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Graphical method for computing the determinant and inverse of a matrix. Generating functions for harmonic oscillator integrals

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Abstract. A graph G with n vertices is associated with the $n\times n$ matrix x. Det x and x_{ij}^{-1} are expressed in terms of sums over sets of subgraphs of G. The method is used to compute generating functions for products of overlaps involving harmonic oscillator wavefunctions.

1. Introduction

The method of calculating determinants and inverses of matrices that we present in § 2 is a graphical transcription of well known formulae. The method turns out to be very convenient for matrices with many zero elements. We illustrate the method in § 3 by computing generating functions for products of integrals over harmonic oscillator wavefunctions. We expose two ways of calculating these generating functions, one which is essentially the method of Birtwistle (1977) and the other which uses ideas from Bargmann (1962, reprinted in Biedenharn and Van Dam 1965, pp 300–16) and is better in the case when the harmonic oscillators have the same frequency. These generating functions are expressed in terms of determinants and inverses of matrices with many zeros, so that our method is useful.

2. Graphical method for computing det x and x^{-1}

We consider an $n\times n$ complex matrix $x=\Lambda-P$, where Λ is diagonal ($\Lambda_{ij}=0$ if $i\neq j$) and where P has zeros on the diagonal: $P_{ii}=0$ $(1\leqslant i\leqslant n)$. To P we associate a graph G consisting of n vertices, noted by V_i $(1\leqslant i\leqslant n)$, and where an arrow, noted by (ij), goes from V_i to V_j for each $P_{ij}\neq 0$. Two examples of graphs corresponding to calculations in § 3 are drawn on figures 1 and 2. We define *path* $[abc\ldots de]$ as the ordered sequences of arrows $(ab),(bc),\ldots,(de)$ and of the k $(k\geqslant 1)$ vertices $V_a, V_b\ldots V_e$. Thus $[a]$ is a path with no arrow. *Circuit* $(abc\ldots de)$ consists of the ordered cycles of the k $(k\geqslant 2)$ arrows $(ab),(bc)\ldots(de)$, (ea), and of vertices $V_a, V_b\ldots V_e$. Circuits (abc), (bca) and (cab) are identical. A set of m $(m\geqslant 0)$ circuits $C_1\ldots C_m$, such that each vertex of $C_1\ldots C_m$ appears only once in the set $\{C_1\ldots C_m\}$ is called a *closed diagram*. We denote the closed diagram composed of zero circuit by J. A set of one path T and m $(m\geqslant 0)$ circuits $C_1\ldots C_m$ such that each vertex of T,

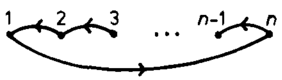

Figure 1. G_1 graph of matrix P, equation (19).

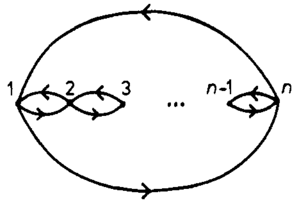

Figure 2. G_2 graph of matrix P, equation (15).

$C_1 \ldots C_m$ appears only once in the set $\{T, C_1 \ldots C_m\}$ is called an *open diagram*. We denote the set of the closed (open) diagrams of G by K (Ω), and by Ω_{ij} the set of the open diagrams with a path of the form $[i \ldots j]$.

For the graph of figure 2 (with $n = 4$), the nine closed diagrams of K are drawn on figure 3 and Ω_{11}, Ω_{12} and Ω_{13} are represented in figure 4.

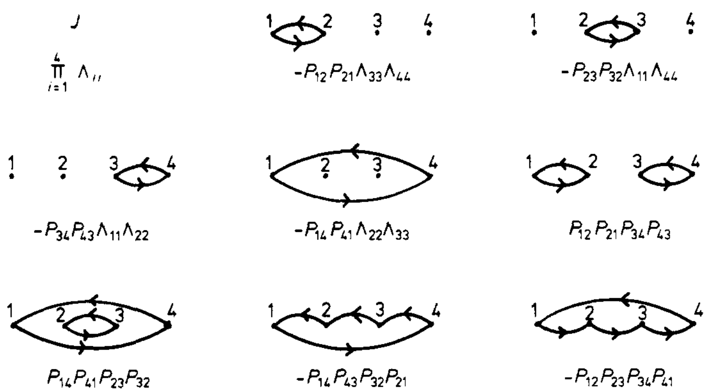

Figure 3. K: the nine closed diagrams of G_2 ($n = 4$) and values of $M(D)$.

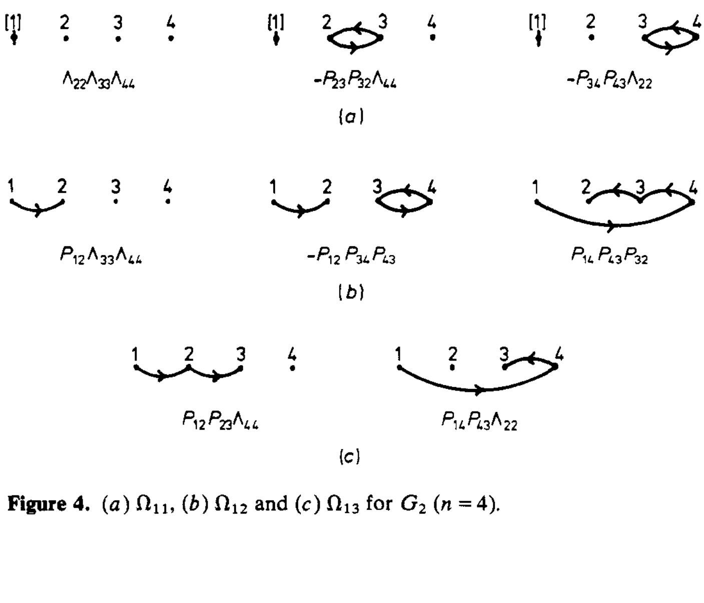

Figure 4. (a) Ω_{11}, (b) Ω_{12} and (c) Ω_{13} for G_2 ($n = 4$).

For each diagram D we denote by $\mathscr{A}(D)$ ($\mathscr{V}(D)$) the set of arrows (vertices) composing the path and/or circuits of D.

If D is a closed or open diagram with m circuits we define

$$M(D)=(-1)^m\Big(\prod_{(ij)\in\mathscr{A}(D)} P_{ij}\Big)\Big(\prod_{k\notin\mathscr{V}(D)} \Lambda_{kk}\Big).$$

In particular: $M(J)=\Pi_{i=1}^{n}\Lambda_{ii}$. Other examples of $M(D)$ are given in figures 3 and 4.

Now we have the following results:

$$\det(\Lambda-P)=\sum_{D\in K} M(D) \tag{1}$$

and

$$(\Lambda-P)_{ij}^{-1}=\frac{\Sigma_{T\in\Omega_{ij}} M(T)}{\Sigma_{D\in K} M(D)}. \tag{2}$$

Indeed, (1) is the graphical transcription of

$$\det x=\sum_{\sigma\in S_n}\epsilon(\sigma)x_{1\sigma(1)}x_{2\sigma(2)}\ldots x_{n\sigma(n)}.$$

As an example, for the permutation of $1\ldots n$, $\sigma=(123)(45)(6)\ldots(n)$, written as a product of cyclic permutations, we have

$$\epsilon(\sigma)x_{1\sigma(1)}x_{2\sigma(2)}\ldots x_{n\sigma(n)}$$
$$=[-(-x_{12})(-x_{23})(-x_{31})][-(-x_{45})(-x_{54})][x_{66}]\ldots[x_{nn}]=M(D)$$

where D is the closed diagram composed of circuits (123) and (45).

Equation (2) is the graphical transcription of

$$(x^{-1})_{ij}=\frac{X_{ij}}{\det x}$$

where X_{ij} is the co-factor of x_{ji} in $\det x$.

If one has to calculate

$$\boldsymbol{v}\,.\,(\Lambda-P)^{-1}\boldsymbol{w}=\sum_{i=1}^{n}\sum_{j=1}^{n} v_i(\Lambda-P)_{ij}^{-1}w_j$$

where $\boldsymbol{v}=(v_1\ldots v_n)$ and $\boldsymbol{w}=(w_1\ldots w_n)$ are two vectors of C^n, it is convenient to put $M'(T)=v_iM(T)w_j$ if $T\in\Omega_{ij}$. Then:

$$\boldsymbol{v}\,.\,(\Lambda-P)^{-1}\boldsymbol{w}=\frac{\Sigma_{T\in\Omega} M'(T)}{\Sigma_{D\in K} M(D)}. \tag{3}$$

Let us emphasise that the interest of equations (1)–(3) is greater when the matrix P is sparse. The diagrams are then easily enumerated and the method described makes the calculations much easier, especially when formal (rather than numerical) expressions are required.

3. Generating functions for products of harmonic oscillator overlaps

3.1. Generating function for the harmonic oscillator wavefunctions

We denote the normalised one-dimensional harmonic oscillator functions by

$$|m\rangle = \frac{a^{\dagger m}}{\sqrt{m!}}|0\rangle \tag{4}$$

with

$$a^{\dagger} = \sqrt{\left(\frac{\omega}{2}\right)}r - \frac{\mathrm{i}}{\sqrt{(2\omega)}}P \tag{5}$$

(see Messiah 1959).

The coherent state (Glauber 1963)

$$|Z, \omega\rangle = \mathrm{e}^{a^{\dagger}\bar{Z}}|0\rangle = \sum_{m=0}^{\infty} \frac{\bar{Z}^m}{\sqrt{m!}}|m\rangle \tag{6}$$

where $Z = x + \mathrm{i}y \in C$, $\bar{Z} = x - \mathrm{i}y$ serves as a generating function for the states of equation (4). In the r representation, state (6) is:

$$\langle r|Z, \omega\rangle = (\omega/\pi)^{1/4} \exp[-\tfrac{1}{2}(\omega r^2 + \bar{Z}^2) + \sqrt{(2\omega)}r\bar{Z}]. \tag{7}$$

The functions of the harmonic oscillator centred at $-d$ are given by

$$|m, \omega, d\rangle = \mathrm{e}^{\mathrm{i}pd}|m\rangle. \tag{8}$$

3.2. Generating functions $S_n(t)$ for products of overlaps

Birtwistle (1977) has given a general method for calculating generating functions of the type:

$$S_n(t) = \sum_{m_1, m_2 \ldots m_n \geq 0} \prod_{i=1}^{n} \langle m_i, \omega_i, d_i|m_{i+1}, \omega_{i+1}, d_{i+1}\rangle t_i^{m_i} \tag{9}$$

($n \geq 2$), $t = (t_1 \ldots t_n) \in C^n$ (when t is sufficiently small, all integrals in the following converge) and where, as in the following, we identify labels 1 and $n+1$. These generating functions provide a means for evaluating chain integrals like $\langle a|b\rangle\langle b|c\rangle\langle c|a\rangle$, and sums of such integrals (Mnatsakanyan 1971).

Introducing the operator:

$$Q(t, \omega) = \sum_{m=0}^{\infty} |m\rangle\langle m|t^m \tag{10}$$

we have:

$$Q(t, \omega) = \int \mathrm{d}\mu_1(Z)|Z, \omega\rangle\langle Zt, \omega| \tag{11}$$

$\mathrm{d}\mu_1(Z) = \pi^{-1}\,\mathrm{e}^{-Z\bar{Z}}\,\mathrm{d}x\,\mathrm{d}y$ is integrated over R^2, following the notation from Bargmann (1962). Equation (9) then reads:

$$S_n(t) = \mathrm{Tr}\, Q_1 Q_2 \ldots Q_n \tag{12}$$

$$Q_k = \mathrm{e}^{\mathrm{i}pd_k}Q(t_k, \omega_k)\,\mathrm{e}^{-\mathrm{i}pd_k} \qquad (1 \leq k \leq n).$$

3.2.1. Calculation of $S_n(t)$: method A. We sketch here the method of Birtwistle for computing $S_n(t)$. The trace in equation (12) is computed in the r representation:

$$S_n(t)=\int \langle r_n|Q_1|r_1\rangle\langle r_1|Q_2|r_2\rangle \ldots \langle r_{n-1}|Q_n|r_n\rangle \, \mathrm{d}^n r \tag{13}$$

$r=(r_1 \ldots r_n)$ is integrated over R^n and

$$\langle r_{k-1}|Q_k|r_k\rangle = \langle r_{k-1}+d_k|Q(t_k, \omega_k)|r_k+d_k\rangle.$$

The matrix element $\langle x|Q(t, \omega)|y\rangle$ can be easily computed from equations (11) and (7), by carrying out integrations similar to the ones studied in the remainder of this section:

$$\langle x|Q(t, \omega)|y\rangle = (\omega/\pi)^{1/2}(1-t^2)^{-1/2} \exp\{\omega[2xyt-(1+t^2)(x^2+y^2)/2]/(1-t^2)\}. \tag{14}$$

Using equation (10) and the expression of the harmonic oscillator function in terms of Hermite polynomials equation (14) is seen to be nothing else than the Mehler formula (Bateman and Erdélyi 1955, equation (14)). Equation (13) is of the form:

$$S_n(t)=\int A \exp[-\boldsymbol{r}\cdot(\Lambda-P)\boldsymbol{r}+\boldsymbol{b}\cdot\boldsymbol{r}+c]\, \mathrm{d}^n\boldsymbol{r}/\pi^{n/2} \tag{15}$$

$$A=\prod_{i=1}^{n} [\omega_i/(1-t_i^2)]^{1/2}.$$

Λ is the $n \times n$ diagonal matrix:

$$\Lambda_{kk}=\frac{1}{2}\left(\frac{\omega_k(1+t_k^2)}{1-t_k^2}+\frac{\omega_{k+1}(1+t_{k+1}^2)}{1-t_{k+1}^2}\right) \qquad (1 \leqslant k \leqslant n).$$

P is the symmetric $n \times n$ matrix, with all elements equal to zero but:

$$P_{k,k+1}=P_{k+1,k}=\frac{\omega_{k+1}t_{k+1}}{1-t_{k+1}^2} \qquad (1 \leqslant k \leqslant n), \text{ if } n>2$$

$$P_{12}=P_{21}=\frac{\omega_1 t_1}{1-t_1^2}+\frac{\omega_2 t_2}{1-t_2^2} \qquad \text{if } n=2$$

$\boldsymbol{b}$ is the n vector:

$$b_k=-\frac{\omega_k d_k(1-t_k)}{1+t_k}-\frac{\omega_{k+1}d_{k+1}(1-t_{k+1})}{1-t_{k+1}} \qquad (1 \leqslant k \leqslant n)$$

$$c=\sum_{k=1}^{n} -\omega_k \frac{1-t_k}{1+t_k} d_k^2$$

and where the cyclic condition $n+1 \equiv 1$ is used.

The integral in equation (15) is calculated in equation (10) of Birtwistle (1977):

$$S_n(t)=A[\det(\Lambda-P)]^{-1/2} \exp[\tfrac{1}{4}\boldsymbol{b}\cdot(\Lambda-P)^{-1}\boldsymbol{b}+c]. \tag{16}$$

The expressions in equation (16) can be easily computed by the method of § 2 with the graph of figure 2 and diagrams like those in figures 3 and 4. But instead of giving explicit results for equation (16), we turn to another method for computing $S_n(t)$ (equation (12)).

3.2.2. Calculation of $S_n(t)$: method B. Using equation (11) we get for the trace in equation (12):

$$S_n(t)=\int \mathrm{d}\mu_n(\zeta) \prod_{k=1}^{n} \langle Z_k\, t_k, \omega_k|\mathrm{e}^{\mathrm{i}p(d_{k+1}-d_k)}|Z_{k+1}, \omega_{k+1}\rangle \tag{17}$$

where $\zeta=(Z_1,\ldots,Z_n)\in C^n$, $\mathrm{d}\mu_n(\zeta)=\Pi_{k=1}^n \mathrm{d}\mu_1(Z_k)$ and $n+1\equiv 1$. The matrix elements in equation (17) are:

$$\langle Z,\omega|\mathrm{e}^{\mathrm{i}pd}|Z',\omega'\rangle$$
$$=(\cos\theta)^{1/2}\exp[\sin\theta(Z^2-\bar{Z}'^2)/2+\cos\theta Z\bar{Z}'$$
$$+\cos\theta(\sqrt{\omega}\, d\bar{Z}'-\sqrt{\omega'}\, dZ)/\sqrt{2}-\cos\theta\sqrt{\omega\omega'}\, d^2/4] \tag{18}$$

where $\sin\theta=(\omega-\omega')/(\omega+\omega')$, $\cos\theta=2\sqrt{\omega\omega'}/(\omega+\omega')$.

The integral in equation (17) is thus seen to be similar to that in equation (15), but now the integration is over R^{2n}, so that in general the computation of $S_n(t)$ is simpler from equation (15). However when the oscillators have the same frequency $\omega_k=\omega$ $(1\leqslant k\leqslant n)$ in equation (18) we have $\sin\theta=0$, so that equation (17) is of the form:

$$S_n(t)=\int \mathrm{d}\mu_n(\zeta)\exp(\bar{\boldsymbol{\zeta}}\,.\,P\boldsymbol{\zeta}+\boldsymbol{v}\,.\,\boldsymbol{\zeta}+\bar{\boldsymbol{\zeta}}\,.\,\boldsymbol{w}+c) \tag{19}$$

where P is the $n\times n$ complex matrix with all elements zero except $P_{k+1,k}=t_k$ $(1\leqslant k\leqslant n)$;

$$v_k=-t_k(d_{k+1}-d_k)\sqrt{\omega/2};\qquad w_{k+1}=(d_{k+1}-d_k)\sqrt{\omega/2}\qquad (1\leqslant k\leqslant n);$$

$$c=\sum_{k=1}^{n}-\omega(d_{k+1}-d_k)^2/4;\qquad n+1\equiv 1.$$

The integral in equation (19) can be computed by the method of the appendix of Bargmann (1962, reprinted in Biedenharn and Van Dam 1965, pp 315–6):

$$S_n(t)=[\det(1-P)]^{-1}\exp[\boldsymbol{v}\,.\,(1-P)^{-1}\boldsymbol{w}+c] \tag{20}$$

Here again, the expressions in equation (20) can be computed by the method of § 2, from equations (1) and (3). The graph of P is drawn in figure 1. There are only two closed diagrams, so that from equation (1):

$$\det(1-P)=1-t_1t_2\ldots t_n.$$

Each of the sets Ω_{ij} contains only one open diagram, so that:

$$\boldsymbol{v}\,.\,(1-P)^{-1}\boldsymbol{w}=[\det(1-P)]^{-1}\sum_{i,j=1}^{n}-\frac{\omega}{2}(d_{j+1}-d_j)(d_i-d_{i-1})\prod_{k=i}^{j}t_k$$

with the conventions that $\Pi_{k=i}^j t_k=(\Pi_{k=1}^n t_k)(\Pi_{k=1}^j t_k)$ if $i>j$ and $d_0=d_n$, $d_{n+1}=d_1$.

4. Conclusion

Other fields of application of the graphical method can be found. For example, the generating function for coupling–recoupling coefficients of SU(2), such as the $3nj$ and njm coefficients, has been expressed by an equation like equation (20) (Labarthe

1975), where P is a $2n \times 2n$ matrix of the form

$$\begin{bmatrix} A & B \\ C & \tilde{A} \end{bmatrix}$$

A, B and C being $n \times n$ matrices such that: $\tilde{B} = -B$, $\tilde{C} = -C$, the tilde denoting the transposed matrix.

In this case, introducing the graph of the coupling–recoupling coefficient (El Baz 1969), which has branches instead of arrows, so that paths go over the branches in two directions, it was shown that:

$$\det(1-P) = \Big(\sum_{D \in K} M(D)\Big)^2$$

where K is the set of the closed diagrams. For the exponent also there is a formula like equation (3).

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