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LETTER TO THE EDITOR

Factorization relations and Wigner's rotation matrices

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Abstract. A factorization formula for the squared Wigner rotation function is derived. General properties of the coefficients and special cases are discussed. The connection with recent factorization relations for vibrational transition probabilities in harmonic and anharmonic oscillators is studied.

Factorization formulae are known in the theory of inelastic collisions from initially excited states, reflecting the fact that the essential dynamics of a process is independent of the initial state, which enters only in a statistical manner. The most popular factorization relation appears in rotational transitions of diatomic molecules by collisions under sudden conditions. Here the transition probabilities for rotational transitions $j \to j'$ are related by [1, 2]

$$P(j' \leftarrow j) = \sum_{j''=|j'-j|}^{j'+j} C^{\rm rot}_{j'j''j}\, P(j'' \leftarrow 0) \tag{1}$$

to the rotational transition probabilities for transitions $0 \to j''$ out of the rotational ground state. The weight coefficients

$$C^{\rm rot}_{j'j''j} = (2j'+1)\begin{pmatrix} j' & j'' & j \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{2}$$

are unaffected by the dynamical quantities determining the collision process. Note that the same factorization formula is valid for differential and integral state-to-state cross sections and also for transition rates [1]. The mechanism underlying the factorization relation is most clearly demonstrated in a classical version of the factorization equation [3, 4].

A similar factorization relation has been derived recently for vibrational transitions under sudden conditions [5] and, more generally, for the celebrated linearly forced harmonic oscillator [6] as well as an anharmonic model [6].

In the present letter we derive a similar factorization relation for the square of the Wigner functions (or Wigner's rotation matrices). It is shown that these results directly yield the vibrational factorization relations without any further dynamical consideration, thus underlining their purely algebraic nature.

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The Wigner function, $D^j_{m\,m'}(\phi,\vartheta,\xi)$ [7, 8, 9], may be represented as a product of three functions depending on a single angle

$$D^j_{m\,m'}(\phi,\vartheta,\xi) = \mathrm{e}^{-\mathrm{i}m\phi}\, d^j_{m\,m'}(\vartheta)\, \mathrm{e}^{-\mathrm{i}m'\xi} \tag{3}$$

where $d^j_{m\,m'}$ is a real function. The explicit form of the Wigner function $d^j_{m\,m'}$ is given by [7, 8]

$$\begin{aligned} d^j_{m\,m'}(\vartheta) &= [(j+m')!\,(j-m')!\,(j+m)!\,(j-m)!\,]^{(1/2)} \\ &\times \sum_\nu \frac{(-1)^\nu}{(j-m-\nu)!\,(j+m'-\nu)!\,(\nu+m-m')!\,\nu!} \\ &\times \left(\cos(\vartheta/2)\right)^{2j+m'-m-2\nu} \left(-\sin(\vartheta/2)\right)^{m-m'+2\nu} \end{aligned} \tag{4}$$

with $-j \leqslant m,\ m' \leqslant j$.

The square

$$\tilde{P}^j_{m'\,m}(\vartheta) = \left|D^j_{m'\,m}(\phi,\vartheta,\xi)\right|^2 = \left|d^j_{m'\,m}(\vartheta)\right|^2 \tag{5}$$

can be easily interpreted in terms of the vector model as the probability that a vector of length $\sqrt{j(j+1)}$ and projection m on a Z-axis leads to a projection m' on an axis Z' with the same origin, but inclined by an angle ϑ (see, e.g. [7, chapter 3.6] and [10]).

For the following considerations it is convenient to shift the indices by defining $n = j - m$ and $n' = j - m'$ and

$$P^j_{n'\,n}(\vartheta) := \tilde{P}^j_{j-n'\,j-n}(\vartheta)\,. \tag{6}$$

For the special case $n = 0$ we have

$$P^j_{n''\,0}(\vartheta) = \frac{(2j)!}{(2j-n'')!\,n''!}\left(\cos(\vartheta/2)\right)^{4j-2n''}\left(\sin(\vartheta/2)\right)^{2n''} \tag{7}$$

and the explicit expression (4) yields

$$\begin{aligned} P^j_{n'\,n}(\vartheta) &= (2j-n')!\,n'!\,(2j-n)!\,n!\left(\cos(\vartheta/2)\right)^{4j-2n+2n'}\left(\sin(\vartheta/2)\right)^{2n'-2n} \\ &\times \sum_\mu \left(-\tan^2(\vartheta/2)\right)^\mu \sum_{l=0}^{\mu} \frac{1}{l!\,(n-l)!\,(2j-n'-l)!\,(l-n+n')!} \\ &\times \frac{1}{(\mu-l)!\,(n-\mu+l)!\,(2j-n'-\mu+l)!\,(\mu-l-n+n')!}\,. \end{aligned} \tag{8}$$

The desired factorization formula is now obtained by replacing the index μ by $\mu = n'' + n' - n$ and using (7), which immediately yields

$$P^j_{n'\,n}(\vartheta) = \sum_{n''} C^j_{n\,n''\,n'}\, P^j_{n''\,0}(\vartheta) \tag{9}$$

where the coefficients are given by

$$C^{j}_{n' n'' n} = (-1)^{s} \sum_{i} \binom{n''}{i-n'} \binom{n}{i-n''} \binom{n'}{i-n} \frac{(2j-n')!\,(2j-n'')!\,(2j-n)!}{(2j)!\,(2j-i)!\,(2j-s+i)!} \tag{10}$$

with $s = n+n'+n''$. The range of the summation indices for the non-zero coefficients is limited by

$$|n'-n| \leqslant n'' \leqslant \min(n+n', 4j-n-n') \tag{11}$$

$$\max(n, n', n'', 2j-s) \leqslant i \leqslant \min(n+n', n''+n, n'+n'', 2j). \tag{12}$$

Equation (9) closely resembles the rotational factorization relation (1). It expresses the probabilities that an angular momentum making a projection $m = j-n$ on a Z-axis will be found making a projection $m' = j-n$ on the rotated Z'-axis in terms of those probabilities for finding a Z'-projection $m'' = j-n''$ for an initial Z-projection j, i.e. a maximum orientation along this axis. It is remarkable that the knowledge of this set of numbers, i.e. the magnitudes of a single row of the rotation matrix, is sufficient to generate all other probabilities. Let us note that the weight coefficients $C^{j}_{n' n'' n}$ are purely algebraic quantities and independent of the angle of inclination ϑ. Let us furthermore note that these weight coefficients can be negative as well as positive depending on the parity of the states involved, and that their magnitude can exceed unity, thus complicating a purely geometric or classical interpretation of the factorization relation (9) as in the case of the formula (1) for rotational transition probabilities.

Some useful properties of the coefficients $C^{j}_{n'' n' n}$ appearing in the factorization formula should be noted:

(i) The coefficients are symmetric in all lower indices

$$C^{j}_{n' n'' n} = C^{j}_{n' n n''} = C^{j}_{n n'' n'} = \ldots \tag{13}$$

as is obvious from (10).

(ii) If one of the lower indices vanishes the coefficients are diagonal and equal to unity, e.g.

$$C^{j}_{n' n'' 0} = \delta_{n' n''}\,. \tag{14}$$

The factorization formula (9) reduces to an identity in this case.

(iii) Integrating the factorization relation (9) and using the orthogonality of the Wigner functions yields the normalization relation

$$\sum_{n'} C^{j}_{n' n'' n} = \sum_{n} C^{j}_{n' n'' n} = \sum_{n''} C^{j}_{n' n'' n} = 1\,. \tag{15}$$

(iv) As a consequence of symmetry and range (11) the $C^j_{n_1\,n_2\,n_3}$ vanish unless all indices satify the triangular rule

$$|n_i - n_j| \leqslant n_k \leqslant \min\,(n_i + n_j, 4j - n_i - n_j) \qquad i,j,k \in (1,2,3)\,. \tag{16}$$

(v) The coefficients have the additional symmetry

$$C^j_{n'\,n''\,n} = C^j_{2j-n'\;2j-n''\;n} \tag{17}$$

which follows directly from (10).

In the following we discuss two applications of the factorization formula (9). First the same relation has been derived for the probabilities $P_{n'n}$ for vibrational transition $n \to n'$ in a forced anharmonic (Morse) oscillator [6]

$$P_{n'n} = \sum_{n''} C^{(N)}_{n'n''n}\, P_{n''0} \tag{18}$$

which is treated in an algebraic model following Levine and Wulfmann [11]. In this model $N+1$ is the number of vibrational states of the anharmonic oscillator. The coefficients can be identified by $C^{(N)}_{n'n''n} = C^j_{n'n''n}$, with $N = 2j$ which is simply a consequence of the identical algebras underlying both cases.

Let us now consider the limit $j \to \infty$ and $\vartheta \to 0$, where $\varrho = 2j\tan^2(\vartheta/2)$ remains finite. Note that in the anharmonic oscillator reinterpretation this is the harmonic oscillator limit $N \to \infty$. In this limit we have [12, 13]

$$\lim_{j\to\infty} P^j_{n'\,n}(\vartheta) = \frac{n!}{n'!}\,\varrho^{n'-n}\,\mathrm{e}^{-\varrho}\,\left[L^{n'-n}_n(\varrho)\right]^2 \tag{19}$$

and the coefficients simplify to

$$\lim_{j\to\infty} C^j_{n'\,n''\,n} = (-1)^s \sum_i \binom{n''}{i-n'}\binom{n}{i-n''}\binom{n'}{i-n} \tag{20}$$

and the factorization formula

$$P_{n'n} = \sum_{n''} C_{n'n''n}\, P_{n''0} \tag{21}$$

for the forced harmonic oscillator [5, 6] is obtained. In this limit the properties (i)–(iii) remain valid for the coefficients $C_{n'\,n''\,n}$ in same form . Some simplifications of the other properties and a further relation are listed:

(iv′) For non-vanishing $C_{n_1\,n_2\,n_3}$ the inequality (iv) simplifies to the triangular rule

$$|n_i - n_j| \leqslant n_k \leqslant n_i + n_j \qquad i,j,k \in (1,2,3)\,. \tag{22}$$

(v′) The symmetry relation (v) is meaningless.

(vi′) The coefficients $C_{n'n''n}$ satisfy the additional sum rule†

$$\sum_{n''} n'' C_{n'n''n}$$

$$= \Bigg\{(-1)^{n'+n} \times \sum_k \binom{n'}{k-n} \sum_{n''} (-1)^{n''}(n''+1) \binom{n''}{k-n'} \binom{n}{k-n''}\Bigg\} - 1$$

$$= \Bigg\{(-1)^{n'+n} \times \sum_k (-1)^k (k-n'+1) \binom{n'}{k-n} \sum_\mu (-1)^\mu \binom{n}{\mu} \binom{k+1-\mu}{k+1-n'}\Bigg\} - 1$$

$$= \Bigg\{\sum_\kappa (-1)^{\kappa-1} \frac{(\kappa+n')(\kappa+n)}{(1-\kappa)!\,\kappa!}\Bigg\} - 1 = n' + n \qquad (23)$$

with $\mu = k - n''$ and $\kappa = k + 1 - (n' + n)$.

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† Equation (23) has been derived in [6, Appendix A], which contains, however, some misprints.