Contributed Paper VIth International Colloquium on Group Theory in Physics
Tubingen, July 1977

MOLIEN FUNCTION AND CALCULATION OF INVARIANT POLYNOMIALS FOR SPACE GROUPS*

Marko V. Jarić and Joseph L. Birman
Physics Department
City College, C. U. N. Y.
New York, New York 10031

Abstract

We have developed an algorithm for the computation of the Molien function (generating for the multiplicity of the identity representation in the symmetrized n^{th} power of representation Γ of group G) and used it to compute the Molien function for irreducible representations of crystal space groups. The calculation is illustrated upon some irreducible representations of the crystal space groups. In particular, a case of interest is some irreducible representations of the crystal space group O_h^3-Pn3m. Quartic invariants are exhibited for irreducible representations *X(j) and *R(j) j= 1,2,3,4 of O_h^3.

As given in standard texts such as Burnside the Molien function $M(\Gamma,G;z)$ for a finite group G is the generating function for the multiplicity c_{n1} with which the trivial representation Γ^{1+} is contained in the symmetrized n^{th} power of representation Γ of G.(1) Writing the formal power series whose coefficients are c_{n1} one has

$$M(\Gamma,G;z) = \sum_{n=0}^{\infty} c_{n1}z^{n} = \frac{1}{|G|} \sum_{g} \frac{1}{\det[1-z\Gamma(g)]} \qquad (1)$$

the sum is over all elements $g \in G$. In (1) $c_{01} \equiv 1$.

We found two very useful algorithms for $M(\Gamma,G;z)$ which are computationally easy to use, and which only require characters: $\chi(g) \equiv \mathrm{Tr}\,\Gamma(g)$. These are:

$$M(\Gamma,G;z) = \frac{1}{|G|} \sum_{g} \exp\Big(\sum_{\ell=1}^{\infty} z^{\ell}\, \chi(g^{\ell})/\ell\Big) \qquad (2)$$

---

*Supported in part by grants: NSF DMR76-20641 - AOL and CUNY-FRAP - 11453.

and

$$M(\Gamma,G;z) = \frac{1}{|G|} \sum_{g} \prod_{j=1}^{p} [1 - z\gamma_j(g)]^{-\delta_j} \qquad (3)$$

where g^{ℓ} is the element which is the ℓ^{th} power of g. In (3) we define δ_j as the subduction coefficient for Γ of G upon irreducible representation γ_j of (cyclic) Abelian group A generated by g. Thus if g has period p,

$$\gamma_j(g) = \exp(2\pi ij/p) \qquad j=1,\dots p$$

and

$$\delta_j = (1/|A|) \sum_{m=1}^{p} \gamma_j(g^m) \, {}^{*}\chi(g^m)$$

Now we can summarize the use of these fomulae for irreducible representation Γ of a space group (some additional details are given in references 1 and 2). Let G be a space group, then $g \equiv (\phi|t)$ where $t = R + \tau$, with R a lattice, and τ a fractional, translation. For subgroup A we take $A = \{g, g^2, \dots, g^{pN} = (e|0)\}$ where $\phi^p = e$ and N is the order of translation group $N = |T|$. Also the point group of G is defined as G/T = P. An irreducible representation $\Gamma^{*\vec{k}n}$ of G is obtained by inducing from irreducible representation $\Gamma^{(\vec{k})(n)}$ of $G(\vec{k})$. Let us write

$$G = G(\vec{k}) + g_2\, G(\vec{k}) + \dots + g_s\, G(\vec{k})$$

where $g_\sigma = (\phi_\sigma|\tau_\sigma)$, σ = 1,...s, and g_σ is a coset representative in G but <u>not</u> in G(k). Note that it is always assumed that a "canonical" decomposition exists so that a particular τ_σ goes with ϕ_σ. Now define $\{\phi\}^\mu \equiv \sum_{\lambda=0}^{\mu-1} \phi^\lambda$ (sum of powers of φ) and the lattice translations $R_\mu \equiv \{\phi\}^\mu t - \tau_\mu$ and $R_{\mu\sigma} \equiv \phi^\mu \tau_\sigma + \tau_\mu - \tau_\sigma - \phi_\sigma \tau_{\mu\sigma}$ where $\tau_{\mu\sigma}$ is the fractional associated with rotation $\phi_\sigma^{-1}\phi^\mu\phi_\sigma$. Then the Molien function for $\Gamma^{*k\,n}$ can be written

$$M(*\vec{k}n;G;z) = \frac{1}{|P|} \sum_{k} c_k\, \bar{m}(*\vec{k}n, g_k; z)$$

where c_k is the order of class $\mathcal{C}_k$ of P, and

$$\bar{m}(*\vec{k}n,\ g_k;z) = \frac{1}{N} \sum_{t\in T} \prod_{\nu=0}^{p-1} \prod_{\sigma=1}^{s} [1 - z\gamma_{\sigma p}(\omega_p)^{\nu}]^{-\delta_{\nu\sigma}}$$

where

$$\omega_p = \exp(2\pi i/p)$$

$$\gamma_{\sigma\mu} = \exp(i\vec{k}_\sigma \cdot (\vec{R}_\mu + \vec{R}_{\mu\sigma})/p)$$

$$\delta_{\nu\sigma} = 1/p \sum_{\mu=1}^{p} (\omega_p^*)^{\mu\nu} (\gamma_{\sigma p}^*)^{\mu} (\gamma_{\sigma\mu})^{p} \dot{\chi}^{(\vec{k})(n)} (\phi_\sigma^{-1} \phi^\mu \phi_\sigma | \vec{\tau}_{\mu\sigma})$$

all quantitites should be calculated for the element $(\phi_k|\tau_k)$, $t\in T$; the dotted character $\dot{\chi}^{(k(n)}(h)$ is defined as

$$\dot{\chi}^{(\vec{k})(n)}(h) = \begin{cases} \chi^{(\vec{k})(n)}(h) & \text{if } h\in G(\vec{k}); \\ 0 & \text{, otherwise.} \end{cases}$$

We computed the Molien function for the irreducible representations $*\Gamma j\pm$, j=1, ..., 5; *Xn, n=1,...4; and *Rn, n=1,...4 of O_h^3-Pn3M. Results are tabulated elsewhere.(2) Also given is the result for the "physically irreducible" representation *R2 ⊕ *R3.

To illustrate an application we have separately computed the quartic (4th degree) polynomial invariants for each of the above representations of O_h^3. These are invariants comprised of symmetrized products of powers of the basis functions $\{\psi_j\}$ of the irreducible representations. The quartic invariants are given in Table 1.

Table 1

Representation	Fourth Degree Invariant Polynomial*
*X1 *X2	$\sum_{i=1}^{3} (\psi_i^4 + \bar{\psi}_i^4)$
	$\sum_{i=1}^{3} \psi_i^2 \bar{\psi}_i^2$
	$\sum_{i<j} [\psi_i^2 \psi_j^2 + \bar{\psi}_i^2 \psi_j^2 + \psi_i^2 \bar{\psi}_j^2 + \bar{\psi}_i^2 \bar{\psi}_j^2]$
	$\sum_{i<j} \psi_i \bar{\psi}_i \psi_j \bar{\psi}_j$
	$\sum_{(ijk)} (\psi_i^2 + \bar{\psi}_i^2)(\psi_j \bar{\psi}_j - \psi_k \bar{\psi}_k)$
*X3 *X4	$\sum_{i=1}^{3} (\psi_i^4 + \bar{\psi}_i^4)$
	$\sum_{i=1}^{3} \bar{\psi}_i^2 \psi_i^2$
	$\sum_{i \neq j} \psi_i^2 \bar{\psi}_j^2$
	$\sum_{i<j} \psi_i \bar{\psi}_i \psi_j \bar{\psi}_j$
	$\sum_{(ijk)} (\psi_i^2 + \bar{\psi}_i^2)(\psi_j \bar{\psi}_j - \psi_k \bar{\psi}_k)$
	$\sum_{i<j} [\psi_i^2 \psi_j^2 + \bar{\psi}_i^2 \bar{\psi}_j^2]$
*R1	$\psi_1^4 + \psi_2^4$, $\psi_1^2 \psi_2^2$
*R2 *R3	$\psi_1^2 \psi_2^2$
*R2 ⊕ *R3	$\psi_1^2 \psi_2^2 + \psi_3^2 \psi_4^2 - 2\psi_1 \psi_2 \psi_3 \psi_4$
	$\psi_1^2 \psi_4^2 + \psi_2^2 \psi_3^2 + 2\psi_1 \psi_2 \psi_3 \psi_4$
	$\psi_1^4 + \psi_2^4 + \psi_3^4 + \psi_4^4 + 2(\psi_1^2 \psi_3^2 + \psi_2^2 \psi_4^2)$
	$(\psi_1^2 - \psi_3^2) \psi_2 \psi_4 + (\psi_2^2 - \psi_4^2) \psi_1 \psi_3$

Table 1 continued

*R4	$\sum_{i=1}^{3} (\psi_1^4 + \bar{\psi}_2^{\,4})$
	$\sum_{i=1}^{3} \psi_i^2 \bar{\psi}_i^{\,2}$
	$\psi_1^2 \bar{\psi}_2^{\,2} + \psi_2^2 \bar{\psi}_3^{\,2} + \psi_3^{\,2} \bar{\psi}_1^{\,2}$
	$\bar{\psi}_1^{\,2} \psi_2^2 + \bar{\psi}_2^{\,2} \psi_3^2 + \bar{\psi}_3^{\,2} \psi_1^2$
	$\sum_{i<j} [\psi_i^2 \psi_j^2 + \bar{\psi}_i^{\,2} \bar{\psi}_j^{\,2}]$
	$\sum_{i<j} \psi_i \bar{\psi}_i \psi_j \bar{\psi}_j$

*(i j k) means cyclic permutation of (123).

References

(1) W. Burnside, Theory of Groups of Finite Order (Dover, New York 1952) and references to Molien's papers therein.

(2) M.V. Jarić and J.L. Birman, J. Math. Phys. 18, 1456, 1459, (cf. Errata) (1977).