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Oscillator Wigner functions

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Abstract. A closed expression is obtained for the n-dimensional Wigner oscillator function and a diagrammatic technique is developed for finding the explicit dependence of the function on Euler angles at any dimension n.

1. Introduction

By oscillator Wigner functions (OWF) we will understand the matrix elements of the operator of finite rotations over Cartesian wavefunctions of the isotropic oscillator.

Such objects are interesting in that they determine the transformation law of the Cartesian wavefunctions of the isotropoic oscillator in a rotating coordinate system. Further, we shall deal just with this aspect of OWF, although they may turn out to be useful in particular problems. Thus, in studying the vibrational transitions in multi-atomic molecules, in some cases the OWF coincide with the overlap integrals defining the intensity of vibrational bands (Doktorov *et al* 1976).

The paper is organised as follows. First the two-dimensional OWF are introduced. Then, OWF of arbitrary dimensionality are constructed in this basis and a diagrammatic technique is developed, which allows us to define the explicit dependence of these functions on Euler angles.

2. Two dimensions

For the transition from one coordinate system $S(x, y)$ to another $S(x', y')$ rotated by an angle α, the Cartesian wavefunctions of a circular oscillator are transformed by the orthogonal matrix‡

$$|j+m', j-m'; x', y'\rangle = \sum_{m=-j}^{j} \langle j+m, j-m; x, y|j+m', j-m'; x', y'\rangle|j+m, j-m; x, y\rangle. \tag{1}$$

Let us expand coefficients of this transformation over the polar wavefunctions with the same energy. Since $E^{\mathrm{Car}} = 2j+1$, $E^{\mathrm{pol}} = 2p+|M|+1$, where p is a non-negative integer, and M the azimuthal quantum number, then $p = j-|M|/2$ at equal energies, so

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‡ We choose the system of units: $\hbar = m = \omega = 1$; angles φ and φ' in systems S and S' are related by $\varphi' = \varphi + \alpha$.

that $-2j \leqslant M \leqslant 2j$ and hence

$$\begin{aligned}\langle j+m, j-m; x, y | j+m', j-m'; x', y'\rangle \\ &= \sum_{k=-j}^{j} \langle j+m, j-m; x, y | j-|k|, 2k; r, \varphi\rangle \, e^{2ik\alpha} \\ &\quad \times \langle j-|k|, 2k; r, \varphi' | j+m', j-m'; x', y'\rangle.\end{aligned}$$

In this formula the coefficients of transition from Cartesian to polar wavefunctions have been calculated by Pogosyan and Ter-Antonyan (1979) and are as follows:

$$\langle j+m, j-m; x, y | j-|k|, 2k; r, \varphi\rangle = (-\mathrm{i})^{j-m}(-1)^{j-|k|} d^{j}_{k,m}(\pi/2),$$

the Wigner d-functions with their phases being defined according to Edmonds (1957). Using this result and the addition theorem for d-functions, we obtain the transformation law

$$|j+m', j-m'; x', y'\rangle = \sum_{m=-j}^{j} d^{j}_{m',m}(2\alpha) |j+m, j-m; x, y\rangle. \tag{2}$$

It is easy to verify that at $m' = -j$ and $\alpha = \pi/4$ we arrive at the known addition theorem for Hermite polynomials. For $\alpha = \pi/4$ formula (2) has been derived in Pogosyan and Ter-Antonyan (1979). Note also that formula (2) results in the integral representation of d-functions via the normalised Hermite function

$$\begin{aligned}d^{j}_{m',m}(\varphi) &= \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y \, \bar{H}_{j+m}(x) \bar{H}_{j-m}(y) \bar{H}_{j+m'}\left(x \cos\frac{\varphi}{2} - y \sin\frac{\varphi}{2}\right) \\ &\quad \times \bar{H}_{j-m}\left(-x \sin\frac{\varphi}{2} + y \cos\frac{\varphi}{2}\right).\end{aligned}$$

The explicit form of transformation (2) can be established without passing to the polar wavefunctions, but by considering relation (1) at large x and y and substituting the Hermite polynomials by the corresponding highest powers of arguments.

3. Three and four dimensions

The Wigner oscillator functions for $n \geqslant 3$ can be calculated, as above, passing first to the spherical basis and then making a two-dimensional rotation. However, even at $n = 3$ the transition coefficients are rather cumbersome (Pogosyan and Ter-Antonyan 1978) and can no longer be summed by the known addition theorems for d-functions and Clebsch–Gordon coefficients. Therefore, we perform here all calculations directly in terms of Cartesian wavefunctions.

The form of an n-dimensional finite-rotation operator is naturally defined by the number of angles used for transition from one point on the sphere to another. In the Cartesian basis the most simple rotations are in separate coordinate planes, as each of such rotations transforms a pair of one-dimensional oscillator functions by the law (2).

An arbitrary n-dimensional rotation is known to be equivalent to a sequence of such 'elementary' rotations at $n(n-1)/2$ Euler angles, chosen in a definite manner.

In the three-dimensional case the finite rotation operator is expressed in terms of the Euler angles θ_1^2, θ_2^2, θ_1^2:

$$\hat{G}(3) = \hat{G}_{21}(\theta_1^2)\hat{G}_{32}(\theta_2^2)\hat{G}_{21}(\theta_1^1). \tag{3}$$

Indices of the operators $\hat{G}_{j+1,j}$ label the coordinate plane in which a rotation occurs, and the rotation is taken to be positive from the $(j+1)$ axis to the j axis. Since the wavefunctions in the systems $S(x, y, z)$ and $S'(x', y', z')$ are related to the same energy, the non-zero matrix elements are $\langle j+m, j-m, n-2j|\hat{G}(3)|j'+m', j'-m', n-2j'\rangle$. Expressing by (3) the operator $\hat{G}(3)$ in terms of operators $\hat{G}_{j+1,j}$ and separating the rotation in the plane (x, y) by the angle θ_1^1, we obtain

$$\begin{aligned}
&\langle j+m, j-m, n-2j|\hat{G}(3)|j'+m', j'-m', n-2j'\rangle \\
&\quad = \sum_{j''=0}^{n/2} \sum_{m''=-j''}^{j''} \langle j+m, j-m, n-2j|\hat{G}_{21}(\theta_1^2)\hat{G}_{32}(\theta_2^2)|j''+m'', j''-m'', n-2j''\rangle \\
&\qquad \times \langle j''+m'', j''-m'', n-2j''|\hat{G}_{21}(\theta_1^1)|j'+m', j'-m', n-2j'\rangle.
\end{aligned}$$

The rotation $\hat{G}_{21}(\theta_1^1)$ does not affect the coordinate z; therefore the latter matrix element differs from zero only at $j''=j'$ and thus there is no longer summation over j''. The coefficient containing the product of two rotation operators is simplified to a linear combination of products of matrix elements of the operators $\hat{G}_{21}(\theta_1^2)$ and $\hat{G}_{32}(\theta_2^2)$, and with analogous selection rules we have

$$\begin{aligned}
&\langle j+m, j-m, n-2j|\hat{G}(3)|j'+m', j'-m', n-2j'\rangle \\
&\quad = \sum_{m''=-j'}^{j'} \sum_{\tilde{m}=-j}^{j} \langle j+m, j-m|\hat{G}_{21}(\theta_1^2)|j+\tilde{m}, j-\tilde{m}\rangle \\
&\qquad \times \langle j-\tilde{m}, n-2j|\hat{G}_{32}(\theta_2^2)|j'-m'', n-2j'\rangle \\
&\qquad \times \langle j'+m'', j'-m''|\hat{G}_{21}(\theta_1^1)|j'+m', j'-m'\rangle \delta_{j+\tilde{m},j'+m''}.
\end{aligned}$$

Then, changing summation over m'' and $\tilde{m}$ to summation over $t=j'+m''$ and $k=j+\tilde{m}$ and using the relation (resulting from (2))

$$\begin{aligned}
&\langle j+m, j-m; x_k, x_{k+1}|j'+m', j'-m'; x'_k, x'_{k+1}\rangle \\
&\quad = \langle j+m, j-m|\hat{G}_{k+1,k}(\alpha)|j'+m', j'-m'\rangle = d^j_{m',m}(2\alpha),
\end{aligned} \tag{4}$$

we arrive at the explicit expression for the three-dimensional oscillator Wigner function

$$\begin{aligned}
&\langle j+m, j-m, n-2j|\hat{G}(3)|j'+m', j'-m', n-2j'\rangle \\
&\quad = \sum_{t=0}^{2\min(j,j')} d^j_{t-j,m}(2\theta_1^2) d^{(n-t)/2}_{2j'-(n+t)/2,2j-(n+t)/2}(2\theta_1^2) d^{j'}_{m',t-j'}(2\theta_1^1).
\end{aligned} \tag{5}$$

The limits of summation over t may be not written explicitly if t is assumed to run only over those values at which the absolute value of lower t-independent indices of d-functions does not exceed that of upper indices.

As is clear from (3), at $\theta_2^2=0$ there is a pure rotation in the plane (x, y) by an angle $\theta_1^1+\theta_1^2$, and at $\theta_1^1=\theta_1^2=0$ the same rotation in the plane (z, y) by an angle θ_2^2, so in these cases expression (4) should turn into the d-function with arguments $2(\theta_1^1+\theta_1^2)$ and $2\theta_1^2$, respectively. The validity of this transition is easily verified with the use of $d^j_{m,m'}(0)=\delta_{mm'}$ and the addition theorem.

The four-dimensional rotation is given by six Euler angles and the operator $\hat{G}(4)$ is expressed through the operators of rotation in coordinate planes by the formula (Vilenkin 1968)

$$\hat{G}(4)=\hat{G}_{21}(\theta_1^3)\hat{G}_{32}(\theta_2^3)\hat{G}_{43}(\theta_3^3)\hat{G}_{21}(\theta_1^2)\hat{G}_{32}(\theta_2^2)\hat{G}_{21}(\theta_1^1). \tag{6}$$

The Wigner oscillator function is calculated analogously:

$$\begin{aligned}\langle j+m, j-m, k-2j, n-k|\hat{G}(4)|j'+m', j'-m', k'-2j', n-k'\rangle \\ =\sum_{\mu,\sigma,\lambda} d^{j'}_{m',\sigma-j'}(2\theta_1^1)d^{\mu}_{\sigma-\mu,\lambda-\mu}(2\theta_1^2)d^{(k'-\sigma)/2}_{2j'-(k'+\sigma)/2,2j-(k'+\sigma)/2}(2\theta_2^2) \\ \times d^{j}_{\lambda-j,m}(2\theta_1^3)d^{(k-\lambda)/2}_{2\mu-(k+\lambda)/2,2j-(k+\lambda)/2}(2\theta_2^3)d^{n/2-\mu}_{k'-\mu-n/2,k-\mu-n/2}(2\theta_1^3).\end{aligned} \tag{7}$$

As for the limits of t-summation, see the comment after formula (5). At $\theta_1^3=\theta_2^3=\theta_3^3=0$ the rotation (6) becomes three-dimensional and formula (7) reduces to (5).

4. n dimensions

Consider now the n-dimensional case. The operator of finite n-dimensional rotations $\hat{G}(n)$ can be represented by the following product of rotation operators in the coordinate planes (Vilenkin 1968):

$$\hat{G}(n)=\hat{G}^{(n-1)}(\theta_1^{n-1},\ldots,\theta_{n-1}^{n-1})\ldots\hat{G}^{(1)}(\theta_1^1), \tag{8}$$

$$\hat{G}^{(k)}(\theta_1^k,\ldots,\theta_k^k)=\hat{G}_{21}(\theta_1^k)\ldots\hat{G}_{k+1,k}(\theta_k^k). \tag{9}$$

From formula (8) it follows that the n-dimensional oscillator Wigner function can be expressed in terms of the matrix elements of operators (9) as follows:

$$\begin{aligned}\langle N_1,\ldots,N_n|\hat{G}(n)|N_1',\ldots,N_1',\ldots,N_n'\rangle \\ =\sum_{p_1^{(n-1)}\ldots p_{(n-1)}^{(n-1)}}\cdots\sum_{p_1^{(2)}p_2^{(2)}}\langle N_1,\ldots,N_n|\hat{G}^{(n-1)}|p_1^{(n-1)}\ldots p_{n-1}^{(n-1)},N_n'\rangle \\ \times\langle p_1^{(n-1)},\ldots,p_{n-1}^{(n-1)}|\hat{G}^{(n-2)}|p_1^{(n-2)},\ldots,p_{n-2}^{(n-2)}N_{n-1}'\rangle\ldots \\ \times\langle p_1^{(2)},p_2^{(2)}|\hat{G}^{(1)}|N_1',N_2'\rangle\end{aligned} \tag{10}$$

with $p_1^{(i)}+\ldots+p_i^{(i)}=N_1'+\ldots+N_i'$.

In the notation

$$p_1^{(1)}=N_1'; \qquad p_i^{(n)}=N_i,\ i=1,2,\ldots,n,$$

expression (10) can be rewritten in a more compact form:

$$\begin{aligned}\langle N_1,\ldots,N_n|\hat{G}(n)|N_1',\ldots,N_n'\rangle \\ =\sum_{p_1^{(i)},\ldots,p_i^{(i)}}\prod_{j=1}^{n-1}\langle p_1^{(j+1)},\ldots,p_{j+1}^{(j+1)}|\hat{G}^{(j)}(\theta_1^j,\ldots,\theta_j^j)|p_1^{(j)},\ldots,p_j^{(j)},N_{j+1}'\rangle.\end{aligned} \tag{11}$$

With the help of (9), we single out the rightmost factor of the product of the operators of rotation in coordinate planes and make use of the expression (resulting from (2))

$$\begin{aligned}
\hat{G}_{j+1,j}(\theta_j^j)|p_j^{(j)}, N'_{j+1}\rangle
&= \sum_m \left\langle \frac{p_j^{(j)}+N'_{j+1}}{2}+m, \frac{p_j^{(j)}+N'_{j+1}}{2}-m \middle| \hat{G}_{j+1,j}(\theta_j^j) \middle| p_j^{(j)}, N'_{j+1} \right\rangle \\
&\quad \times \left| \frac{p_j^{(j)}+N'_{j+1}}{2}-m, \frac{p_j^{(j)}+N'_{j+1}}{2}+m \right\rangle
\end{aligned}$$

where summation over m is in the limits $2|m| \leqslant p_j^{(j)}+N'_{j+1}$. Carrying the state vector $\langle p_{j+1}^{(j+1)}|$ out of the product of the first $(j-1)$ operators of rotation in the coordinate planes, and using the condition of orthonormalisation of one-dimensional oscillator wavefunctions, we arrive at the relation

$$\begin{aligned}
&\langle p_1^{(j+1)}, \ldots, p_{j+1}^{(j+1)}| \prod_{l=1}^{j} \hat{G}_{l+1,l}(\theta_l^j)|p_1^{(j)}, \ldots, p_j^{(j)}, N'_{j+1}\rangle \\
&\quad = \langle p_j^{(j)}+N'_{j+1}-p_{j+1}^{(j+1)}, p_{j+1}^{(j+1)}|\hat{G}_{j+1,j}(\theta_j^j)|p_j^{(j)}, N'_{j+1}\rangle \\
&\quad \times \langle p_1^{(j+1)}, \ldots, p_j^{(j+1)}| \prod_{l=1}^{j-1} \hat{G}_{l+1,l}(\theta_l^j)|p_1^{(j)}, \ldots, p_{j-1}^{(j)}, p_j^{(j)}+N'_{j+1}-p_{j+1}^{(j+1)}\rangle.
\end{aligned}$$

Further decreasing the number of multipliers in the product of rotation operators, after $(j-1)$ steps we find

$$\begin{aligned}
&\langle p_1^{(j+1)}, \ldots, p_{j+1}^{(j+1)}| \prod_{l=1}^{j} \hat{G}_{l+1,l}(\theta_l^j)|p_1^{(j)} \ldots p_j^{(j)}, N'_{j+1}\rangle \\
&\quad = \prod_{k=1}^{j} \langle J_{jk}+\mathcal{M}_{jk}, J_{jk}-\mathcal{M}_{jk}|\hat{G}_{j-k+2}(\theta_{j-k+1}^j)|J_{jk}+\mathcal{M}'_{jk}, J_{jk}-\mathcal{M}'_{jk}\rangle.
\end{aligned} \tag{12}$$

The quantities J_{jk}, $\mathcal{M}_{jk}$ and $\mathcal{M}'_{jk}$ are defined in the following manner:

$$2J_{jk} = N'_{j+1} + \sum_{\nu=j-k+1}^{j} p_\nu^{(j)} - \sum_{\nu=j-k+2}^{j+1} p_\nu^{(j+1)} + p_{j-k+2}^{(j+1)},$$

$$2\mathcal{M}_{jk} = N'_{j+1} + \sum_{\nu=j-k+1}^{j} p_\nu^{(j)} - \sum_{\nu=j-k+2}^{j+1} p_\nu^{(j+1)} - p_{j-k+2}^{(j+1)},$$

$$2\mathcal{M}_{jk} = \sum_{\nu=1}^{j-k+1} p_\nu^{(j)} - \sum_{\nu=1}^{j-k+2} p_\nu^{(j+1)} + p_{j-k+1}^{(j)}.$$

Now with formula (4) we arrive at the final result

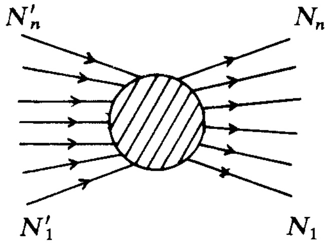
$$\langle N_1, \ldots, N_4|\hat{G}(n)|N'_1, \ldots, N'_n\rangle = \sum_{p_1^{(i)},\ldots,p_i^{(i)}} \prod_{j=1}^{n-1} \prod_{k=1}^{j} d^{J_{jk}}_{\mathcal{M}_{jk},\mathcal{M}'_{jk}}(2\theta_{j-k+1}^j). \tag{13}$$

As can be verified, formula (13) at $n = 2, 3$ and 4 reduces to (4), (5) and (7), respectively.

5. Graphs

The results obtained can be made much more transparent through the following analogy. The operator $\hat{G}(n)$ relates states $|N_1, \ldots, N_n; X_1, \ldots, X_n\rangle$ and $|N'_1, \ldots, N'_n;$

$X_1, \ldots, X_n\rangle$; therefore, the matrix element $\langle N_1, \ldots, N_n|\hat{G}(n)|N'_1, \ldots, N'_n\rangle$ can be interpreted as the 'amplitude of transition of a system' from state N' to state N, and this amplitude can be associated with the diagram

$\langle N_1, \ldots, N_n|\hat{G}(n)|N'_1, \ldots, N'_n\rangle =$ 

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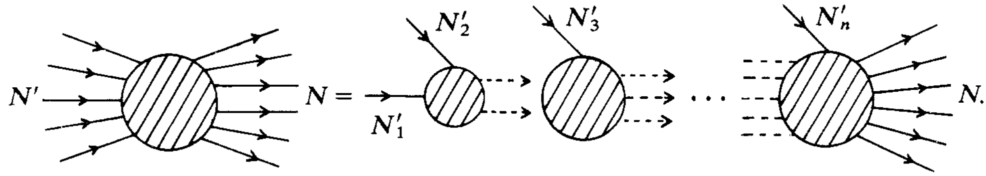
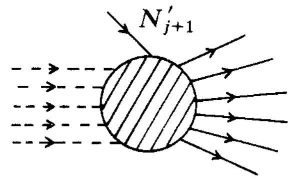
In such an interpretation the expression (10) of the matrix element of the operator $\hat{G}(n)$ over the matrix elements of the operators $\hat{G}^{(j)}$ is graphically represented by a sequence of 'transitions'



(14)

Summation is implied over broken lines; intermediate blocks with one full line correspond to the matrix elements of operators $\hat{G}^{(j)}$:

$$\langle p_1^{(j+1)}, \ldots, p_{j+1}^{(j+1)}|\hat{G}^{(j)}(\theta_1^j, \ldots, \theta_j^j)|p_1^{(j)}, \ldots, p_j^{(j)}, N'_{j+1}\rangle \qquad (15)$$

$= p^{(j)}$ 

$p^{(j+1)}$.

According to the condition preceding formula (11), at $j = 1$ and $j = n$ these blocks become, respectively, the first and the last blocks of expansion (14). Each block obeys the conservation law

$$p_1^{(j+1)} + \ldots + p_{j+1}^{(j+1)} = p_1^j + \ldots + p_j^j + N'_{j+1}.$$

The graphical expansion (14) and expression (12) allow the transition amplitude $\langle N|\hat{G}(n)|N'\rangle$ to be represented by the amplitudes of elementary transitions of two lines into two lines (see figure 1).

In this diagram the number of intersections (elementary blocks) equals $n(n-1)/2$; this means that rotation in the coordinate plane by a certain Euler angle is associated with each of such blocks. The number of summations in formula (13) equals $(n-1)$ $(n-2)/2$ and coincides with the number of elementary loops in the diagram of figure 2.

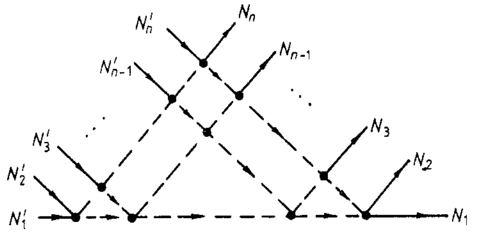


Figure 1. Diagram representing the n-dimensional oscillator Wigner function by d-functions dependent on angles of rotations in the coordinate planes.

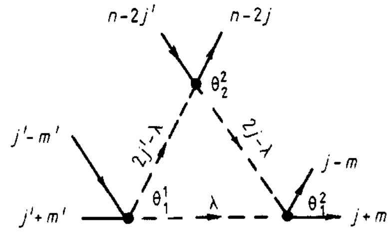
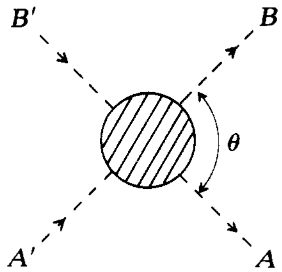


Figure 2. Diagram for the three-dimensional oscillator Wigner function.

According to formula (4), to each intersection there corresponds the amplitude of the elementary 'transition'



$$= \langle A, B|\hat{G}(\theta)|A', B'\rangle = d^{(A+B)/2}_{(A'-B')/2,(A-B)/2}(2\theta). \tag{16}$$

The operator $\hat{G}(\theta)$ in (16) should be supplied with indices of the coordinate axes defining the plane in which the rotation occurs. We have omitted these indices since they are unambiguously defined by the very diagram of figure 1.

The procedure of calculation is as follows. For each n we draw the corresponding diagram, mark the Euler angles, and place the indices for all lines. The number of non-fixed indices should be equal to the number of elementary loops of the diagram. Further, with each intersection we associate the d-function of the angle 'attached' to this intersection. Indices of the d-function obey the rule (16) and the summation is carried out over non-fixed indices, over those values for which the d-function is meaningful. The latter condition has been discussed earlier in connection with formula (5).

Let us exemplify this procedure for $n = 3, 4$. Choosing the indices of wavefunctions as in § 3, we arrive at the diagrams drawn in figures 2 and 3.

The formulated rules for those diagrams give rise to the formulae (5) and (7).

Thus the diagrammatic method reduces the problem of calculating the Wigner oscillator function to simple geometrical constructions.

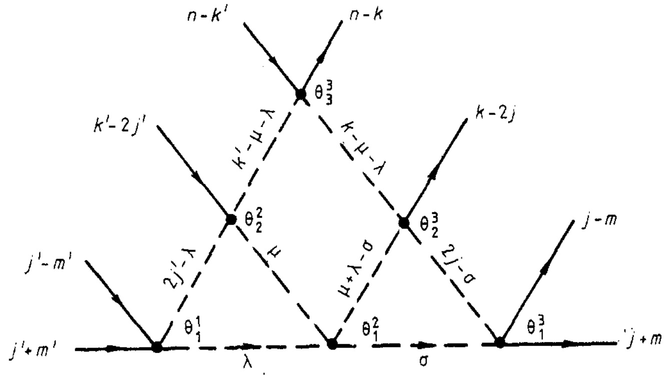


Figure 3. Diagram for the four-dimensional oscillator Wigner function.

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