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A generalized Molien function for field theoretical Hamiltonians

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A generating function, or Molien function, the coefficients of which give the number of independent polynomial invariants in G, has been useful in the Landau and renormalization group theories of phase transitions. Here a generalized Molien function for a field theoretical Hamiltonian (with short-range interactions) of the most general form invariant in a group G is derived. This form is useful for more general renormalization group calculations. Its Taylor series is calculated to low order for the $F\Gamma_2^-$ representation of the space group $R\,\bar{3}c$ and also for the $l = 1$ (faithful) representation of SO(3).

I. INTRODUCTION

The idea of a generating function, sometimes known as a Molien function,[1] the coefficients in the Taylor's series expansion of which give meaningful information about a particular group, has proven[2–4] to be very useful in constructing free energies for use in the Landau theory of structural and magnetic phase transitions in solids. In Ref. 5, it was shown that an effective Hamiltonian or field theoretical Hamiltonian could be constructed for structural phase transitions of the form

$$H(c) = \sum_{m=0}^{\infty} \frac{1}{m!} \int \cdots \int d\,\mathbf{k}_1 \cdots d\,\mathbf{k}_m (2\pi)^{-(m-1)d}$$
$$\times \delta(\mathbf{k}_1 + \cdots + \mathbf{k}_m) \sum_{L_m} H^m_{L_m}(\mathbf{k}_1,\ldots,\mathbf{k}_m)$$
$$\times c_{l_1}(\mathbf{k}_1) \cdots c_{l_m}(\mathbf{k}_m), \tag{1}$$

leading to a free energy of

$$F = -\frac{1}{\beta} \ln \int Dc\, e^{-H(c)}.$$

Here $\int Dc$ indicates a functional integration over the collection of $c_i(\mathbf{k})$ and $\mathbf{k}$ ranges continuously over a sphere with $k < \Lambda$, the cutoff parameter. L_m is the compound index $l_1 l_2 \cdots l_m$.

Furthermore, the form of $H(c)$ must be invariant when

$$c_i(\mathbf{k}) \to c_j(S^{-1}\mathbf{k}) D_{ji}(g), \tag{2}$$

or equivalently, when $\mathbf{k} \to S\,\mathbf{k}$, $H^m \to H^m D^m(g)$, where $g = (S\,|\,\mathbf{t} + \mathbf{t})$ is a space group element in G, the space group of the higher symmetry phase. It would be desirable if a generating function could be found for the more general field theoretical or Landau–Ginzburg–Wilson Hamiltonian of Eq. (1), given Eq. (2). In Ref. 6 the authors pointed out that a term not previously considered, but present in the most general invariant free energy form, contributes significantly to renormalization group behavior. A generalized Molien function for the H of Eq. (1) would be of aid in other such general considerations. Also, the $D(g)$ of Eq. (2) could be replaced by a general representation of any compact group, particularly any unitary compact group, and the following analysis would hold, if the group mean is suitably defined. (This does not take into account the antiunitary θ or complex conjugation, but a generalization is easily accomplished to include it.)

II. DERIVATION AND CALCULATION

Define a function $F(s,t)$, analytic in s,t, such that if

$$F(s,t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} c_{nm} s^n t^m,$$

then c_{nm} will be the number of invariants of order n in the components of $\mathbf{k}$ and order m in c in $H(c)$. To find $F(s,t)$ we pursue a method which is motivated by procedures contained in Refs. 1, 2, and 7. The invariance group of a term in Eq. (1) includes the symmetry of Eq. (2) and in addition each term must be invariant under any exchange of indices, either on k or c. Such an invariance group is known formally as a wreath product; however, here we need only recognize the existence of both kinds of symmetries. The condition that a term of given order be invariant will be taken to mean that it transforms identically under an arbitrary product of a transformation g in G, and one in S_m, call it π, where S_m is the symmetric group in m objects. Note that the essential symmetry is in $\mathbf{k}$ space. One can be misled in attempting to find invariant forms in real space.[5,6]

To find the number of invariants of given order n and m we construct a general basis of the right order and find the subduction frequency of the identity representation on the representation induced by this basis.

For $m = 0$, there is only one basis functional, i.e., a constant, independent of c and k, hence

$$c_{n0} = \delta_{n0}. \tag{3}$$

For $m = 1$, the basis functionals in Eq. (1) are[5]

$$\Psi_{l_1} = c_{l_1}(0).$$

The permutational invariance subgroup is just S_1 so that

$$c_{n1} = \underset{g}{M} \sum_i D_{ii}(g)\delta_{n0} = \underset{g}{M}\, \chi(g)\delta_{n0}, \tag{4}$$

where

$$\underset{g}{M} = \frac{1}{|G|} \sum_{g \in G}$$

is the group mean, or its suitable generalization to an infinite group.

For $m \geq 2$, define a vector $\mathbf{a}$ in $N^{(m-1)d}$, the $(m-1)d$ th Cartesian product of N, the set of non-negative integers, with components a_{ij}, $i = 1,2,\ldots,m-1$, and $j = 1,2,\ldots,d$, such that $\Sigma_{ij} a_{ij} = n$. Here d is the spatial dimension. Then a basis of functionals of order n,m in H, with $m \geq 2$, will have inte-

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grands of the form

$$\Psi(\mathbf{a},L_m)=\prod_{i=1}^{m-1}\prod_{j=1}^{d}(k_{ij})^{a_{ij}}c_{l_1}(\mathbf{k}_1)\times c_{l_2}(\mathbf{k}_2)\cdots c_{l_m}(\mathbf{k}_m),$$

where $\mathbf{k}_m=-\mathbf{k}_1-\cdots-\mathbf{k}_{m-1}$ and k_{ij} is the jth component of $\mathbf{k}_i$. This particular Ψ has the advantage of already being symmetric in the k_{ij} for a fixed i. No sums are implied here or in the aftermath.

Suppose the basis of the $\mathbf{k}_i$ has been chosen so that $gk_{ij}=\rho_j k_{ij}$, where ρ_j is an eigenvalue of $V(g)$, a matrix in the vector representation of G. Then

$$g\Psi(\mathbf{a},L_m)=\prod_{ij}(\rho_j)^{a_{ij}}(k_{ij})^{a_{ij}}\sum_{L'_m}D_{l_1l'_1}(g)\cdots\times D_{l_ml'_m}(g)c_{l'_1}(\mathbf{k}_1)\cdots c_{l'_m}(\mathbf{k}_m).$$

Further,

$$\begin{aligned}\pi g\Psi(\mathbf{a},L_m)&=\prod_{ij}(\rho_j)^{a_{ij}}(k_{\bar\pi(i)j})^{a_{ij}}D_{l_1l'_{\bar\pi(1)}}(g)\cdots D_{l_ml'_{\bar\pi(m)}}(g)c_{l'_{\bar\pi(1)}}(\mathbf{k}_{\bar\pi(1)})\cdots c_{l'_{\bar\pi(m)}}(\mathbf{k}_{\bar\pi(m)})\\&=\prod_{ij}(\rho_j)^{a_{ij}}(k_{\bar\pi(i)j})^{a_{ij}}D_{l_1l'_{\bar\pi(1)}}(g)\cdots D_{l_ml'_{\bar\pi(m)}}(g)c_{l'_1}(\mathbf{k}_1)\cdots c_{l'_m}(\mathbf{k}_m).\end{aligned}$$

Here $\bar\pi=\pi^{-1}$.

Now suppose that $\bar\pi(q)=m$. Then in the above expression there occurs a factor

$$\begin{aligned}(k_{\bar\pi(q)j})^{a_{qj}}&=(-k_{1j}-k_{2j}-\cdots-k_{m-1\,j})^{a_{qj}}\\&=(-1)^{a_{qj}}\sum a_{qj}!(a_{qj1}!\cdots a_{qjm-1}!)^{-1}\times(k_{l_j})^{a_{ij}}\cdots(k_{m-1\,j})^{a_{qjm-1}},\end{aligned}$$

where the sum is over all $a_{qji}\geq 0$ such that

$$\sum_{i=1}^{m-1}a_{qji}=a_{qj}.$$

Writing

$$\pi g\psi(\mathbf{a},L_m)=\sum_{a'L'_m}\Gamma(\mathbf{a},L_m;\mathbf{a}',L'_m)(\pi g)\psi(\mathbf{a}',L'_m),$$

we see that

$$\begin{aligned}\Gamma(\mathbf{a},L_m;\mathbf{a}',L'_m)=\prod_j(-1)^{a_{qj}}a_{qj}!\prod_i(\rho_j)^{a_{ij}}&\times(a_{qji}!)^{-1}\,\delta(a'_{ij}-a_{\pi(i)j}-a_{qji})\\&\times D_{l_il'_{\bar\pi(i)}}(g),\end{aligned}\tag{5}$$

where all restrictions on the a_{ij} and a_{qji} as noted before hold, and we have defined $\mathrm{a}_{mj}=0$ for all j. In this we have written

$$\prod_{ij}(k_{\bar\pi(i)j})^{a_{ij}}=\prod_{ij}(k_{ij})^{a_{\pi(i)j}},$$

where appropriate and $\delta(n)$ is the Kronecker delta δ_{n0}.

We can then form the trace of Eq. (5) to find the character of Γ, giving

$$\begin{aligned}\operatorname{tr}\Gamma(\pi g)=\sum_{aL_m}\prod_j(-1)^{a_{qj}}a_{qj}!\prod_i(\rho_j)^{a_{\pi(i)j}}&\\\times(a_{qji}!)^{-1}\,\delta(a_{ij}-a_{\pi(i)j}-a_{qji})D_{l_il_{\bar\pi(i)}}(g).&\end{aligned}\tag{6}$$

Now the sum over the L_m gives a factor, if π (and hence $\bar\pi$) has cycle structure $(\nu_1,\nu_2,\ldots,\nu_m)$,

$$(\chi(g))^{\nu_1}(\chi(g^2))^{\nu_2}\cdots(\chi(g^m))^{\nu_m},$$

which follows by writing

$$\prod_i D_{l_il_{\bar\pi(i)}}(g)=D_{l_1l_{\bar\pi(1)}}(g)\cdots D_{l_{\bar\pi(\nu_s-1)(1)}l_1}(g)\cdots,$$

if, for example, 1 lies in a cycle of length ν_s, etc.

To carry out conveniently the sum over $\mathbf{a}$ we use the fact that a Kronecker delta $\delta(n)$ may be represented by

$$\delta(n)=\frac{1}{2\pi i}\oint_c dz\,z^{-(n+1)},\tag{7}$$

where the contour c includes the origin. With this we can extend the sum over $\mathbf{a}$ in Eq. (6) to all $\mathbf{a}\in N^{(m-1)d}$, by including $\delta(n-\Sigma a_{ij})$ in this form. Then

$$\begin{aligned}\operatorname{tr}\Gamma(\pi g)=\frac{1}{2\pi i}\oint_c dz\,z^{-(n+1)}\sum_a\prod_j(-1)^{a_{qj}}a_{qj}!&\times\prod_i\frac{1}{a_{qji}!}(\rho_j)^{a_{ij}}z^{a_{ij}}\,\delta(a_{ij}-a_{\pi(i)j}-a_{qji})\\&\times\prod_l(\chi(g^l))^{\nu_l}.\end{aligned}\tag{8}$$

Now suppose m lies in cycle of length l in π, i.e., $(q\cdots sm)$. The Kronecker delta in the sum over $\mathbf{a}$ in Eq. (8) constrains $a_{ij}\geq a_{\pi(i)j}$. Then

$$a_{qj}\geq a_{\pi(q)j}\geq a_{\pi^2(q)j}\geq\cdots\geq a_{sj}\geq a_{mj}=0,$$

such that

$$a_{\pi^{u-1}(q)j}-a_{\pi^u(q)j}=a_{qj\pi^{u-1}(q)}.$$

Note that $s=\pi^{l-2}(q)$. Also, for l_i in another cycle in $\pi=(l_1l_2\cdots l_t)$, the Kronecker delta restricts the sum to all a_{ij} such that

$$a_{i_1j}\geq a_{i_2j}\geq\cdots\geq a_{i_tj}\geq a_{i_1j},$$

which implies that they are all equal.

The portion of Eq. (8) involving a_{ij}, i in the cycle containing m, is then

$$\begin{aligned}\prod_j\sum_{a_{qj}=0}^{\infty}(-1)^{a_{qj}}a_{qj}!(z\rho_j)^{a_{qj}}\sum_{a_{\pi(q)j}=0}^{a_{qj}}\frac{(z\rho_j)^{a_{\pi(q)j}}}{(a_{qj}-a_{\pi(q)j})!}&\times\sum_{a_{\pi^2(q)j}=0}^{a_{\pi(q)j}}\frac{(z\rho_j)^{a_{\pi^2(q)j}}}{(a_{\pi(q)j}-a_{\pi^2(q)j})!}\\&\cdots\sum_{a_{\pi^{l-2}(q)j}=0}^{a_{\pi^{l-3}(q)j}}\frac{(z\rho_j)^{a_{\pi^{l-2}(q)j}}}{(a_{\pi^{l-3}(q)j}-a_{\pi^{l-2}(q)j})!(a_{\pi^{l-2}(q)j})!}.\end{aligned}\tag{9}$$

Noting that

$$\sum_{i=0}^{p}\frac{x^i}{(p-i)!i!}=\frac{1}{p!}\sum_{i=0}^{p}\binom{p}{i}x^i1^{p-i}=\frac{(1+x)^p}{p!}$$

and performing the last $l-2$ sums in Eq. (9), it becomes

$$\prod_j \sum_{a_{qj}} (-1)^{a_{qj}} (z\rho_j)^{a_{qj}} (1+z\rho_j(1+z\rho_j(\cdots(1+z\rho_j))))^{a_{qj}}$$

$$= \prod_j (1+z\rho_j(\cdots(1+z\rho_j)))^{-1}$$

$$= \prod_j \Big(\sum_{i=0}^{l-1} (z\rho_j)^i\Big)^{-1}$$

$$= \prod_j \frac{1-z\rho_j}{1-(z\rho_j)^l}. \tag{10}$$

Furthermore the contribution to Eq. (8) from the sum over **a** for the cycles of length r [if the length of $(q\cdots sm)$ is not r] is [where $p=\nu_r r-(r-1)=(\nu_r-1)r+1$]

$$\prod_j \sum_{a_{i_1 j}=0}^{\infty} (z\rho_j)^{ra_{i_1 j}} \cdots \sum_{a_{i_p j}=0}^{\infty} (z\rho_j)^{ra_{i_p j}}$$

$$= \prod_j (1-z^r(\rho_j)^r)^{-\nu_r}$$

$$= \det(I-z^r V^r(g))^{-\nu_r}. \tag{11}$$

Combining the results of Eqs. (6)–(11) we have

$$\operatorname{tr} \Gamma(\pi g) = \frac{1}{2\pi i}\oint_c dz\, z^{-(n+1)} \det(I-zV(g)) \times \prod_{i=1}^{m} \det(I-z^i V^i(g))^{-\nu_i} (\chi(g^i))^{\nu_i}. \tag{12}$$

The contribution $c_{nm}(g)$ of the element g to c_{nm} is given by the number of times $\Gamma(\pi g)$ contains the identity representation of S_m. From Eq. (12) it is clear that $\operatorname{tr}\Gamma(\pi g)$ is a class function on S_m in that it depends only on the cycle structure of π. The number of elements in a class (ν) is $m!\Pi_i(i^{\nu_i}\nu_i!)^{-1}$ so that

$$c_{nm}(g) = \underset{\pi}{M} \operatorname{tr}\Gamma(\pi g) = \sum_{(\nu)} \frac{1}{2\pi i}\oint_c dz\, z^{-(n+1)} \times \det(I-zV(g)) \prod_i \left(\frac{\chi(g^i)}{i\det(I-z^iV^i(g))}\right)^{\nu_i} \frac{1}{\nu_i!}, \tag{13}$$

where the sum over (ν) is restricted to all (ν) such that $\Sigma_i i\nu_i = m$ as i ranges from 1 to m. Using Eq. (7) to constrain the ν_i and then summing over all (ν) leaves Eq. (13)

$$c_{nm}(g) = \left(\frac{1}{2\pi i}\right)^2 \oint\oint dz\, du\, z^{-(n+1)} u^{-(m+1)} \times \det(I-zV(g)) \prod_i \sum_{\nu_i} \frac{1}{\nu_i!}\left(\frac{u^i\chi(g^i)}{i\det(I-z^iV^i(g))}\right)^{\nu_i}$$

$$= (2\pi i)^{-2} \oint\oint dz\, du\, z^{-(n+1)} u^{-(m+1)} \times \det(I-zV(g)) \exp\left(\sum_{i=1}^{m} \frac{u^i\chi(g^i)}{i\det(I-z^iV^i(g))}\right). \tag{14}$$

Equation (14) was derived for $m\geq 2$ but can be extended to $m=1$. This may be seen by noting that

$$\frac{1}{2\pi i}\oint du\, u^{-(m+1)} f(u) = \frac{1}{m!}\frac{df^m(u)}{du^m}\bigg|_{u=0}. \tag{15}$$

When Eq. (15) is applied to Eq. (14) for $m=1$, one obtains Eq. (4). Note, however, that Eq. (14), when $m=0$, gives

$$c_{n0}(g) = \frac{1}{n!}\frac{d^n}{ds^n}\det(I-sV(g))|_{s=0}, \tag{16}$$

rather than Eq. (3).

From Eq. (15) one can quickly see that the summation in Eq. (14) on i can be extended to infinity. This fact also then allows us to recognize Eq. (14) as just the coefficient of $s^n t^m$ in the power series

$$F'(s,t,g) = \sum_{nm} c_{nm}(g) s^n t^m,$$

if we identify

$$F'(s,t,g) = \det(I-sV(g)) \exp\left(\sum_{i=1}^{\infty} \frac{t^i\chi(g^i)}{i\det(I-s^iV^i(g))}\right).$$

Taking into account the discrepancy between Eqs. (3) and (16), and since

$$c_{nm} = \underset{g}{M}\, c_{nm}(g),$$

it then follows that

$$F(s,t) = \underset{g}{M}\, F(s,t,g),$$

where

$$F(s,t,g) = F'(s,t,g) - \det(I-sV(g)) + 1$$

or

$$F(s,t) = 1 + \underset{g}{M} \det(I-sV(g)) \times \left[\exp\left(\sum_{i=1}^{\infty} \frac{t^i\chi(g^i)}{i\det(I-s^iV^i(g))}\right) - 1\right]. \tag{17}$$

It does not appear at present that Eq. (17) can be simplified further. As a check set $s=0$ in Eq. (17), leaving

$$F(0,t) = \underset{g}{M} \exp\left(\sum_{i=1}^{\infty} \operatorname{tr}\left(\frac{t^iD(g)^i}{i}\right)\right) = \underset{g}{M} \exp(-\operatorname{tr}\ln(I-tD(g))) = \underset{g}{M} \det(I-tD(g))^{-1},$$

which one recognizes as the expression for the simple Molien function.[2]

Equation (17) still is not entirely satisfactory for general calculations. However, it is useful in finding particular terms of arbitrary order m and n. This is so particularly if one uses computer algebra to perform the expansion. Indeed, for most representations of a space group G of interest, there are a finite number of $D(g)$ and $V(g)$ and one can readily find $F(s,t)$ to any desired order in s,t.

As an example, for the $F\Gamma_2^-$ representation of $R\,\bar{3}c$ (notation is that of Ref. 8)

$$F(s,t) = 1 + t^2(1 + 4s^2 + 9s^4 + 16s^6 + \cdots) + t^3(s + 10s^3 + 42s^5 + \cdots) + t^4(2 + 14s^2 + 103s^4 + \cdots) + t^5(3s + 50s^3 + \cdots) + t^6(3 + 31s^2 + \cdots) + \cdots,$$

where the computer algebra MACSYMA[9] has been employed.

As an example of the application of Eq. (17) to an infinite group, apply it to the faithful, or $l = 1$, representation of SO(3). The calculation is greatly simplified by noting that $F(s,t,g)$ is a class function, since it involves only similarity invariant traces and determinants. Then the sum over g reduces to an integral over the rotation angle, with an appropriate weighting factor. The result is

$$F(s,t) = 1 + (1 + s + 2s^2 + s^3 + 2s^4 + \cdots)t^2 + (s + s^2 + 5s^3 + \cdots)t^3 + (1 + s + 6s^2 + \cdots)t^4 + (s + \cdots)t^5 + (1 + \cdots)t^6 + \cdots.$$

Thus, for example, this representation has a Lifshitz invariant, i.e., $c_{12} = 1$.

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