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Continuous Point Groups

A simple derivation of the closed formula for the reduction of representations

Following the paper by one of us (*1*) three interesting communications on the reduction of representations of continuous point groups have appeared recently in *this Journal* (*2–4*). We would also like to make some further comments on the topic. They are motivated by the impression that we have been apparently unaware of the fact that a closed formula *does* also exist for the reduction of representations of continuous point groups. This reads (*5*)

$$a_i = \frac{\sum_R \int \chi(R)\chi^i(R)\mathrm{d}R}{\sum_R \int \mathrm{d}R} \tag{1}$$

where the integration is taken over the range of the continuously changing parameter R (in this case the azimuthal angle ϕ), and the summation goes over the classes of distinct, discrete operations. Other symbols in eqn. (1) have the usual meaning.

Equation (1) is (not easily) derived from the extension of the great orthogonality theorem to continuous groups (*6*).

While just calling the attention to the general omission of eqn. (1) should be intrinsically interesting, we should also like to present a derivation of it starting from the well-known corresponding formula for finite groups, i.e.

$$a_i = \frac{\sum_R \chi(R)\chi^i(R)}{h} \tag{2}$$

where h is the order of the group.

Let us first consider the finite, axial C_n group. It consists of the elements (symmetry operations) $\{C_n, C_n{}^2, C_n{}^3, \ldots, C_n{}^n \equiv E\}$. It is a one-parameter group, the parameter being the angle ϕ. The order of the group is n.

The rotation angle is given in general by

$$\phi_k = k(2\pi/n),\ k = 1, 2, \ldots, n$$

and the minimal step in ϕ is evidently

$$\phi_k + 1 - \phi_k = 2\pi/n \tag{3}$$

Equation (2) takes in this case the form

$$a_i = \frac{1}{n}\sum_{\phi_k} \chi(C(\phi_k))\,\chi^i(C(\phi_k))$$

$$= \frac{1}{2\pi}\sum_{\phi_k} \chi(C(\phi_k))\chi^i(C(\phi_k))\,(2\pi/n) \tag{4}$$

In the limit, when $n \to \infty$, $(\phi_{k+1} - \phi_k) \to \mathrm{d}\phi$, and this combined with eqns. (3) and (4) yields for C_∞

$$a_i = (1/2\pi)\int_0^{2\pi} \chi(C(\phi))\chi^i(C(\phi))\mathrm{d}\phi$$

Let us now extend this result to $C_{\infty v}$, by starting with C_{nv}. Here one has a new class of element, the infinite reflection planes σ_v. The group order is $2n$ and the infinite reflection planes are also characterized by the angle ϕ. So, eqn. (2) takes the form

$$a_i = (1/2n)\left\{\sum_{\phi_k} \chi(C(\phi_k))\chi^i(C(\phi_k)) + \sum_{\phi_k}\chi(\sigma_v(\phi_k))\chi^i(\sigma_v(\phi_k))\right\}$$

which upon multiplying and dividing by 2π, becomes in the limit as $n \to \infty$

$$a_i = (1/4\pi)\left\{\int_0^{2\pi} \chi(C(\phi))\chi^i(C(\phi))\mathrm{d}\phi + \int_0^{2\pi}\chi(\sigma_v(\phi))\chi^i(\sigma_v(\phi))\mathrm{d}\phi\right\} \tag{5}$$

which is the explicit form of eqn. (1) for $C_{\infty v}$. For example (a) of (1) this yields

$$a_{\Sigma^+} = (1/4\pi)\left\{\int_0^{2\pi} (2 + 2\cos\phi)\cdot 1\cdot \mathrm{d}\phi + \int_0^{2\pi} 2\cdot 1\cdot \mathrm{d}\phi\right\} = 2$$

$$a_{\Pi} = (1/4\pi)\left\{\int_0^{2\pi} (2 + 2\cos\phi)\cdot 2\cos\phi\cdot \mathrm{d}\phi + \int_0^{2\pi} 2\cdot 0\cdot \mathrm{d}\phi\right\} = 1$$

as it must be.

For $D_{\infty h}$ one starts from D_{nh}. One first realizes that the elements of the D_h's axial groups are for any point group classifiable in four sets of distinct operations, namely proper rotations, improper rotations, binary axes and symmetry, vertical planes. The angle ϕ serves to label and distinguish among different operations within the same set. For example, in D_{3h} (order of the group = 12 = 4 × 3) the sets are

$$\{C_3(2\pi/3), C_3(4\pi/3), C_3(2\pi) \equiv E\}$$
$$\{S_3(2\pi/3), S_3(4\pi/3), S_3(2\pi) \equiv \sigma_h\}$$
$$\{C_2(2\pi/3), C_2(4\pi/3), C_2(2\pi)\}$$
$$\{\sigma_v(2\pi/3), \sigma_v(4\pi/3), \sigma_v(2\pi)\}$$

and from eqn. (2)

$$a_i = (1/4\cdot 3)\left\{\sum_{\phi_k} \chi(C_3(\phi_k))\chi^i(C_3(\phi_k)) + \ldots\right\}$$

where only the terms from the first set have been explicitly written, and the summations go through $\phi_k = 2\pi/3, 4\pi/3, 2\pi$. For D_{nh} one should have instead symbolically

$$a_i = (1/4n)\left\{\sum_{\phi_k}^{\mathrm{p.r.}}(\ ) + \sum_{\phi_k}^{\mathrm{i.r.}}(\ ) + \sum_{\phi_k}^{C_2}(\ ) + \sum_{\phi_k}^{\sigma_v}(\ )\right\}$$

where p.r., i.r., C_2 and σ_v above the Σs mean summation over the proper rotations, over the improper rotations, over the binary axes, and over the symmetry planes, respectively, and ( ) means the pertinent $\chi(R)\chi^i(R)$ products. Equation (6) can be written in a more convenient fashion, i.e.

$$a_i = (1/8\pi)\sum_{\mathrm{sets}}\sum_{\phi_k}(\ )\,(2\pi/n)$$

and in the limit, i.e. for $D_{\infty h}$

$$a_i = (1/8\pi)\sum_{\mathrm{sets}}\int_0^{2\pi} \chi(R)\chi^i(R)\,\mathrm{d}\phi$$

The four sets in $D_{\infty h}$ are $\{E, C(\phi)\}$, $\{i, S(\phi)\}$, $\{C_2\}$, and $\{\sigma_v\}$ so explicitly in example (b) of (1)

$$a_{\Sigma_g{}^+} = (1/8\pi)\left\{\int_0^{2\pi} 4\cos^2\phi\cdot 1\cdot \mathrm{d}\phi + \int_0^{2\pi} 4\cos^2\phi\cdot 1\cdot \mathrm{d}\phi + \int_0^{2\pi} 0\cdot 1\cdot \mathrm{d}\phi + \int_0^{2\pi} 0\cdot 1\cdot \mathrm{d}\phi\right\} = 1$$

Here we have taken for the $\Pi_g \otimes \Pi_g$ representation: $\chi(C(\phi)) = \chi(S\phi) = 4\cos^2\phi$, $\chi(C_2) = \chi(\sigma_v) = 0$. In the same way one easily gets $a_{\Sigma_g{}^-} = 1$ and $a_{\Delta_g} = 1$. For other cases, the following relationships are useful

$$\int_0^{2\pi} \cos k\phi \cdot \cos 1\phi \cdot \mathrm{d}\phi = \pi\delta_{k1}$$

where δ_{k1} is the Kronecker delta, and

$$\int_0^{2\pi} \cos k\phi\ \mathrm{d}\phi = 0 \text{ for } k \text{ integer.}$$

It should be noted that the proof above presented of eqn.

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(1) is rigorous enough for the usual representations of the point groups. For these the characters $\chi(R)$ are continuous and bounded over the range of R and the limiting processes considered converge. In general one can be sure that the characters are bounded for unitary finite-dimensional representations. In fact let $a_{ij}(R)$ be the element belonging to the ith-row and jth-column of the matrix representing the element $g(R)$ in a unitary finite-dimensional representation. The unitarity implies

$$\sum_j a_{ij(R)}a^*{}_{kj(R)} = \delta_{ik}$$

and taking $i = k$

$$|a_{ii}|^2 + \sum_{j \neq i} |a_{ij}|^2 = 1$$

wherefrom one gets $|a_{ii}| \leq 1$. This means in turn that

$$|\chi(R)| = \left|\sum_i a_{ii}\right| \leq \sum_i |a_{ii}| \leq n$$

n being the dimension of the representation.

Nonetheless, it would be wrong to infer from these considerations that the general theory of continuous groups can be drawn from that of the finite groups. Lie group theory has a structure and richness which goes far beyond the scope of the simpler discrete groups framework.

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