{L}(k)$ are related by

$$\{\gamma_j \mid V(\gamma_j)+R_n\} = \varepsilon(j,n)\{\gamma_j \mid V(\gamma_j)\} , \tag{11.1b}$$

$$\varepsilon(j,n) = \varepsilon(n) = \exp(-ik\cdot R_n) . \tag{11.1c}$$

To avoid notational clumsiness, we use the same symbol $\{\gamma \mid V(\gamma)\}$ to denote both the group element and the corresponding operator or representative matrix in $\mathscr{L}(k)$.

Equation (11.1b) shows that in the rep space $\mathscr{L}(k)$ the little group $G(k)$ has only $|G_0(k)|$ linearly independent operators $\{\gamma_i \mid V(\gamma_i)\}$, $i = 1,2,\ldots,|G_0(k)|$.

Using Eqs. (9.8), (9.10), and (11.1b), we obtain the multiplication relation for these independent operators,

$$\{\gamma_i \mid V(\gamma_i)\}\{\gamma_j \mid V(\gamma_j)\} = \mu(i,j)\{\gamma_{ij} \mid V(\gamma_{ij})\} , \tag{11.2a}$$

$$\mu(i,j) = \exp(-ik\cdot R_{ij}) = \exp\{-ik\cdot[V(\gamma_i)+\gamma_i V(\gamma_j)-V(\gamma_{ij})]\} . \tag{11.2b}$$

By identifying $\mathscr{L}(k)$, $|G_0(k)|$, $\{\gamma_i \mid V(\gamma_i)\}$, and $\mu(i,j)$ with L, $|g|$, R_i, and $\eta(i,j)$, respectively, in Sec. I.C, we see that all the distinct operators $\varepsilon(i,n)\{\gamma_i \mid V(\gamma_i)\}$ form a rep group

$$G_k = \{\{\gamma_i \mid V(\gamma_i)\} : i = 1,2,\ldots,|G_0(k)|\}_m , \tag{11.2c}$$

where m is an integer depending on k (see discussion below).

The rep group G_k can be regarded as a faithful rep of an abstract group $\hat{G}_k$. The abstract group could be, for example, the so-called central extension $\overline{G}^{k^*}$ defined by Schur (see Bradley and Cracknell, 1972). Notice that what is called the representation group by Döring (1959) and Birman (1974) is just another name for the central extension, and thus differs from our definition for the rep group.

From Eq. (11.1b) it is clear that the IRB of the little group $G(k)$ in the space $\mathscr{L}(k)$ is identical to the IRB of the rep group G_k; their representation matrices are related by

$$D^{(\mathbf{k})(\nu)}(\{\gamma \mid \mathbf{V}(\gamma)+\mathbf{R}_n\})=e^{-i\mathbf{k}\cdot\mathbf{R}_n}D^{(\mathbf{k})(\nu)}(\{\gamma \mid \mathbf{V}(\gamma)\}) , \tag{11.3}$$

where $(\mathbf{k})(\nu)$ is the label for the irrep of $\mathbf{G}(\mathbf{k})$ or $\mathbf{G}_\mathbf{k}$. It is to be noted that, in this paper, the symbol $D^{(j)}(X)$ is always regarded as the representative matrix of an operator X with respect to a certain basis labeled by the index j, and $D^{(j)}(Y)$ is that for another operator Y, while X and Y may belong to *different* groups. This notation is consistent with the convention used in quantum mechanics and is very convenient.

The irrep $D^{(\mathbf{k})(\nu)}(\{\gamma \mid \mathbf{c}\})$ is called the small rep of the little group $\mathbf{G}(\mathbf{k})$.

If the wave vector $\mathbf{k}$ is a point of symmetry, then $\mathbf{k}$ is of the form

$$\mathbf{k}=\frac{1}{m}(m_1\mathbf{b}_1+m_2\mathbf{b}_2+m_3\mathbf{b}_3) , \tag{11.4a}$$

where m and m_i are integers. In such a case, the phase factor $\mu(i,j)$ in Eq. (11.2b) is of the form

$$\mu(i,j)=\exp(-i\mathbf{k}\cdot\mathbf{R}_{ij}) =\exp(2\pi li/m), \quad l=0,1,\ldots . \tag{11.4b}$$

Hence the rep group $\mathbf{G}_\mathbf{k}$ is an m-fold covering group of $\mathbf{G}_0(\mathbf{k})$ with the elements

$$e^{2\pi li/m}\{\gamma_j \mid \mathbf{V}(\gamma_j)\}, \quad j=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| , \quad l=0,1,\ldots,m-1 . \tag{11.4c}$$

Nevertheless, if $\mathbf{k}$ is a line (or plane) of symmetry, for instance if $\mathbf{k}$ is of the form

$$k=\frac{1}{m'}(m_1\mathbf{b}_1+m_2\mathbf{b}_2)+p_3\mathbf{b}_3 , \tag{11.4d}$$

where p_3 is an arbitrary number, say an irrational number, then the phase factor $\mu(i,j)$ will not have the simple form of Eq. (11.4b). It is thus seen that the factor system μ has the unpleasant feature that the integer $m=|\mathbf{G}_\mathbf{k}|/|\mathbf{G}_0(\mathbf{k})|$ depends on the wave vector $\mathbf{k}$ and may become very large for $\mathbf{k}$ in a line (or plane) of symmetry. To avoid this trouble, we proceed to the next section.

B. The rep group $\mathbf{G}'_\mathbf{k}$

Let us make the following gauge transformation for the group elements of $\mathbf{G}(\mathbf{k})$:

$$R_i\equiv\{\gamma_i \mid V(\gamma_i)\}' =\exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]\{\gamma_i \mid \mathbf{V}(\gamma_i)\} . \tag{11.5}$$

This transformation seems to have been used for the first time in the context of studying the degeneracies of electronic energy bands in crystals by Kovalev and Lyubarskii (1958). It follows from Eq. (11.2a) that in the space $\mathscr{L}(\mathbf{k})$ we have

$$R_iR_j=\eta(i,j)R_{ij} , \tag{11.6a}$$

$$\eta(i,j)=\exp\{-i\mathbf{k}\cdot[\gamma_i\mathbf{V}(\gamma_j)-\mathbf{V}(\gamma_j)]\} . \tag{11.6b}$$

According to Eq. (10.3),

$$\gamma_i^{-1}\mathbf{k}=\mathbf{k}+\mathbf{K}_{\gamma_i} , \tag{11.6c}$$

where $\mathbf{K}_{\gamma_i}$ is a reciprocal lattice vector. Thus

$$\eta(i,j)=\exp[-i\mathbf{K}_{\gamma_i}\cdot\mathbf{V}(\gamma_j)] . \tag{11.6d}$$

With Eqs. (9.2b) and (11.6d), the phase factor $\eta(j,k)$ is of the form

$$\eta(j,k)=\exp(2\pi ia_{jk}/m), \quad m=2,3,4,6 , \tag{11.7}$$

where a_{jk} is an integer depending on j and k. Therefore, in the space $\mathscr{L}(\mathbf{k})$, the $m\,|\mathbf{G}_0(\mathbf{k})|$ operators

$$R_j^{(l)}=\exp(2\pi li/m)R_j, \quad j=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| , \quad l=0,1,\ldots,m-1 , \tag{11.8}$$

form a rep group designated as

$$\mathbf{G}'_\mathbf{k}=\{R_i : i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\}_m . \tag{11.9}$$

The rep group $\mathbf{G}'_\mathbf{k}$ is an m-fold covering group of the point group $\mathbf{G}_0(\mathbf{k})$ where the integer m depends only on what kind of fractional translation the space group $\mathbf{G}$ has and takes only four possible values, 2, 3, 4, and 6, for all 230 space groups.

Since R_i differs from $\{\gamma_i \mid \mathbf{V}(\gamma_i)\}$ only by the phase factor $\exp[i\mathbf{k}\cdot\mathbf{V}(\gamma_i)]$, the groups $\mathbf{G}'_\mathbf{k}$, $\mathbf{G}_\mathbf{k}$, and $\mathbf{G}(\mathbf{k})$ have identical irreducible bases, and their matrices, upon using Eqs. (11.3) and (11.5), are related to one another by

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i \mid \mathbf{V}(\gamma_i)\})=e^{-i\mathbf{k}\cdot\mathbf{V}(\gamma_i)}D^{(\mathbf{k})(\nu)}(R_i) , \tag{11.10a}$$

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i \mid \mathbf{c}_i\})=e^{-i\mathbf{k}\cdot\mathbf{c}_i}D^{(\mathbf{k})(\nu)}(R_i) , \tag{11.10b}$$

where $D^{(\mathbf{k})(\nu)}(R_i)$ is the irreducible matrix for the element R_i of the rep group $\mathbf{G}'_\mathbf{k}$.

For notational convenience, we often use $\Delta(\gamma_i)$ to denote the matrix $D^{(\mathbf{k})(\nu)}(R_i)$, i.e.,

$$\Delta(\gamma_i)\equiv D^{(\mathbf{k})(\nu)}(R_i)=D^{(\mathbf{k})(\nu)}(\{\gamma_i \mid \mathbf{V}(\gamma_i)\}') . \tag{11.11a}$$

Equation (11.10b) then reads

$$D^{(\mathbf{k})(\nu)}(\{\gamma_i \mid \mathbf{c}_i\})=e^{-i\mathbf{k}\cdot\mathbf{c}_i}\Delta(\gamma_i) . \tag{11.10c}$$

It follows from Eqs. (11.6a) and (11.11a) that

$$\Delta(\gamma_i)\Delta(\gamma_j)\equiv\eta(i,j)\Delta(\gamma_i\gamma_j) . \tag{11.11b}$$

Δ is called the projective irrep of the point group $\mathbf{G}_0(\mathbf{k})$, the ray rep (Hamermesh, 1962), the multiplier rep (Maradudin and Vosko, 1968), or the loaded or weighted rep (Lyubarskii, 1957; Kovalev, 1961).

In summary, the problem of finding the irreps of an infinite group $\mathbf{G}(\mathbf{k})$ is converted into finding that of the rep group $\mathbf{G}_\mathbf{k}$ or $\mathbf{G}'_\mathbf{k}$. For those wave vectors $\mathbf{k}$ which are lines or planes of symmetry, we must work with the rep group $\mathbf{G}'_\mathbf{k}$, while for those $\mathbf{k}$ which are points of symmetry, we can work either with the group $\mathbf{G}_\mathbf{k}$ or with $\mathbf{G}'_\mathbf{k}$. However, the multiplication relation (11.6a) for $\mathbf{G}'_\mathbf{k}$ is

much simpler than that for $\mathbf{G}_\mathbf{k}$; in the following we shall work only with the rep group $\mathbf{G}'_\mathbf{k}$, irrespective of points of symmetry or line (planes) of symmetry.

The $|\mathbf{G}_0(\mathbf{k})|$ functions

$$\psi_j \equiv R_j \exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{r}], \quad j=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})| , \tag{11.12a}$$

carry the rep space $\mathscr{L}(\mathbf{k})$ for $\mathbf{G}'_\mathbf{k}$, which coincides with the space $\mathscr{L}(\mathbf{k})$ of Eq. (10.7b). The group space of the rep group $\mathbf{G}'_\mathbf{k}$ is denoted by

$$L(\mathbf{k})=\{R_i : i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|\} . \tag{11.12b}$$

The spaces $\mathscr{L}(\mathbf{k})$ and $L(\mathbf{k})$ are isomorphic, and it is more convenient to work with the latter. In the following we work mainly with $L(\mathbf{k})$.

C. Special cases of the rep group $\mathbf{G}'_\mathbf{k}$

The following four cases need to be considered separately.

(1) For a general $\mathbf{k}$ point. This is a trivial case, since now $\mathbf{G}'_\mathbf{k}=\mathbf{G}_\mathbf{k}=\{\varepsilon\}$.

(2) For the symmorphic space group, or the nonsymmorphic space group whose little group $\mathbf{G}(\mathbf{k})$ is symmorphic for the wave vector $\mathbf{k}$ under consideration. For these cases, $\mathbf{V}(\gamma)\equiv 0$, and according to Eqs. (11.2b) and (11.6d) the phase factor $\mu(i,j)=\eta(i,j)=1$, hence

$$\mathbf{G}_\mathbf{k}=\mathbf{G}'_\mathbf{k}=G_0(\mathbf{k}) , \tag{11.13}$$

i.e., the rep group $\mathbf{G}'_\mathbf{k}$ (or $\mathbf{G}_\mathbf{k}$) is identical to the point group $\mathbf{G}_0(\mathbf{k})$, whose irreps are already known. In passing we point out that in such cases the space $L(\mathbf{k})=\{R_i\}=\{\gamma_i\}$ is the regular rep space of the point group $\mathbf{G}_0(\mathbf{k})$.

(3) For an interior point of a Brillouin zone. When the wave vector $\mathbf{k}$ is not on the surface of the Brillouin zone, the only possibility for $\gamma\mathbf{k}=\mathbf{k}+\mathbf{K}_m$ is that $\mathbf{K}_m=0$, i.e.,

$$\gamma\mathbf{k}=\mathbf{k} . \tag{11.14}$$

Comparing this with Eq. (11.6c), we know that now $\mathbf{K}_\gamma\equiv 0$, and the phase factor in Eq. (11.6a) is again equal to one, $\eta(i,j)\equiv 1$. Therefore, the rep group $\mathbf{G}'_\mathbf{k}$ is isomorphic to the point group $\mathbf{G}_0(\mathbf{k})=\{\gamma_i\}$. Suppose $D^{(\nu)}$ is the irrep of the point group $\mathbf{G}_0(\mathbf{k})$. Then the irrep of the rep group $\mathbf{G}'_\mathbf{k}$ is

$$D^{(\mathbf{k})(\nu)}(R_i)=D^{(\nu)}(\gamma_i) . \tag{11.15a}$$

while the irrep of the little group $\mathbf{G}(\mathbf{k})$ is [Eq. (11.10b)]

$$D^{(\mathbf{k})(\nu)}(\{\gamma\,|\,\mathbf{c}\})=e^{-i\mathbf{k}\cdot\mathbf{c}}D^{(\nu)}(\gamma) . \tag{11.15b}$$

Observe that, for the origin point $\mathbf{k}=0$, we again have

$$\mathbf{G}_\mathbf{k}=\mathbf{G}'_\mathbf{k} , \tag{11.16}$$

i.e., the distinction between $\mathbf{G}_\mathbf{k}$ and $\mathbf{G}'_\mathbf{k}$ disappears.

It should also be noted that for the case of interior points, although the rep group $\mathbf{G}'_\mathbf{k}$ and the point group $\mathbf{G}_0(\mathbf{k})$ have identical irreps (11.15a), their irreducible bases do not coincide. For example, if

$$\varphi^{(\nu)}_{\mathbf{k},a}=\sum_i u^{(\nu)}_{a,i}\gamma_i\psi_\mathbf{k} \tag{11.17a}$$

is the irreducible basis of $\mathbf{G}_0(\mathbf{k})$, where $u^{(\nu)}_{a,i}$ are coefficients and $\psi_\mathbf{k}=\exp[i(\mathbf{k}+\mathbf{K}_n)\cdot\mathbf{r}]$, then the corresponding irreducible basis of $\mathbf{G}'_\mathbf{k}$ is

$$\psi^{(\nu)}_{\mathbf{k},a}=\sum_i u^{(\nu)}_{a,i}\{\gamma_i\,|\,\mathbf{V}(\gamma_i)\}'\psi_\mathbf{k} . \tag{11.17b}$$

(4) For a point on the surface of a Brillouin zone and for nonsymmorphic little groups. For cases (1)—(3) above, the irreps of the rep group $\mathbf{G}'_\mathbf{k}$ can be directly taken over from those of the point group $\mathbf{G}_0(\mathbf{k})$. The only case for which the irreps of $\mathbf{G}'_\mathbf{k}$ cannot be obtained in this way and have to be worked out anew is when the wave vector $\mathbf{k}$ is on the surface of a Brillouin zone and its little group $\mathbf{G}(\mathbf{k})$ is nonsymmorphic.

The whole machinery for constructing irreps for the rep group has been worked out in Secs. II—VII. All the formulas there can be applied to the rep group $\mathbf{G}'_\mathbf{k}$ with $|\mathbf{g}|$ replaced by $|\mathbf{G}_0(\mathbf{k})|$. Before going into detail on the application of the general theory to the specific group $\mathbf{G}'_\mathbf{k}$, let us discuss briefly one of the conventional methods for constructing the irreps of $\mathbf{G}(\mathbf{k})$, the projective-rep method.

D. The projective-rep method

We recapitulate the main points of Schur's theory on projective representations (Schur, 1904,1907,1911; Birman, 1974; Bradley and Cracknell, 1972) as follows. Our starting point is still Eq. (11.11b). Under the gauge transformation

$$\Delta'(\gamma_i)=C_i\Delta(\gamma_i) , \tag{11.18}$$

with $|C_i|=1$, Eq. (11.11b) becomes

$$\Delta'(\gamma_i)\Delta'(\gamma_j)=\eta'(i,j)\Delta'(\gamma_i\gamma_j) , \tag{11.19a}$$

$$\eta'(i,j)=\frac{C_iC_j}{C_{ij}}\eta(i,j) . \tag{11.19b}$$

The factor systems η and η' are said to belong to the same class. We need study only one factor system for each class. One of Schur's basic theorems is the following: The number of classes of factor systems of a finite group $\mathbf{g}$ is finite, denoted by m, and every projective rep is equivalent to a unitary one with a factor system in the same class.

Let $\mathbf{g}^*$ be the central extension of $\mathbf{g}$ with an Abelian group $\mathbf{A}$ of order m such that $\mathbf{A}$ is an invariant subgroup of $\mathbf{g}^*$ and $\mathbf{A}$ is contained in the center of $\mathbf{g}^*$. (The center of a group is the set of all elements each of which is in a class by itself.)

Another basic theorem of Schur is the following: All the projective irreps of $\mathbf{g}$ are vector irreps of $\mathbf{g}^*$ subduced on $\mathbf{g}$.

The central extension $\mathbf{g}^*$ of minimum order producing all the distinct projective irreps of $\mathbf{g}$ is called the "rep"

group (here we added the quotation marks to differentiate Schur's usage from our definition of the rep group).

To obtain projective irreps belonging to a given factor system η of Eq. (11.7), we can construct the "rep" group $\mathbf{g}^*$ as follows: Form $m \mid \mathbf{g} \mid$ pairs of elements (γ_j, l), each pair with a γ_j from $\mathbf{g}$ and an l from the cyclic group Z_m of integers $0, 1, \ldots, m-1$; the group product of Z_m is defined as addition modulo m. The multiplication rule for $\mathbf{g}^*$ is defined by

$$(\gamma_j, l)(\gamma_k, l') = (\gamma_j \gamma_k, l + l' + a_{jk}) . \tag{11.20}$$

All the projective irreps of $\mathbf{g}$ for the factor system η can be found from the vector rep of $\mathbf{g}^*$.

Now let us return to the little co-group $\mathbf{g} = \mathbf{G}_0(\mathbf{k})$. Its central extension is $\mathbf{g}^* = \mathbf{G}_0(\mathbf{k})^*$, or $\overline{\mathbf{G}}^{\mathbf{k}^*}$ in Bradley and Cracknell's notation. The relation between the central extension $\mathbf{G}_0(\mathbf{k})^*$ and our rep group $\mathbf{G}'_{\mathbf{k}}$ is clear when we note that from Eqs. (11.6a), (11.7), and (11.8) we have

$$R_j^{(l)} R_k^{(l')} = \exp[2\pi i (l + l')/m] R_j R_k$$
$$= \exp[2\pi i (l + l' + a_{jk})/m] R_{jk} = R_{jk}^{(l'')} , \tag{11.21a}$$

$$l'' = l + l' + a_{jk} . \tag{11.21b}$$

Comparing Eq. (11.20) with Eqs. (11.21), we see that there is a one-to-one correspondence between (γ_j, l) and $R_j^{(l)}$; therefore $\mathbf{G}_0(\mathbf{k})^*$ is isomorphic to $\mathbf{G}'_{\mathbf{k}}$. Being an abstract group, the central extension $\mathbf{G}_0(\mathbf{k})^*$ is just the abstract group $\hat{\mathbf{G}}'_{\mathbf{k}}$ with the rep group $\mathbf{G}'_{\mathbf{k}}$ as its faithful representation.

Several approaches are available for constructing projective irreps of a point group belonging to a given factor system.

1. Döring's approach

Taking the simplest factor systems, i.e., taking as many phase factors $\eta(i,j) = 1$ as possible, Döring was able to construct all the different projective irreps of the 32 point groups (Döring, 1959). However, Döring's irreps are usually not associated with the factor system (11.6d) we need for constructing the irreps of the little group $\mathbf{G}(\mathbf{k})$, and a gauge transformation [Eq. (11.18)] is required to correct the factor system. Therefore, Döring's table for the projective irreps of point groups is not in a form that permits direct application of his projective irreps to space groups. This is the reason why the projective-rep method was less widespread, before Kovalev's table (1961) was published, than the little-group method due to Herring (1942). Herring's method is based on the factor group $\mathbf{G}(\mathbf{k})/\mathbf{T}(\mathbf{k})$, where $\mathbf{T}(\mathbf{k})$ is a subgroup of all lattice translations through vectors $\mathbf{R}$ for which $\exp(-i\mathbf{k}\cdot\mathbf{R}) = 1$.

2. Kovalev and Lyubarskii's approach

From Eqs. (11.11b) and (11.6d), we obtain a set of matrix equations for the generators of $\mathbf{G}_0(\mathbf{k})$. With the help of $\sum_\nu h_\nu^2 = \mid \mathbf{G}_0(\mathbf{k}) \mid$, we can determine the projective irreducible matrices for these generators on a case-by-case basis (Lyubarskii, 1957). The whole projective rep of $\mathbf{G}_0(\mathbf{k})$ results from matrix multiplication. The disadvantage of this approach is that it is very tedious. Based on this method, tables of the projective irreps have been constructed for the little co-groups corresponding to most of the symmetry points in the Brillouin zone for all 230 space groups (Kovalev, 1961).

3. Bradley and Cracknell's approach

Bradley and Cracknell (1972) published extensive character tables for all abstract groups that may appear as the central extension groups $\mathbf{G}_0(\mathbf{k})^*$ or $\hat{\mathbf{G}}'_{\mathbf{k}}$. However, out of the N inequivalent irreps of $\mathbf{G}_0(\mathbf{k})^*$, only n are acceptable irreps for the little group $\mathbf{G}(\mathbf{k})$ in the space $\mathscr{L}(\mathbf{k})$. By requiring that

$$D(\gamma_j, l) = \Delta(\gamma_j) \exp(2\pi i l/m) , \tag{11.22}$$

for all j and l, Bradley and Cracknell could determine which irreps of $\mathbf{G}_0(\mathbf{k})^*$ were acceptable for $\mathbf{G}(\mathbf{k})$. They also listed the irreducible matrices for the generators of the little group $\mathbf{G}(\mathbf{k})$.

The disadvantage of this approach is that we have to work with groups of large order, which can be as high as 192 for the cubic system. Since all we need are the acceptable reps, the labor involved in constructing all the N irreps of $\mathbf{G}_0(\mathbf{k})^*$ or $\hat{\mathbf{G}}'_{\mathbf{k}}$ seems disproportionate.

4. Dirl's approach

The projective irreps constructed by the previous approaches are arbitrary, i.e., they do not fit into a specific classification scheme. In practice, as in the investigation of compatibility for space groups, one needs to construct projective irreps of the little co-group $\mathbf{G}_0(\mathbf{k})$ in the $\mathbf{G}_0(\mathbf{k}) \supset \mathbf{G}_0(\mathbf{k}')$ classification, where $\mathbf{k}$ is a point lying on the surface of the Brillouin zone and $\mathbf{k}' = \varepsilon\mathbf{k}$, $0 < \varepsilon < 1$, is a point of lower symmetry.

A successive induction procedure has been established by Dirl (1977) to construct the required $\mathbf{G}_0(\mathbf{k}) \supset \mathbf{G}_0(\mathbf{k}')$ projective irreps. However, the formulation is rather formidable and defies a brief recapitulation here. The interested reader is referred to Dirl's original paper.

The projective irreps of the little co-group have also been obtained by Sahni and Venkataraman (1970) by inducing from those of a subgroup of prime order starting from an invariant cyclic subgroup.

XII. THE CSCO AND CHARACTERS OF THE REPRESENTATION GROUP $\mathbf{G}'_{\mathbf{k}}$

A. The group table of $\mathbf{G}'_{\mathbf{k}}$

Although the rep group $\mathbf{G}'_{\mathbf{k}}$ is of order $m \mid \mathbf{G}_0(\mathbf{k}) \mid$, its multiplication rule is totally determined by the multipli-

cation relation among the $|\mathbf{G}_0(\mathbf{k})|$ active elements R_ρ, $\rho=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|$, which is referred to as the group table of $\mathbf{G}'_\mathbf{k}$.

The group table of $\mathbf{G}'_\mathbf{k}$ can easily be constructed from the group table $\gamma_\rho\gamma_\sigma=\gamma_{\rho\sigma}$ of the little co-group $\mathbf{G}_0(\mathbf{k})$ by replacing γ's with R's and multiplying the $(\rho\sigma)$ entry with the phase factor,

$$\eta(\rho,\sigma)=\exp[-i(\gamma_\rho^{-1}\mathbf{k}-\mathbf{k})\cdot\mathbf{V}(\gamma_\sigma)] . \tag{12.1a}$$

Since phase factors $\eta(\rho,\sigma)$ are crucial for the whole process of analysis, we give a simple formula for calculating them. To this end, we introduce the following notations. Let

$$\mathbf{b}=(\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3),\quad \mathbf{t}=(\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3) ,$$
$$\mathbf{p}=(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3),\quad \tau_\sigma=(\tau_{\sigma1},\tau_{\sigma2},\tau_{\sigma3}) , \tag{12.1b}$$

The wave vector $\mathbf{k}$ and the nonprimitive translation $\mathbf{V}(\gamma_\sigma)$ can be expressed as

$$\mathbf{k}=\mathbf{p}\cdot\mathbf{b}=p_1\mathbf{b}_1+p_2\mathbf{b}_2+p_3\mathbf{b}_3 ,$$
$$\mathbf{V}(\gamma_\sigma)=\tau_\sigma\cdot\mathbf{t}=\tau_{\sigma1}\mathbf{t}_1+\tau_{\sigma2}\mathbf{t}_2+\tau_{\sigma3}\mathbf{t}_3 . \tag{12.1c}$$

Obviously, under rotations, (p_1,p_2,p_3) transforms as $(\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3)$, while $(\tau_{\sigma1},\tau_{\sigma2},\tau_{\sigma3})$ transforms as $(\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3)$. Furthermore

$$\gamma_\rho^{-1}\mathbf{k}=\gamma_\rho^{-1}(\mathbf{p}\cdot\mathbf{b})=\mathbf{p}\cdot(\gamma_\rho^{-1}\mathbf{b})=\mathbf{p}_\rho\cdot\mathbf{b} ,$$
$$\mathbf{p}_\rho=\gamma_\rho\mathbf{p}=(p_{\rho1},p_{\rho2},p_{\rho3}) . \tag{12.1d}$$

The transformed vector $\mathbf{p}_\rho=\gamma_\rho\mathbf{p}$ can be found from Table 3.2 in Bradley and Cracknell (1972) by replacing the $\mathbf{t}_i$'s with $\mathbf{p}_i$'s. Using Eqs. (12.1a), (12.1c), and (12.1d) we finally obtain

$$\eta(\rho,\sigma)=\exp[-2\pi i(\mathbf{p}_\rho-\mathbf{p})\cdot\tau_\sigma] , \tag{12.2a}$$

where

$$(\mathbf{p}_\rho-\mathbf{p})\cdot\tau_\sigma=\sum_{i=1}^{3}(p_{\rho i}-p_i)\tau_{\sigma i} . \tag{12.2b}$$

B. Classes and class operators of the rep group $\mathbf{G}'_\mathbf{k}$

On the basis of the group table of $\mathbf{G}'_\mathbf{k}$, it is easy to determine the classes of $\mathbf{G}'_\mathbf{k}$. In this process the following observation is of help.

Suppose for the point group $\mathbf{G}_0(\mathbf{k})$ we have

$$\gamma_j\gamma_i\gamma_j^{-1}=\gamma_k .$$

Then for the group $\mathbf{G}'_\mathbf{k}$ we shall have

$$R_jR_iR_j^{-1}=e^{2\pi il/m}R_k . \tag{12.3}$$

This shows that if γ_i and γ_k belong to the same class of the point group $\mathbf{G}_0(\mathbf{k})$, then R_i and $R_k^{(l)}$ may belong to the same class of $\mathbf{G}'_\mathbf{k}$, while if γ_i and γ_k do not belong to the same class of $\mathbf{G}_0(\mathbf{k})$, then $R_i^{(l)}$ and $R_k^{(l')}$ for any l and l' will never belong to the same class of $\mathbf{G}'_\mathbf{k}$.

It should be pointed out that, for an abstract group, we never choose the identity operator as a member of the CSCO except for the trivial identity group (consisting of only one element), whereas for the rep group, it may happen that there is only one linearly independent class operator for a nontrivial rep group. In such a case the identity operator must be the linearly independent class operator and is the CSCO of this nontrivial rep group. Examples of finding the CSCO of $\mathbf{G}'_\mathbf{k}$ are given in Sec. XIV.A.

C. The characters of $\mathbf{G}'_\mathbf{k}$

Although the rep group $\mathbf{G}'_\mathbf{k}$ has N classes, all we need are the characters of the n classes whose class operators are linearly independent. The character of the remaining class is either zero, for a null class operator, or a factor times one of the n known characters. For example, if $C_i=\mu C_j$, then $\chi_i=\mu\chi_j$, where μ is a constant factor.

The procedure for obtaining the characters of the rep group $\mathbf{G}'_\mathbf{k}$ by the EFM is given in Sec. VII.C. Here it is sufficient to mention that by working with the rep group $\mathbf{G}'_\mathbf{k}$ rather than the abstract group $\hat{\mathbf{G}}'_\mathbf{k}$ [or $\mathbf{G}_0(\mathbf{k})^*$], we can reduce the order of the eigenequations for the characters from N to n. From the known fact that $(N)_{\max}=32$, while $(n)_{\max}=11$ for the single-valued representations of the 230 space groups (Bradley and Cracknell, 1972), we can fully appreciate the importance of this simplification.

We can use the eigenvalues ν of the CSCO of $\mathbf{G}'_\mathbf{k}$ to label irreps of the rep group $\mathbf{G}'_\mathbf{k}$ or of the little group $\mathbf{G}(\mathbf{k})$. However, to follow the customary notation (Birman, 1974), we prefer to use $(\mathbf{k})(\nu)$ as label of the irreps of $\mathbf{G}'_\mathbf{k}$ or $\mathbf{G}(\mathbf{k})$.

XIII. THE IRREDUCIBLE BASIS AND MATRICES OF $\mathbf{G}'_\mathbf{k}$

A. The CSCO-II and CSCO-III of $\mathbf{G}'_\mathbf{k}$

To decompose the group space $L(\mathbf{k})$ of $\mathbf{G}'_\mathbf{k}$, we need to introduce a suitable group chain $\mathbf{G}'_\mathbf{k}\supset\mathbf{G}'_s$, which can be assumed to be a canonical one without loss of generality. For simplicity in exposition, here $\mathbf{G}'_s$ is assumed to be simply a subgroup of $\mathbf{G}'_\mathbf{k}$ instead of a subgroup chain, i.e.,

$$\mathbf{G}'_s=\{R_s\},\quad R_s=\{\gamma_s\,|\,\mathbf{V}(\gamma_s)\}' . \tag{13.1}$$

We also need the intrinsic group $\overline{\mathbf{G}}'_\mathbf{k}$ of the rep group $\mathbf{G}'_\mathbf{k}$ defined by Eq. (4.11a), i.e.,

$$\overline{R}_iR_j=R_jR_i \text{ for any } R_j\in L(\mathbf{k}) . \tag{13.2}$$

$\overline{\mathbf{G}}'_\mathbf{k}$ and $\mathbf{G}'_\mathbf{k}$ are commutative and anti-isomorphic. Corresponding to the subgroup $\mathbf{G}'_s$ of $\mathbf{G}'_\mathbf{k}$ is the intrinsic subgroup

$$\overline{\mathbf{G}}'_s=\{\overline{R}_s\} \tag{13.3}$$

of $\overline{\mathbf{G}}'_{\mathbf{k}}$. Let C and $C(s)$ be the CSCO of $\mathbf{G}'_{\mathbf{k}}$ and $\mathbf{G}'_s$, respectively; then $\overline{C}$ and $\overline{C}(s)$ are the CSCO of $\overline{G}'_k$ and $\overline{G}'_s$, respectively, where $\overline{C}$ and $\overline{C}(s)$ are obtained from C and $C(s)$ by replacing the elements of $\mathbf{G}'_{\mathbf{k}}$ with the corresponding intrinsic group elements. Furthermore, we still have $\overline{C}=C$.

If $K=(C,C(s),\overline{C}(s))$ is a CSCO in the $|\mathbf{G}_0(\mathbf{k})|$-dimensional space $L(\mathbf{k})$, then K is the CSCO-III of $\mathbf{G}'_{\mathbf{k}}$, while $M=(C,C(s))$ is the CSCO-II of $\mathbf{G}'_{\mathbf{k}}$.

The intrinsic group $\overline{\mathbf{G}}(\mathbf{k})$ of the little group $\mathbf{G}(\mathbf{k})$ is defined by

$$\overline{\mathbf{G}}(\mathbf{k})=\{\overline{\{\gamma_i\,|\,\mathbf{V}(\gamma_i)+\mathbf{R}_n\}},i=1,2,\ldots,|\mathbf{G}_0(\mathbf{k})|,\mathbf{R}_n\in L\} \tag{13.4a}$$

with

$$\overline{\{\gamma_i\,|\,\mathbf{c}\}}=e^{-i\mathbf{k}\cdot\mathbf{c}}\overline{R}_i,\quad \mathbf{c}=V(\gamma_i)+\mathbf{R}_n\ . \tag{13.4b}$$

The eigenvector of the CSCO-III of $\mathbf{G}'_{\mathbf{k}}$ in the space $L(\mathbf{k})$ is denoted by $P_a^{(\mathbf{k})(\nu)b}$. Equation (6.1a) now reads

$$\begin{bmatrix} C \\ C(s) \\ \overline{C}(s) \end{bmatrix} P_a^{(\mathbf{k})(\nu)b}=\begin{bmatrix} \nu \\ a \\ b \end{bmatrix} P_a^{(\mathbf{k})(\nu)b},\quad a,b=a_1,a_2,\ldots,a_{h_\nu}\ . \tag{13.5}$$

The eigenvector $P_a^{(\mathbf{k})(\nu)b}$ is a linear combination of R_i,

$$P_a^{(\mathbf{k})(\nu)b}=\sum_i^{|\mathbf{G}_0(\mathbf{k})|} u_{ab,i}^{(\mathbf{k})(\nu)}R_i\ . \tag{13.6}$$

Equations (6.3), (6.5), and (6.9) still hold under the substitutions

$$|\mathbf{g}|\rightarrow|\mathbf{G}_0(\mathbf{k})|,\quad u_{\nu ab,i}\rightarrow u_{ab,i}^{(\mathbf{k})(\nu)}\ . \tag{13.7}$$

Then the coefficients $u_{ab,i}^{(\mathbf{k})(\nu)}$ are the solutions to Eq. (6.5).

The eigenvector $P_a^{(\mathbf{k})(\nu)b}$, for $a,b=a_1,\ldots,a_{h_\nu}$ constitutes the $\mathbf{G}'_{\mathbf{k}}\supset\mathbf{G}'_s$ and $\overline{\mathbf{G}}'_{\mathbf{k}}\supset\overline{\mathbf{G}}'_s$ IRB. Equation (6.3) shows that the number of times that the irrep $(\mathbf{k})(\nu)$ of $\mathbf{G}'_{\mathbf{k}}$ appears in the space $L(\mathbf{k})$ is equal to its dimension h_ν.

One of the advantages of the EFM for constructing the IRB or irreps of $\mathbf{G}(\mathbf{k})$ is that the subgroup chain used to classify the IRB or irrep can be chosen at will without the restriction that the subgroup has to be an invariant subgroup of $\mathbf{G}(\mathbf{k})$ as in Dirl's method (Dirl, 1977). For example, in the case studied by Dirl, we can choose $\mathbf{G}'_s=\mathbf{G}'_{\mathbf{k}'}$, $\mathbf{k}'=\varepsilon\mathbf{k}$, $0<\varepsilon<1$, where $\mathbf{G}'_{\mathbf{k}'}$ is the rep group corresponding to the little group $\mathbf{G}(\mathbf{k}')$. If $\mathbf{G}'_{\mathbf{k}}\supset\mathbf{G}'_{\mathbf{k}'}$ is not a canonical subgroup chain, then in addition to the CSCO of $\mathbf{G}'_{\mathbf{k}'}$ we need to seek extra operators to form the operator set $C(s)$. (See Sec. V.B.)

However, if for some circumstances we are only interested in obtaining irreps of $\mathbf{G}(\mathbf{k})$ without the requirement that they be in a certain classification scheme, then we pay attention only to the operator set $C(s)$, without bothering about its related subgroup chain. In such cases, the eigenvalue of $C(s)$ is used merely to distinguish between the components of an irreducible basis, and $C(s)$ can be chosen differently for different irreps. The choice of $C(s)$ can be arbitrary so long as its eigenvalues can provide enough labels for the basis vectors of the same irrep. It is always desirable that $C(s)$ contain as few operators as possible. For example, for two-dimensional irreps the possible choice of $C(s)$ is a (plane) reflection operator σ, or a twofold rotation C_2; for irreps with $h_\nu=3$ (4) it is a threefold (fourfold) rotation C_3 (C_4); and for irreps with $h_\nu=6$, it is (C_{2x},C_{2y},I) or (C_{31}^{+},I), where I is the inversion.

B. The irreps of $\mathbf{G}'_{\mathbf{k}}$ and the projective irreps of $\mathbf{G}_0(\mathbf{k})$

With the standard phase choice for the eigenvectors $P_a^{(\mathbf{k})(\nu)b}$, the irreducible matrix elements of $\mathbf{G}'_{\mathbf{k}}$ are simply related to the coefficients $u_{ab,i}^{(\mathbf{k})(\nu)}$ by [cf. Eq. (6.23)]

$$D_{ab}^{(\mathbf{k})(\nu)}(R_i)=\Delta_{ab}^{(\nu)}(\gamma_i)=\left[\frac{|\mathbf{G}_0(\mathbf{k})|}{h_\nu}\right]^{1/2}(u_{ab,i}^{(\mathbf{k})(\nu)})^*\ . \tag{13.8}$$

By solving the eigenequation (6.5), we can obtain all the irreps $D^{(\mathbf{k})(\nu)}$ of G'_k, i.e., the projective irreps $\Delta^{(\nu)}$ of the little co-group $\mathbf{G}_0(\mathbf{k})$.

The rule for determining the phases of $P_a^{(\mathbf{k})(\nu)b}$ so that Eq. (13.8) holds is identical to that given in Sec. VI.C under the substitution (13.7).

From Eqs. (6.26) and (13.8) we get the two orthogonal theorems for the projective irreps of $\mathbf{G}_0(\mathbf{k})$,

$$\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}\sum_i^{|\mathbf{G}_0(\mathbf{k})|}\Delta_{ab}^{(\nu)}(\gamma_i)^*\Delta_{a'b'}^{(\nu')}(\gamma_i)=\delta_{\nu\nu'}\delta_{aa'}\delta_{bb'}\ , \tag{13.9a}$$

$$\sum_\nu^n\sum_{a,b}^{h_\nu}\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}\Delta_{ab}^{(\nu)}(\gamma_i)^*\Delta_{ab}^{(\nu)}(\gamma_j)=\delta_{ij}\ . \tag{13.9b}$$

Inserting Eq. (13.8) into Eq. (13.6), we get the normalized generalized projection operator,

$$P_a^{(\mathbf{k})(\nu)b}=\left[\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}\right]^{1/2}\sum_i^{|\mathbf{G}_0(\mathbf{k})|}D_{ab}^{(k)(\nu)}(R_i)^*R_i \tag{13.10}$$

for the rep group $\mathbf{G}'_{\mathbf{k}}$. The generalized projection operator for the rep group $\mathbf{G}'_{\mathbf{k}}$ or for the little group $\mathbf{G}(\mathbf{k})$ is

$$P_{ab}^{(\mathbf{k})(\nu)}=\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}\sum_i^{|\mathbf{G}_0(\mathbf{k})|}D_{ab}^{(\mathbf{k})(\nu)}(R_i)^*R_i\ . \tag{13.11a}$$

Using Eqs. (11.5) and (11.10a), we can rewrite Eq. (13.11a)

$$P_{ab}^{(\mathbf{k})(\nu)}=\frac{h_\nu}{|\mathbf{G}_0(\mathbf{k})|}\sum_i^{|\mathbf{G}_0(\mathbf{k})|}D_{ab}^{(\mathbf{k})(\nu)}(\{\gamma_i\,|\,\mathbf{V}(\gamma_i)\})^*\times\{\gamma_i\,|\,\mathbf{V}(\gamma_i)\}\ . \tag{13.11b}$$

C. The irreducible basis of $\mathbf{G}(\mathbf{k})$

The $\mathbf{G}'_{\mathbf{k}}\supset\mathbf{G}'_s$ and $\overline{\mathbf{G}}'_{\mathbf{k}}\supset\overline{\mathbf{G}}'_s$ IRB in the rep space $\mathscr{L}(\mathbf{k})$ is simply given by

TABLE VII. The group table of the rep group $\mathbf{G}'_W$ for the space group O_h^7.

η_ρ	$\{\varepsilon \mid 0\}'$	$\{C_{2x} \mid 0\}'$	$\{C_{2d} \mid \tau\}'$	$\{C_{2f} \mid \tau\}'$	$\{\sigma_y \mid \tau\}'$	$\{\sigma_z \mid \tau\}'$	$\{S_{4x}^- \mid 0\}$	$\{S_{4x}^+ \mid 0\}$
1	1	2	3	4	5	6	7	8
−1	2	1	−4	−3	−6	−5	8	7
i	3	4	$i1$	$i2$	$i7$	$i8$	5	6
$-i$	4	3	$-i2$	$-i1$	$-i8$	$-i7$	6	5
−1	5	6	−8	−7	−1	−2	4	3
1	6	5	7	8	2	1	3	4
i	7	8	$i6$	$i5$	$i3$	$i4$	2	1
$-i$	8	7	$-i5$	$-i6$	$-i4$	$-i3$	1	2

$$\psi_{\mathbf{k},a}^{(\nu)b}=P_a^{(\mathbf{k})(\nu)b}\psi_{\mathbf{k}}(\mathbf{x}) = \sum_i^{|\mathbf{G}_0(\mathbf{k})|} u_{ab,i}^{(\mathbf{k})(\nu)}\psi_i \ . \tag{13.12}$$

Notice that $\psi_{\mathbf{k},a}^{(\nu)b}$ is also the $\mathbf{G}(\mathbf{k})\supset\mathbf{G}(s)$ and $\overline{\mathbf{G}}(\mathbf{k})\supset\overline{\mathbf{G}}(s)$ IRB, where $\mathbf{G}(s)$ is the subgroup of the little group $\mathbf{G}(\mathbf{k})$, which has $\mathbf{G}'_s$ of Eq. (13.1) as its rep group.

Under the action of the element $\{\gamma \mid \mathbf{c}\}$ of $\mathbf{G}(\mathbf{k})$ [$\overline{\{\gamma \mid \mathbf{c}\}}$ of $\overline{\mathbf{G}}(\mathbf{k})$], $\psi_{\mathbf{k},a}^{(\nu)b}$ only changes its "external" (intrinsic) quantum number a (b) [cf. Eqs. (6.22)],

$$\{\gamma \mid \mathbf{c}\}\psi_{\mathbf{k},a}^{(\nu)b}=\sum_{a'} D_{a'a}^{(\mathbf{k})(\nu)}(\{\gamma \mid \mathbf{c}\})\psi_{\mathbf{k},a'}^{(\nu)b} \ , \tag{13.13a}$$

$$\overline{\{\gamma \mid \mathbf{c}\}}\psi_{\mathbf{k},a}^{(\nu)b}=\sum_{b'} D_{bb'}^{(k)(\nu)}(\{\gamma \mid \mathbf{c}\})\psi_{\mathbf{k},a}^{(\nu)b'} \ , \tag{13.13b}$$

The h_ν sets of IRB of $\mathbf{G}(\mathbf{k})$, $\{\psi_{\mathbf{k},a}^{(\nu)b}: a=1,2,\ldots,h_\nu\}$, $b=1,2,\ldots,h_\nu$, which carry h_ν equivalent (or identical, under the standard phase choice) irreps of $\mathbf{G}(\mathbf{k})$, are distinguished by the intrinsic quantum number b.

XIV. EXAMPLES: THE POINT W OF O_h^7 AND THE POINT R OF O_h^3

In this section, we give several examples of the application of the EFM for obtaining the characters and irreps of the rep group $\mathbf{G}'_{\mathbf{k}}$. From these it is then trivial to obtain the characters and small reps of the little group $\mathbf{G}(\mathbf{k})$ by using Eq. (11.10b).

Since the cases (1)—(3) in Sec. XI.C are trivial, we treat here only case (4), i.e., when $\mathbf{k}$ is a surface point and the little group $\mathbf{G}(\mathbf{k})$ is nonsymmorphic.

The notation for space-group operators follows that used by Bradley and Cracknell (1972).

A. Seeking the CSCO and characters

1. The point W of the space group O_h^7

The vector $\mathbf{p}$ for the point W is

$$\mathbf{p}=(\tfrac{1}{2}\ \tfrac{1}{4}\ \tfrac{3}{4}) \ . \tag{14.1}$$

O_h^7 belongs to the face-centered cubic Γ_c^f with the generators

$$\{C_{2z} \mid 0\},\ \{C_{2x} \mid 0\},\ \{C_{31}^+ \mid 0\} \ ,$$
$$\{C_{2a} \mid \tau\},\ \{I \mid \tau\},\ \tau=(\tfrac{1}{4}\ \tfrac{1}{4}\ \tfrac{1}{4}) \ . \tag{14.2}$$

The little co-group is

$$\mathbf{G}_0(W)=D_{2d}=(\varepsilon,C_{2x},C_{2d},C_{2f},\sigma_y,\sigma_z,S_{4x}^-S_{4x}^+) \ ,$$
$$|\mathbf{G}_0(W)|=8 \ . \tag{14.3}$$

Using Eq. (12.2a) and Bradley and Cracknell's Table 3.2 under the heading "cubic Γ_c^f," we can calculate the phase factor,

$$\eta_\rho=\exp[-2\pi i(\gamma_\rho\mathbf{p}-\mathbf{p})\cdot\tau] \ , \tag{14.4}$$

as shown in the first column of Table VII. $\eta_\rho=\pm1,\pm i$. Hence the representation group $\mathbf{G}'_W$ is a fourfold covering group of D_{2d}.

If we take up the group table of D_{2d}, and multiply the

TABLE VIII. The class structure of $\mathbf{G}'_W$.

$R_i R_j^{-1} R_i R_j$ \ R_j	1	2	3	4	5	6	7	8
1	1	1	1	1	1	1	1	1
2	2	2	−2	−2	−2	−2	2	2
3	3	−3	3	−3	$-i4$	$i4$	$-i4$	$i4$
4	4	−4	−4	4	$i3$	$-i3$	$-i3$	$i3$
5	5	−5	$i6$	$-i6$	5	−5	$-i6$	$i6$
6	6	−6	$-i5$	$i5$	−6	6	$-i5$	$i5$
7	7	7	$i8$	$i8$	$i8$	$i8$	7	7
8	8	8	$-i7$	$-i7$	$-i7$	$-i7$	8	8

$(\rho\sigma)$ entries by the phase factor η_ρ for those columns σ which have the nonprimitive translation τ, then we get the group table of the representation group $\mathbf{G}'_W$, as shown in Table VII.

By multiplying the jth column of Table VII from the left with the element R_j^{-1} we obtain the class structure of G'_W shown in Table VIII.

From Table VIII it is easily seen that $\mathbf{G}'_W$ has 14 classes with the class operators

$$\begin{aligned} &C_1=R_1,\ C_1'=iR_1,\ C_1''=-iR_1,\ C_1'''=-R_1\ , \\ &C_2=R_2-R_2,\ C_2'=iC_2,\ C_3=R_3-R_3+iR_4-iR_4\ , \\ &C_3'=iC_3,\ C_4=R_5-R_5+iR_6-iR_6,\ C_4'=iC_4\ , \\ &C_5=R_7+iR_8,\ C_5'=iC_5,\ C_5''=-iC_5,\ C_5'''=-C_5\ . \end{aligned} \tag{14.5}$$

However, only the class operators C_1 and C_5 are linearly independent. Hence $n=2$. Using Table VII, we can easily establish the multiplication relation for the class operators C_1 and C_5,

$$C_5\begin{bmatrix} C_1 \\ C_5 \end{bmatrix}=\begin{bmatrix} 0 & 1 \\ 2i & 0 \end{bmatrix}\begin{bmatrix} C_1 \\ C_5 \end{bmatrix}\ . \tag{14.6a}$$

Then the representation matrix of C_5 in the class space is

$$\mathscr{D}(C_5)=\begin{bmatrix} 0 & 2i \\ 1 & 0 \end{bmatrix}\ . \tag{14.6b}$$

By diagonalizing $\mathscr{D}(C_5)$, we know that C_5 has two distinct eigenvalues $\nu=\pm(1+i)$; therefore C_5 is a CSCO-I of $\mathbf{G}'_W$. We could use the eigenvalues $\pm(1+i)$ to label the two irreps of $\mathbf{G}'_W$, but we prefer to use the conventional symbols W_1 and W_2 to label them.

The eigenvectors of $\mathscr{D}(C_5)$ with the normalization (7.15c) (remembering that $g_1=1$ and $g_5=2$) are

$$\begin{aligned} &\nu=1+i,\ \mathbf{q}^{(W_1)}=\sqrt{1/8}(2,1-i)\ , \\ &\nu=-(1+i),\ \mathbf{q}^{(W_2)}=\sqrt{1/8}(2,-1+i)\ . \end{aligned} \tag{14.7}$$

From Eqs. (7.16) and (14.7) we get the characters of the classes C_1 and C_5. Using Eq. (14.5) we in turn get the characters of the remaining classes. The complete character table is shown in Table IX.

2. The point R of O_h^3

The vector $\mathbf{p}$ for the point R is

$$\mathbf{p}=(\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2})\ . \tag{14.8}$$

The group O_h^3 belongs to the simple cubic lattice with the generators

$$\begin{aligned} &\{C_{2z}\,|\,0\},\ \{C_{2x}\,|\,0\},\ \{C_{2a}\,|\,\boldsymbol{\tau}\}\ , \\ &\{C_{31}^{+}\,|\,0\},\ \{I\,|\,0\},\ \boldsymbol{\tau}=(\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2})\ . \end{aligned} \tag{14.9}$$

The little co-group is the point group O_h of order 48, and the little group $\mathbf{G}(\mathbf{k})$ is the space group itself.

In the same manner we can construct the multiplication table of the representation group $\mathbf{G}'_R$, which is a twofold covering group of O_h. Because of space limitations, we do not reproduce the table here, but only mention a technical point, namely that only one-fourth (i.e., a 24×24 array) of the group table of $\mathbf{G}'_R$, which only involves the proper rotations, is required.

The group $\mathbf{G}'_R$ has $N=14$ classes and $n=4$ linearly independent class operators, which are

$$\begin{aligned} &C_1=\varepsilon,\ C_2=C_{2x}+C_{2y}+C_{2z}\ , \\ &C_3=\sum_{i=1}^{4}(C_{3i}^{+}+C_{3i}^{-}),\ C_4=\sum_{i=1}^{4}(C_{3i}^{+}-C_{3i}^{-})I\ , \end{aligned} \tag{14.10}$$

where α is the abbreviation of $\{\alpha\,|\,0\}$.

The multiplication relations of these class operators are listed in Table X. From Eq. (3.7) and Table X we get

$$\begin{aligned} \mathscr{D}(C_2)&=\begin{bmatrix} 0 & 3 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}\ , \\ \mathscr{D}(C_3)&=\begin{bmatrix} 0 & 0 & 8 & 0 \\ 0 & 0 & 8 & 0 \\ 1 & 3 & 4 & 0 \\ 0 & 0 & 0 & -4 \end{bmatrix}\ , \\ \mathscr{D}(C_4)&=\begin{bmatrix} 0 & 0 & 0 & -8 \\ 0 & 0 & 0 & -8 \\ 0 & 0 & 0 & 4 \\ 1 & 3 & -4 & 0 \end{bmatrix}\ . \end{aligned} \tag{14.11}$$

The eigenvalues of the matrix $\mathscr{D}(C_2)$ are found to be

$$\lambda_2=-1\ \text{(singlet)},\ 3\ \text{(triplet)}\ .$$

The occurrence of degeneracy means that C_2 is not a CSCO-I of $\mathbf{G}'_R$. We try another matrix, say $\mathscr{D}(C_4)$. Its eigenvalues are

TABLE IX. The character table of the representation group $\mathbf{G}'_W$ for the space group O_h^7.

		Class													
ν	(ν)	1	1′	1″	1‴	2	2′	3	3′	4	4′	5	5′	5″	5‴
$1+i$	W_1	2	$2i$	$-2i$	-2	0	0	0	0	0	0	$1+i$	$-1+i$	$1-i$	$-1-i$
$-(1+i)$	W_2	2	$2i$	$-2i$	-2	0	0	0	0	0	0	$-1-i$	$1-i$	$-1+i$	$1+i$

TABLE X. Multiplication relations for the class operator of the rep group G'_R.

C_1	C_2	C_3	C_4
C_2	$3C_1+2C_2$	$3C_3$	$3C_4$
C_3	$3C_3$	$4C_3+8C_1+8C_2$	$-4C_4$
C_4	$3C_4$	$-4C_4$	$4C_3-8C_1-8C_2$

$$\lambda_4=0 \text{ (doublet)}, \ \pm 4\sqrt{3}i \text{ (singlet)} . \tag{14.2}$$

Thus C_4 is also not a CSCO-I of $\mathbf{G}'_R$. However, taken together, $C=(C_2,C_4)$ is a CSCO-I of G'_R, since by diagonalizing the matrices $\mathscr{D}(C_2)$ and $\mathscr{D}(C_4)$ simultaneously, we find four distinct sets of eigenvalues. The eigenvalues and eigenvectors are

$$\begin{aligned}
&\nu=(\lambda_2,\lambda_4)\\
&=(3,0), && \mathbf{q}^{(R_1)}=\sqrt{1/48}(2,2,2,0) ,\\
&=(3,4\sqrt{3}i), && \mathbf{q}^{(R_2)}=\sqrt{1/48}(2,2,-1,-\sqrt{3}i) ,\\
&=(3,-4\sqrt{3}i), && \mathbf{q}^{(R_3)}=\sqrt{1/48}(2,2,-1,\sqrt{3}i) ,\\
&=(3,-4\sqrt{3}i), && \\
&=(-1,0), && \mathbf{q}^{(R_4)}=\sqrt{1/48}(6,-2,0,0) .
\end{aligned} \tag{14.13}$$

The character vectors $\boldsymbol{\chi}^{(\nu)}$ of $\mathbf{G}'_R$ are simply related to the vector $\mathbf{q}^{(\nu)}$ in Eq. (14.13) by

$$\boldsymbol{\chi}^{(\nu)}=\sqrt{48}(\mathbf{q}^{(\nu)})^* . \tag{14.14}$$

From the foregoing examples, one can see clearly the power of the eigenfunction method. For both cases, the class numbers are 14. If one uses the conventional method, one needs to solve nonlinear algebraic equations of order 14, which is totally out of the question for hand calculation. By using the eigenfunction method, one reduces the problem to that of solving linear algebraic equations of order 2 or 4, which can easily be done by hand.

B. Seeking the CSCO-I from the existing character table

As will be seen in Sec. XVIII, the CSCO-I is crucial for obtaining the Clebsch-Gordan coefficient of a space group. For a group about which we know nothing except its group table, we can use the foregoing method to obtain the CSCO-I and characters of the group simultaneously. However, if the character table of a group is known, as is the case for all point groups and the 230 space groups, it is trivial to find the CSCO-I of the group by the method given in Sec. VII.C.

Now let us try to find the CSCO-I for the rep group $\mathbf{G}'_X$ of the space group O_h^7. The vector $\mathbf{p}$ for the point X is

$$\mathbf{p}=(\tfrac{1}{2}\ \tfrac{1}{2}\ 0) .$$

From Table T159 of Kovalev (1961), with slight changes in notation, we can write down the characters of the rep group $\mathbf{G}'_X$. We enter the characters of those elements whose characters are not identically zero in Table XI.

It is seen that $\{C_{2a}\,|\,\tau\}'$ and $-\{C_{2b}\,|\,\tau\}'$ belong to the same class, and $\{\sigma_{da}\,|\,0\}$ and $\{\sigma_{db}\,|\,0\}$ belong to the same class. Furthermore, according to Eq. (6.47), Table XI after deleting the sixth and eighth columns is (accidently) the eigenvalue table of the class operators. Hence we see that the class operators

$$\begin{aligned}
C_1&=\{C_{2a}\,|\,\tau\}'-\{C_{2b}\,|\,\tau\}' ,\\
C_2&=\{\sigma_{da}\,|\,0\}+\{\sigma_{db}\,|\,0\} ,
\end{aligned} \tag{14.15}$$

have $n=4$ distinct sets of eigenvalues as shown in the first column of Table XI. Therefore, (C_1,C_2) is a CSCO-I of $\mathbf{G}'_X$.

C. Constructing irreps of the rep group $\mathbf{G}'_k$

1. The point W of O_h^7

With $n=2$, and $|\mathbf{G}_0(W)|=8$, Eq. (6.3) reads

$$8=2^2+2^2 . \tag{14.16}$$

Therefore, the eight-dimensional rep produced by the space $L(W)$ can be decomposed into two inequivalent irreps with dimension 2, each occurring twice. We choose

$$(C(s),\bar{C}(s))=(R_7,\bar{R}_7) . \tag{14.17}$$

The matrices of the operator R_7 and $\bar{R}_7$ in the space $L(W)$ can be read out from the seventh row and seventh

TABLE XI. Character table of the rep group $\mathbf{G}'_X$ for the space group O_h^7.

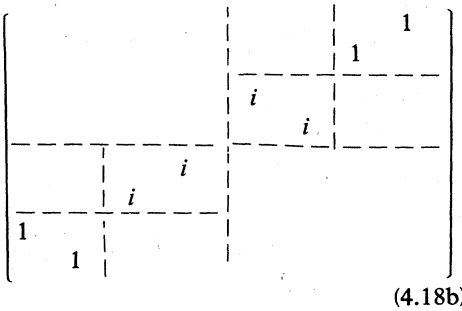
(C_1,C_2)	(ν)	$\{\varepsilon\,\|\,0\}'$	$\{C_{2z}\,\|\,0\}'$	$\{C_{2a}\,\|\,\tau\}'$	$\{C_{2b}\,\|\,\tau\}'$	$\{\sigma_{da}\,\|\,0\}'$	$\{\sigma_{db}\,\|\,0\}'$
(0,2)	X_1	2	2	0	0	2	2
(0,−2)	X_2	2	2	0	0	−2	−2
(2i,0)	X_3	2	−2	2i	−2i	0	0
(−2i,0)	X_4	2	−2	−2i	2i	0	0

[a] X_i are related to Kovalev's $\hat{\tau}^i$ by $X_1\to\hat{\tau}^3$, $X_2\to\hat{\tau}^4$, $X_3\to\hat{\tau}^2$, $X_4\to\hat{\tau}^1$.

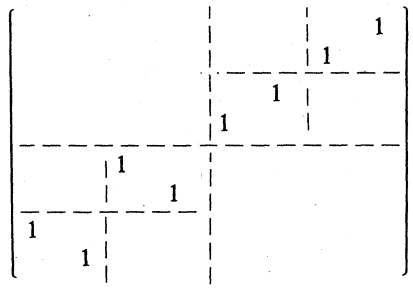
column, respectively, of Table VII,

$$D(R_7)=(7,8,i6,i5,i3,i4,2,1)\ ,$$
$$D(\bar{R}_7)=(78564321)\ , \tag{14.18a}$$

where the shorthand notations stand for

$D(R_7)=$ 

(4.18b)

$D(\bar{R}_7)=$ 

These matrices are very much like the ordinary regular rep matrices, in that in each row and each column there is only one nonvanishing element.

The element $R_7=\{S_{4x}^{-}\mid 0\}$ obeys the algebraic equation $(R_7)^4=1$. Hence the eigenvalues of R_7 are easily found to be $\pm 1,\pm i$ without the necessity of solving the secular equation. The same applies to the eigenvalues of $\bar{R}_7$.

Substituting the eigenvalues $a,b=\pm 1,\pm i$ into the eigenequations of $D(R_7)$ and $D(\bar{R})$, we obtain eight simultaneous eigenvectors of $(R_7,\bar{R}_7)$ corresponding to the eight distinct sets of eigenvalues, $(a,b)=(1,1),(i,1),(1,i)(i,i),(-1,-1),(-i,-1)(-1,-i),(-i,-i)$. Therefore, $(R_7,\bar{R}_7)$ is already a CSCO-III of group $\mathbf{G}'_W$, and the CSCO-I of $\mathbf{G}'_W$ is redundant in decomposing the rep space $L(\mathbf{k})$. Of course it happens only by accident. If we had chosen $(C(s),\bar{C}(s))=(R_2,\bar{R}_2)$, the CSCO-III of $\mathbf{G}'_W$ would have had to include the CSCO-I of $\mathbf{G}'_W$. Hence a suitable choice of $C(s)$ can save lots of labor.

The eigenvectors are listed in Table XII.

From Eq. (6.1d) or (13.5) we know that the first four vectors in Table XII belong to an irrep labeled by W_1, and the other four vectors belong to another irrep labeled by W_2.

The phases of the eigenvectors in Table XII are determined by the three steps given in Sec. VI.C. The phases for the first, fourth, fifth, and eighth rows are determined by step (1). The phases of the second and sixth rows can be chosen arbitrarily according to step (2). The phases of the third and seventh rows are determined by step (3). For example, from the first and second rows of Table XII as well as from Table VII, we can evaluate

$$D_{12}^{(W_1)}(R_3)=\langle\psi_1^{(W_1)1}\mid R_3\mid\psi_i^{(W_1)1}\rangle$$
$$=\tfrac{1}{4}\langle 1+2+7+8\mid 3\mid 3+4+5+6\rangle=i\ ,$$

where we used obvious abbreviations. Therefore, the coefficient in front of R_3 in the third row $\psi_1^{(W_1)b=2}\equiv\psi_1^{(W_1)i}$ must be proportional to $D_{12}^{(W_1)}(R_3)^*=-i$.

Our result in Table XII differs from that of Bradley

TABLE XII. The irreducible bases and irreps of the rep group $\mathbf{G}'_W$ for the space group O_h^7.

$\psi_a^{(\nu)b}$	N		$\{\varepsilon\mid 0\}'$ R_1	$\{C_{2x}\mid 0\}'$ R_2	$\{C_{2d}\mid 0\}'$ R_3	$\{C_{2f}\mid\tau\}'$ R_4	$\{\sigma_y\mid\tau\}'$ R_5	$\{\sigma_z\mid\tau\}'$ R_6	$\{S_{4x}^{-}\mid 0\}'$ R_7	$\{S_{4x}^{+}\mid 0\}'$ R_8
$\psi_1^{(W_1)1}$	$\frac{1}{2}$	D_{11}^*	1	1					1	1
$\psi_i^{(W_1)1}$	$\frac{1}{2}$	D_{21}^*			1	1	1	1		
$\psi_1^{(W_1)i}$	$\frac{1}{2}$	D_{12}^*			$-i$	i	-1	1		
$\psi_i^{(W_1)i}$	$\frac{1}{2}$	D_{22}^*	1	-1					$-i$	i
$\psi_{-1}^{(W_2)-1}$	$\frac{1}{2}$	D_{11}^*	1	1					-1	-1
$\psi_{-i}^{(W_2)-1}$	$\frac{1}{2}$	D_{21}^*			1	1	-1	-1		
$\psi_{-1}^{(W_2)-i}$	$\frac{1}{2}$	D_{12}^*			$-i$	i	1	-1		
$\psi_{-i}^{(W_2)-i}$	$\frac{1}{2}$	D_{22}^*	1	-1					i	$-i$
$\Delta^{(W_1)}(\gamma_i)=D^{(W_1)}(R_i)$			$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$	$\begin{bmatrix}0&i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-1\\1&0\end{bmatrix}$	$\begin{bmatrix}0&1\\1&0\end{bmatrix}$	$\begin{bmatrix}1&0\\0&i\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-i\end{bmatrix}$
$\Delta^{(W_2)}(\gamma_i)=D^{(W_2)}(R_i)$			$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$	$\begin{bmatrix}0&i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&-i\\1&0\end{bmatrix}$	$\begin{bmatrix}0&1\\-1&0\end{bmatrix}$	$\begin{bmatrix}0&-1\\-1&0\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&-i\end{bmatrix}$	$\begin{bmatrix}-1&0\\0&i\end{bmatrix}$

and Cracknell (1972, p. 168) in phase choice. However, if we let the basis vectors in Table XII undergo the transformations

$$\psi_i^{(W_1)1}\to\omega\psi_i^{(W_1)1},\quad \psi_{-i}^{(W_2)-1}\to\omega\psi_{-i}^{(W_2)-1},$$
$$\psi_1^{(W_1)i}\to -i\omega\psi_1^{(W_1)i},\quad \psi_{-1}^{(W_2)-i}\to -i\omega\psi_{-1}^{(W_2)-i},$$
$$\omega=e^{-3\pi i/4},$$

the two results become identical.

2. The point R of O_h^3

From Eq. (14.13) it is known that the rep group $\mathbf{G}'_R$ has three two-dimensional and one six-dimensional irreps. Let us construct the six-dimensional rep $D^{(R_4)}$. According to Eq. (14.13), $D^{(R_4)}$ corresponds to the single root -1 of the class operator,

$$C_2=C_{2x}+C_{2y}+C_{2z}\ . \tag{14.19}$$

Thus for our purposes, we can take C_2 as the CSCO-I of $\mathbf{G}'_R$. The operator sets $C(s)$ and $\bar{C}(s)$ are chosen as

$$C(s)=(I,C_{2x},C_{2y}),\quad \bar{C}(s)=(\bar{I},\bar{C}_{2x},\bar{C}_{2y})\ . \tag{14.20}$$

The advantage of choosing inversion I as an element of $C(s)$ is that under this choice, I and $\bar{I}$ are diagonal with the eigenvalues ±1. The linear combination coefficients u_i and $u_{i'}$ in front of the elements R_i and $R_{i'}=R_iI$ are thus related to each other by

$$u_{i'}=\pm u_i,\quad i=1,2,\ldots,24 \text{ for } \bar{I}=\begin{cases}+1\\-1\end{cases}. \tag{14.21}$$

As a consequence, the number of sought-for coefficients is immediately reduced from 48 to 24, and to find them, again only one-fourth (i.e., a 24×24 array) of the group table of $\mathbf{G}'_R$ is sufficient.

From the relevant one-fourth of the group table of $\mathbf{G}'_R$, we can immediately write down the eigenequations of the operators C_2, I, C_{2x}, C_{2y}, $\bar{I}$, $\bar{C}_{2x}$, and $\bar{C}_{2y}$. For hand calculation, we can substitute the eigenvalues -1 for C_2, and ±1 for the remaining six operators in the corresponding eigenequations and find their simultaneous eigenvectors. It is easily found that nonvanishing eigenvectors are obtainable only for the following six sets of eigenvalues of $C(s)=(I,C_{2x},C_{2y})$ or $\bar{C}(s)=(\bar{I},\bar{C}_{2x},\bar{C}_{2y})$:

$$(1,1,-1),(1,-1,1),(1,-1,-1),(-1,1,-1),(-1,-1,1),(-1,-1,-1)\ . \tag{14.22}$$

The ordering in Eq. (14.22) corresponds to the index $a,b=1,2,\ldots,6$. After adjusting the phases of the eigenvectors as in previous example, by using Eq. (13.8) we can write down the representation matrices:

$$\begin{array}{llll}
\{\varepsilon\,|\,0\}=(1\,2\,3\,4\,5\,6), & \{C_{2x}\,|\,0\}=(1\,\bar2\,\bar3\,4\,\bar5\,\bar6), & \{C_{2y}\,|\,0\}=(\bar1\,2\,\bar3\,\bar4\,5\,\bar6), & \{C_{2z}\,|\,0\}=(\bar1\,\bar2\,3\,\bar4\,\bar5\,6),\\
\{C_{4x}^-\,|\,\tau\}'=(4\,\bar6\,\bar5\,\bar1\,3\,\bar2), & \{C_{4y}^-\,|\,\tau\}'=(6\,\bar5\,\bar4\,3\,2\,1), & \{C_{4z}^-\,|\,\tau\}'=(5\,4\,6\,2\,1\,\bar3), & \{C_{4x}^+\,|\,\tau\}'=(4\,6\,5\,\bar1\,3\,2),\\
\{C_{4y}^+\,|\,\tau\}'=(\bar6\,\bar5\,4\,3\,2\,\bar1), & \{C_{4z}^+\,|\,\tau\}'=(\bar5\,\bar4\,6\,\bar2\,\bar1\,\bar3), & \{C_{31}^-\,|\,0\}=(3\,1\,2\,6\,\bar4\,\bar5), & \{C_{32}^-\,|\,0\}=(\bar3\,1\,\bar2\,\bar6\,\bar4\,5),\\
\{C_{33}^-\,|\,0\}=(\bar3\,\bar1\,2\,\bar6\,4\,\bar5), & \{C_{34}^-\,|\,0\}=(3\,\bar1\,\bar2\,6\,4\,5), & \{C_{31}^+\,|\,0\}=(2\,3\,1\,\bar5\,\bar6\,4), & \{C_{32}^+\,|\,0\}=(2\,\bar3\,\bar1\,5\,6\,\bar4),\\
\{C_{33}^+\,|\,0\}=(\bar2\,3\,\bar1\,5\,\bar6\,\bar4), & \{C_{34}^+\,|\,0\}=(\bar2\,\bar3\,1\,5\,6\,4), & \{C_{2a}\,|\,\tau\}'=(\bar5\,4\,\bar6\,\bar2\,1\,3), & \{C_{2b}\,|\,\tau\}'=(5\,\bar4\,\bar6\,2\,\bar1\,3),\\
\{C_{2c}\,|\,\tau\}'=(6\,5\,4\,\bar3\,\bar2\,\bar1), & \{C_{2d}\,|\,\tau\}'=(\bar4\,6\,\bar5\,1\,3\,\bar2), & \{C_{2e}\,|\,\tau\}'=(\bar6\,5\,\bar4\,3\,\bar2\,1), & \{C_{2f}\,|\,\tau\}'=(\bar4\,\bar6\,5\,1\,\bar3\,2).
\end{array} \tag{14.23}$$

The parentheses here stand for matrices as exemplified by

$$(4\,\bar6\,\bar5\,\bar1\,3\,\bar2)=\begin{vmatrix} & & & -1 & 0 & 0\\ & \mathbf{0} & & 0 & 0 & -1\\ & & & 0 & -1 & 0\\ 1 & 0 & 0 & & & \\ 0 & 0 & -1 & & \mathbf{0} & \\ 0 & -1 & 0 & & & \end{vmatrix}. \tag{14.24}$$

Multiplying the matrices in Eq. (14.23) by $D(I)=(1\,2\,3\,\bar4\,\bar5\,\bar6)$, we get the representation matrices for the other 24 elements of $\mathbf{G}'_R$.

It should be pointed out that the choices of the operator set $C(s)$, the CSCO-II $M=(C,C(s))$, and CSCO-III $K=(C,C(s),\bar{C}(s))$ are not unique. We can choose each of them to consist of a single operator. For example, in the above case we can choose $C(s)$ as

$$\mathscr{C}(s)=3I+2C_{2x}+C_{2y}\ .$$

It has six distinct eigenvalues, 4, 2, 0, -2, -4, and -6, corresponding to the six sets of eigenvalues in Eq. (14.22). We can also choose

$$7\mathscr{C}(s)+5\overline{\mathscr{C}}(s)$$

in place of the operator set $(I,C_{2x},C_{2y},\bar{I},\bar{C}_{2x},\bar{C}_{2y})$, which has 36 distinct eigenvalues $(7a+5b)$, with $a,b=0$, ±2, ±4, and -6. Clearly, for computer calculation, the fewer the operators to be diagonalized simultaneously the better. However, for hand calculation, this is not necessarily so, as can be seen from the above example.

XV. IRREDUCIBLE BASIS AND REPRESENTATIONS OF THE SPACE GROUP

A. The induced rep

We first factorize the space group $\mathbf{G}$ into left cosets with respect to the little group $\mathbf{G}(\mathbf{k})$,

$$\mathbf{G}=\mathbf{G}(\mathbf{k})+\{\beta_2\,|\,\mathbf{V}(\beta_2)\}\mathbf{G}(\mathbf{k})+\cdots +\{\beta_q\,|\,V(\beta_q)\}\mathbf{G}(\mathbf{k})\ . \tag{15.1}$$

Suppose that $\psi^{(\nu)}_{\mathbf{k},a}$ is an IRB of the little group $\mathbf{G}(\mathbf{k})$ and let us define

$$\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\{\beta_\sigma\,|\,\mathbf{V}(\beta_\sigma)\}\psi^{(\nu)}_{\mathbf{k},a}\ , \qquad \sigma=1,2,\ldots,q;a=1,2,\ldots,h_\nu\ , \tag{15.2}$$

with the convention that $\{\beta_1\,|\,\mathbf{V}(\beta_1)\}=\{\varepsilon\,|\,0\}$. The q wave vectors

$$\mathbf{k}_\sigma=\beta_\sigma\mathbf{k},\quad \sigma=1,2,\ldots,q \tag{15.3a}$$

form what is called a star, or set of mutually inequivalent $\mathbf{k}$ vectors

$$*\mathbf{k}=(\mathbf{k}_1,\mathbf{k}_2,\ldots,\mathbf{k}_q)\ , \tag{15.3b}$$

with $\mathbf{k}_1\equiv\mathbf{k}$. The wave vector $\mathbf{k}$ is called the canonical wave vector (Birman, 1974). Any one of the q wave vectors can serve as the canonical wave vector. If $\mathbf{k}$ is a general point in the Brillouin zone, then $\mathbf{k}$ is called a general star, otherwise it is called a special star.

The space

$$\mathscr{L}(\mathbf{k}_\sigma)=\{\psi^{(\nu)}_{\mathbf{k}_\sigma a}:a=1,2,\ldots,h_\nu\} \tag{15.3c}$$

is isomorphic to the space $\mathscr{L}(\mathbf{k})$, or to the group space $L(\mathbf{k})$ of the rep group $\mathbf{G}'_{\mathbf{k}}$. Clearly, the space $\mathscr{L}(*k)$ defined by Eq. (10.2c) is decomposed into a direct sum of the q spaces $\mathscr{L}(\mathbf{k}_\sigma)$ isomorphic to one another,

$$\mathscr{L}(*\mathbf{k})=\sum_{\sigma=1}^{q}\oplus\mathscr{L}(\mathbf{k}_\sigma)\ . \tag{15.3d}$$

Let us apply an element $\{\alpha\,|\,\mathbf{a}\}$ of $\mathbf{G}$ to Eq. (15.2),

$$\{\alpha\,|\,\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\psi^{(\nu)}_{\mathbf{k},a}\ . \tag{15.4}$$

$\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,V_\sigma\}$ must be an element of $\mathbf{G}$ and must belong to one and only one coset, say the τth coset, i.e.,

$$\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}=\{\beta_\tau\,|\,\mathbf{V}_\tau\}\{\gamma\,|\,\mathbf{c}\}\ . \tag{15.5}$$

Assembling Eqs. (15.2), (15.5), and (13.13a), we obtain

$$\{\alpha\,|\,\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\{\beta_\tau\,|\,\mathbf{V}_\tau\}\sum_b D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma\,|\,\mathbf{c}\})\psi^{(\nu)}_{\mathbf{k},b} =\sum_b D^{(k)(\nu)}_{ba}(\{\gamma\,|\,\mathbf{c}\})\psi^{(\nu)}_{\mathbf{k}_\tau b}\ , \tag{15.6}$$

where $D^{(\mathbf{k})(\nu)}(\{\gamma\,|\,\mathbf{c}\})$ is the irreducible matrix of the little group $\mathbf{G}(\mathbf{k})$. Therefore, the qh_ν functions $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ carry a rep for the space group $\mathbf{G}$, which is called the induced rep and denoted by $D^{(*\mathbf{k})(\nu)}$ (Birman, 1974) or $D^{(\mathbf{k})(\nu)}{\uparrow}\mathbf{G}$ (Bradley and Cracknell, 1972). It will be proved in Sec. XVI.B that the induced rep $D^{(*\mathbf{k})(\nu)}$ is an irrep of the space group $\mathbf{G}$.

The induced rep is of qh_ν dimension, and its matrix elements can be expressed as

$$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha\,|\,\mathbf{a}\})=\langle\psi^{(\nu)}_{\mathbf{k}_\tau b}\,|\,\{\alpha\,|\,\mathbf{a}\}\,|\,\psi^{(\nu)}_{\mathbf{k}_\sigma a}\rangle\ . \tag{15.7a}$$

Define

$$R_{\bar\tau\alpha\sigma}\equiv\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\ . \tag{15.7b}$$

It follows from Eqs. (15.2) and (15.7a) that

$$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha\,|\,\mathbf{a}\})=\langle\psi^{(\nu)}_{\mathbf{k},b}\,|\,R_{\bar\tau\alpha\sigma}\,|\,\psi^{(\nu)}_{\mathbf{k},a}\rangle\ . \tag{15.7c}$$

According to the left coset decomposition (15.1), we know that $R_{\bar\tau\alpha\sigma}$ is either an element of the little group $\mathbf{G}(\mathbf{k})$ or a coset representative $\{\beta\,|\,\mathbf{V}(\beta)\}$ times an element of $\mathbf{G}(\mathbf{k})$. For the former, the right-hand side of Eq. (15.7c) is just the irreducible matrix element of $\mathbf{G}(\mathbf{k})$, and for the latter, Eq. (15.7c) must vanish, since $R_{\bar\tau\alpha\sigma}=\{\beta\,|\,\mathbf{V}(\beta)\}\times\{\gamma\,|\,\mathbf{c}\}$ will change the wave vector $\mathbf{k}$ into $\mathbf{k}_\beta$, while $\mathbf{k}$ is the label for the irreps of the translational group $\mathbf{T}$, and the bases belonging to different irreps of $\mathbf{T}$ are orthogonal. Hence Eq. (15.7c) can be expressed as

$$D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha\,|\,\mathbf{a}\})=D^{(\mathbf{k})(\nu)}_{ba}(R_{\bar\tau\alpha\sigma}) =D^{(\mathbf{k})(\nu)}_{ba}(\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\})\ . \tag{15.7d}$$

[Recall our convention about the representation matrix symbol $D(X)$, stated after Eq. (11.3).]

It is convenient to write the $qh_\nu\times qh_\nu$ matrix $D^{(*\mathbf{k})(\nu)}$ in block decomposition form (Birman, 1974),

$$D^{(*\mathbf{k})(\nu)}(\{\alpha\,|\,\mathbf{a}\})=\begin{bmatrix} D^{(*\mathbf{k})(\nu)}_{(11)} & \cdots & D^{(*\mathbf{k})(\nu)}_{(1q)} \\ \vdots & & \vdots \\ D^{(*\mathbf{k})(\nu)}_{(q1)} & \cdots & D^{(*\mathbf{k})(\nu)}_{(qq)} \end{bmatrix}, \tag{15.8a}$$

where

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\})=D^{(\mathbf{k})(\nu)}(\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\{\alpha\,|\,\mathbf{a}\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}) \tag{15.8b}$$

is a $(h_\nu\times h_\nu)$ matrix. According to Eq. (15.5), for given $\{\alpha\,|\,\mathbf{a}\}$ and σ there is only a unique τ that enables $R_{\bar\tau\alpha\sigma}$ to belong to the little group $\mathbf{G}(\mathbf{k})$. As a consequence, in each row and each column of the block form (15.8a), only one matrix block differs from zero. Another way of saying this is that for given σ and τ, only those elements of $\mathbf{G}$ which satisfy

$$\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\}=\{\beta_\tau\,|\,\mathbf{V}_\tau\}\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_m\}\times\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1},\quad \gamma\in\mathbf{G}_0(\mathbf{k}) \tag{15.8c}$$

have the nonzero submatrices

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})=D^{(\mathbf{k})(\nu)}(\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_m\})\ . \tag{15.8d}$$

Notice that there is a one-to-one correspondence between α and γ on the one hand, and $\mathbf{R}_n$ and $\mathbf{R}_m$ on the other hand.

Kunert and Suffczynski (1982) have written a program for computing the full matrices $D^{(*\mathbf{k})(\nu)}$ for space groups with body-centered-cubic lattices. They first calculate the matrices for the generators of the group, and then use matrix multiplication to get all the matrices. In the following, we shall give a simpler algorithm for the full matrices.

B. A simple algorithm for full rep matrices

So far we have only recapitulated the result given by Birman (1974). To go further, we note that Eq. (15.8d), though simple in appearance, is not the best form for practical construction of the full matrices of a space group. In the following, we rewrite it in a more appropriate form.

From Eq. (15.8b) we have

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\}) = D^{(\mathbf{k})(\nu)}(\{\beta_\tau^{-1}\alpha\beta_\sigma\,|\,\beta_\tau^{-1}(\alpha\mathbf{V}_\sigma-\mathbf{V}_\tau+\mathbf{a})\})\ . \tag{15.8e}$$

With the help of Eq. (11.10c), this becomes

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\}) = \exp[-i\mathbf{k}_\tau\cdot(\alpha\mathbf{V}_\sigma-\mathbf{V}_\tau+\mathbf{a})] \times \mathscr{D}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\})\ . \tag{15.9a}$$

where

$$\mathscr{D}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\}) \equiv \Delta(\beta_\tau^{-1}\alpha\beta_\sigma)\ , \tag{15.9b}$$

with the convention

$$\Delta(\beta_\tau^{-1}\alpha\beta_\sigma)=0 \quad \text{if } \beta_\tau^{-1}\alpha\beta_\sigma \notin \mathbf{G}_0(\mathbf{k})\ . \tag{15.9c}$$

In other words,

$$\Delta(\beta_\tau^{-1}\alpha\beta_\sigma)=0 \tag{15.10a}$$

unless

$$\beta_\tau^{-1}\alpha\beta_\sigma=\gamma\ , \tag{15.10b}$$

or

$$\alpha\beta_\sigma=\beta_\tau\gamma\ . \tag{15.10c}$$

Multiplying Eq. (15.10c) from the right by $\mathbf{k}$, we obtain another form of condition (15.10b):

$$\alpha\mathbf{k}_\sigma \doteq \mathbf{k}_\tau\ . \tag{15.10d}$$

Setting $\{\alpha\,|\,\mathbf{a}\}=\{\varepsilon\,|\,\mathbf{R}_n\}$, from Eq. (15.10d) we must have $\sigma=\tau$, while from Eq. (15.9) we have

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\varepsilon\,|\,\mathbf{R}_n\}) = \delta_{\tau\sigma}e^{-i\mathbf{k}_\tau\cdot\mathbf{R}_n}\Delta(\varepsilon) = \delta_{\tau\sigma}e^{-i\mathbf{k}_\tau\cdot\mathbf{R}_n}\mathbf{I}_\nu\ , \tag{15.11}$$

where $\mathbf{I}_\nu$ is the $h_\nu\times h_\nu$ unit matrix.

Hence we see that the translation $\{\varepsilon\,|\,\mathbf{R}_n\}$ is represented by the diagonal matrix

$$D^{(*\mathbf{k})(\nu)}(\{\varepsilon\,|\,\mathbf{R}_n\}) = \begin{bmatrix} e^{-i\mathbf{k}_1\cdot\mathbf{R}_n}\mathbf{I}_\nu & & 0 \\ & \ddots & \\ 0 & & e^{-i\mathbf{k}_q\cdot\mathbf{R}_n}\mathbf{I}_\nu \end{bmatrix}\ . \tag{15.12}$$

Equation (15.9) gives a very convenient formula for constructing irreps of the space group $\mathbf{G}$ from the irreps $\Delta(\gamma)=D^{(\mathbf{k})(\nu)}(\{\gamma\,|\,\mathbf{V}(\gamma)\}')$ of the rep group $\mathbf{G}'_\mathbf{k}$. The procedure for obtaining irreps of $\mathbf{G}$ can be summarized as follows.

(1) Following our procedure for Eq. (15.8a), we first introduce a matrix $\mathscr{D}(\{\alpha\,|\,\mathbf{a}\})$, whose $(\sigma\tau)$ block is the matrix $\mathscr{D}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\})$ defined by Eq. (15.9b). To obtain $\mathscr{D}(\{\alpha\,|\,\mathbf{a}\})$, let us build up an array with q rows labeled by $\varepsilon,\beta_2^{-1},\ldots,\beta_q^{-1}$ and q columns labeled by $\varepsilon,\beta_2,\ldots,\beta_q$,

$$\mathscr{D}(\{\alpha\,|\,\mathbf{a}\}) = \begin{array}{c} \\ \varepsilon \\ \beta_2^{-1} \\ \vdots \\ \beta_\tau^{-1} \\ \vdots \\ \beta_q^{-1} \end{array} \begin{array}{c} \begin{array}{ccccccc} \varepsilon & \beta_2 & \cdots & \beta_\sigma & \cdots & \beta_q \end{array} \\ \begin{bmatrix} & & & 0 & & \\ & & & 0 & & \\ & & & \vdots & & \\ 0 & 0 & \cdots & \Delta(\gamma) & \cdots & 0 \\ & & & \vdots & & \\ & & & 0 & & \end{bmatrix} \end{array} \quad \text{for } \beta_\tau^{-1}\alpha\beta_\sigma=\gamma\ . \tag{15.13}$$

Utilizing the point-group multiplication table, we form the products $\beta_\tau^{-1}\alpha\beta_\sigma$ for given τ with varying $\sigma=1,2,\ldots$. In each step we check whether $\beta_\tau^{-1}\alpha\beta_\sigma$ is an element of the point group $\mathbf{G}_0(\mathbf{k})$. If not, we put a zero (an $h_\nu\times h_\nu$ null matrix) in the $(\tau\sigma)$ block; if yes, e.g., $\beta_\tau^{-1}\alpha\beta_\sigma=\gamma$, then we put $\Delta(\gamma)$ into the $(\tau\sigma)$ block and zero for all the remaining entries in the τth row and σth column. We repeat this process for each $\tau=1,2,\ldots,q$.

(2) Multiplying the nonzero matrices $\Delta(\gamma)$ in Eq. (15.13) by the appropriate phase factors $\exp[-i\mathbf{k}_\tau\cdot(\alpha\mathbf{V}_\sigma-\mathbf{V}_\tau+\mathbf{a})]$, we immediately get the sought-for matrix $D^{(*\mathbf{k})(\nu)}(\{\alpha\,|\,\mathbf{a}\})$.

(3) The following symmetries (15.14) of the matrix $\mathscr{D}(\{\alpha\,|\,\mathbf{a}\})$ can be used either to save work or to check the calculation.

From Eq. (15.9b) it is seen that if

$$\mathscr{D}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\})=\Delta(\gamma),\quad \gamma=\beta_\tau^{-1}\alpha\beta_\sigma\ , \tag{15.14a}$$

then

$$\mathscr{D}_{(\sigma\tau)}(\{\alpha\,|\,\mathbf{a}\}^{-1})=\Delta(\gamma^{-1})\ . \tag{15.14b}$$

Furthermore, if $\alpha=\alpha^{-1}$, we have

$$\mathscr{D}_{(\sigma\tau)}(\{\alpha\,|\,\mathbf{a}\})=\Delta(\gamma^{-1})\ , \tag{15.14c}$$

since

$$\mathscr{D}_{(\sigma\tau)}(\{\alpha\,|\,\mathbf{a}\})=\Delta(\beta_\sigma^{-1}\alpha\beta_\tau)=\Delta((\beta_\tau^{-1}\alpha\beta_\sigma)^{-1}) .$$

For examples of these symmetries, see Eqs. (19.10) and (19.21).

From the foregoing discussion we see clearly that in the process of constructing irreps of the space group we are able to avoid tedious space-group multiplication, and only the much simpler point-group multiplication is required.

Another point that deserves pointing out is that the choice of the coset representative $\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}$ is arbitrary, i.e., any element in a coset can be chosen as the representative of that coset. Different choices of the representatives correspond to different conventions for relative phases between the basis vectors $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ with different σ. For practical purposes, it is always desirable to choose elements that do not associate with nonprimitive translations as the coset representatives, since under such a choice Eq. (15.9) is simplified as follows:

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\alpha\,|\,\mathbf{a}\})=e^{-i\mathbf{k}_\tau\cdot\mathbf{a}}\Delta(\beta_\tau^{-1}\alpha\beta_\sigma) , \tag{15.15}$$

suitable for $\mathbf{V}(\beta_\sigma)=\mathbf{V}(\beta_\tau)=0$.

C. The $\mathbf{G}\supset\mathbf{G}(\mathbf{k}_\sigma)\supset\mathbf{G}(s_\sigma)\supset\mathbf{T}$ irreducible basis

Finally let us take a look at the meaning of the irreducible basis vectors $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ of the space group $\mathbf{G}$. We have already seen that $\psi^{(\nu)}_{\mathbf{k},a}$ is the $\mathbf{G}\supset\mathbf{G}(\mathbf{k})\supset\mathbf{G}(s)\supset\mathbf{T}$ irreducible basis and obeys the eigenequations

$$\begin{bmatrix} C \\ C(s) \\ \hat{\mathbf{k}} \end{bmatrix}\psi^{(\nu)}_{\mathbf{k},a}=\begin{bmatrix} \nu \\ a \\ \mathbf{k} \end{bmatrix}\psi^{(\nu)}_{\mathbf{k},a} , \tag{15.16}$$

where C and $C(s)$ are the CSCO-I of the rep groups $\mathbf{G}'_\mathbf{k}$ and $\mathbf{G}'_s$, respectively, and $\hat{\mathbf{k}}=-i\nabla$ is the CSCO-I of $\mathbf{T}$. Since the little group $\mathbf{G}(\mathbf{k})$ and the rep group $\mathbf{G}'_\mathbf{k}$ have common irreducible bases and common irrep labels, for convenience in exposition, we shall refer to the CSCO-I C of $\mathbf{G}'_\mathbf{k}$ in Secs. XV–XVII as the CSCO-I of the little group $\mathbf{G}(\mathbf{k})$; similarly, the CSCO-I $C(s)$ of $\mathbf{G}'_s$ will be referred to as the CSCO-I of the subgroup $\mathbf{G}(s)$ of $\mathbf{G}(\mathbf{k})$.

As in Eq. (10.3) we may define the little group $\mathbf{G}(\mathbf{k}_\sigma)$ for the wave vector $\mathbf{k}_\sigma=\beta_\sigma\mathbf{k}$ such that under the rotations of the rotational part of $\mathbf{G}(\mathbf{k}_\sigma)$, the wave vector $\mathbf{k}_\sigma$ is invariant modulo a reciprocal lattice vector. Clearly the relation between the groups $\mathbf{G}(\mathbf{k}_\sigma)$ and $\mathbf{G}(\mathbf{k})$ is

$$\mathbf{G}(\mathbf{k}_\sigma)=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\mathbf{G}(\mathbf{k})\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1} . \tag{15.17a}$$

Suppose $\{\alpha\,|\,\mathbf{a}\}$ is an element of $\mathbf{G}(\mathbf{k}_\sigma)$; then $\{\alpha\,|\,\mathbf{a}\}$ is necessarily of the form

$$\{\alpha\,|\,\mathbf{a}\}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_n\}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1} . \tag{15.18a}$$

From Eqs. (15.18a) and (15.6) we have

$$\{\alpha\,|\,\mathbf{a}\}\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\sum_b D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_n\})\psi^{(\nu)}_{\mathbf{k}_\sigma b} , \tag{15.18b}$$

that is, $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ is the irreducible basis of the group $\mathbf{G}(\mathbf{k}_\sigma)$. Furthermore, as in Eq. (15.17a) we define

$$\mathbf{G}(s_\sigma)\equiv\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\mathbf{G}(s)\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1} . \tag{15.17b}$$

Clearly $\mathbf{G}(s_\sigma)$ is a subgroup of $\mathbf{G}(\mathbf{k}_\sigma)$. According to Eq. (15.17), the CSCO-I of $\mathbf{G}(\mathbf{k}_\sigma)$ and $\mathbf{G}(s_\sigma)$ are

$$\begin{aligned} C(\mathbf{k}_\sigma)&=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}C\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1} , \\ C(s_\sigma)&=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}C(s)\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1} . \end{aligned} \tag{15.19}$$

With Eqs. (15.2), (15.16), and (15.19) we have

$$\begin{bmatrix} C(\mathbf{k}_\sigma) \\ C(s_\sigma) \\ \hat{\mathbf{k}} \end{bmatrix}\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\begin{bmatrix} \nu \\ a \\ \mathbf{k}_\sigma \end{bmatrix}\psi^{(\nu)}_{\mathbf{k}_\sigma a} . \tag{15.20}$$

Hence we see that the partner (or component) $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ of the irreducible basis of a space group $\mathbf{G}$ is the $\mathbf{G}\supset\mathbf{G}(\mathbf{k}_\sigma)\supset\mathbf{G}(s_\sigma)\supset\mathbf{T}$ irreducible basis. In other words, the group chains used to classify the irreducible basis vectors of a space group $\mathbf{G}$ vary with the components. This is quite different from the usual case (e.g., the permutation group, rotation group, or unitary group), where the same group chain is always used to classify all the components in a given irrep of the group.

XVI. DECOMPOSITION OF REGULAR REPRESENTATION OF A SPACE GROUP

A. Born-Karman boundary conditions

In order to adapt the criteria of irreducibility for a finite group to a space group, we impose the so-called Born-Karman cyclic boundary conditions, so that the space group becomes a finite group. The Born-Karman conditions require (see, for example, Birman, 1974) that we choose three large real positive numbers N_1, N_2, and N_3 such that the points in crystal space defined by $\mathbf{r}$ and $\mathbf{r}+2N_i\mathbf{t}_i$, $i=1,2,3$, are identical and therefore the translation vectors $\mathbf{R}_n$ satisfy the cyclic conditions

$$\begin{aligned} \mathbf{R}_n+2N_1\mathbf{t}_1&=\mathbf{R}_n+2N_2\mathbf{t}_2 \\ &=\mathbf{R}_n+2N_3\mathbf{t}_3=\mathbf{R}_n . \end{aligned} \tag{16.1}$$

In this way the translation group $\mathbf{T}$ becomes a finite group with the elements

$$\begin{aligned} &\mathbf{R}_n=n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3 , \\ &-N_i\le n_i\le N_i-1 . \end{aligned} \tag{16.2}$$

The order of $\mathbf{T}$ is denoted by N and

$$N=8N_1N_2N_3 , \tag{16.3}$$

while the space group $\mathbf{G}$ also becomes a finite group with the elements

$$\{\alpha_i \mid \mathbf{V}(\alpha_i)+\mathbf{R}_n\},\quad i=1,2,\ldots,|\mathbf{G}_0|\ ,\quad n=12,\ldots,N\ , \tag{16.4}$$

where $\mathbf{R}_n$ are given by Eq. (16.2). The order of $\mathbf{G}$ is

$$|\mathbf{G}|=N|\mathbf{G}_0|\ , \tag{16.5a}$$

and the order of the little group $\mathbf{G}(\mathbf{k})$ is

$$|\mathbf{G}(\mathbf{k})|=N|\mathbf{G}_0(\mathbf{k})|\ . \tag{16.5b}$$

The irreducible rep of $\mathbf{T}$ is still of the form (9.22)

$$D^{(\mathbf{k})}(\{\varepsilon \mid \mathbf{R}_n\})=\exp(-i\mathbf{k}\cdot\mathbf{R}_n)\ . \tag{16.6}$$

However, the wave vector $\mathbf{k}$ is now discrete. The values of $\mathbf{k}$ in Eq. (9.23) are determined by the boundary conditions $D^{(\mathbf{k})}(\{\varepsilon \mid 2N_j\mathbf{t}_j\})=1$, i.e.,

$$\exp(-4\pi i N_j p_j)=1,\quad j=1,2,3\ . \tag{16.7}$$

Hence

$$p_i=\frac{l_i}{2N_i},\quad i=1,2,3\ , \tag{16.8a}$$

where l_i are integers and satisfy

$$-N_i\le l_i\le N_i-1\ . \tag{16.8b}$$

The $N=8N_1N_2N_3$ inequivalent wave vectors $\mathbf{k}$ define N inequivalent irreps of the translation group $\mathbf{T}$.

The first Brillouin zone can be defined as the set of these N points $\mathbf{k}$. The N wave vector $\mathbf{k}$ in the zone are grouped into distinct and disjoint stars $*\mathbf{k}$, each containing $q(\mathbf{k})$ wave vectors. It is clear that

$$\sum_{\mathbf{k}}1=\sum_{*\mathbf{k}}q(\mathbf{k})=N=8N_1N_2N_3\ . \tag{16.9}$$

B. Regular representation of a space group

Suppose $\psi(\mathbf{x})$ is a function without any translational or rotational symmetries. Applying the $|\mathbf{G}|$ elements in (16.4) of a space group $\mathbf{G}$ to $\psi(\mathbf{x})$ results in $|\mathbf{G}|$ linearly independent functions $\psi_{n,\alpha_i}(\mathbf{x})$ which span the regular rep space $\mathscr{L}_G$ for the space group $\mathbf{G}$,

$$\mathscr{L}_G=\{\psi_{n,\alpha_i}(\mathbf{x}):n=1,2,\ldots,N,\ i=1,2,\ldots,|\mathbf{G}_0|\}\ . \tag{16.10a}$$

$$\psi_{n,\alpha_i}(\mathbf{x})=\{\varepsilon \mid \mathbf{R}_n\}\{\alpha_i \mid \mathbf{V}(\alpha_i)\}\psi(\mathbf{x})\ . \tag{16.10b}$$

Our task is to decompose completely this $|\mathbf{G}|$-dimensional space into $|\mathbf{G}|$ one-dimensional spaces, each associated with an irreducible basis vector of $\mathbf{G}$.

With the projection operators (9.27) of the translation group $\mathbf{T}$,

$$P^{(\mathbf{k})}=\left[\frac{1}{N}\right]^{1/2}\sum_{n=1}^{N}e^{i\mathbf{k}\cdot\mathbf{R}_n}\{\varepsilon \mid \mathbf{R}_n\}\ , \tag{16.11}$$

where $\mathbf{k}$ runs over all the N values in Eq. (16.8), the regular rep space $\mathscr{L}_G$ is decomposed into a direct sum of N subspaces $\mathscr{L}^{\mathbf{k}_\tau}$:

$$\mathscr{L}_G=\sum_{*\mathbf{k}}\sum_{\tau=1}^{q(\mathbf{k})}\mathscr{L}^{\mathbf{k}_\tau}\ , \tag{16.12a}$$

$$\mathscr{L}^{\mathbf{k}_\tau}=\{\psi_{\alpha_i}^{\mathbf{k}_\tau}(\mathbf{x}):i=1,2,\ldots,|\mathbf{G}_0|\}\ , \tag{16.12b}$$

where

$$\psi_{\alpha_i}^{\mathbf{k}_\tau}(\mathbf{x})=\{\alpha_i \mid \mathbf{V}(\alpha_i)\}P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})\ . \tag{16.12c}$$

The $|\mathbf{G}_0|$-dimensional space $\mathscr{L}^{\mathbf{k}_\tau}$ is isomorphic to the space $\mathscr{L}(*\mathbf{k})$ of Eq. (10.2c), and when $\tau=1$, $\mathscr{L}^{\mathbf{k}_\tau}$ is again designated by $\mathscr{L}(*\mathbf{k})$. In analogy with Eq. (15.3d), the space $\mathscr{L}^{\mathbf{k}_\tau}$ can be further decomposed into $q(\mathbf{k})$ eigenspaces $\mathscr{L}^{\mathbf{k}_\tau}(\mathbf{k}_\sigma)$ of $\{\varepsilon \mid \mathbf{R}_n\}$, all isomorphic to the space $\mathscr{L}(\mathbf{k})$,

$$\mathscr{L}^{\mathbf{k}_\tau}=\sum_{\sigma=1}^{q(\mathbf{k})}\mathscr{L}^{\mathbf{k}_\tau}(\mathbf{k}_\sigma),\quad |\mathbf{k}_\sigma|=|\mathbf{k}_\tau|\ . \tag{16.13}$$

It is easily seen that if $\psi(\mathbf{x})$ were a Bloch function

$$\psi(\mathbf{x})=\psi_{\mathbf{k}}(\mathbf{x})=\exp[i(\mathbf{k}+\mathbf{K}_m)\cdot\mathbf{x}]\ , \tag{16.14}$$

then the space $\mathscr{L}_G$ would shrink into $\mathscr{L}(*\mathbf{k})$. Another way of stating this result is that by applying the $N|\mathbf{G}_0|$ elements of a space group $\mathbf{G}$ to a function that has translational symmetries (or equivalently, has a definite wave vector $\mathbf{k}$), we can only generate $|\mathbf{G}_0|$ linearly independent functions, which is just the case discussed in Secs. X–XIV.

The function $P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})$ belongs to the wave vector $\mathbf{k}_\tau$. We can use the projection operator $P_a^{(\mathbf{k}_\tau)(\nu)b}$ of the group $\mathbf{G}(\mathbf{k}_\tau)$ to project out of $P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})$ the $\mathbf{G}(\mathbf{k}_\tau)\supset\mathbf{G}(s_\tau)\supset\mathbf{T}$ irreducible basis,

$$\psi_{\mathbf{k}_\tau a}^{(\nu)\mathbf{k}_\tau b}=P_a^{(\mathbf{k}_\tau)(\nu)b}P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})\ , \tag{16.15a}$$

$$P_a^{(\mathbf{k}_\tau)(\nu)b}=\{\beta_\tau \mid \mathbf{V}_\tau\}P_a^{(\mathbf{k})(\nu)b}\{\beta_\tau \mid \mathbf{V}_\tau\}^{-1}\ , \tag{16.15b}$$

where $P_a^{(\mathbf{k})(\nu)b}$ is the projection operator for the rep group $\mathbf{G}'_{\mathbf{k}}$ or $\mathbf{G}_{\mathbf{k}}$ [see Eq. (13.10)]. Furthermore, from $\mathbf{k}_\sigma=\beta_\sigma\beta_\tau^{-1}\mathbf{k}_\tau$ and Eq. (15.2) we have

$$\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\{\beta_\sigma \mid \mathbf{V}_\sigma\}\{\beta_\tau \mid \mathbf{V}_\tau\}^{-1}\psi_{\mathbf{k}_\tau a}^{(\nu)\mathbf{k}_\tau b}\ . \tag{16.16a}$$

When we use Eq. (16.15), it becomes

$$\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\{\beta_\sigma \mid \mathbf{V}_\sigma\}P_a^{(\mathbf{k})(\nu)b}\{\beta_\tau \mid \mathbf{V}_\tau\}^{-1}P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})\ . \tag{16.16b}$$

The right-hand side of Eq. (16.16b) tells us that $P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})$ belongs to the wave vector $\mathbf{k}_\tau$; after the action of $\{\beta_\tau \mid \mathbf{V}_\tau\}^{-1}$, it belongs to the wave vector $\mathbf{k}$; the projection operator $P_a^{(\mathbf{k})(\nu)b}$ of the little group $\mathbf{G}(\mathbf{k})$ projects out of it the irreducible basis vector $\psi_{\mathbf{k},a}^{(\nu)\mathbf{k}_\tau b}$; finally the coset representative $\{\beta_\sigma \mid \mathbf{V}_\sigma\}$ transforms it into the basis vector $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$.

According to Eq. (15.6), the system of functions $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ for $\sigma=1,2,\ldots,q(\mathbf{k})$, $a=1,2,\ldots,h_\nu(\mathbf{k})$, with fixed $\mathbf{k}_\tau$ and b, carries a rep (the induced rep) of dimension

TABLE XIII. The spaces $\mathscr{L}_G$, $\mathscr{L}(*\mathbf{k})$, $\mathscr{L}(\mathbf{k})$ and their basis vectors.

space	$\mathscr{L}_G=\sum_{*\mathbf{k}}\sum_{\sigma,\tau=1}^{q(\mathbf{k})}\oplus\mathscr{L}^{\mathbf{k}_\tau}(\mathbf{k}_\sigma)$[a]
dimension	$N\lvert\mathbf{G}_0\rvert=\sum_{*\mathbf{k}}\sum_{\sigma,\tau=1}^{q(\mathbf{k})}\sum_{\nu=1}^{n}[h_\nu(\mathbf{k})]^2$
reducible basis:	$\psi_{\alpha_i}^{\mathbf{k}_\tau}(\mathbf{x})$, $\tau=1,2,\ldots,q(\mathbf{k})$, for all possible $*\mathbf{k}$, $i=1,2,\ldots,\lvert\mathbf{G}_0\rvert$;
IRB:	$\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$, $\nu=1,2,\ldots,n$; $a,b=1,2,\ldots,h_\nu(\mathbf{k})$; $\sigma,\tau=1,2,\ldots,q(\mathbf{k})$, for all $*\mathbf{k}$

space	$\mathscr{L}(*\mathbf{k})=\sum_{\sigma=1}^{q(\mathbf{k})}\oplus\mathscr{L}(\mathbf{k}_\sigma)$
dimension	$\lvert\mathbf{G}_0\rvert=\sum_{\sigma=1}^{q(\mathbf{k})}\sum_{\nu=1}^{n}[h_\nu(\mathbf{k})]^2$
reducible basis:	$\psi_{\alpha_i\mathbf{k}}=\{\alpha_i\mid\mathbf{V}(\alpha_i)\}\psi_{\mathbf{k}}$, $i=1,2,\ldots,\lvert\mathbf{G}_0\rvert$;
IRB:	$\psi_{\mathbf{k}_\sigma a}^{(\nu)b}$, $\nu=1,2,\ldots,n$; $a,b=1,2,\ldots,h_\nu(\mathbf{k})$; $\sigma=1,2,\ldots,q(\mathbf{k})$

space	$\mathscr{L}(\mathbf{k})=\sum_{\nu=1}^{n}\oplus\mathscr{L}_\nu(\mathbf{k})$[b]
dimension	$\lvert\mathbf{G}_0(\mathbf{k})\rvert=\sum_{\nu=1}^{n}[h_\nu(\mathbf{k})]^2$
reducible basis:	$\psi_{\gamma_i\mathbf{k}}=\{\gamma_i\mid\mathbf{V}(\gamma_i)\}\psi_{\mathbf{k}}(\mathbf{x})$, $i=1,2,\ldots,\lvert G_0(\mathbf{k})\rvert$;
IRB:	$\psi_{\mathbf{k},a}^{(\nu)b}$, $\nu=1,2,\ldots,n$; $a,b=1,2,\ldots,h_\nu(\mathbf{k})$

[a]The space $\mathscr{L}^{\mathbf{k}_\tau}(\mathbf{k}_\sigma)$ is isomorphic to the space $\mathscr{L}(\mathbf{k})=\mathscr{L}^{\mathbf{k}_1}(\mathbf{k}_1)$.
[b]$\mathscr{L}_\nu(\mathbf{k})$ is the eigenspace of the CSCO-I of $\mathbf{G}(\mathbf{k})$ in the space $\mathscr{L}(\mathbf{k})$.

$q(\mathbf{k})\cdot h_\nu(\mathbf{k})$ for the space group $\mathbf{G}$. Now we move on to prove that this rep is an irreducible representation of $\mathbf{G}$, and the irreps $D^{(*\mathbf{k})(\nu)}$ with all possible $*\mathbf{k}$ and ν form a complete set of inequivalent irreps. For this purpose it suffices to show that the sum of squares of the dimensions of all the irreps $D^{(*\mathbf{k})(\nu)}$ equals the order of the space group $\mathbf{G}$. This is easily done as follows:

$$\begin{aligned}\sum_{*\mathbf{k}}\sum_{\nu=1}^{n}[q(\mathbf{k})h_\nu(\mathbf{k})]^2&=\sum_{\mathbf{k}}q(\mathbf{k})\sum_{\nu=1}^{n}[h_\nu(\mathbf{k})]^2\\&=\sum_{\mathbf{k}}q(\mathbf{k})\lvert\mathbf{G}_0(\mathbf{k})\rvert\\&=\sum_{\mathbf{k}}\lvert\mathbf{G}_0\rvert=N\lvert\mathbf{G}_0\rvert\ ,\end{aligned}\tag{16.17}$$

where in the first and last steps we used Eq. (16.9), and in the second step used Eq. (6.3), i.e., the irreducibility of the ray rep $\Delta^{(\nu)}$ of the little co-group $\mathbf{G}_0(\mathbf{k})$. According to Eq. (16.5a), $N\lvert\mathbf{G}_0\rvert$ is just the order of the space group $\mathbf{G}$. Hence the proof is finished.

To summarize, the $\lvert\mathbf{G}\rvert$-dimensional regular rep space of a space group $\mathbf{G}$ is decomposed into $\lvert\mathbf{G}\rvert$ one-dimensional spaces spanned by each of the irreducible basis vectors $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ given in Eq. (16.16b), for all possible stars $*\mathbf{k}$ and all possible values of (σ,a) and (τ,b). The subscript (σ,a) serves as the component index, while the superscript (τ,b) serves as the multiplicity label; both range from 1 to the dimension $q(\mathbf{k})\cdot h_\nu(\mathbf{k})$ of the irrep $D^{(*\mathbf{k})(\nu)}$, i.e., each irrep $D^{(*\mathbf{k})(\nu)}$ occurs $q(\mathbf{k})\cdot h_\nu(\mathbf{k})$ times. For ease of reference, the basis vectors before and after reductions for the spaces $\mathscr{L}_G\mathscr{L}(*\mathbf{k})$ and $\mathscr{L}(\mathbf{k})$ are listed in Table XIII.

XVII. THE CSCO-III OF A SPACE GROUP G AND ORTHOGONAL THEOREMS FOR THE FULL MATRICES

A. The intrinsic space group $\overline{\mathbf{G}}$

We have now completed the main steps in finding the irreducible basis of a space group. In order to have a better understanding of the physical meaning of the basis vectors $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$, especially the meaning of their multiplicity label $(\mathbf{k}_\tau,b)$, let us introduce the intrinsic group $\overline{\mathbf{G}}$ of the space group $\mathbf{G}$. In Eq. (13.2) we defined the intrinsic group $\overline{\mathbf{G}}'_{\mathbf{k}}$ of the rep group $\mathbf{G}'_{\mathbf{k}}$, and then extended it into

the intrinsic group $\overline{\mathbf{G}}(\mathbf{k})$ of the little group $\mathbf{G}(\mathbf{k})$ [Eq. (13.4a)]. Alternatively, we can define the group $\overline{\mathbf{G}}(\mathbf{k})$ as follows: The intrinsic group $\overline{\mathbf{G}}(\mathbf{k})$ is an operator group with the elements (operators) $\overline{\{\gamma\,|\,\mathbf{c}\}}$ defined in the $|\mathbf{G}(\mathbf{k})|$-dimensional group space of the little group $\mathbf{G}(\mathbf{k})$ through

$$\overline{\{\gamma\,|\,\mathbf{c}\}}\overline{\{\gamma'\,|\,\mathbf{c}'\}}=\overline{\{\gamma'\,|\,\mathbf{c}'\}}\overline{\{\gamma\,|\,\mathbf{c}\}} \quad \text{for any } \{\gamma'\,|\,\mathbf{c}'\}\in\mathbf{G}(\mathbf{k})\ . \tag{17.1}$$

$\overline{\mathbf{G}}(\mathbf{k})$ is anti-isomorphic and commutative with the group $\mathbf{G}(\mathbf{k})$. Symbolically, we write

$$[\overline{\mathbf{G}}(\mathbf{k}),\mathbf{G}(\mathbf{k})]=0\ . \tag{17.2}$$

Likewise, we can define the intrinsic group $\overline{\mathbf{G}}$ of the space group $\mathbf{G}$ as an operator group with the elements $\overline{\{\alpha\,|\,\mathbf{a}\}}$ defined in the $|\mathbf{G}|$-dimensional group space of $\mathbf{G}$ through

$$\overline{\{\alpha\,|\,\mathbf{a}\}}\overline{\{\beta\,|\,\mathbf{b}\}}=\overline{\{\beta\,|\,\mathbf{b}\}}\overline{\{\alpha\,|\,\mathbf{a}\}} \text{ for any } \{\beta\,|\,\mathbf{b}\}\in\mathbf{G}\ . \tag{17.3}$$

$\overline{\mathbf{G}}$ is anti-isomorphic and commutative with the space group $\mathbf{G}$. Symbolically,

$$[\overline{\mathbf{G}},\mathbf{G}]=0\ . \tag{17.4}$$

It must be stressed that although $\mathbf{G}(\mathbf{k})$ is a subgroup of $\mathbf{G}$, the intrinsic group $\overline{\mathbf{G}}(\mathbf{k})$ is not a subgroup of the "total" intrinsic group $\overline{\mathbf{G}}$. It is easy to see this from the following arguments. If $\overline{\mathbf{G}}(\mathbf{k})$ were a subgroup of $\overline{\mathbf{G}}$, then according to Eq. (17.4) we would have

$$[\overline{\mathbf{G}}(\mathbf{k}),\mathbf{G}]=0\ ,$$

while according to Eq. (17.2), $\overline{\mathbf{G}}(\mathbf{k})$ only commutes with the subgroup $\mathbf{G}(\mathbf{k})$ of $\mathbf{G}$ rather than the whole group $\mathbf{G}$. Hence $\overline{\mathbf{G}}(\mathbf{k})$ cannot be a subgroup of $\overline{\mathbf{G}}$. Of course there exists a subgroup of the "total" intrinsic group $\overline{\mathbf{G}}$ which is also anti-isomorphic and commutative with $\mathbf{G}(\mathbf{k})$; however, this subgroup of $\overline{\mathbf{G}}$ is useless to the subsequent discussion and will not be mentioned any more. What is needed of the subgroups of $\overline{\mathbf{G}}$ is the intrinsic translation group $\overline{\mathbf{T}}$. Its elements $\overline{\{\varepsilon\,|\,\mathbf{R}_n\}}$ commute with any elements of $\mathbf{G}$

$$[\overline{\{\varepsilon\,|\,\mathbf{R}_n\}},\{\alpha\,|\,\mathbf{a}\}]=0 \text{ for any } \{\alpha\,|\,\mathbf{a}\}\in\mathbf{G}\ . \tag{17.5}$$

According to Sec. IX.C, the CSCO of the translation group $\mathbf{T}$ is $\{\varepsilon\,|\,\mathbf{R}_n\}$ or simply the momentum operator $\hat{\mathbf{k}}$. The CSCO of the intrinsic translation group $\overline{\mathbf{T}}$ is then $\overline{\{\varepsilon\,|\,\mathbf{R}_n\}}$, or simply the "intrinsic momentum operator" $\hat{\bar{\mathbf{k}}}$, which commutes with any operator $\{\alpha\,|\,\mathbf{a}\}$ of $\mathbf{G}$,

$$[\hat{\bar{\mathbf{k}}},\{\alpha\,|\,\mathbf{a}\}]=0\ . \tag{17.6}$$

The CSCO-I of the space group $\mathbf{G}$ cannot easily be found due to the complex nature of its class operators. Nevertheless, from

$$\{\alpha\,|\,\mathbf{a}\}\{\varepsilon\,|\,\mathbf{R}_n\}\{\alpha\,|\,\mathbf{a}\}^{-1}=\{\varepsilon\,|\,\alpha\mathbf{R}_n\}\ , \tag{17.7}$$

we know that

$$\mathscr{C}=\sum_{i=1}^{|\mathbf{G}_0|}\{\varepsilon\,|\,\alpha_i\mathbf{R}_n\} \tag{17.8}$$

is a translational class operator of the space group $\mathbf{G}$ and therefore can be chosen as one of the operators making up the CSCO-I of the space group. As we shall see in a moment, the operator $\mathscr{C}$ is all that we need of the CSCO-I of $\mathbf{G}$.

Applying the operator $\mathscr{C}$ to the basis vector $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ we have

$$\mathscr{C}\psi^{(\nu)}_{\mathbf{k}_\sigma a}=\lambda^{(*\mathbf{k})}\psi^{(\nu)}_{\mathbf{k}_\sigma a}\ ; \tag{17.9a}$$

that is, the basis vector $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ is an eigenfunction of $\mathscr{C}$ with the eigenvalue

$$\lambda^{(*\mathbf{k})}=|\mathbf{G}_0(\mathbf{k})|\sum_{\tau=1}^{q}\exp(-i\mathbf{k}_\tau\cdot\mathbf{R}_n)\ , \tag{17.9b}$$

which is a constant for any member of the basis $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$, and thus is a function of the star $*\mathbf{k}$. One could have used $\lambda^{(*\mathbf{k})}$ as one of the labels for the irreps of the space group if one wished, but of course the simpler label $(*\mathbf{k})$ is always preferred.

Combining Eqs. (15.20) and (17.9) we know that $\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}$ is simultaneously the eigenfunction of the operator $\mathscr{C}$ and the CSCO $C(\mathbf{k}_\sigma)$, $C(s_\sigma)$, and $\hat{\mathbf{k}}$ of the subgroups $\mathbf{G}(\mathbf{k}_\sigma)$, $\mathbf{G}(s_\sigma)$, and $\mathbf{T}$, respectively,

$$\mathrm{col}(\mathscr{C},C(\mathbf{k}_\sigma),C(s_\sigma),\hat{\mathbf{k}})\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}=\mathrm{col}(\lambda^{(*\mathbf{k})},\nu,a,\mathbf{k}_\sigma)\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}\ , \tag{17.10a}$$

where $\mathrm{col}(a,b,\ldots)$ denotes a column vector.

According to Eq. (4.10b), the CSCO of the space group $\mathbf{G}$ and its intrinsic group $\overline{\mathbf{G}}$ are equal; therefore $\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}$ is also an eigenfunction of the CSCO of $\overline{\mathbf{G}}$. In other words, it is also an irreducible basis vector of the intrinsic group $\overline{\mathbf{G}}$. Now we are going to show that $\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}$ is indeed simultaneously the eigenfunction of the operators $\overline{\mathscr{C}}=\mathscr{C}$, and the CSCO $\overline{C}(\mathbf{k}_\sigma)$, $\overline{C}(s_\sigma)$, and $\hat{\bar{\mathbf{k}}}$ of the intrinsic groups $\overline{G}(\mathbf{k}_\sigma)$, $\overline{G}(s_\sigma)$, and $\overline{\mathbf{T}}$, respectively:

$$\mathrm{col}(\overline{\mathscr{C}},\overline{C}(\mathbf{k}_\sigma),\overline{C}(s_\sigma),\hat{\bar{\mathbf{k}}})\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}=\mathrm{col}(\lambda^{(*\mathbf{k})},\nu,b,\mathbf{k}_\tau)\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}\ . \tag{17.10b}$$

The intrinsic group $\overline{\mathbf{G}}(\mathbf{k}_\sigma)$ and its subgroup $\overline{\mathbf{G}}(s_\sigma)$ are defined by

$$\begin{bmatrix}\overline{\mathbf{G}}(\mathbf{k}_\sigma)\\ \overline{\mathbf{G}}(s_\sigma)\end{bmatrix}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\begin{bmatrix}\overline{\mathbf{G}}(\mathbf{k})\\ \overline{\mathbf{G}}(s)\end{bmatrix}\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}^{-1}\ . \tag{17.11a}$$

Therefore, their CSCO-II's are

$$\begin{bmatrix}\overline{C}(\mathbf{k}_\sigma)\\ \overline{C}(s_\sigma)\end{bmatrix}=\{\beta_\sigma\,|\,V_\sigma\}\begin{bmatrix}\overline{C}\\ \overline{C}(s)\end{bmatrix}\{\beta_\sigma\,|\,V_\sigma\}^{-1}\ . \tag{17.11b}$$

Applying the operators $\bar{C}(\mathbf{k}_\sigma)$ and $\bar{C}(s_\sigma)$ to $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ in Eq. (16.16b), we have

$$\begin{bmatrix}\bar{C}(\mathbf{k}_\sigma)\\ \bar{C}(s_\sigma)\end{bmatrix}\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}\begin{bmatrix}\bar{C}\\ \bar{C}(s)\end{bmatrix}P_a^{(\mathbf{k})(\nu)b}$$

$$\times\{\beta_\tau\,|\,V_\tau\}^{-1}P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})\ . \qquad (17.12a)$$

Using $\bar{C}=C$ [see Eq. (4.10b)] and Eq. (13.5), it becomes

$$\begin{bmatrix}\bar{C}(\mathbf{k}_\sigma)\\ \bar{C}(s_\sigma)\end{bmatrix}\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\begin{bmatrix}\nu\\ b\end{bmatrix}\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\ . \qquad (17.12b)$$

Hence $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ is the eigenfunction of both $\bar{C}(\mathbf{k}_\sigma)$ and $\bar{C}(s_\sigma)$.

Now we come to the last operator, the intrinsic momentum operator $\hat{\bar{\mathbf{k}}}$. The action of an intrinsic operator $\overline{\{\alpha\,|\,\mathbf{a}\}}$ of $\bar{\mathbf{G}}$ on the configuration functions depends on the choice of the so-called "intrinsic state" (Chen and Gao, 1982). From among the $N\,|\,\mathbf{G}_0\,|$ functions $\psi_{n,\alpha}(\mathbf{x})$ in the regular rep space of $\mathbf{G}$, we can choose any one, say $\psi(\mathbf{x})$, as the intrinsic state and define the action of the intrinsic elements $\overline{\{\alpha\,|\,\mathbf{a}\}}$ on it to be equal to that of the group elments $\{\alpha\,|\,\mathbf{a}\}$,

$$\overline{\{\alpha\,|\,a\}}\psi(\mathbf{x})=\{\alpha\,|\,\mathbf{a}\}\psi(\mathbf{x})\ \text{ for any }\ \overline{\{\alpha\,|\,\mathbf{a}\}}\in\bar{\mathbf{G}}\ . \qquad (17.13)$$

The choice of the intrinsic state is arbitrary, but once chosen, it should be kept fixed through the whole analysis. The operation of the intrinsic element $\overline{\{\alpha\,|\,\mathbf{a}\}}$ on any other functions $\psi_{n,\beta}=\{\beta\,|\,\mathbf{V}(\beta)+\mathbf{R}_n\}\psi(\mathbf{x})$ is unambiguously dictated by Eqs. (17.3) and (17.13), i.e.,

$$\overline{\{\alpha\,|\,\mathbf{a}\}}\psi_{n,\beta}(\mathbf{x})=\{\beta\,|\,\mathbf{V}(\beta)+\mathbf{R}_n\}\{\alpha\,|\,\mathbf{a}\}\psi(\mathbf{x})\ . \qquad (17.14)$$

With this preliminary knowledge, let us apply the intrinsic momentum operator $\hat{\bar{\mathbf{k}}}$ to Eq. (16.16b),

$$\hat{\bar{\mathbf{k}}}\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}P_a^{(\mathbf{k})(\nu)b}\{\beta_\tau\,|\,V_\tau\}^{-1}P^{(\mathbf{k}_\tau)}\hat{\bar{\mathbf{k}}}\psi(\mathbf{x})\ , \qquad (17.15)$$

where we used Eq. (17.6). Due to Eq. (17.13), the operator $\hat{\bar{\mathbf{k}}}$ in front of $\psi(\mathbf{x})$ can be replaced by $\hat{\mathbf{k}}$. Using the fact that the operator $\hat{\mathbf{k}}$ commutes with the projection operator of the translation group and that the function $P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})$ belongs to the wave vector $\mathbf{k}_\tau$, we have

$$P^{(\mathbf{k}_\tau)}\hat{\mathbf{k}}\psi(\mathbf{x})=\hat{\mathbf{k}}P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})=\mathbf{k}_\tau P^{(\mathbf{k}_\tau)}\psi(\mathbf{x})\ . \qquad (17.16)$$

Combining Eq. (17.15) with (17.16), we get

$$\hat{\bar{\mathbf{k}}}\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\mathbf{k}_\tau\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\ . \qquad (17.17)$$

Therefore, $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ is an eigenfunction of the intrinsic momentum operator $\hat{\bar{\mathbf{k}}}$ with the eigenvalue $\mathbf{k}_\tau$.

To summarize, Eq. (17.10b) shows that $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ is the irreducible basis of the intrinsic group $\bar{\mathbf{G}}$ in the $\bar{\mathbf{G}}\supset\bar{\mathbf{T}}$ and $\bar{\mathbf{G}}(\mathbf{k}_\sigma)\supset\bar{\mathbf{G}}(s_\sigma)$ classification scheme, with $(*\mathbf{k})(\nu)$ as the irrep label and $(\mathbf{k}_\tau b)$ as the component label.

B. The CSCO-II and CSCO-III of G

Combining Eqs. (17.10a) and (17.10b), we have the simultaneous eigenequations

$$\mathrm{col}(\mathscr{C},C(\mathbf{k}_\sigma),\hat{\mathbf{k}},C(s_\sigma),\hat{\bar{\mathbf{k}}},\bar{C}(s_\sigma))\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$$
$$=\mathrm{col}(\lambda^{(*\mathbf{k})},\nu,\mathbf{k}_\sigma,a,\mathbf{k}_\tau,b)\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\ . \qquad (17.18)$$

We claim that

$$K=(\mathscr{C},C(\mathbf{k}_\sigma),\hat{\mathbf{k}},C(s_\sigma),\hat{\bar{\mathbf{k}}},\bar{C}(s_\sigma)) \qquad (17.19)$$

is a CSCO-III of the space $\mathbf{G}$, while

$$M=(\mathscr{C},C(\mathbf{k}_\sigma),\hat{\mathbf{k}},C(s_\sigma)) \qquad (17.20)$$

is a CSCO-II of $\mathbf{G}$. This claim is easily supported by noting that, according to the completeness condition Eq. (16.17), the operator K has $|\,\mathbf{G}\,|$ distinct sets of eigenvalues and that it contains a "Casimir operator" $\mathscr{C}$ of the space group $\mathbf{G}$. K is a complete set of commuting operators in the group space of $\mathbf{G}$. Therefore, its eigenfunctions $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ are all nondegenerate and form an orthonormal and complete set

$$\langle\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\,|\,\psi_{\mathbf{k}'_{\sigma'}a'}^{(\nu')\mathbf{k}'_{\tau'}b'}\rangle=\delta_{*\mathbf{k}*\mathbf{k}'}\delta_{\sigma\sigma'}\delta_{\tau\tau'}\delta_{\nu\nu'}\delta_{aa'}\delta_{bb'}\ ,$$
$$\sum_{*\mathbf{k}\nu\sigma a\tau b}|\,\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\rangle\langle\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}\,|=1\ . \qquad (17.21)$$

The irreducible basis $\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}$ can be expressed in terms of the reducible basis $\psi_{n,\alpha}(\mathbf{x})$ of Eq. (16.10) as

$$\psi_{\mathbf{k}_\sigma a}^{(\nu)\mathbf{k}_\tau b}=\sum_{n,\alpha}U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}\psi_{n,\alpha}(\mathbf{x})\ . \qquad (17.22)$$

The coefficients $U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}$ then obey the unitarity conditions:

$$\sum_{n,\alpha}U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}(U_{\sigma'a'\tau'b',n\alpha}^{(*\mathbf{k}')(\nu')})^*=\delta_{*\mathbf{k}*\mathbf{k}'}\delta_{\sigma\sigma'}\delta_{\tau\tau'}\delta_{\nu\nu'}\delta_{aa'}\delta_{bb'}\ ,$$
$$\sum_{*\mathbf{k}\nu\sigma a\tau b}U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}(U_{\sigma a\tau b,n'\alpha'}^{(*\mathbf{k})(\nu)})^*=\delta_{nn'}\delta_{\alpha\alpha'}\ . \qquad (17.23)$$

C. The orthogonal theorems for the full rep matrices

In analogy with Eq. (13.8), the coefficients $U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}$ are related to the irreducible matrix elements of $\mathbf{G}$ by

$$U_{\sigma a\tau b,n\alpha}^{(*\mathbf{k})(\nu)}=\left[\frac{qh_\nu}{|\,\mathbf{G}\,|}\right]^{1/2}D_{\sigma a,\tau b}^{(*\mathbf{k})(\nu)}(\{\dot{\alpha}\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})^*\ . \qquad (17.24)$$

Inserting Eq. (17.24) into Eq. (17.23), we obtain the two orthogonal theorems for the irreducible matrix elements of the space group $\mathbf{G}$:

$$\frac{qh_\nu}{|\mathbf{G}|}\sum_{n\alpha} D^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})^* D^{(*\mathbf{k}')(\nu')}_{\sigma' a',\tau' b'}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})=\delta_{*\mathbf{k}*\mathbf{k}'}\delta_{\sigma\sigma'}\delta_{\tau\tau'}\delta_{\nu\nu'}\delta_{aa'}\delta_{bb'}\,,$$

$$\sum_{*\mathbf{k}\nu\sigma a\tau b}\frac{qh_\nu}{|\mathbf{G}|}D^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})^* D^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}(\{\alpha'\,|\,\mathbf{V}(\alpha')+\mathbf{R}_{n'}\})=\delta_{nn'}\delta_{\alpha\alpha'}\,. \tag{17.25}$$

D. The generalized projection operator of G

The projection operator for the space group $\mathbf{G}$ is given by

$$P^{(*\mathbf{k})(\nu)\tau b}_{\sigma a}=\left[\frac{qh_\nu}{|\mathbf{G}|}\right]^{1/2}\sum_{n\alpha} D^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})^*\,\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\}\,. \tag{17.26}$$

By applying this to a general function $\psi(\mathbf{x})$, we get the $\mathbf{G}\supset\mathbf{G}(\mathbf{k}_\sigma)\supset\mathbf{G}(s_\sigma)\supset\mathbf{T}$, $\overline{\mathbf{G}}\supset\overline{\mathbf{T}}$, $\overline{\mathbf{G}}(\mathbf{k}_\sigma)\supset\overline{\mathbf{G}}(s_\sigma)$ irreducible basis,

$$\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}=P^{(*\mathbf{k})(\nu)\tau b}_{\sigma a}\psi(\mathbf{x})\,. \tag{17.27}$$

However, we have already obtained a simpler expression for the same basis, as shown in Eq. (16.16b). Are these two seemingly quite different expressions, Eqs. (16.16b) and (17.27), identical? Of course they have to be so, as is shown in the following. Using Eqs. (15.8c) and (15.8d), as well as the remark following them, we can multiply Eq. (17.26) by $(qh_\nu/|\mathbf{G}|)^{1/2}$ and recast it in the form

$$P^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}=\frac{qh_\nu}{|\mathbf{G}|}\sum_{n\alpha} D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\})\{\alpha\,|\,\mathbf{V}(\alpha)+\mathbf{R}_n\}^{-1}$$

$$=\frac{qh_\nu}{|\mathbf{G}|}\sum_{m\gamma} D^{(\mathbf{k})(\nu)}_{ba}(\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_m\})\{\beta_\sigma\,|\,V_\sigma\}\{\gamma\,|\,\mathbf{V}(\gamma)+\mathbf{R}_m\}^{-1}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\,. \tag{17.28}$$

From $q/|\mathbf{G}|=1/[\,|\mathbf{G}_0(\mathbf{k})|\,N]$ and Eq. (13.11) we have

$$P^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}P^{(\mathbf{k})(\nu)}_{ab}\mathscr{P}^{(\mathbf{k})}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\,, \tag{17.29}$$

where

$$\mathscr{P}^{(\mathbf{k})}=\left[\frac{1}{N}\right]^{1/2}P^{(\mathbf{k})}=\frac{1}{N}\sum_{n=1}^{N}e^{i\mathbf{k}\cdot\mathbf{R}_n}\{\varepsilon\,|\,\mathbf{R}_n\}\,.$$

Furthermore,

$$\mathscr{P}^{(\mathbf{k})}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}=\frac{1}{N}\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}\{\varepsilon\,|\,\mathbf{R}_n\}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}$$

$$=\frac{1}{N}\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\{\varepsilon\,|\,\beta_\tau\mathbf{R}_n\}$$

$$=\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\mathscr{P}^{(\mathbf{k}_\tau)}\,. \tag{17.30}$$

Inserting Eq. (17.30) into Eq. (17.29) we immediately get

$$P^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}=\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}P^{(\mathbf{k})(\nu)}_{ab}\{\beta_\tau\,|\,\mathbf{V}_\tau\}^{-1}\mathscr{P}^{(\mathbf{k}_\tau)}\,. \tag{17.31}$$

This is exactly what is required by Eq. (16.16b).

Equation (17.29) is in the form of Eq. (6.37) and is identical with the factored irreducible symmetry operator (FISO) derived by Folland [1979, Eq. (22)]. Explicit results for the FISO's and symmetry-adapted functions are also given by him for the diamond-structure space group and double space group.

In analogy with Eq. (13.13), we have

$$\{\alpha\,|\,\mathbf{a}\}\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}=\sum_{a'}D^{(*\mathbf{k})(\nu)}_{\sigma' a',\sigma a}(\{\alpha\,|\,\mathbf{a}\})\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_{\sigma'}a'}\,, \tag{17.32a}$$

$$\overline{\{\alpha\,|\,\mathbf{a}\}}\psi^{(\nu)\mathbf{k}_\tau b}_{\mathbf{k}_\sigma a}=\sum_{b'}D^{(*\mathbf{k})(\nu)}_{\tau b,\tau' b'}(\{\alpha\,|\,\mathbf{a}\})\psi^{(\nu)\mathbf{k}_\tau b'}_{\mathbf{k}_\sigma a}\,. \tag{17.32b}$$

Thus an element of $\mathbf{G}$ can never change the intrinsic quantum numbers $\mathbf{k}_\tau$ and b, while an element of the intrinsic group $\overline{\mathbf{G}}$ can never change the "external" quantum numbers $\mathbf{k}_\sigma$ and a.

E. The intrinsic wave vector

Finally let us try to elucidate the meaning of the intrinsic wave vector $\mathbf{k}_\tau$ in Eq. (17.17). We first recall what we did for the rotation-group case (Chen, Wang, and Gao, 1983). The projection operator $P^{(J)}_{MK}$ of SO_3 is simultaneously an eigenvector of the CSCO-III of SO_3 [cf. Eq. (1.7)],

$$\mathrm{col}(J^2,J_z,\bar{J}_z)P^{(J)}_{MK}=\mathrm{col}(J(J+1),M,K)P^{(J)}_{MK}\,, \tag{17.33a}$$

$$P^{(J)}_{MK}=\frac{2J+1}{8\pi^2}\int\sin\beta\,d\alpha\,d\beta\,d\gamma D^{(J)}_{MK}(\alpha\beta\gamma)^* R(\alpha\beta\gamma)\,. \tag{17.33b}$$

In the nuclear collective-rotation model (Bohr and Mottelson, 1969), we know that the intrinsic state of a deformed nucleus does not have a definite angular momentum, but does have a definite z component, say Ω, of the angular momentum in the intrinsic frame. Let $\Phi_\Omega(\mathbf{x})$ be such an intrinsic state. According to Eq. (50) in Chen, Wang, and Gao (1983),

$$P^{(J)}_{MK}\Phi_\Omega(\mathbf{X})=\delta_{K\Omega}\Psi^{(J)K}_M . \tag{17.34}$$

$\Psi^{(J)K}_M$ gives the nuclear wave function in the adiabatic approximation. Equation (17.34) shows that the z component K of the total angular momentum $\mathbf{J}$ in the intrinsic frame equals the z component Ω of the angular momentum possessed by the intrinsic state $\Phi_\Omega(\mathbf{X})$. This means that there are no nuclear collective rotations about the symmetry axis (i.e., the z axis in the intrinsic frame) of a nucleus. Each intrinsic quantum number K characterize a rotational energy band of the nucleus.

Now we turn back to the space-group case. In much the same way we can obtain the following results. Suppose $\varphi_{\mathbf{k}_i}(\mathbf{x})$ is an electron wave function which does not have a definite space-group symmetry but does have a definite wave vector (or momentum) $\mathbf{k}_i$. Let such a state be called the "intrinsic state" of an electron. Out of the projection operator $P^{(*\mathbf{k})(\nu)}_{\sigma a\tau b}$, we can build a "bunch" of states $\psi^{(\nu)\mathbf{k}_i b}_{\mathbf{k}_\sigma a}$ by

$$P^{(*\mathbf{k})(\nu)}_{\sigma a,\tau b}\varphi_{\mathbf{k}_i}(\mathbf{x})=\delta_{\mathbf{k}_\tau\mathbf{k}_i}\psi^{(\nu)\mathbf{k}_i b}_{\mathbf{k}_\sigma a} . \tag{17.35}$$

This shows that the intrinsic wave vectors $\mathbf{k}_i$ of these states are all equal to the wave vector $\mathbf{k}_i$ of the "intrinsic state" of the electron. Therefore, all these states in the "bunch" are characterized by the same intrinsic wave vector $\mathbf{k}_i$. It is not known whether the energies of an electron in a crystal are grouped into bands characterized by the intrinsic wave vectors as the energies of a deformed nucleus are characterized by the intrinsic z component of the angular momentum.

XVIII. THE CLEBSCH-GORDAN COEFFICIENTS OF SPACE GROUPS

A. The CG series

Suppose that $D^{(*\mathbf{k})(\nu)}$ and $D^{(*\mathbf{k}')(\nu')}$ are two irreps of a space group $\mathbf{G}$. The Kronecker product of these two irreps can be reduced into a direct sum of the irreps of $\mathbf{G}$,

$$D^{(*\mathbf{k})(\nu)}\otimes D^{(*\mathbf{k}')(\nu')}=\sum_{*\mathbf{k}''}\sum_{\nu''}\oplus(*\mathbf{k}\nu*\mathbf{k}'\nu' \mid *\mathbf{k}''\nu'')\times D^{(*\mathbf{k}'')(\nu'')} , \tag{18.1}$$

where $(*\mathbf{k}\nu*\mathbf{k}'\nu' \mid *\mathbf{k}''\nu'')$ is an integer and is the number of times that the irrep $D^{(*\mathbf{k}'')(\nu'')}$ occurs in the Kronecker product rep. Equation (18.1) is referred to as the Clebsch-Gordon series of the space group, and the integer $(*\mathbf{k}\nu*k'\nu' \mid *k''\nu'')$ is called the reduction coefficient (Birman, 1974) or the multiplicity. [We note that the integer $(*\mathbf{k}\nu*\mathbf{k}'\nu' \mid *\mathbf{k}''\nu'')$ is called the Clebsch-Gordan coefficient by Bradley and Cracknell (1972), but we reserve the name "Clebsch-Gordan coefficient" for the unitary transformation coefficient of Eq. (18.3b).]

Several methods are available for calculating the space-group reduction coefficient (Birman, 1962,1974; Hsieh and Chen, 1964; Bradley and Cracknell, 1972; Dirl, 1976b; van den Broek, 1979a). A complete and explicit set of tables for the reduction coefficients has been published (Davies and Cracknell, 1979,1980; Cracknell and Davies, 1979).

Let $\psi^{(\nu)}_{\mathbf{k}_\sigma a}$ and $\psi^{(\nu')}_{\mathbf{k}'_{\sigma'}a'}$ be the basis vectors carrying the irreps $D^{(*\mathbf{k})(\nu)}$ and $D^{(*\mathbf{k}')(\nu')}$, respectively. The CG coefficients of the space group are defined as the expansion coefficients in the following equation:

$$\psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''}=\sum_{\sigma a\sigma' a'}\left[\begin{array}{cc|c}\nu\mathbf{k}\nu'\mathbf{k}' & & \nu''\mathbf{k}'' \quad \theta\\ \sigma a\sigma' a' & & \sigma'' a''\end{array}\right]\psi^{(\nu)}_{\mathbf{k}_\sigma a}\psi^{(\nu')}_{\mathbf{k}'_{\sigma'}a'} ,$$

$$\theta=1,2,\ldots,(*\mathbf{k}\nu*\mathbf{k}'\nu' \mid *\mathbf{k}''\nu'') , \tag{18.2}$$

where θ is the multiplicity label. The inverse of Eq. (18.2) is

$$\psi^{(\nu)}_{\mathbf{k}_\sigma a}\psi^{(\nu')}_{\mathbf{k}'_{\sigma'}a'}=\sum_{\nu''\mathbf{k}''\sigma''a''\theta}\left[\begin{array}{cc|c}\nu\mathbf{k} & \nu'\mathbf{k}' & \nu''\mathbf{k}''\theta\\ \sigma a & \sigma' a' & \sigma'' a''\end{array}\right]\psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''} . \tag{18.3a}$$

The CG coefficients can be expressed as

$$\left[\begin{array}{cc|c}\nu\mathbf{k} & \nu'\mathbf{k}' & \nu''\mathbf{k}''\theta\\ \sigma a & \sigma' a' & \sigma'' a''\end{array}\right]=\langle\psi^{(\nu)}_{\mathbf{k}_\sigma a}\psi^{(\nu')}_{\mathbf{k}'_{\sigma'}a'} \mid \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''}\rangle . \tag{18.3b}$$

Using

$$\langle\psi^{(\nu)}_{\mathbf{k}_\sigma a}\psi^{(\nu')}_{\mathbf{k}'_{\sigma'}a'} \mid \{\varepsilon \mid \mathbf{R}_n\} \mid \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a''}\rangle=e^{-i\mathbf{k}''_{\sigma''}\cdot\mathbf{R}_n}C$$

$$=\langle\{\varepsilon \mid -\mathbf{R}_n\}(\psi^{(\nu)}_{\mathbf{k}_\sigma a}\psi^{(\nu)}_{\mathbf{k}'_{\sigma'}a'}) \mid \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma''}a'}\rangle=e^{-i(\mathbf{k}_\sigma+\mathbf{k}'_{\sigma'})\cdot\mathbf{R}_n}C ,$$

where C is the abbreviation for the CG coefficient (18.3b); we know that the CG coefficient vanishes unless

$$\mathbf{k}_\sigma+\mathbf{k}'_{\sigma'}-\mathbf{k}''_{\sigma''}=\mathbf{K}_m . \tag{18.4}$$

According to Eq. (18.4) we can introduce the wavevector selection rule,

$$*\mathbf{k}\otimes *\mathbf{k}'=\sum_{*\mathbf{k}''}(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')*\mathbf{k}'' . \tag{18.5}$$

The integers $(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')$ are referred to as the wavevector reduction coefficients. Plainly we have

$$(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'') = (*\mathbf{k}'*\mathbf{k} \mid *\mathbf{k}'') \ . \tag{18.6}$$

Assuming that there are q, q', and q'' points in the stars $*\mathbf{k}$, $*\mathbf{k}'$, and $*\mathbf{k}''$, respectively, it follows from Eq. (18.5) that

$$qq' = \sum_{*\mathbf{k}''} (*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')q'' \ . \tag{18.7}$$

A simple prescription for determining the wave-vector reduction coefficients is given by Birman (1962).

B. The calculation of the CG coefficients

Setting $\sigma''=1$ in Eq. (18.2), we have

$$\psi^{(\nu'')\theta}_{\mathbf{k}''a''} = \sum_{\sigma a \sigma' a'} \left[\begin{matrix} \nu\mathbf{k}\nu'\mathbf{k}' \\ \sigma a \sigma' a' \end{matrix} \middle| \begin{matrix} \nu''\mathbf{k}''\theta \\ 1a'' \end{matrix} \right] | \sigma a \sigma' a' \rangle \ , \tag{18.8a}$$

where

$$| \sigma a \sigma' a' \rangle \equiv \psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma'} a'} \ . \tag{18.8b}$$

Since $\psi^{(\nu'')\theta}_{\mathbf{k}''a''}$ is the irreducible basis of the rep group $\mathbf{G}'_{\mathbf{k}''}$, it is necessarily an eigenvector of the CSCO-II $(C, C(s))$ of the group $\mathbf{G}'_{\mathbf{k}''}$:

$$\begin{bmatrix} C \\ C(s) \end{bmatrix} \psi^{(\nu'')\theta}_{\mathbf{k}''a''} = \begin{bmatrix} \nu'' \\ a'' \end{bmatrix} \psi^{(\nu'')\theta}_{\mathbf{k}''a''} \ , \tag{18.9a}$$

or, written in matrix form,

$$\begin{bmatrix} M(C) \\ M(C(s)) \end{bmatrix} U^{(\nu'')\theta}_{\mathbf{k}''a''} = \begin{bmatrix} \nu'' \\ a'' \end{bmatrix} U^{(\nu'')\theta}_{\mathbf{k}''a''} \tag{18.9b}$$

where $M(C)$ and $M(C(s))$ are the representatives of the operators C and $C(s)$ in the uncoupled representation with the basis $| \sigma a \sigma' a' \rangle$, and the vector

$$U^{(\nu'')\theta}_{\mathbf{k}''a''} = \left\{ \left[\begin{matrix} \nu\mathbf{k}\nu'\mathbf{k}' \\ \sigma a \sigma' a' \end{matrix} \middle| \begin{matrix} \nu''\mathbf{k}''\theta \\ 1a'' \end{matrix} \right] \right\} \tag{18.10}$$

is the representative of $\psi^{(\nu'')\theta}_{\mathbf{k}''a''}$; (ν'', a'') is the eigenvalue of $(C, C(s))$. In other words, the CG coefficients (18.10) result from a diagonalization of the matrices $M(C)$ and $M(C(s))$ simultaneously. To calculate $M(C)$ and $M(C(S))$, we must first calculate the matrices $M(\{\gamma'' \mid \mathbf{c}''\}')$ for the group elements $\{\gamma'' \mid \mathbf{c}''\}'$ contained in the CSCO-II of $\mathbf{G}'_{\mathbf{k}''}$. In this section, to avoid notational clumsiness, we use the abbreviation

$$\{\gamma'' \mid \mathbf{c}''\} = \{\gamma'' \mid \mathbf{V}(\gamma'')\} \ . \tag{18.11}$$

From $\{\gamma'' \mid \mathbf{c}''\}' = e^{i\mathbf{k}''\cdot\mathbf{c}''} \{\gamma'' \mid \mathbf{c}''\}$, we have

$$M(\{\gamma'' \mid \mathbf{c}''\}') = e^{i\mathbf{k}''\cdot\mathbf{c}''} M(\{\gamma'' \mid \mathbf{c}''\}) \ . \tag{18.12}$$

The matrix elements of $M(\{\gamma'' \mid \mathbf{c}''\})$ can be expressed as

$$\begin{aligned} M_{\tau b \tau' b', \sigma a \sigma' a'}(\{\gamma'' \mid \mathbf{c}''\}) &= \langle \tau b \tau' b' \mid \{\gamma'' \mid \mathbf{c}''\} \mid \sigma a \sigma' a' \rangle \\ &= D^{(*\mathbf{k})(\nu)}_{\tau b, \sigma a}(\{\gamma'' \mid \mathbf{c}''\}) D^{(*\mathbf{k}')(\nu')}_{\tau' b', \sigma' a'}(\{\gamma'' \mid \mathbf{c}''\}) \ , \end{aligned} \tag{18.13a}$$

or in the form of a direct product of the matrices,

$$M(\{\gamma'' \mid \mathbf{c}''\}) = D^{(*\mathbf{k})(\nu)}(\{\gamma'' \mid \mathbf{c}''\}) \otimes D^{(*\mathbf{k}')(\nu')}(\{\gamma'' \mid \mathbf{c}''\}) \ . \tag{18.13b}$$

The matrices $D^{(*\mathbf{k})(\nu)}(\{\gamma'' \mid \mathbf{c}''\})$ and $D^{(*\mathbf{k}')(\nu')}(\{\gamma'' \mid \mathbf{c}''\})$ can be evaluated from the irreps of the rep groups $\mathbf{G}'_{\mathbf{k}}$ and $\mathbf{G}'_{\mathbf{k}'}$ by using Eq. (15.9) or (15.15), while the matrices $M(C)$ and $M(C(s))$ can be evaluated by using Eq. (18.13). From the secular equations of $M(C)$ and $M(C(s))$, we can get the eigenvalues $(\nu'' a'')$ and their degeneracies. If the degeneracy of the eigenvalue $(\nu'' a'')$ is d, then it implies that the reduction coefficient is

$$(*\mathbf{k}\nu *\mathbf{k}'\nu') \mid *\mathbf{k}''\nu'') = d \ . \tag{18.14}$$

Substituting the eigenvalue (ν'', a'') into Eq. (18.9b), we can get d orthogonal eigenvectors,

$$U^{(\nu'')\theta}_{\mathbf{k}''a''} = \left\{ \left[\begin{matrix} \nu\mathbf{k}\nu'\mathbf{k}' \\ \sigma a \sigma' a' \end{matrix} \middle| \begin{matrix} \nu''\mathbf{k}''\theta \\ 1a'' \end{matrix} \right] \right\}, \quad \theta = 1, 2, \ldots, d \ , \tag{18.15}$$

where the component index for the vector U is $(\sigma a \sigma' a')$.

C. Relative phase of the CG coefficients

To ensure that the CG coefficients (18.10) with the same ν'', $\mathbf{k}''$, and θ, but different a'' have the correct relative phase, we can use the following technique.

Suppose the matrix element of an element $\{\gamma'' \mid \mathbf{c}''\}'$ of $\mathbf{G}'_{\mathbf{k}''}$ has the property

$$| D^{(\mathbf{k}'')(\nu'')}_{b''a''}(\{\gamma'' \mid \mathbf{c}''\}') | = 1 \ , \tag{18.16}$$

for a specific b'' and a''. Then we have

$$\{\gamma'' \mid \mathbf{c}''\}' \psi^{(\nu'')\theta}_{\mathbf{k}''a''} = D^{(\mathbf{k}'')(\nu'')}_{b''a''}(\{\gamma'' \mid \mathbf{c}''\}') \psi^{(\nu'')\theta}_{\mathbf{k}''b''} \ . \tag{18.17}$$

Now suppose the d orthogonal eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''a''}$, $\theta = 1, 2, \ldots, d$, with a definite ν'' and a'' have been obtained from Eq. (18.9b). Then it follows from Eq. (18.17) that the b'' component of the CG coefficient can be found through the formula

$$\begin{aligned} U^{(\nu'')\theta}_{\mathbf{k}''b''} = &[D^{(\mathbf{k}'')(\nu'')}_{b''a''}(\{\gamma'' \mid \mathbf{c}''\}')]^{-1} \\ &\times M(\{\gamma'' \mid \mathbf{c}''\}') U^{(\nu'')\theta}_{\mathbf{k}''a''} \ . \end{aligned} \tag{18.18}$$

Hence it is only necessary to find the d orthogonal eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''a''}$, $\theta = 1, 2, \ldots, d$, for a specific ν'' and a''; all the other eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''b''}$, $b'' \neq a''$, with the correct relative phases, can be found in turn from Eq. (18.18) by choosing in each step an element $\{\gamma'' \mid \mathbf{c}''\}'$ that obeys the condition (18.16).

The matrix elements of irreps for the rep group $\mathbf{G}'_{\mathbf{k}}$ are usually very simple, i.e., requirement (18.16) can always

be met by a certain element $\{\gamma'' \mid \mathbf{c}''\}'$. Even if it were not so, we could still use a slightly different formula, such as (7.6), to evaluate all the components of the CGC successively.

D. The full CG coefficients of space groups

Up to now we have found only the CG coefficients $U^{(\nu'')\theta}_{\mathbf{k}''a''}$ corresponding to $\sigma''=1$. It follows from Eq. (15.2) that the CG coefficients

$$U^{(\nu'')\theta}_{\mathbf{k}''\sigma''a''}=\left\{\begin{pmatrix}\nu\mathbf{k}\nu'\mathbf{k}' \\ \sigma a\sigma' a'\end{pmatrix}\middle|\begin{matrix}\nu''\mathbf{k}''\theta \\ \sigma'' a''\end{matrix}\right\} \tag{18.19}$$

for $\sigma''\neq 1$ can be found from $U^{(\nu'')\theta}_{\mathbf{k}''a''}$ by the formula

$$\begin{aligned}U^{(\nu'')\theta}_{\mathbf{k}''\sigma''a''}&=M(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})U^{(\nu'')\theta}_{\mathbf{k}''a''}\\&=D^{(*\mathbf{k})(\nu)}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})\otimes D^{(*\mathbf{k}')(\nu')}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})U^{(\nu'')\theta}_{\mathbf{k}''a''}\ ,\end{aligned} \tag{18.20}$$

where $\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\}$ is the coset representative of the space group $\mathbf{G}$ with regard to the little group $\mathbf{G}(\mathbf{k}'')$:

$$\mathbf{G}=\sum_{\sigma''=1}^{q''}\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\}\mathbf{G}(\mathbf{k}'')\ . \tag{18.21}$$

Equation (18.20) can be rewritten as

$$\begin{pmatrix}\nu\mathbf{k}\nu'\mathbf{k}' \\ \tau b\tau' b'\end{pmatrix}\begin{matrix}\nu''\mathbf{k}''\theta \\ \sigma'' a''\end{matrix}=\sum_{aa'}D^{(*\mathbf{k})(\nu)}_{\tau b,\sigma a}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})D^{(*\mathbf{k}')(\nu')}_{\tau' b',\sigma' a'}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})\begin{pmatrix}\nu\mathbf{k}\nu'\mathbf{k}' \\ \sigma a\sigma' a'\end{pmatrix}\begin{matrix}\nu''\mathbf{k}''\theta \\ 1a''\end{matrix}\ . \tag{18.22}$$

Observe that there is no summation over σ and σ', on the right-hand side of Eq. (18.22), since the index σ (σ') is uniquely specified by τ (τ') and $\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\}$, for which the submatrix

$$D^{(*\mathbf{k})(\nu)}_{(\tau\sigma)}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\})(D^{(*\mathbf{k}')(\nu')}_{(\tau'\sigma')}(\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\}))$$

does not vanish.

E. Some remarks

The following remarks should be added in regard to the eigenfunction method for evaluating CG coefficients of space groups.

(1) Here we only need to know *a priori* the wave-vector selection rule (which is easy to work out), but not the CG series.

(2) However, if the CG series is known *a priori,* the eigenvalues ($\nu''a''$) can be found easily from the relation between the eigenvalues and characters (6.47), and thus the work of solving the secular equation is saved. Of course this point is important only for hand calculation.

(3) For computer calculation, the CSCO-II of $\mathbf{G}'_{\mathbf{k}''}$ can be appropriately chosen so that it consists of only a single operator (see Sec. VIII.A or XIV.C).

(4) It seems at first sight that the order of the eigenequation (18.9b) is equal to $(qh_\nu)\times(q'h_{\nu'})$. But actually, due to the wave-vector selection rule (18.4), the order of Eq. (18.9b) is much smaller.

F. Summary of the eigenfunction method for space-group CG coefficients

The scheme for obtaining the CG coefficients of space groups can be summarized as follows.

(1) Determine the wave-vector selection rule.

(2) Pick out one star $*\mathbf{k}''$ among those for which the wave-vector reduction coefficients $(*\mathbf{k}*\mathbf{k}'\mid *\mathbf{k}'')\geq 1$ and the CG coefficients are to be calculated.

(3) Choose the canonical wave vectors $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$.

(4) For each of the canonical wave vectors, choose appropriate coset representatives of $\mathbf{G}$,

$$\begin{aligned}\mathbf{G}&=\sum_{\sigma}\oplus\{\beta_\sigma\mid \mathbf{V}_\sigma\}\mathbf{G}(\mathbf{k})\ ,\\ \mathbf{G}&=\sum_{\sigma'}\oplus\{\beta_{\sigma'}\mid \mathbf{V}_{\sigma'}\}\mathbf{G}(\mathbf{k}')\ ,\\ \mathbf{G}&=\sum_{\sigma''}\oplus\{\beta_{\sigma''}\mid \mathbf{V}_{\sigma''}\}\mathbf{G}(\mathbf{k}'')\ ,\end{aligned} \tag{18.23}$$

and find all the $\mathbf{k}$ points in the stars $*\mathbf{k}$ and $*\mathbf{k}'$ according to

$$\begin{aligned}&\mathbf{k}_\sigma=\beta_\sigma\mathbf{k},\quad \sigma=1,2,\ldots,q\ ,\\ &\mathbf{k}'_{\sigma'}=\beta_{\sigma'}\mathbf{k}',\quad \sigma'=1,2,\ldots,q'\ .\end{aligned} \tag{18.24}$$

To simplify calculation, in the following we always choose as the coset representatives elements whose nonprimitive translations are zero, i.e., we assume

$$\mathbf{V}_\sigma=\mathbf{V}_{\sigma'}=\mathbf{V}_{\sigma''}=0\ . \tag{18.25}$$

(5) Determine all the index pairs $(\sigma\sigma')$ which satisfy

$$\mathbf{k}_\sigma+\mathbf{k}'_{\sigma'}=\mathbf{k}''+\mathbf{K}_m\ . \tag{18.26}$$

For convenience in exposition, in the following we assume that there exist only two such pairs, $(\sigma\sigma')$ and $(\tau\tau')$.

(6) Using the eigenfunction method of Sec. XIII, or consulting an existing table, e.g., the Kovalev (1961) table, find the irreps $D^{(\mathbf{k})(\nu)}$, $D^{(\mathbf{k}')(\nu')}$, and $D^{(\mathbf{k}'')(\nu'')}$ for the rep groups $\mathbf{G}'_{\mathbf{k}}$, $\mathbf{G}'_{\mathbf{k}'}$, and $\mathbf{G}'_{\mathbf{k}''}$, respectively.

(7) Construct the irreducible matrices $D^{(*\mathbf{k})(\nu)}(\{\gamma''\,|\,\mathbf{V}(\gamma'')\})$ and $D^{(*k')(\nu')}(\{\gamma''\,|\,\mathbf{V}(\gamma'')\})$ for the elements $\{\gamma''\,|\,\mathbf{V}(\gamma'')\}$ of the group $\mathbf{G}_{\mathbf{k}''}$, from which the CSCO-II of $\mathbf{G}_{\mathbf{k}''}$ is composed. However, only the submatrices related to the indices σ, τ, (σ',τ'), instead of the full matrices $D^{(*\mathbf{k})(\nu)}$ ($D^{(*\mathbf{k}')(\nu')}$), are required to determine the CG coefficients, e.g.,

$$[D^{(*\mathbf{k})(\nu)}(\{\gamma''\,|\,\mathbf{V}(\gamma'')\})]=\begin{matrix}&\tau&\sigma\\ \tau\\ \sigma\end{matrix}\begin{bmatrix} D_{(\tau\tau)} & D_{(\tau\sigma)}\\ D_{(\sigma\tau)} & D_{(\sigma\sigma)}\end{bmatrix},$$

$$[D^{(*\mathbf{k}')(\nu')}(\{\gamma''\,|\,\mathbf{V}(\gamma'')\})]=\begin{matrix}&\tau'&\sigma'\\ \tau'\\ \sigma'\end{matrix}\begin{bmatrix} D'_{(\tau'\tau')} & D'_{(\tau'\sigma')}\\ D'_{(\sigma'\tau')} & D'_{(\sigma'\sigma')}\end{bmatrix}, \tag{18.27a}$$

where the bold square brackets denote a submatrix, and

$$D_{(\tau\sigma)}=\exp[-i\mathbf{k}_\tau\cdot\mathbf{V}(\gamma'')]\Delta(\beta_\tau^{-1}\gamma''\beta_\sigma)\,,$$
$$D'_{(\tau'\sigma')}=\exp[-i\mathbf{k}'_{\tau'}\cdot\mathbf{V}(\gamma'')]\Delta(\beta_{\tau'}^{-1}\gamma''\beta_{\sigma'})\,, \tag{18.27b}$$

from Eq. (15.15).

(8) With the help of Eq. (18.13b), construct the representation matrix of $\{\gamma''\,|\,\mathbf{V}(\gamma'')\}$ in the uncoupled rep,

$$M(\{\gamma''\,|\,\mathbf{V}(\gamma'')\}')=\begin{matrix}&\tau\tau'&\sigma\sigma'\\ \tau\tau'\\ \sigma\sigma'\end{matrix}\begin{bmatrix} D_{(\tau\tau)}\otimes D'_{(\tau'\tau')} & D_{(\tau\sigma)}\otimes D'_{(\tau'\sigma')}\\ D_{(\sigma\tau)}\otimes D'_{(\sigma'\tau')} & D_{(\sigma\sigma)}\otimes D'_{(\sigma'\sigma')}\end{bmatrix}. \tag{18.28a}$$

Then form the matrix

$$M(\{\gamma''\,|\,\mathbf{V}(\gamma'')\}')=\exp[i\mathbf{k}''\cdot\mathbf{V}(\gamma'')]M(\{\gamma''\,|\,\mathbf{V}(\gamma'')\})\,. \tag{18.28b}$$

The ordering for rows or columns in the matrix M is as follows:

$$|\tau 1\tau' 1\rangle\cdots|\tau 1\tau' h_{\nu'}\rangle, |\tau 2\tau' 1\rangle\cdots|\tau 2\tau' h_{\nu'}\rangle\cdots|\tau h_\nu\tau' h_{\nu'}\rangle\,,$$
$$|\sigma 1\sigma' 1\rangle\cdots|\sigma 1\sigma' h_{\nu'}\rangle, |\sigma 2\sigma' 1\rangle\cdots|\sigma 2\sigma' h_{\nu'}\rangle\cdots|\sigma h_\nu\sigma' h_{\nu'}\rangle\,. \tag{18.29}$$

Suppose the class operator C_i is contained in the CSCO-II of $\mathbf{G}'_{\mathbf{k}''}$. By adding up the matrices $M(\{\gamma''\,|\,\mathbf{V}(\gamma'')\}')$ for all $\{\gamma''\,|\,\mathbf{V}(\gamma'')\}$ belonging to the class i, we obtain the matrix $M(C_i)$. In this way we can obtain the matrices $M(C)$ and $M(C(s))$ of the CSCO-II of $\mathbf{G}'_{\mathbf{k}''}$.

(9) By diagonalizing the matrices $M(C)$ and $M(C(s))$ simultaneously, we get the eigenvalues $(\nu''a'')$ and their degeneracies $d=(*\mathbf{k}\nu *\mathbf{k}'\nu'\,|\,*\mathbf{k}''\nu'')$. Or equivalently, we first diagonalize the matrix $M(C)$ and get the eigenvalues ν'' and the corresponding degeneracies $m_{\nu''}$. Then the reduction coefficient $(*\mathbf{k}\nu *\mathbf{k}'\nu'\,|\,*\mathbf{k}''\nu'')=m_{\nu''}/h_{\nu''}$; $h_{\nu''}$ is the dimension of the irrep $D^{(\mathbf{k}'')(\nu'')}$ of $\mathbf{G}'_{\mathbf{k}''}$.

For each ν'' and a specific but arbitrarily chosen a'', find the eigenvectors $U^{(\nu'')\theta}_{\mathbf{k}''a''}$, $\theta=1,2,\ldots,d$.

(10) Using Eq. (18.18), obtain all the CG coefficients belonging to $\sigma''=1$.

(11) Using Eq. (18.22), obtain the CG coefficients for $\sigma''\neq 1$.

(12) Pick out another star $*\mathbf{k}''$, choose its canonical wave vector $\mathbf{k}''$ and coset representatives $\{\beta_{\sigma''}\,|\,\mathbf{V}_{\sigma''}\}$, then return to step (5) and go through to the end.

A program in FORTRAN based on the EFM is now being written for computing space-group CG coefficients (Zheng, 1985).

XIX. EXAMPLES: OBTAINING SPACE-GROUP CLEBSCH-GORDAN COEFFICIENTS

In this section, following the prescription in Sec. XVIII step by step, we shall give two examples of calculations for the CG coefficients of the nonsymmorphic space group O_h^7.

A. The CG coefficients of O_h^7 for $*X(1)\otimes *X(2)\to *X(\nu'')$

(1) The wave-vector selection rule is easily found:

$$*X\otimes *X=3\Gamma+2*X\,. \tag{19.1}$$

(2) Pick out $*\mathbf{k}''=*X$.

(3) The canonical wave vectors are chosen as

$$\mathbf{k}=\mathbf{k}'=\mathbf{k}''=\mathbf{k}_z=(\tfrac{1}{2}\,\tfrac{1}{2}\,0)\,, \tag{19.2}$$

with $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$ as basis.

Notice that the choice in Eq. (19.2) is different from that given by Berenson, Itzkan, and Birman (1975). They choose

$$\mathbf{k}=\mathbf{k}_x,\quad \mathbf{k}'=\mathbf{k}_y,\quad \mathbf{k}''=\mathbf{k}_z\,. \tag{19.3}$$

(4) The coset representatives of O_h^7 with respect to the little group $\mathbf{G}(X)$ are chosen to be

$$\{\beta_2\,|\,\mathbf{V}_2\}=\{C_{31}^+\,|\,0\},\quad \{\beta_3\,|\,\mathbf{V}_3\}=\{C_{31}^-\,|\,0\}\,. \tag{19.4}$$

Under the rotation C_{31}^+, the wave vectors $\mathbf{k}_x$, $\mathbf{k}_y$, and $\mathbf{k}_z$ transform among themselves cyclically.

The star X contains three $\mathbf{k}$ points, $\mathbf{k}_\sigma=\beta_\sigma\mathbf{k}$,

$$\mathbf{k}_1=\mathbf{k}=\mathbf{k}_z=(\tfrac{1}{2}\,\tfrac{1}{2}\,0)\,,$$
$$\mathbf{k}_2=\mathbf{k}_x=(0\,\tfrac{1}{2}\,\tfrac{1}{2})\,, \tag{19.5}$$
$$\mathbf{k}_3=\mathbf{k}_y=(\tfrac{1}{2}\,0\,\tfrac{1}{2})\,.$$

TABLE XIV. The ray irreps $\Delta^{X_i}(\gamma)$ for the little co-group $\mathbf{G}_0(\mathbf{X})$, i.e., the irreps of the rep group $\mathbf{G}'_X$. $\Delta^{X_2}=\delta^{(2)}\Delta^{X_1}$, $\Delta^{X_4}=\delta^{(4)}\Delta^{X_3}$; $X_1\to\hat{\tau}^3$, $X_2\to\hat{\tau}^4$, $X_3\to\hat{\tau}^2$, $X_4\to\hat{\tau}^1$, where $\hat{\tau}^i$ are the labels used by Kovalev. From Kovalev (1961).

	(C_1,C_2)	$C(s)$		ε	C_{2y}	C_{2z}	C_{2x}	C_{4z}^-	C_{4z}^+	C_{2a}	C_{2b}	I	σ_y	σ_z	σ_x	S_{4z}^+	S_{4z}^-	σ_{da}	σ_{db}
X_1	(0,2)	$\left.\begin{matrix}1\\-1\end{matrix}\right\}$		ε	φ	ε	φ	λ	λ	κ	κ	κ	λ	κ	λ	φ	φ	ε	ε
X_2	(0,−2)	$\left.\begin{matrix}1\\-1\end{matrix}\right\}$	$\delta^{(2)}$	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$-$	$-$	$-$	$-$	$-$	$-$	$-$	$-$
X_3	(2i,0)	$\left.\begin{matrix}-i\\i\end{matrix}\right\}$		ε	λ	$-\varepsilon$	$-\lambda$	λi	$-\lambda i$	εi	$-\varepsilon i$	κ	$-\varphi$	$-\kappa$	φ	φi	$-\varphi i$	$-\kappa i$	κi
X_4	(−2i,0)	$\left.\begin{matrix}-i\\i\end{matrix}\right\}$	$\delta^{(4)}$	$+$	$-$	$+$	$-$	$+$	$+$	$-$	$-$	$+$	$-$	$+$	$-$	$+$	$+$	$-$	$-$

(5) From Eq. (19.5) it is readily seen that

$$\mathbf{k}_x+\mathbf{k}_y=\mathbf{k}_z+(001). \tag{19.6}$$

Hence the index pairs are $(\tau\tau')=(23)$ and $(\sigma\sigma')=(32)$.

(6) The ray or projective irreps $\Delta^{X_i}(\gamma)$ for the little co-group $\mathbf{G}_0(\mathbf{X})$ are given in Kovalev (1961), Table T159. We relist them here in Table XIV.

In Table XIV and in the following we often use the symbols

$$\varepsilon=\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad \lambda=\begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad \varphi=\begin{bmatrix}0&1\\1&0\end{bmatrix},$$
$$\kappa=\begin{bmatrix}0&1\\-1&0\end{bmatrix},\quad \mu=\begin{bmatrix}1&0\\0&i\end{bmatrix}. \tag{19.7}$$

(7) From Eq. (14.15) we know that CSCO-I of the group $\mathbf{G}'_X$ is

$$C=(C_1,C_2),\quad C_1=\{C_{2a}\,|\,\boldsymbol{\tau}\}'-\{C_{2b}\,|\,\boldsymbol{\tau}\}',$$
$$C_2=\{\sigma_{da}\,|\,0\}+\{\sigma_{ab}\,|\,0\}\,. \tag{19.8}$$

The eigenvalues of (C_1,C_2) are listed in Table XIV. Furthermore, from this table it is seen that apart from the identity the only elements whose matrices are always diagonalized for the irreps X_1–X_4 are $\{C_{4z}^+\,|\,\boldsymbol{\tau}\}'$ and $\{C_{4z}^-\,|\,\boldsymbol{\tau}\}'$. Hence either $\{C_{4z}^+\,|\,\boldsymbol{\tau}\}'$ or $\{C_{4z}^-\,|\,\boldsymbol{\tau}\}'$ can be taken as the operator $C(s)$, whose eigenvalues are used to distinguish the two basis vectors of the irreps X_1–X_4. We choose

$$C(s)=\{C_{4z}^+\,|\,\boldsymbol{\tau}\}'\,. \tag{19.9}$$

The eigenvalues of $C(s)$ listed in Table XIV are inferred from the diagonal elements of the matrices $\Delta^{X_j}(C_{4z}^+)$.

Using Eq. (15.9) or (18.27) and Table XIV, we can easily construct the space-group rep $D^{(*X)(\nu)}$. For example,

$$\mathscr{D}(\{C_{4z}^+\,|\,\boldsymbol{\tau}\})=\begin{array}{c}\\ \varepsilon\\ C_{31}^-\\ C_{31}^+\end{array}\begin{array}{c}\begin{array}{ccc}\varepsilon & C_{31}^+ & C_{31}^-\end{array}\\ \begin{bmatrix}\Delta(C_{4z}^+) & 0 & 0\\ 0 & 0 & \Delta(C_{2a})\\ 0 & \Delta(C_{4z}^-) & 0\end{bmatrix}\end{array}, \tag{19.10a}$$

$$D^{(*X)(j)}(\{C_{4z}^+\,|\,\boldsymbol{\tau}\})=-i\mathscr{D}(\{C_{4z}^+\,|\,\boldsymbol{\tau}\})$$
$$=\begin{bmatrix}-\lambda i&0&0\\0&0&-\kappa i\\0&-\lambda i&0\end{bmatrix},\quad j=1,2\,. \tag{19.10b}$$

Similarly we have

$$D^{(*X)(j)}(\{C_{2a}\,|\,\boldsymbol{\tau}\})=\begin{bmatrix}-\kappa i&0&0\\0&0&-\lambda i\\0&-\lambda i&0\end{bmatrix},$$

$$D^{(*X)(j)}(\{C_{2b}\,|\,\tau\})=\begin{bmatrix}-\kappa i & 0 & 0\\ 0 & 0 & -\kappa i\\ 0 & -\kappa i & 0\end{bmatrix},$$
$$D^{(*X)(j)}(\{\sigma_{da}\,|\,0\})=(-1)^{j+1}\begin{bmatrix}\varepsilon & 0 & 0\\ 0 & 0 & \varphi\\ 0 & \varphi & 0\end{bmatrix}, \tag{19.10c}$$
$$D^{(*X)(j)}(\{\sigma_{db}\,|\,0\})=(-1)^{j+1}\begin{bmatrix}\varepsilon & 0 & 0\\ 0 & 0 & \varepsilon\\ 0 & \varepsilon & 0\end{bmatrix},\quad j=1,2\ .$$

(8) From Eqs. (18.28) and (19.10) we have

$$M(C_1)=M(\{C_{2a}\,|\,\tau\}')-M(\{C_{2b}\,|\,\tau\}')$$
$$=\begin{array}{c}\\23\\32\end{array}\begin{array}{c}\begin{array}{ccc}23 & & 32\end{array}\\ \begin{bmatrix}0 & -\lambda & \kappa\\ & -\kappa & \lambda\\ -\lambda & \kappa & 0\\ -\kappa & \lambda & \end{bmatrix}\end{array}(i)\ , \tag{19.11a}$$

$$M(C_2)=-\begin{bmatrix}0 & \varepsilon & \varphi\\ & \varphi & \varepsilon\\ \varepsilon & \varphi & 0\\ \varphi & \varepsilon & \end{bmatrix}, \tag{19.11b}$$

$$M(C(s))=i\begin{bmatrix}0 & 0 & \lambda\\ & -\lambda & 0\\ \kappa & 0 & 0\\ 0 & -\kappa & \end{bmatrix},$$

$$M(\{C_{2a}\,|\,\tau\}')=i\begin{bmatrix}0 & -\lambda & 0\\ & 0 & \lambda\\ -\lambda & 0 & 0\\ 0 & \lambda & \end{bmatrix}, \tag{19.11c}$$

$$M(\{\sigma_a\,|\,0\})=\begin{bmatrix}0 & 0 & \varphi\\ & \varphi & 0\\ 0 & \varphi & 0\\ \varphi & 0 & \end{bmatrix}.$$

By setting $(\tau\tau')=(23)$, $(\sigma\sigma')=(32)$, and $h_\nu=h_{\nu'}=2$ in Eq. (18.29), we obtain the ordering of the product basis vectors

$$|x1y1\rangle,\ |x1y2\rangle,\ |x2y1\rangle,\ |x2y2\rangle,$$
$$|y1x1\rangle,\ |y1x2\rangle,\ |y2x1\rangle,\ |y2x2\rangle, \tag{19.12}$$

where $|xayb\rangle$ represents the vector $|\psi^{(X_1)}_{\mathbf{k}_x a}\psi^{(X_2)}_{\mathbf{k}_y b}\rangle$.

(9) The eigenvalues of $M(C_1)$ and $M(C_2)$ are found to be

$$(C_1,C_2)=(0,2),\ (0,-2),\ (2i,0),\ (-2i,0)\ ,$$

and each has the degeneracy 2. By comparing with Table XIV we get the CG series

$$*X(1)\otimes *X(2)=*X(1)\oplus *X(2)\oplus *X(3)\oplus *X(4)\ . \tag{19.13}$$

The eigenvalues of $M(C(s))$ are found to be ±1, $\pm i$. Substituting the four sets of eigenvalues of $(C_1,C_2,C(s))$—(0,2,1), (0,−2,1), (2i,0,−i), and (−2i,0,−i)—into the eigenequation (18.9), we obtain the four eigenvectors listed in the odd rows of Table XV. They are the CG coefficients for the first components $a''=1$.

(10) On the basis of Eq. (18.18) and Table XIV, the second component of the CG coefficients can be expressed as

$$U^{(X_j)}_{\mathbf{k}_z 2}=\frac{M(\{C_{2a}\,|\,\tau\}')}{\Delta^{(X_j)}_{21}(C_{2a})}U^{(X_j)}_{\mathbf{k}_z 1}$$
$$=-M(\{C_{2a}\,|\,\tau\}')U^{(X_j)}_{\mathbf{k}_z 1},\quad j=1,2\ ,$$
$$U^{(x_j)}_{\mathbf{k}_z 2}=\frac{M(\{\sigma_{da}\,|\,0\})}{\Delta^{(X_j)}_{21}(\sigma_{da})}U^{(X_j)}_{\mathbf{k}_z 1} \tag{19.14}$$
$$=i(-1)^j M(\{\sigma_{da}\,|\,0\})U^{(X_j)}_{\mathbf{k}_z 1},\quad j=3,4\ .$$

With Eqs. (19.14) and (19.11c), as well as the odd rows in Table XV, we can find $U^{(X_j)}_{\mathbf{k}_z 2}$, e.g.,

$$U^{(X_3)}_{\mathbf{k}_z 2}=\frac{i}{\sqrt{8}}\begin{bmatrix}&&&&&&&1\\&&&&&&1&\\&&&&&1&&\\&&&&1&&&\\&&&1&&&&\\&&1&&&&&\\&1&&&&&&\\1&&&&&&&\end{bmatrix}\begin{bmatrix}1\\-1\\1\\-1\\-1\\-1\\1\\1\end{bmatrix}$$
$$=\frac{1}{\sqrt{8}}\begin{bmatrix}i\\i\\-i\\-i\\-i\\i\\-i\\i\end{bmatrix}. \tag{19.15}$$

The CG coefficients $U^{(X_j)}_{\mathbf{k}_z 2}$ are listed in the even rows of Table XV.

(11) In order to obtain the CG coefficients with $\sigma''\neq1$, we in general need to use Eq. (18.22). However, for the case where

$$*\mathbf{k}=*\mathbf{k}'=*\mathbf{k}''\ ,$$
$$\{\beta_\sigma\,|\,\mathbf{V}_\sigma\}=\{\beta_{\sigma'}\,|\,\mathbf{V}_{\sigma'}\}=\{\beta_{\sigma''}\,|\,\mathbf{V}_{\sigma''}\}\ , \tag{19.16}$$

it is a very simple matter to obtain the CG coefficients

TABLE XV. The CG coefficients $\langle {}^{\mathbf{k}\nu\gamma\mathbf{k}'}_{\alpha\sigma\alpha'} | {}^{X(j)}_{k_z''} \rangle$ of O_h^7 for $*X(1)\otimes *X(2)$ and $\sigma''=1$. $xayb$ signifies $\mathbf{k}_x a \mathbf{k}_y b$, etc.

	(C_1C_2)	$C(s)$	N	$x1y1$	$x1y2$	$x2y1$	$x2y2$	$y1x1$	$y1x2$	$y2x1$	$y2x2$
$X(1)$	(0,2)	1	$(\frac{1}{8})^{1/2}$	1	$-i$	$-i$	1	-1	i	i	-1
		-1	$(\frac{1}{8})^{1/2}$	$-i$	1	1	$-i$	i	-1	-1	i
$X(2)$	(0,−2)	1	$(\frac{1}{8})^{1/2}$	1	i	i	1	1	i	i	1
		-1	$(\frac{1}{8})^{1/2}$	i	1	1	i	i	1	1	i
$X(3)$	(2i,0)	$-i$	$(\frac{1}{8})^{1/2}$	1	-1	1	-1	-1	-1	1	1
		i	$(\frac{1}{8})^{1/2}$	i	i	$-i$	$-i$	$-i$	i	$-i$	i
$X(4)$	(−2i,0)	$-i$	$(\frac{1}{8})^{1/2}$	1	1	-1	-1	1	-1	1	-1
		i	$(\frac{1}{8})^{1/2}$	i	$-i$	i	$-i$	i	i	$-i$	$-i$

with $\sigma''\neq 1$ from those with $\sigma''=1$. For example, in our case here for $\sigma''=2$, $\{\beta_{\sigma''} \mid \mathbf{V}_{\sigma''}\}=C_{31}^{+}$,

$$\psi_{\mathbf{k}_x}^{X(1)} = C_{31}^{+}\psi_{\mathbf{k}_z}^{X(1)}$$
$$= (\tfrac{1}{8})^{1/2}(\mid y\,1z\,1\rangle - i \mid y\,1z\,2\rangle - i \mid y\,2z\,1\rangle$$
$$+ \mid y\,2z\,2\rangle - \mid z\,1y\,1\rangle + i \mid z\,1y\,2\rangle$$
$$+ i \mid z\,2y\,1\rangle + \mid z\,2y\,2\rangle) .$$

Hence the CG coefficients for $\sigma''=2$ and 3 result from a cyclic permutation of x, y, and z in Table XV.

Similarly, by letting $*\mathbf{k}=\Gamma$, we can get the CG coefficients for $*X(1)\otimes *X(2)\rightarrow\Gamma(\nu'')$.

Both Saulevich *et al.* (1970) and Berenson *et al.* (1975) have calculated the CG coefficients of O_h^7 for $*X(1)\otimes *X(2)$, and discrepancies were found, as pointed out in the latter paper. Our result supports that of Berenson *et al.*

B. The CG coefficients of O_h^7 for $*X(1)\otimes *W(1)\rightarrow *\Delta(\nu'')$

We now turn to a more general example for which the three wave-vector stars $*\mathbf{k}$, $*\mathbf{k}'$, and $*\mathbf{k}''$ are all different and the multiplicity may be larger than one.

(1) The wave-vector selection rule is easily found (Birman, 1962):

$$*X\otimes *W = 2*\Delta + *W . \tag{19.17a}$$

(2) Pick out $*\mathbf{k}''=*\Delta$.

(3) The canonical wave vectors are chosen to be

$$\text{Star } X\text{: } \mathbf{k}=(\tfrac{1}{2}\,\tfrac{1}{2}\,0) ,$$
$$\text{Star } W\text{: } \mathbf{k}'=(\tfrac{1}{2}\,\tfrac{1}{4}\,\tfrac{3}{4}) , \tag{19.17b}$$
$$\text{Star } \Delta\text{: } \mathbf{k}''=(\tfrac{1}{4}\,\tfrac{1}{4}\,0) .$$

(4) The coset representatives and $\mathbf{k}_\sigma$ for star X are identical with Eqs. (19.4) and (19.5), while the coset representatives $\{\beta_{\sigma'} \mid \mathbf{V}_{\sigma'}\}$ and $\mathbf{k}'_{\sigma'}$ for star W are listed in Table XVI.

It should be noted although the wave vector, e.g., $\mathbf{k}'=(\frac{1}{2}\,-\frac{1}{4}\,\frac{1}{4})$, is equivalent to $(\frac{1}{2}\,\frac{3}{4}\,\frac{1}{4})$, the former is *not replaceable* by the latter; otherwise errors will be incurred.

(5) From

$$\mathbf{k}_2+\mathbf{k}'_5=\mathbf{k}''+(011) ,$$
$$\mathbf{k}_3+\mathbf{k}'_\sigma=\mathbf{k}''+(001) , \tag{19.18}$$

it is seen that the index pairs are $(\tau\tau')=(25)$ and $(\sigma\sigma')=(36)$.

(6) The irreps $D^{(X)(\nu)}$ and $D^{(W)(\nu')}$ are given in Tables XIV and XII, respectively.

(7) Δ is an internal point, hence its representation group $\mathbf{G}'_\Delta$ is isomorphic to the little co-group, the point group C_{4v}. From Table III we see that among the three class operators (C_3,C_4,C_5), any two can serve as the CSCO-I C of C_{4v}. Here let us choose $C=(C_3,C_4)$. Besides, we

TABLE XVI. The coset representatives $\{\beta_{\sigma'}|\mathbf{V}_{\sigma'}\}$ and $\mathbf{k}'_{\sigma'}$ for star W.

σ'	1	2	3	4	5	6
$\{\beta_{\sigma'}\|\mathbf{V}_{\sigma'}\}$	$\{\varepsilon\|0\}$	$\{C_{2y}\|0\}$	$\{C_{31}^{+}\|0\}$	$\{C_{33}^{+}\|0\}$	$\{C_{31}^{-}\|0\}$	$\{C_{32}^{-}\|0\}$
$\mathbf{k}'_{\sigma'}$	$(\frac{1}{2}\ \frac{1}{4}\ \frac{3}{4})$	$(\frac{1}{2}\ -\frac{1}{4}\ \frac{1}{4})$	$(\frac{3}{4}\ \frac{1}{2}\ \frac{1}{4})$	$(\frac{1}{4}\ \frac{1}{2}\ -\frac{1}{4})$	$(\frac{1}{4}\ \frac{3}{4}\ \frac{1}{2})$	$(-\frac{1}{4}\ \frac{1}{4}\ \frac{1}{2})$

choose $C(s)=\sigma_y$; this corresponds to choosing (x,y) as the basis vectors of the two-dimensional irrep of C_{4v}. Due to the isomorphism between G'_Δ and C_{4v}, the CSCO-I of G'_Δ is

$$C=(C_3,C_4),\quad C_3=\{C_{4z}^{+}|\tau\}'+\{C_{4z}^{-}|\tau\}',$$
$$C_4=\{\sigma_x|\tau\}'+\{\sigma_y|\tau\}', \tag{19.19}$$

and the operator $C(s)$ is

$$C(s)=\{\sigma_y|\tau\}'. \tag{19.20}$$

By means of Eq. (18.27) and Tables XIV and XII, we can construct the following submatrices:

$$[D^{(*X)(1)}(\{C_{4z}^{+}|\tau\})]=\begin{matrix}&2&3\\2&0&\kappa\\3&\lambda&0\end{matrix}(-i),$$

$$[D^{(*X)(1)}(\{C_{4z}^{-}|\tau\})]=-i\begin{bmatrix}0&\lambda\\\kappa&0\end{bmatrix},$$

$$[D^{(*X)(1)}(\{\sigma_x|\tau\})]=-i\begin{bmatrix}\kappa&0\\0&\lambda\end{bmatrix},$$

$$[D^{(*X)(1)}(\{\sigma_y|\tau\})]=-i\begin{bmatrix}\lambda&0\\0&\kappa\end{bmatrix},$$

$$[D^{(*W)(1)}(\{C_{4z}^{+}|\tau\})]=\begin{matrix}&5&6\\5&0&-\mu i\\6&\mu^*&0\end{matrix}e^{-\pi i/4},$$

$$[D^{(*W)(1)}(\{C_{4z}^{-}|\tau\})]=e^{-\pi i/4}\begin{bmatrix}0&-\mu^* i\\\mu&0\end{bmatrix},$$

$$[D^{(*W)(1)}(\{\sigma_x|\tau\})]=e^{-\pi i/4}\begin{bmatrix}\kappa i&0\\0&-\kappa\end{bmatrix},$$

$$[D^{(*W)(1)}(\{\sigma_y|\tau\})]=e^{-\pi i/4}\begin{bmatrix}-\varphi i&0\\0&\varphi\end{bmatrix}. \tag{19.21}$$

The 2×2 matrices $\kappa,\lambda,\ldots,$ are defined in Eq. (19.7).

(8) Using Eqs. (18.28) and (19.21), we obtain

$$M(\{C_{4z}^{+}|\tau\}')=\begin{matrix}&25&36\\25&0&\begin{bmatrix}0&-1\\1&0\end{bmatrix}\mu\\36&\begin{bmatrix}-i&0\\0&i\end{bmatrix}\mu^*&0\end{matrix},$$

$$M(\{C_{4z}^{-}|\tau\}')=\begin{bmatrix}0&\begin{bmatrix}-1&0\\0&1\end{bmatrix}\mu^*\\\begin{bmatrix}0&-i\\i&0\end{bmatrix}\mu&0\end{bmatrix},$$

$$M(\{\sigma_x|\tau\}')=\begin{bmatrix}\begin{bmatrix}0&1\\-1&0\end{bmatrix}\kappa&0\\0&\begin{bmatrix}i&0\\0&-i\end{bmatrix}\kappa\end{bmatrix},$$

$$M(\{\sigma_y|\tau\}')=\begin{bmatrix}\begin{bmatrix}-1&0\\0&1\end{bmatrix}\varphi&0\\0&\begin{bmatrix}0&-i\\i&0\end{bmatrix}\varphi\end{bmatrix}. \tag{19.22}$$

By setting $(\tau\tau')=(25)$, $(\sigma\sigma')=(36)$, and $h_\nu=h_{\nu'}=2$ in Eq. (18.29), we get the ordering for the eight product basis vectors:

$$|2151\rangle,\ |2152\rangle,\ |2251\rangle,\ |2252\rangle,$$
$$|3161\rangle,\ |3162\rangle,\ |3261\rangle,\ |3262\rangle. \tag{19.23}$$

(9) The eigenvalues of the matrices $M(C_3)=M(\{C_{4z}^{+}|\tau\}')+M(\{C_{4z}^{-}|\tau\}')$ and $M(C_4)=M(\{\sigma_x|\tau\}')+M(\{\sigma_y|\tau\}')$ are found to be

$$\text{Single roots: } (2,2),(2,-2),(-2,2),(-2,-2);$$
$$\text{Quartet root: } (0,0), \tag{19.24}$$

which corresponds, according to Table III, to the point group reps A_1, A_2, B_1, B_2, and E, respectively. The first four are one dimensional, and the last one is two dimensional. We use $\Delta(1)$—$\Delta(5)$ to denote the corresponding reps for the group G'_Δ. The degeneracy 4 divided by the dimensionality 2 gives the number of times that the irrep $\Delta(5)$ occurs in the rep $*X(1)\otimes *W(1)$. Therefore, we have the CG series.

TABLE XVII. The CG coefficients $\left(\begin{smallmatrix} X(1)W(1) & \Delta(\nu'')\theta \\ \sigma a\ \sigma' a' & 1a'' \end{smallmatrix}\right)$ of O_h^7 for $*X(1)\otimes *W(1)$ and $\sigma''=1$.

					$\sigma a\sigma' a'$								
	(C_3,C_4)		$C(s)$	θ	N	$\lvert 2151\rangle$	$\lvert 2152\rangle$	$\lvert 2251\rangle$	$\lvert 2252\rangle$	$\lvert 3161\rangle$	$\lvert 3162\rangle$	$\lvert 3261\rangle$	$\lvert 3262\rangle$
$\Delta(1)$	A_1	(2,2)			$(\frac{1}{8})^{1/2}$	1	−1	1	1	1	$-i$	1	i
$\Delta(2)$	A_2	(2,−2)			$(\frac{1}{8})^{1/2}$	1	1	1	−1	−1	$-i$	−1	i
$\Delta(3)$	B_1	(-2,2)			$(\frac{1}{8})^{1/2}$	1	−1	1	1	−1	i	−1	$-i$
$\Delta(4)$	B_2	(-2,−2)			$(\frac{1}{8})^{1/2}$	1	1	1	−1	1	i	1	$-i$
$\Delta(5)$	E	(0,0)	1	1	$\frac{1}{2}$	1	−1	−1	−1				
			−1	1	$\frac{1}{2}$					1	$-i$	−1	$-i$
$\Delta(5)$	E	(0,0)	1	2	$\frac{1}{2}$					1	i	−1	i
			−1	2	$\frac{1}{2}$	1	1	−1	1				

$$*X(1)\otimes *W(1)$$
$$=*\Delta(1)\oplus *\Delta(2)\oplus *\Delta(3)\oplus *\Delta(4)\oplus 2*\Delta(5)\ . \quad (19.25)$$

For the first four single roots, we can immediately find the corresponding eigenvectors, as listed in the first four rows of Table XVII. For the quartet root (0,0), a further diagonalization of the matrix $M(C(s))$ is required. Its eigenvalues $a''=1$ and -1 correspond to the first and second components of the rep $\Delta(5)$, respectively. When we substitute the eigenvalues (0,0,1) of $(C_3,C_4,C(s))$ into their eigenequations, a degeneracy of 2 remains. Consequently there exist two linearly independent solutions. The two orthogonal eigenvectors can be chosen as

$$U_{\mathbf{k}'',1}^{(\theta=1)}=\tfrac{1}{2}(1,-1,-1,-1,0,0,0,0)\ ,$$
$$U_{\mathbf{k}'',1}^{(\theta=2)}=\tfrac{1}{2}(0,0,0,0,1,i,-1,i)\ . \quad (19.26)$$

(10) It is known that the matrix for the element C_{4z} in the rep E of C_{4v} is

$$D^{(E)}(C_{4z}^{+})=\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\ . \quad (19.27)$$

Hence Eq. (18.18) now reads

$$U_{\mathbf{k}''2}^{(\theta)}=\frac{1}{D_{21}^{(E)}(C_{4z}^{+})}M(\{C_{4z}^{+}\mid\tau\}')U_{\mathbf{k}''1}^{(\theta)}\ . \quad (19.28)$$

From Eqs. (19.22) and (19.26)—(19.28) we can calculate $U_{\mathbf{k}''2}^{(\theta)}$; the result is listed in Table XVII.

(11) Using Eq. (18.22), we can get the CG coefficients with $\sigma''\neq 1$ which are not listed here.

XX. OTHER METHODS FOR OBTAINING SPACE-GROUP CLEBSCH-GORDAN COEFFICIENTS

In recent years there has been a remarkable number of papers devoted to the space-group CGC. They mainly fall into the following three categories.

A. Berenson's method

The Koster method (see Sec. VII.E) has been used to calculate the space-group CGC by Berenson and Birman (1975) and Berenson *et al.* (1975). Similar discussions were presented by Litvan and Zak (1969), Saulevich *et al.* (1970), Sakata (1974), and Cornwell (1970). To facilitate comparison, we use Berenson's notation,

$$U_{\sigma a\sigma' a',\sigma'' a''}^{(\theta)}=\left(\begin{array}{cc|c}\mathbf{k}\nu & \mathbf{k}'\nu' & \mathbf{k}''\nu''\theta\\ \sigma a & \sigma' a' & \sigma'' a''\end{array}\right) \quad (20.1)$$

for the CGC and use $U(\sigma\sigma'\sigma'')$ to denote the submatrix of the $(\sigma\sigma'\sigma'')$ block, with aa' as the row index and a'' as the column index; we refer to $U(111)$ as the principle-block CGC.

Equation (7.34a) now reads

$$\langle \sigma a \sigma' a' \mid P^{(*\mathbf{k}'')(\nu'')}_{\sigma'' a'', \tau'' b''} \mid \tau b \tau' b' \rangle = \sum_{\theta} U^{(\theta)}_{\sigma a \sigma' a', \sigma'' a''} (U^{(\theta)}_{\tau b \tau' b', \tau'' b''})^* \ . \tag{20.2a}$$

From Eq. (17.26) we have

$$\langle \sigma a \sigma' a' \mid P^{(*\mathbf{k}'')(\nu'')}_{\sigma'' a'', \tau'' b''} \mid \tau b \tau' b' \rangle = \frac{q'' h_{\nu''}}{N \mid \mathbf{G}_0 \mid} \sum_{\{\alpha \mid \mathbf{a}\}} D^{(*\mathbf{k})(\nu)}_{\sigma a, \tau b}(\{\alpha \mid \mathbf{a}\}) D^{(*\mathbf{k}')(\nu')}_{\sigma' a', \tau' b'}(\{\alpha \mid \mathbf{a}\}) D^{(*\mathbf{k}'')(\nu'')}_{\sigma'' a'', \tau'', b''}(\{\alpha \mid \mathbf{a}\})^* \ , \tag{20.2b}$$

where $\{\alpha \mid \mathbf{a}\}$ $[=\{\alpha \mid \mathbf{V}(\alpha)+\mathbf{R}_n\}]$ is to be summed over all the $N \mid \mathbf{G}_0 \mid$ elements of $\mathbf{G}$.

Using Eqs. (15.8e) and (15.9a) and the irreducibility of the rep of the translation group $\mathbf{T}$, we have

$$\frac{1}{N} \sum_{n} \exp[-i(\mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} - \mathbf{k}''_{\sigma''}) \cdot \mathbf{R}_n] = \begin{cases} 0 & \text{for } \mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} - \mathbf{k}''_{\sigma''} \neq \mathbf{K}_m \\ 1 & \text{for } \mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} - \mathbf{k}''_{\sigma''} = \mathbf{K}_m \end{cases} \ . \tag{20.3}$$

Equation (20.2b) becomes

$$\langle \sigma a \sigma' a' \mid P^{(*\mathbf{k}'')(\nu'')}_{\sigma'' a'', \tau'' b''} \mid \tau b \tau' b' \rangle = \frac{h_{\nu''}}{\mid G_0(\mathbf{k}'') \mid} \sum_{\alpha} D^{(\mathbf{k})(\nu)}_{ab}(\{\gamma_{\sigma\tau} \mid \mathbf{V}_{\sigma\tau}\}) D^{(\mathbf{k}')(\nu')}_{a'b'}(\{\gamma_{\sigma'\tau'} \mid \mathbf{V}_{\sigma'\tau'}\})$$
$$\times D^{(\mathbf{k}'')(\nu'')}_{a''b''}(\{\gamma_{\sigma''\tau''} \mid \mathbf{V}_{\sigma''\tau''}\})^* \ , \tag{20.2c}$$

where

$$\gamma_{\sigma\tau} = \beta_\sigma^{-1} \alpha \beta_\tau, \quad \mathbf{V}_{\sigma\tau} = \beta_\sigma^{-1}(\alpha \mathbf{V}_\tau - \mathbf{V}_\sigma + \mathbf{V}_\alpha) \ . \tag{20.2d}$$

It is to be noted that throughout this section Eq. (18.26) is always assumed to hold, and the convention mentioned after Eq. (11.3) is used, i.e., if $\gamma \notin \mathbf{G}_0(\mathbf{k})$, then $D^{(\mathbf{k})(\nu)}(\{\gamma \mid \mathbf{V}_\gamma\}) = 0$. Equations similar to (20.2d) can be written for $\gamma_{\sigma'\tau'}$, $\mathbf{V}_{\sigma'\tau'}$, $\gamma_{\sigma''\tau''}$, and $\mathbf{V}_{\sigma''\tau''}$.

For the principle-block CGC, from Eqs. (20.2a) and (20.2c) we have

$$\frac{h_{\nu''}}{\mid \mathbf{G}_0(\mathbf{k}'') \mid} \sum_{\alpha} D^{(\mathbf{k})(\nu)}_{ab}(\{\alpha \mid \mathbf{V}_\alpha\}) D^{(\mathbf{k}')(\nu')}_{a'b'}(\{\alpha \mid \mathbf{V}_\alpha\}) D^{(\mathbf{k}'')(\nu'')}_{a''b''}(\{\alpha \mid \mathbf{V}_\alpha\})^* = \sum_{\theta} U^{(\theta)}_{1a\,1a',1a''} (U^{(\theta)}_{1b\,1b',1b''})^* \ , \tag{20.4}$$

where α is to be summed over those elements belonging simultaneously to the groups $\mathbf{G}_0(\mathbf{k})$, $\mathbf{G}_0(\mathbf{k}')$, and $\mathbf{G}_0(\mathbf{k}'')$.

The non-principle-block CGC can be obtained by the following procedure. Consider the point-group operator β_Σ, which changes simultaneously $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$ into $\mathbf{k}_\sigma$, $\mathbf{k}'_{\sigma'}$, and $\mathbf{k}''_{\sigma''}$ modulo a reciprocal lattice vector, i.e.,

$$\beta_\Sigma \mathbf{k} \doteq \mathbf{k}_\sigma, \quad \beta_\Sigma \mathbf{k}' \doteq \mathbf{k}'_{\sigma'}, \quad \beta_\Sigma \mathbf{k}'' \doteq \mathbf{k}''_{\sigma''} \ . \tag{20.5}$$

Due to $\beta_\Sigma \mathbf{k} \doteq k_\sigma$, $\{\beta_\Sigma \mid \mathbf{V}_\Sigma\}$ is necessarily in the σth coset in Eq. (15.1). Thus we must have

$$\{\beta_\Sigma \mid \mathbf{V}_\Sigma\} = \{\beta_\sigma \mid \mathbf{V}_\sigma\}\{\gamma_k \mid \mathbf{c}_k\} \ , \tag{20.6a}$$

where $\{\gamma_k \mid \mathbf{c}_k\} \in \mathbf{G}(\mathbf{k})$. Using Eqs. (20.6a) and (15.2) we obtain

$$\{\beta_\Sigma \mid \mathbf{V}_\Sigma\}^{-1} \psi^{(\nu)}_{\mathbf{k}_\sigma a} = \sum_{b} D^{(\mathbf{k})(\nu)}_{ab}(\{\gamma_k \mid \mathbf{c}_k\})^* \psi^{(\nu)}_{\mathbf{k},b} \ . \tag{20.7}$$

Analogously we have

$$\{\beta_\Sigma \mid \mathbf{V}_\Sigma\} = \{\beta_{\sigma'} \mid \mathbf{V}_{\sigma'}\}\{\gamma_{k'} \mid \mathbf{c}_{k'}\} \ ,$$
$$\{\beta_\Sigma \mid \mathbf{V}_\Sigma\} = \{\beta_{\sigma''} \mid \mathbf{V}_{\sigma''}\}\{\gamma_{k''} \mid \mathbf{c}_{k''}\} \ , \tag{20.6b}$$

where $\{\gamma_{k'} \mid \mathbf{c}_{k'}\}$ and $\{\gamma_{k''} \mid \mathbf{c}_{k''}\}$ belong to the groups $\mathbf{G}(\mathbf{k}')$ and $\mathbf{G}(\mathbf{k}'')$, respectively.

The CGC in Eq. (18.3b) can be expressed as

$$U^{(\theta)}_{\sigma a \sigma' a', \sigma'' a''} = \langle \{\beta_\Sigma \mid \mathbf{V}_\Sigma\}^{-1} (\psi^{(\nu)}_{\mathbf{k}_\sigma a} \psi^{(\nu')}_{\mathbf{k}'_{\sigma' a'}}) \mid \{\beta_\Sigma \mid \mathbf{V}_\Sigma\}^{-1} \psi^{(\nu'')\theta}_{\mathbf{k}''_{\sigma'' a''}} \rangle \ . \tag{20.8a}$$

With the help of Eqs. (20.6) and (20.7), we finally get

$$U^{(\theta)}(\sigma\sigma'\sigma'') = D^{(\mathbf{k})(\nu)}(\{\gamma_k \mid \mathbf{c}_k\}) \otimes D^{(\mathbf{k}')(\nu')}(\{\gamma_{k'} \mid \mathbf{c}_{k'}\}) U^{(\theta)}(111) D^{(\mathbf{k}'')(\nu'')}(\{\gamma_{k''} \mid \mathbf{c}_{k''}\})^{-1} \ . \tag{20.8b}$$

The above method has been used to calculate the CGC for $*X \otimes *X$ of the space groups O_h^7 and O_h^5 (Berenson *et al.*, 1975), as well as for O_h^9 and O_h^{10} (Kunert and Suffczynski, 1980; Suffczynski and Kunert, 1982). Sakata used a similar method (see Sec. VII.E) for calculating the CGC of the double space group $\bar{D}_{4h}^{14}$. Kowalczyk *et al.* (1980) have also written a program for calculating the principle-block CGC.

B. Dirl's method

This method is based on Schindler, Mirman, and Dirl's approach (Sec. VII.E). Equations (7.39a)—(7.40) can easily be transposed to the space-group CGC (Dirl, 1979c, 1979d) [cf. Eqs. (7.39a), (7.39b), and (7.40b), respectively]

$$|*\mathbf{k}''\nu'',\theta=(\tau b\tau' b')\tau'' b''\rangle = N_{\tau b\tau' b'}^{(k''\nu'')\tau'' b''} P_{\tau'' b'',\tau' b''}^{(*\mathbf{k}'')(\nu'')} |\tau b\tau' b'\rangle \ , \tag{20.9a}$$

$$N_{\tau b\tau' b'}^{(k''\nu'')\tau'' b''} = |\langle \tau b\tau' b' | P_{\tau'' b'',\tau' b''}^{(*\mathbf{k}'')(\nu'')} |\tau b\tau' b'\rangle|^{-1/2} \ , \tag{20.9b}$$

$$U_{\sigma a\sigma' a',\sigma'' a''}^{\theta=(\tau b\tau' b')} = N_{\tau b\tau' b'}^{(k''\nu'')\tau'' b''} \langle \sigma\sigma' a' | P_{\sigma'' a'',\tau'' b''}^{(*\mathbf{k}'')(\nu'')} |\tau b\tau' b'\rangle \ , \tag{20.10}$$

where the matrix elements of $P_{\sigma'' a'',\tau'' b''}^{(*\mathbf{k}'')(\nu'')}$ are given by Eq. (20.2b).

The key problem in using (20.10) to calculate all the CG coefficients of the space group $\mathbf{G}$ is to determine the multiplicity index θ, i.e., to find $(*\mathbf{k}\nu *\mathbf{k}'\nu' | *\mathbf{k}''\nu'')$ sets of indices $\theta=\tau b\tau' b', \bar{\tau}\bar{b}\bar{\tau}'\bar{b}', \ldots$, so that the vectors in Eq. (20.9a) are orthogonal with respect to θ,

$$\begin{aligned}\langle *\mathbf{k}''\nu'',\theta=(\bar{\tau}\bar{b}\bar{\tau}'\bar{b}')\tau'' b'' | *\mathbf{k}''\nu'',\theta=(\tau b\tau' b')\tau'' b''\rangle \\ = N_{\bar{\tau}\bar{b}\bar{\tau}'\bar{b}'}^{(\mathbf{k}''\nu'')\tau'' b''} \langle \bar{\tau}\bar{b}\bar{\tau}'\bar{b}' | P_{\tau'' b'',\tau' b''}^{(*\mathbf{k}'')(\nu'')} |\tau b\tau' b'\rangle \\ = \delta_{(\bar{\tau}\bar{b}\bar{\tau}'\bar{b}')(\tau b\tau' b')} \ .\end{aligned} \tag{20.11}$$

Dirl (1979c,1979d) demonstrated that even for the most complicated case the determination of the multiplicity index requires only the inspection of simple equations. Davies and Dirl (1983) have written a program for the space-group CGC based on Dirl's method. Similar work has been done by van den Broek (1979a), using the double coset approach.

The disadvantages of the previous two methods are that they require a great many irreducible matrix elements and the resulting CGC is in general not adapted to a definite subgroup chain.

C. Gard's method

Gard (1973) took a quite different approach to the space-group CGC. The essential difference lies in the fact that instead of directly reducing the Kronecker product rep for the full space group $\mathbf{G}$, as in the EFM, Berenson, or Dirl method, Gard reduces the Kroenecker product rep for the subgroup $\mathbf{G}_\alpha$ of the little group $\mathbf{G}(\mathbf{k})$; then, through induction, followed by reduction of the induced rep, he obtains the irreps of $\mathbf{G}(\mathbf{k})$; and finally, using induction again, he obtains the irreps of $\mathbf{G}$.

Suppose that we have two subgroup chains $\mathbf{G}\supset\mathbf{G}(\mathbf{k}_1)$ and $\mathbf{G}\supset\mathbf{G}(\mathbf{k}_2)$. The irreps and IRB of $\mathbf{G}(\mathbf{k}_i)$ are denoted as

$$\mathbf{G}(\mathbf{k}_1)\text{: irrep } D^{(\mathbf{k}_1)(\nu_1)}, \quad \text{IRB } \psi_{\mathbf{k}_1 a_1}^{(\nu_1)} = \phi_l \ , \tag{20.12a}$$

$$\mathbf{G}(\mathbf{k}_2)\text{: irrep } D^{(\mathbf{k}_2)(\nu_2)}, \quad \text{IRB } \psi_{\mathbf{k}_2 a_2}^{(\nu_2)} = \psi_m \ . \tag{20.12b}$$

The left coset decomposition of $\mathbf{G}$ with respect to $\mathbf{G}(\mathbf{k}_i)$ is

$$\mathbf{G}=\sum_\tau \oplus s_\tau \mathbf{G}(\mathbf{k}_1) \ , \quad s_\tau=\{\beta_\tau | \mathbf{V}_\tau\} \ , \tag{20.13a}$$

$$\mathbf{G}=\sum_\sigma \oplus s_\sigma \mathbf{G}(\mathbf{k}_2), \quad s_\sigma=\{\beta_\sigma | \mathbf{V}_\sigma\} \ . \tag{20.13b}$$

The double coset decomposition of $\mathbf{G}$ with respect to $\mathbf{G}(\mathbf{k}_1)$ and $\mathbf{G}(\mathbf{k}_2)$ is

$$\mathbf{G}=\sum_\alpha \oplus \mathbf{G}(\mathbf{k}_2) d_\alpha \mathbf{G}(\mathbf{k}_1), \quad d_\alpha=\{\alpha | \mathbf{V}_\alpha\} \ , \tag{20.14}$$

where d_α is called the double coset representative.

Let

$$\mathbf{k}=\alpha\mathbf{k}_1+\mathbf{k}_2 \ . \tag{20.15}$$

The decomposition of $\mathbf{G}$ with respect to $\mathbf{G}(\mathbf{k})$ is

$$\mathbf{G}=\sum_\omega \oplus s_\omega \mathbf{G}(\mathbf{k}), \quad s_\omega=\{\beta_\omega | \mathbf{V}_\omega\} \ . \tag{20.16}$$

Define a group

$$\mathbf{G}_\alpha=\mathbf{G}(\alpha\mathbf{k}_1)\cap\mathbf{G}(\mathbf{k}_2) \ , \tag{20.17a}$$

where $\mathbf{G}(\alpha\mathbf{k}_1)$ is the little group for the wave vector $\alpha\mathbf{k}_1$,

$$\mathbf{G}(\alpha\mathbf{k}_1)=d_\alpha \mathbf{G}(\mathbf{k}_1) d_\alpha^{-1} \ . \tag{20.17b}$$

It can be shown that $\mathbf{G}_\alpha$ is a subgroup of $\mathbf{G}(\mathbf{k})$. The left coset decomposition of $\mathbf{G}(\mathbf{k})$ with respect to $\mathbf{G}_\alpha$ is expressed as

$$\mathbf{G}(\mathbf{k})=\sum_\lambda \oplus q_\lambda^\alpha \mathbf{G}_\alpha \ . \tag{20.18}$$

Therefore, $\mathbf{G}_\alpha$ is the intersection of $\mathbf{G}(\alpha\mathbf{k}_1)$, $\mathbf{G}(\mathbf{k}_2)$, and $\mathbf{G}(\mathbf{k})$. This is the key point that enables us to form the Kronecker product rep $D^{(\alpha\mathbf{k}_1)(\nu_1)}\otimes D^{(\mathbf{k}_2)(\nu_2)}$ of the group G_α, which is obtained from the irreps of $\mathbf{G}(\alpha\mathbf{k}_1)$ and $\mathbf{G}(\mathbf{k}_2)$ subduced to $\mathbf{G}_\alpha$; we then reduce this Kronecker product rep to get the irreps $D^{(\mu)}$ of $\mathbf{G}_\alpha$, and later, through two stages of induction, to get reps of the full space group $\mathbf{G}$.

According to Mackey (1952), the decomposition of the Kronecker product of two induced reps can be expressed as

$$\begin{aligned}(D^{(\mathbf{k}_1)(\nu_1)}\uparrow\mathbf{G})\otimes(D^{(\mathbf{k}_2)(\nu_2)}\uparrow\mathbf{G}) \\ = \sum_\alpha \oplus \{[D_\alpha^{(\mathbf{k}_1)(\nu_1)}(\mathbf{G}_\alpha)\otimes D^{(\mathbf{k}_2)(\nu_2)}(\mathbf{G}_\alpha)]\uparrow\mathbf{G}(\mathbf{k})\}\uparrow\mathbf{G} \ ,\end{aligned} \tag{20.19}$$

where $D^{(\mathbf{k}_1)(\nu_1)}(\mathbf{G}_\alpha)$ is the rep of $\mathbf{G}_\alpha$ subduced from the irrep $D_{(\alpha\alpha)}^{(\mathbf{k}_1)(\nu_1)}$ [see Eq. (15.8b)] of $\mathbf{G}(\alpha\mathbf{k}_1)$: $D_\alpha^{(\mathbf{k}_1)(\nu_1)}(\mathbf{G}_\alpha) = D_{(\alpha\alpha)}^{(\mathbf{k}_1)(\nu_1)}\downarrow\mathbf{G}_\alpha$ with the basis $\{q_\lambda^\alpha\varphi_i\}$, and $D^{(\mathbf{k}_2)(\nu_2)}(\mathbf{G}_\alpha) = D^{(\mathbf{k}_2)(\nu_2)}\downarrow\mathbf{G}_\alpha$ with the basis $\{\psi_j\}$.

The transformation from the uncoupled basis $|s_\tau\varphi_l s_\sigma\psi_m\rangle$ to the IRB $\psi_{\mathbf{k}_\omega a}^{(\nu)\theta}$ of $\mathbf{G}$ can be accomplished through the following three steps.

(1) From the basis $|s_\tau\varphi_l s_\sigma\psi_m\rangle$ to the basis $s_\omega q_\lambda^\alpha | d_\alpha\varphi_i,\psi_j\rangle$:

$$s_\omega q_\lambda^\alpha | d_\alpha\varphi_i,\psi_j\rangle = \sum_{lm} \langle \tau\sigma lm | \alpha\omega\lambda ij\rangle | s_\tau\varphi_l s_\sigma\psi_m\rangle \ , \tag{20.20a}$$

$$\langle \tau\sigma lm \mid \alpha\omega\lambda ij \rangle = D_{li}^{(\mathbf{k}_1)(\nu_1)}(s_\tau^{-1} s_\omega q_\lambda^\alpha d_\alpha) \times D_{mj}^{(\mathbf{k}_2)(\nu_2)}(s_\sigma^{-1} s_\omega q_\lambda^\alpha) . \quad (2.20b)$$

(2) Reduce the Kronecker product of the reps $D_\alpha^{(\mathbf{k}_1)(\nu_1)}$ and $D^{(\mathbf{k}_2)(\nu_2)}$ of the group $\mathbf{G}_\alpha$,

$$| \Phi_s^{(\mu)\tau} \rangle = \sum_{ij} \langle \alpha ij \mid \mu\tau s \rangle \mid d_\alpha \varphi_i, \psi_j \rangle . \quad (20.21)$$

(3) Reduce the induced rep $D^{(\mu)} \uparrow \mathbf{G}(\mathbf{k})$ to get the IRB of $\mathbf{G}(\mathbf{k})$,

$$| \psi_{\mathbf{k},a}^{(\nu)\theta} \rangle = \sum_{s\lambda} \langle \lambda\alpha\mu\tau s \mid \nu\mathbf{k}\theta a \rangle q_\alpha^\lambda \mid \Phi_s^{(\mu)\tau} \rangle . \quad (20.22)$$

Combining Eqs. (20.20)—(20.22) we obtain the space-group CGC,

$$\begin{vmatrix} \mathbf{k}_1\nu_1 & \mathbf{k}_2\nu_2 \\ \tau a_1, & \sigma a_2 \end{vmatrix} \mathbf{k}\nu\theta \\ \omega a \end{vmatrix} \equiv \langle \tau\sigma lm \mid \mathbf{k}\nu\theta\omega a \rangle = \sum_{\lambda ijs} \langle \tau\sigma lm \mid \alpha\omega\lambda ij \rangle \langle \alpha ij \mid \mu\tau s \rangle \times \langle \lambda\alpha\mu\tau s \mid \nu\mathbf{k}\theta a \rangle . \quad (20.23)$$

In general, the group $\mathbf{G}_\alpha$ will be small and step (2) can be easily accomplished. However, step (3) may cause trouble in a general case within the framework of the conventional rep theory. The difficulty can be easily overcome with the help of the EFM, i.e., by using the CSCO of the group $\mathbf{G}(\mathbf{k})$ to decompose the induced rep space.

XXI. CONCLUDING REMARKS

Suppose that the distinct operators or matrices of an abstract discrete group $\hat{\mathbf{G}}$, whose order can be infinite, in a rep space L form a rep group $\mathbf{G}$ of order $m \mid \mathbf{g} \mid$, which is an m-fold covering group of a finite group $\mathbf{g}$; then the problem of seeking the irreps of $\hat{\mathbf{G}}$ (or equivalently, the projective irreps of $\mathbf{g}$) in the space L can be replaced by that of finding the irreps of the rep group $\mathbf{G}$, and the group order is reduced from $\mid \hat{\mathbf{G}} \mid$ (which can be infinite) to $\mid \mathbf{g} \mid$. Therefore, the construction of the irreps of the little group $\mathbf{G}(\mathbf{k})$ is just as easy as that of its little co-group $\mathbf{G}_0(\mathbf{k})$, with the only difference being that the matrix elements of the regular rep for $\mathbf{G}_0(\mathbf{k})$ are either zeros or ones, whereas those for the rep group $\mathbf{G}'_\mathbf{k}$ are either zeros or of the form $\exp(2\pi il/m)$.

The following correspondences are established for a rep group $\mathbf{G}$ or an abstract group $\mathbf{G}$ (since the abstract group is a special case of the rep group).

(1) The irreducible character vector—The complex conjugate of the eigenvector of the CSCO-I of $\mathbf{G}$ in the class space.

(2) The irreducible matrix element vector—The complex conjugate of the eigenvector of the CSCO-III of $\mathbf{G}$ in the group space.

(3) The irreducible basis vector—The eigenvector of the CSCO-II of $\mathbf{G}$ in a reducible space.

(4) The CGC vector—The eigenvector of the CSCO-II of $\mathbf{G}$ in the Kronecker product space.

Based on the above correspondences, a universal method, the eigenfunction method, is set up for calculating the characters, the irreducible basis and matrices, and the CGC adapted to any given subgroup chain. The EFM is suitable for both hand and computer calculation. For computer calculation it is expedient to choose self-adjoint CSCO's, since the diagonalization of Hermitian matrices is much easier than of non-Hermitian matrices. The CSCO's can be easily found for point groups and space groups, and can be chosen to consist of only a single operator. The EFM for obtaining the irreps of the little group $\mathbf{G}(\mathbf{k})$ adapted to any given subgroup chain has been programmed by Zheng (1985).

When the intrinsic group $\overline{\mathbf{G}}$ is introduced, which commutes with and is anti-isomorphic to the group $\mathbf{G}$, the eigenvalue of the CSCO for the intrinsic subgroup chain $\overline{\mathbf{G}}(s)$ provides the multiplicity label for distinguishing the h_ν equivalent irreps of $\mathbf{G}$ that occur in the regular rep of $\mathbf{G}$.

Based on the EFM, an easily programmable algorithm is proposed for computing the space-group CGC. The new features of this method are that (a) the CGC is adapted to any given subgroup chain, (b) the CGC and CG series are obtained simultaneously, and (c) the method involves only a very small number of space-group irreducible matrix elements. The programming work is now being undertaken (Zheng, 1985).

The present paper, together with previous papers (Chen and Gao, 1982; Chen, Wang, and Gao, 1983), provides a unified CSCO approach to the permutation group, point group, space group, and compact Lie group. Potential applications of this approach to magnetic point groups and magnetic space groups remain to be studied.

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