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ON GENERAL TRANSFORMATION BRACKETS FOR HARMONIC OSCILLATOR STATES

P. Kramer* †

Comisión Nacional de Energía Nuclear, México

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ABSTRACT: Certain reduced Wigner coefficients of the unitary group $\mathcal{U}(3)$ are explicitly obtained and used to derive the general transformation bracket for two-particle harmonic oscillator states in a closed form. The result admits a generalization to more than two particles.

1. INTRODUCTION

States of two particles moving in a common harmonic oscillator potential admit in a simple way a transformation to relative and center-of-mass coordinates. These transformations have found a great variety of applications in nuclear and atomic physics. The definition and recursive calculation of the corresponding transformation brackets was discussed by Moshinsky[1], tabulations are due to Brody and Moshinsky[2]. Later on these brackets were identified with representation matrix elements of finite SU(2) rotations by

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* Visiting professor of the International Atomic Energy Agency, Vienna.

† Permanent address: Institut fuer Theoretische Physik, Tuebingen, Germany.

Brody and Moshinsky[3] and by Kaufman and Noack[4]. Generalizations to arbitrary angles which arise for example for two particles of different mass have been discussed by Smirnov[5,6] and Gal[7].

In this paper we derive a closed expression for the general transformation bracket which is believed to be new, conceptually simple and capable of generalizations to states involving more than two particles. For the group theory and notation we refer to an article by Moshinsky and the present author[8].

2. STATES OF ONE AND TWO PARTICLES

The states of a single particle moving in an harmonic oscillator potential may be characterized by the total number of quanta N, the orbital angular momentum L with values $L = N, N-2, \ldots$ and its projection M. The number N replaces the usual quantum number $n = 1/2\,(N-L)$. On introducing the operators[8] (p. 346)

$$\eta_j = (2\hbar)^{-\frac{1}{2}} \left[(m\omega)^{\frac{1}{2}} x_j - i\,(m\omega)^{-\frac{1}{2}} p_j \right], \tag{1}$$

we may define the normalized polynomials[3]

$$P^N_{LM}(\eta) = A_{NL}(\eta \cdot \eta)^{\frac{1}{2}(N-L)}\, \mathcal{Y}_{LM}(\eta), \tag{2}$$

$$A_{NL} = (-)^{\frac{1}{2}(N-L)} \left[\frac{4\pi}{(N+L+1)!!\,(N-L)!!} \right]^{\frac{1}{2}} \tag{3}$$

with $\mathcal{Y}_{LM}$ being a solid spherical harmonic. The polynomial eq. (2) when applied to the ground state

$$|\,0> = \left(\frac{m\omega}{\hbar\pi} \right)^{3/4} \exp\left[-\frac{m\omega}{2\hbar} \sum_{j=1}^{3} (x_j)^2 \right], \tag{4}$$

generates a normalized state of one particle,

$$P^N_{LM}(\eta)\,|\,0> \; = \; <\mathbf{x}\,|\,NLM> . \tag{5}$$

Printers note: As no boldface η was available, an η without lower index is a vector whose components are η_1, η_2, η_3.

The hamiltonian of two particles in a common harmonic oscillator potential admits the unitary symmetry group $\boldsymbol{U}(6)$ acting on the six operators η_j^s, $s = 1, 2$, $j = 1, 2, 3$ (Ref. 8, p. 347). Choosing the subgroups $U(3) \oplus U(3)$ that act separately on the operators belonging to the first and second particle or, alternatively, choosing the direct product $\mathcal{U}(3) \times U(2)$ of unitary groups that act on the lower and upper indices of the operators respectively, one may define two different sets of two-particle states that transform irreducibly under $\boldsymbol{U}(6)$ and the corresponding subgroups. The normalized polynomial which corresponds to the first subgroup is clearly the product

$$P^{N_1}_{L_1 M_1}(\eta^1)\, P^{N_2}_{L_2 M_2}(\eta^2) \,. \tag{6}$$

The normalized polynomial for the second subgroup we denote by

$$P^{[h_1 h_2]\}}_{\Omega L M N_1 N_2}(\eta^1, \eta^2) \,. \tag{7}$$

It is of degree N_s in the components of η^s and characterized by the partition $[h_1 h_2]$ giving the irreducible representation of both $\mathcal{U}(3)$ and $U(2)$. The quantum numbers L and M denote the total orbital angular momentum and its component, and the quantum number Ω was introduced by Bargmann and Moshinsky[9]. The polynomials eq. (6) and (7) when applied to the product of the ground states for both particles generate normalized states of two particles with total number of quanta

$$N = N_1 + N_2 = h_1 + h_2 \,. \tag{8}$$

The polynomials in eq. (6) may be coupled with respect to their angular momenta and related to the polynomials eq. (7) by means of the reduced Wigner coefficients of the group $\mathcal{U}(3)$ with subgroup $\mathbb{O}^+(3)$ (Ref. 8, p. 390),

$$\left[P^{N_1}_{L_1}(\eta^1)\ P^{N_2}_{L_2}(\eta^2) \right]_{LM}$$

$$= \sum_{M_1 M_2} P^{N_1}_{L_1 M_1}(\eta^1)\ P^{N_2}_{L_2 M_2}(\eta^2) < L_1 M_1 L_2 M_2 \mid LM >$$

$$= \sum_{h_1 h_2 \Omega} P^{[h_1 h_2]}_{\Omega L M N_1 N_2}(\eta^1, \eta^2) \left\langle \begin{matrix} [h_1 h_2] \\ \Omega L \end{matrix} \middle| \begin{matrix} [N_1]\,[N_2] \\ L_1 \quad L_2 \end{matrix} \right\rangle . \quad (9)$$

We shall consider a special case of this polynomial identity. Putting $\eta^1 = \eta^2 = \eta$, the polynomial on the right-hand side depends on the single vector η and hence cannot carry a two-rowed partition of $\mathcal{U}(3)$. In this case the only contributions on the right-hand side have $h_2 = 0$, $h_1 = N = N_1 + N_2$, the quantum number Ω is redundant, and the remaining polynomial must be proportional to a one-particle polynomial of the type eq. (2),

$$P^{[N]}_{LMN_1 N_2}(\eta, \eta) = P^{N}_{LM}(\eta)\ B(N_1 N_2 N). \quad (10)$$

The coefficient $B(N_1 N_2 N)$ must be independent of L and M. Equation (9) then becomes

$$\left[P^{N_1}_{L_1}(\eta)\ P^{N_2}_{L_2}(\eta) \right]_{LM}$$

$$= P^{N}_{LM}(\eta)\ B(N_1 N_2 N) \left\langle \begin{matrix} [N] \\ L \end{matrix} \middle| \begin{matrix} [N_1]\,[N_2] \\ L_1 \quad L_2 \end{matrix} \right\rangle . \quad (11)$$

We insert the polynomial eq. (2) into this equation and use an expression for a coupled product of two solid spherical harmonics given by Moshinsky[1] to obtain

$$B(N_1 N_2 N) \left\langle \begin{array}{c|cc} [N] & [N_1] & [N_2] \\ L & L_1 & L_2 \end{array} \right\rangle$$

$$= A_{N_1 L_1} A_{N_2 L_2} A^{-1}_{NL} H(L_1 L_2 L) , \tag{12}$$

$$H(L_1 L_2 L) = \left[\frac{(2L_1 + 1)(2L_2 + 1)}{4\pi(2L + 1)} \right]^{\frac{1}{2}} \langle L_1 0 L_2 0 | L 0 \rangle \tag{13}$$

The Wigner coefficient of $\mathcal{O}^+(3)$ appearing in eq. (13) is given by Edmonds (Ref. 10 p. 50) in terms of powers of factorials. The coefficient $B(N_1 N_2 N)$ can be determined by noting that for $L = N$ there is only one reduced Wigner coefficient which may be chosen as one because of normalization,

$$\left\langle \begin{array}{c|cc} [N] & [N_1] & [N_2] \\ N & L_1 & L_2 \end{array} \right\rangle = \delta_{L_1 N_1} \delta_{L_2 N_2} \ . \tag{14}$$

Evaluating eq. (12) for this case gives

$$B(N_1 N_2 N) = \left[\frac{N!}{N_1 ! N_2 !} \right]^{\frac{1}{2}} \tag{15}$$

and for the reduced Wigner coefficient we finally obtain

$$\left\langle \begin{array}{c|cc} [N] & [N_1] & [N_2] \\ L & L_1 & L_2 \end{array} \right\rangle$$

$$= \left[\frac{N_1 ! N_2 !}{N!} \right]^{\frac{1}{2}} A_{N_1 L_1} A_{N_2 L_2} A^{-1}_{NL} H(L_1 L_2 L) . \tag{16}$$

The factors on the right-hand side of eq. (16) are determined by eqs. (3) and (13) as products of powers of factorials.

3. GENERAL TRANSFORMATION BRACKETS FOR TWO PARTICLES

By means of a 2 x 2 unitary matrix

$$\boldsymbol{u} = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \tag{17}$$

one may introduce the linear transformation

$$\begin{aligned} \eta^1 \to \overline{\eta}^1 &= \eta^1 u_{11} + \eta^2 u_{21} \\ \eta^2 \to \overline{\eta}^2 &= \eta^1 u_{12} + \eta^2 u_{22} \end{aligned} \tag{18}$$

The coefficients in the relation between the coupled polynomials eq. (6) in barred and unbarred operators we define as the general transformation brackets,

$$\begin{aligned} &\left[P^{N_1}_{L_1}(\eta^1 u_{11} + \eta^2 u_{21})\, P^{N_2}_{L_2}(\eta^1 u_{12} + \eta^2 u_{22}) \right]_{LM} \\ &= \sum_{\overline{N}_1 \overline{L}_1 \overline{N}_2 \overline{L}_2} \left\{ \left[P^{\overline{N}_1}_{\overline{L}_1}(\eta^1)\, P^{\overline{N}_2}_{\overline{L}_2}(\eta^2) \right]_{LM} \times \right. \\ &\qquad \left. \times \left\langle \overline{N}_1 \overline{L}_2 \overline{N}_2 \overline{L}_2 L \,\middle|\, R(\boldsymbol{u}) \,\middle|\, N_1 L_1 N_2 L_2 L \right\rangle \right\}. \end{aligned} \tag{19}$$

The general transformation bracket is independent of M (ref. 1) and is zero if $\overline{N}_1 + \overline{N}_2 \neq N_1 + N_2$. Of particular interest for physical applications is the case of an orthogonal matrix,

$$\boldsymbol{u} = \begin{pmatrix} \cos \tfrac{1}{2}\beta & -\sin \tfrac{1}{2}\beta \\ \sin \tfrac{1}{2}\beta & \cos \tfrac{1}{2}\beta \end{pmatrix}. \tag{20}$$

It has been considered by Gal[7] and reduces to the standard bracket defined by Moshinsky[1] on putting $\beta = \pi/2$.

The unitary matrix $\boldsymbol{u}$ is an element of the group $U(2)$ in the direct product $\mathfrak{U}(3) \times U(2)$. As the polynomials eq. (7) provide a basis for an irreducible representation of $U(2)$, they transform under the linear transformation eq. (18) according to the well-known representations of this group whose matrix elements we denote by

$$D^{[h_1 h_2]}_{\overline{N}_1 N_1}(\boldsymbol{u}) \;, \tag{21}$$

taking the degree in the first vector as the row index of the basis. Kaufman and Noack[4] used the relation eq. (9) to rewrite the general transformation bracket as

$$\left\langle \overline{N}_1 \overline{L}_1 \overline{N}_2 \overline{L}_2 L \,\middle|\, R(\boldsymbol{u}) \,\middle|\, N_1 L_1 N_2 L_2 L \right\rangle$$

$$= \sum_{h_1 h_2 \Omega} \left\langle \begin{matrix} [\overline{N}_1] & [\overline{N}_2] \\ \overline{L}_1 & \overline{L}_2 \end{matrix} \,\middle|\, \begin{matrix} [h_1 h_2] \\ \Omega L \end{matrix} \right\rangle D^{[h_1 h_2]}_{\overline{N}_1 N_1}(\boldsymbol{u}) \left\langle \begin{matrix} [h_1 h_2] \\ \Omega L \end{matrix} \,\middle|\, \begin{matrix} [N_1] & [N_2] \\ L_1 & L_2 \end{matrix} \right\rangle .$$

The general usefulness of this expression depends on a knowledge of the reduced Wigner coefficients of $\mathfrak{U}(3)$. As these coefficients are not available in closed form, we shall employ eq. (22) only for the special cases $N_2 = 0$ and $N_1 = 0$. In these cases the second reduced Wigner coefficient on the right-hand side of eq. (22) becomes

$$\delta_{h_1 N_1} \delta_{h_2 0} \delta_{L L_1} \tag{23a}$$

and

$$\delta_{h_1 N_2} \delta_{h_2 0} \delta_{L L_2} \tag{23b}$$

respectively with the consequence that the first reduced Wigner coefficient is of the special type obtained in eq. (15). For the representation matrix elements of $U(2)$ one easily derives

$$D^{[N_1]}_{\overline{N}_1 N_1}(\boldsymbol{u}) = \left[\frac{N_1!}{\overline{N}_1!\,\overline{N}_2!}\right]^{\frac{1}{2}} (u_{11})^{\overline{N}_1} (u_{21})^{\overline{N}_2} \tag{24a}$$

$$D^{[N_2]}_{\overline{N}_1 0}(\boldsymbol{u}) = \left[\frac{N_2!}{\overline{N}_1!\,\overline{N}_2!}\right]^{\frac{1}{2}} (u_{12})^{\overline{N}_1} (u_{22})^{\overline{N}_2} \tag{24b}$$

which leads after some changes of notation to the expressions

$$\begin{aligned} &P^{N_1}_{L_1 M_1}(\eta^1 u_{11} + \eta^2 u_{21}) \\ &= \sum_{N_{11} L_{11} N_{21} L_{21}} \Bigg\{ \left[P^{N_{11}}_{L_{11}}(\eta^1)\; P^{N_{21}}_{L_{21}}(\eta^2) \right]_{L_1 M_1} \\ &\qquad \left\langle \begin{matrix} [N_{11}] & [N_{21}] \\ L_{11} & L_{21} \end{matrix} \middle| \begin{matrix} [N_1] \\ L_1 \end{matrix} \right\rangle \left[\frac{N_1!}{N_{11}!\,N_{21}!}\right]^{\frac{1}{2}} (u_{11})^{N_{11}} (u_{21})^{N_{21}} \Bigg\} , \end{aligned} \tag{25a}$$

$$\begin{aligned} &P^{N_2}_{L_2 M_2}(\eta^1 u_{12} + \eta^2 u_{22}) \\ &= \sum_{N_{12} L_{12} N_{22} L_{22}} \Bigg\{ \left[P^{N_{12}}_{L_{12}}(\eta^1)\; P^{N_{22}}_{L_{22}}(\eta^2) \right]_{L_2 M_2} \\ &\qquad \left\langle \begin{matrix} [N_{12}] & [N_{22}] \\ L_{12} & L_{22} \end{matrix} \middle| \begin{matrix} [N_2] \\ L_2 \end{matrix} \right\rangle \left[\frac{N_2!}{N_{12}!\,N_{22}!}\right]^{\frac{1}{2}} (u_{12})^{N_{12}} (u_{22})^{N_{22}} \Bigg\} . \end{aligned} \tag{25b}$$

Now we may combine the expansions eqs. (25a) and (25b) and recouple the four angular momenta $L_{11}\, L_{12}\, L_{21}\, L_{22}$ according to

$$\left[\left[P^{N_{11}}_{L_{11}}(\eta^1)\; P^{N_{21}}_{L_{21}}(\eta^2)\right]_{L_1} \left[P^{N_{12}}_{L_{12}}(\eta^1)\; P^{N_{22}}_{L_{22}}(\eta^2)\right]_{L_2}\right]_{LM}$$

$$= \sum_{\overline{L}_1 \overline{L}_2} \left\{ \left[\left[P^{N_{11}}_{L_{11}}(\eta^1)\; P^{N_{12}}_{L_{12}}(\eta^1)\right]_{\overline{L}_1} \left[P^{N_{21}}_{L_{21}}(\eta^2)\; P^{N_{22}}_{L_{22}}(\eta^2)\right]_{\overline{L}_2}\right]_{LM} \right.$$

$$\left. \Big\langle (L_{11}L_{12})\, \overline{L}_1\, (L_{21}L_{22})\, \overline{L}_2 L \,\Big|\, (L_{11}L_{21})\, L_1\, (L_{12}L_{22})\, L_2 L \Big\rangle \right\} \tag{26}$$

where

$$\Big\langle (L_{11}L_{12})\, \overline{L}_1\, (L_{21}L_{22})\, \overline{L}_2 L \,\Big|\, (L_{11}L_{21})\, L_1\, (L_{12}L_{22})\, L_2 L \Big\rangle$$

$$= \left[(2\overline{L}_1 + 1)(2\overline{L}_2 + 1)(2L_1 + 1)(2L_2 + 1)\right]^{\frac{1}{2}} \begin{Bmatrix} L & L_1 & L_2 \\ \overline{L}_1 & L_{11} & L_{12} \\ \overline{L}_2 & L_{21} & L_{22} \end{Bmatrix} \tag{27}$$

is a standard recoupling coefficient of the rotation group (Ref. 10 p. 101). The coupled polynomials depending on the same vector on the right-hand side of eq. (26) may be simplified by use of eqs. (11) and (15). Coupling the left-hand polynomials of eqs. (25a) and (25b) to the angular momentum L, carrying out the expansion eq. (25), the recoupling eq. (26) and the simplifications just mentioned, one derives for the general transformation bracket the final result

$$\left\langle \overline{N}_1 \overline{L}_1 \overline{N}_2 \overline{L}_2 L \,\middle|\, R(u) \,\middle|\, N_1 L_1 N_2 L_2 L \right\rangle$$

$$= [\overline{N}_1 ! \overline{N}_2 ! N_1 ! N_2 !]^{\frac{1}{2}} \sum_{N_{11} N_{12} N_{21} N_{22}} [N_{11} ! N_{12} ! N_{21} ! N_{22} !]^{-1}$$

$$\cdot\ (u_{11})^{N_{11}} (u_{12})^{N_{12}} (u_{21})^{N_{21}} (u_{22})^{N_{22}}$$

$$\cdot \sum_{L_{11} L_{12} L_{21} L_{22}} \left\{ \left\langle \begin{matrix} [\overline{N}_1] \\ \overline{L}_1 \end{matrix} \middle| \begin{matrix} [N_{11}] & [N_{12}] \\ L_{11} & L_{12} \end{matrix} \right\rangle \left\langle \begin{matrix} [\overline{N}_2] \\ \overline{L}_2 \end{matrix} \middle| \begin{matrix} [N_{21}] & [N_{22}] \\ L_{21} & L_{22} \end{matrix} \right\rangle \right.$$

$$\left\langle \begin{matrix} [N_{11}] & [N_{21}] \\ L_{11} & L_{21} \end{matrix} \middle| \begin{matrix} [N_1] \\ L_1 \end{matrix} \right\rangle \left\langle \begin{matrix} [N_{12}] & [N_{22}] \\ L_{12} & L_{22} \end{matrix} \middle| \begin{matrix} [N_2] \\ L_2 \end{matrix} \right\rangle$$

$$\left. \left\langle (L_{11} L_{12}) \overline{L}_1 (L_{21} L_{22}) \overline{L}_2 L \,\middle|\, (L_{11} L_{21}) L_1 (L_{12} L_{22}) L_2 L \right\rangle \right\} . \qquad (28)$$

The first sum is restricted by the equalities $N_{11} + N_{12} = \overline{N}_1$, $N_{21} + N_{22} = \overline{N}_2$, $N_{11} + N_{21} = N_1$ and $N_{12} + N_{22} = N_2$.

The reduced Wigner coefficients appearing in eq. (28) are real and given by eq. (16). Equation (28) gives the transformation bracket as a polynomial in the matrix elements u_{st}. Once the coefficients of this polynomial have been calculated for a given choice of $\overline{N}_1 \overline{L}_1 \overline{N}_2 \overline{L}_2 N_1 L_1 N_2 L_2 L$, the transformation bracket is easily determined for all values of these matrix elements.

4. GENERALIZATION TO MORE PARTICLES

The result of the last section admits a generalization to more than two particles. First of all this requires the choice of a coupling scheme. Then each polynomial factor may be expanded in analogy to eq. (25) by means of products of the reduced Wigner coefficients eq. (15). For successive coupling of k particles, this expansion is easily determined as

$$P^{N_s}_{L_s M_s}(\eta^1 u_{1s} + \eta^2 u_{2s} + \eta^3 u_{3s} + \ldots + \eta^k u_{ks})$$

$$= \sum_{N_{1\ldots i,s} L_{1\ldots i,s}} \Bigg\{ \Bigg[\cdot\cdot \Bigg[\Bigg[P^{N_{1s}}_{L_{1s}}(\eta^1)\, P^{N_{2s}}_{L_{2s}}(\eta^2) \Bigg]_{L_{12,s}} P^{N_{3s}}_{L_{3s}}(\eta^3) \Bigg]_{L_{123,s}} \ldots P^{N_{ks}}_{L_{ks}}(\eta^k) \Bigg]_{L_s M_s}$$

$$\left\langle \begin{matrix} [N_{1s}]\,[N_{2s}] \\ L_{1s} \quad L_{2s} \end{matrix} \middle| \begin{matrix} [N_{12,s}] \\ L_{12,s} \end{matrix} \right\rangle \left\langle \begin{matrix} [N_{12,s}]\,[N_{3s}] \\ L_{12,s} \quad L_{3s} \end{matrix} \middle| \begin{matrix} [N_{123,s}] \\ L_{123,s} \end{matrix} \right\rangle \cdot\cdot$$

$$\left\langle \begin{matrix} [N_{1\ldots k-1,s}]\,[N_{ks}] \\ L_{1\ldots k-1,s} \quad L_{ks} \end{matrix} \middle| \begin{matrix} N_s \\ L_s \end{matrix} \right\rangle \left[\frac{N_s!}{N_{1s}!\,N_{2s}!\,N_{3s}!\ldots N_{ks}!} \right]^{\frac{1}{2}}$$

$$(u_{1s})^{N_{1s}} (u_{2s})^{N_{2s}} (u_{3s})^{N_{3s}} \ldots . (u_{ks})^{N_{ks}} \Bigg\} \tag{29}$$

with $L_{12,s}\, L_{123,s} \ldots L_s$ being the intermediate angular momenta and

$$N_{1\ldots i,s} = N_{1\ldots i-1,s} + N_{i,s}\;. \tag{30}$$

In the next step one may couple successively the left-hand sides of eq. (29) for $s = 1 \ldots k$, carry out the expansions and recouple in such a way that all polynomials depending on the same vector are coupled. Again this can be simplified by repeated application of eqs. (11) and (15) which introduces a product of reduced Wigner coefficients and square roots of factorials. Clearly the final result of this general transformation is very similar to eq. (28) as it contains a number of reduced Wigner coefficients of $\mathcal{U}(3)$ along with a general recoupling coefficient of k^2 angular momenta.

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RESUMEN

Se obtienen explícitamente ciertos coeficientes de Wigner reducidos del grupo unitario $\mathcal{U}(3)$ y se usan para obtener en forma cerrada los paréntesis de transformación generales para estados de dos partículas en un oscilador armónico. El resultado se puede generalizar para más de dos partículas.