Talmi-Moshinsky Transformation for 2D Harmonic Oscillator Functions

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The Harmonic Oscillator Functions The harmonic oscillator (HO) functions are the eigenstate wave function of the Hamiltonian

$$H = \frac{1}{2m}\boldsymbol{p}^2 + \frac{1}{2}m\omega^2\boldsymbol{r}^2, \tag{1}$$

where $\boldsymbol{r}$ and $\boldsymbol{p}$ are the coordinate and momentum operator, respectively, $[r_i, p_j] = i\delta_{ij}$. It is convenient to introduce a new parameter $b = \sqrt{m\omega}$ (here we take $\hbar = c = 1$), called the basis energy scale. $\ell = b^{-1}$ is called the natural length of the HO functions.

In the momentum representation, the eigenstate wavefunctions read,

$$\psi_n^m(\boldsymbol{p}) \equiv b^{-1}\sqrt{\frac{4\pi n!}{(n+|m|)!}}\rho^{|m|}e^{-\frac{1}{2}\rho^2}L_n^{|m|}(\rho^2)e^{im\theta}, \tag{2}$$

where $\rho = |\boldsymbol{p}|/b$, $\theta = \arg\boldsymbol{p}$, $L_n^\alpha(x)$ are the generalized Laguerre polynomials. This definition of the HO functions satisfies the orthonormality relations:

$$\int \frac{\mathrm{d}^2\boldsymbol{p}}{(2\pi)^2}\psi_n^{m*}(\boldsymbol{p})\psi_{n'}^{m'}(\boldsymbol{p}) = \delta_{nn'}\delta_{mm'}, \tag{3}$$

$$\sum_{n=0}^{+\infty}\sum_{m=-n}^{n}\psi_n^m(\boldsymbol{p})\psi_n^m(\boldsymbol{p}') = (2\pi)^2\delta^{(2)}(\boldsymbol{p}-\boldsymbol{p}'). \tag{4}$$

The Jacobi Variables Consider a two-body system. Let $\boldsymbol{p}_1$, $\boldsymbol{p}_2$ be the momentum of the two particles respectively, and m_1 and m_2 be the mass of the two particles respectively. The total momentum $\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$. The relative momentum is $\boldsymbol{p} = \frac{m_2}{m_1+m_2}\boldsymbol{p}_1 - \frac{m_1}{m_1+m_2}\boldsymbol{p}_2$. The total mass $M = m_1 + m_2$. The

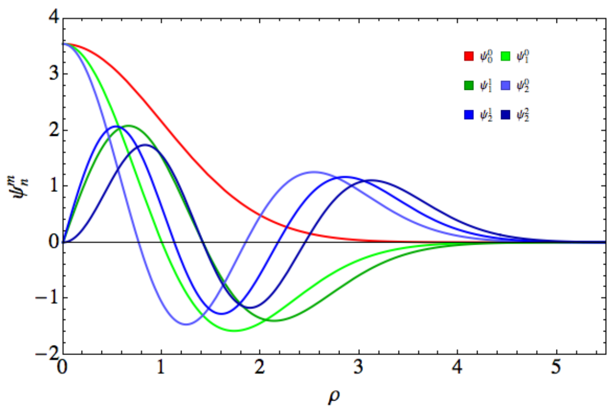


Figure 1: The first few HO functions ($\theta = 0$)

n_1, m_1, n_2, m_2	0,0,0,0	0,-1,0,0	0,0,0,-1	0,1,0,0	0,0,0,1
0,0,0,0	1				
0,-1,0,0		$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$		
0,0,0,-1		$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$		
0,1,0,0				$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
0,0,0,1				$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$

Table 1: The first few TMCs

reduced mass $m = \frac{m_1 m_2}{m_1+m_2}$. Similarly, the center-of-mass coordinate is $\boldsymbol{R} = \frac{m_1}{m_1+m_2}\boldsymbol{r}_1 + \frac{m_2}{m_1+m_2}\boldsymbol{r}_2$. The relative coordinate is $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. It is easy to see $[R_i, P_j] = i\delta_{ij}$ and $[r_i, p_j] = i\delta_{ij}$, $[R_i, p_j] = [r_i, P_j] = 0$, i.e. $\boldsymbol{R}$ is conjugate to $\boldsymbol{P}$ and $\boldsymbol{r}$ to $\boldsymbol{p}$. The procedure can be generalized to the n-body system. The resulted coordinates and momenta are called the Jacobi variables.

The generating Hamiltonian of the two particle system

$$H = \frac{1}{2m_1}\boldsymbol{p}_1^2 + \frac{1}{2}m_1\omega^2\boldsymbol{r}_1^2 + \frac{1}{2m_2}\boldsymbol{p}_2^2 + \frac{1}{2}m_2\omega^2\boldsymbol{r}_2^2, \tag{5}$$

can be expressed in terms of the Jacobi variables,

$$H = \frac{1}{2M}\boldsymbol{P}^2 + \frac{1}{2}M\omega^2\boldsymbol{R}^2 + \frac{1}{2m}\boldsymbol{p}^2 + \frac{1}{2}m\omega^2\boldsymbol{r}^2. \tag{6}$$

The resulted Hamiltonian is two HOs in Jacobi variables, which means the subspaces spanned by the single-particle states are exactly the same as the subspaces spanned by the Jacobi variables. Therefore, the single-particle wave functions can be written as the superposition of the wavefunctions in the Jacobi variables. For the two-body case, we have (Talmi-Moshinsky transformation):

$$\psi_{n_1}^{m_1}(\boldsymbol{p}_1)\psi_{n_2}^{m_2}(\boldsymbol{p}_2) = \sum_{NMnm} C(n_1, m_1, n_2, m_2; N, M, n, m; b_2/b_1)\psi_N^M(\boldsymbol{P})\psi_n^m(\boldsymbol{p}), \tag{7}$$

$$\psi_N^M(\boldsymbol{P})\psi_n^m(\boldsymbol{p}) = \sum_{n_1 m_1 n_2 m_2} C'(N, M, n, m; n_1, m_1, n_2, m_2; b_2/b_1)\psi_{n_1}^{m_1}(\boldsymbol{p}_1)\psi_{n_2}^{m_2}(\boldsymbol{p}_2). \tag{8}$$

The coefficients C and C' are called the Talmi-Moshinsky coefficients (TMCs). Applying Eq. (3),

$$C(n_1, m_1, n_2, m_2; N, M, n, m; b_2/b_1) = \int \frac{\mathrm{d}^2\boldsymbol{p}_1}{(2\pi)^2}\int \frac{\mathrm{d}^2\boldsymbol{p}_2}{(2\pi)^2}\psi_N^{M*}(\boldsymbol{p}_1)\psi_n^{m*}(\boldsymbol{p})\psi_{n_1}^{m_1}(\boldsymbol{p}_1)\psi_{n_2}^{m_2}(\boldsymbol{p}_2) \tag{9}$$

$$C'(n_1, m_1, n_2, m_2; N, M, n, m; b_2/b_1) = \int \frac{\mathrm{d}^2\boldsymbol{p}_1}{(2\pi)^2}\int \frac{\mathrm{d}^2\boldsymbol{p}_2}{(2\pi)^2}\psi_{n_1}^{m_1 *}(\boldsymbol{p}_1)\psi_{n_2}^{m_2 *}(\boldsymbol{p}_2)\psi_N^M(\boldsymbol{p}_1)\psi_n^m(\boldsymbol{p}). \tag{10}$$

It is easy to see,

$$C'(N, M, n, m; n_1, m_1, n_2, m_2; \gamma) = C^*(n_1, m_1, n_2, m_2; N, M, n, m; \gamma). \tag{11}$$

Applying Eq. (3) again,

$$\sum_{NMnm} C^*(n_1, m_1, n_2, m_2; N, M, n, m; \gamma)C(n_1', m_1', n_2', m_2'; N, M, n, m; \gamma) = \delta_{n_1 n_1'}\delta_{m_1 m_1'}\delta_{n_2 n_2'}\delta_{m_2 m_2'}. \tag{12}$$

As the eigen-subspaces can be identified by HO energy $E = \sum_i (2n_i + |m_i| + 1)$ and the magnetic projection $m_J = \sum_i m_i$, $C(n_1, m_1, n_2, m_2; N, M, n, m; \gamma) \propto \delta_{2n_1+|m_1|+2n_2+|m_2|, 2N+|M|+2n+|m|}\delta_{m_1+m_2, M+m}$.

Compute TMCs Let $\bar{\boldsymbol{p}} \equiv \boldsymbol{p}/b$. The exponential generating function of the HO functions $\psi_n^m(\boldsymbol{p})$ is,

$$e^{-\frac{1}{2}\bar{\boldsymbol{p}}^2 + 2\bar{\boldsymbol{p}}\cdot\bar{\boldsymbol{q}} - \bar{\boldsymbol{q}}^2} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{(-1)^n\psi_n^m(\boldsymbol{p})}{\sqrt{4\pi(n+|m|)!n!}}e^{-\mathrm{i}m\phi}\bar{q}^{2n+|m|} \tag{13}$$

where, $\boldsymbol{q}$ is some 2D momentum vector, $\bar{\boldsymbol{q}} = \boldsymbol{q}/b$, $\bar{q} = |\boldsymbol{q}|/b, \phi = \arg \bar{\boldsymbol{q}}$. To prove this relation, we can use the modified Bessel function I_n as a bridge. The series representation of $I_n(z)$ reads [1],

$$e^{z\cos\theta} = \sum_{m=-\infty}^{+\infty} I_m(z) e^{im\theta}. \tag{14}$$

Bessel function J_n is the generating function for the Laguerre polynomial:

$$J_m(2xz) = (xz)^m \, e^{-z^2} \sum_{n=0}^{\infty} \frac{L_n^m(x^2)}{(n+m)!} z^{2n}, \ (n, m \in \mathbb{Z}) \tag{15}$$

Note that $I_n(z) = i^{-n} J_n(iz)$. The above equation can be rewritten as,

$$I_m(2xz) = (xz)^m \, e^{z^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+m)!} L_n^m(x^2) z^{2n}, \ (n, m \in \mathbb{Z}) \tag{16}$$

Combine Eq. (14), Eq. (16) and Eq. (2), Eq. (13) can be easily shown.

Let $\boldsymbol{Q}$ and $\boldsymbol{q}$ be the total and relative momentum for $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Define $\bar{\boldsymbol{p}}_i = \boldsymbol{p}_i/b_i$, $\bar{\boldsymbol{q}}_i = \boldsymbol{q}_i/b_i, \bar{\boldsymbol{P}} = \boldsymbol{P}/B, \bar{\boldsymbol{p}} = \boldsymbol{p}/b, \bar{\boldsymbol{Q}} = \boldsymbol{Q}/B, \bar{\boldsymbol{q}} = \boldsymbol{q}/b$. It is convenient to introduce a phase factor $\delta = \arctan(b_2/b_1)$. Then the relation between the Jacobi variables and the single-particle variables are:

$$\begin{aligned} \bar{\boldsymbol{P}} &= \cos\delta \ \bar{\boldsymbol{p}}_1 + \sin\delta \ \bar{\boldsymbol{p}}_2, \quad \bar{\boldsymbol{p}} = \sin\delta \ \bar{\boldsymbol{p}}_1 - \cos\delta \ \bar{\boldsymbol{p}}_2, \\ \bar{\boldsymbol{Q}} &= \cos\delta \ \bar{\boldsymbol{q}}_1 + \sin\delta \ \bar{\boldsymbol{q}}_2, \quad \bar{\boldsymbol{q}} = \sin\delta \ \bar{\boldsymbol{q}}_1 - \cos\delta \ \bar{\boldsymbol{q}}_2. \end{aligned} \tag{17}$$

Then there holds the identity,

$$\tfrac{1}{2}\bar{\boldsymbol{p}}_1^2 - 2\bar{\boldsymbol{p}}_1 \cdot \bar{\boldsymbol{q}}_1 + \bar{\boldsymbol{q}}_1^2 + \tfrac{1}{2}\bar{\boldsymbol{p}}_2^2 - 2\bar{\boldsymbol{p}}_2 \cdot \bar{\boldsymbol{q}}_2 + \bar{\boldsymbol{q}}_2^2 = \tfrac{1}{2}\bar{\boldsymbol{P}}^2 - 2\bar{\boldsymbol{P}} \cdot \bar{\boldsymbol{Q}} + \bar{\boldsymbol{Q}}^2 + \tfrac{1}{2}\bar{\boldsymbol{p}}^2 - 2\bar{\boldsymbol{p}} \cdot \bar{\boldsymbol{q}} + \bar{\boldsymbol{q}}^2. \tag{18}$$

Therefore,

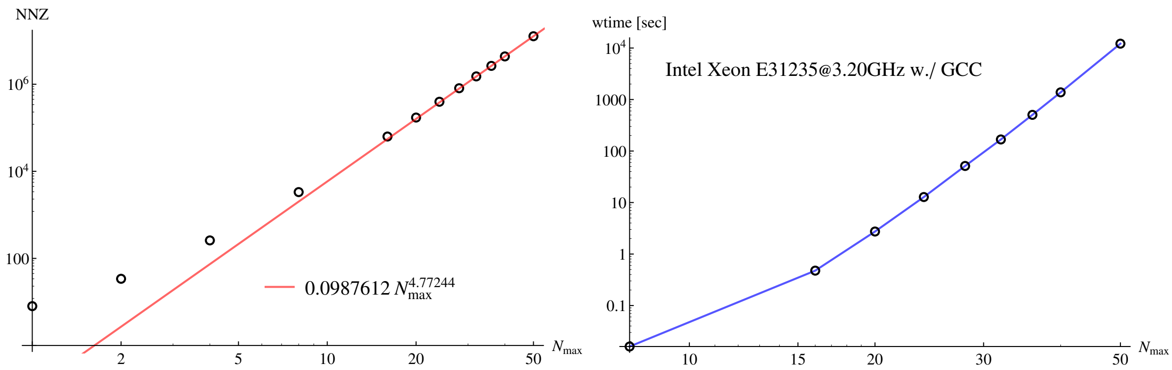
$$\begin{aligned} &\sum_{n_1,m_1,n_2,m_2} \frac{(-1)^{n_1+n_2}}{\sqrt{(n_1+|m_1|)!n_1!(n_2+|m_2|)!n_2!}} \Psi_{n_1}^{m_1}(\boldsymbol{p_1}) \Psi_{n_2}^{m_2}(\boldsymbol{p_2}) e^{-\mathrm{i}m_1\phi_1 - \mathrm{i}m_2\phi_2} \bar{q}_1^{2n_1+|m_1|} \bar{q}_2^{2n_2+|m_2|} \\ = &\sum_{N,M,n,m} \frac{(-1)^{N+n}}{\sqrt{(N+|M|)!N!(n+|m|)!n!}} \Psi_N^M(\boldsymbol{P}) \Psi_n^m(\boldsymbol{p}) e^{-\mathrm{i}M\Phi - \mathrm{i}m\phi} \bar{Q}^{2N+|M|} \bar{q}^{2n+|m|} \end{aligned}$$

Apparently, $\bar{Q}, \bar{q}$ are polynomials of $\bar{q}_1, \bar{q}_2$. And the phases can also be expressed as polynomials of $e^{i\phi_1}$ and $e^{i\phi_2}$, $\bar{Q}e^{-im\Phi} = (\cos\delta \ \bar{q}_1 e^{-i\phi_1} + \sin\delta \ \bar{q}_2 e^{-i\phi_2})^m$, and $\bar{q}e^{-im\phi} = (\sin\delta \ \bar{q}_1 e^{-i\phi_1} - \cos\delta \ \bar{q}_2 e^{-i\phi_2})^m$. Therefore, we can expand right-hand side in terms of $q_1, q_2, e^{\mathrm{i}\phi_1}, e^{\mathrm{i}\phi_2}$, and identify each term on the left-hand side. Then we get,

$$\begin{aligned} C(N, M, n, m; n_1, m_1, n_2, m_2, \tan\delta) &= \delta_{2n_1+|m_1|+2n_2+|m_2|, 2N+|M|+2n+|m|} \delta_{m_1+m_2, M+m} \\ \times (-1)^{N+n+n_1+n_2} (\sin\delta)^{2n_2+|m_2|} &(\cos\delta)^{2n_1+|m_1|} \sqrt{\frac{n_1!n_2!(n_1+|m_1|)!(n_2+|m_2|)!}{N!n!(N+|M|)!(n+|m|)!}} \sum_{\alpha,\beta,\gamma,\lambda,\sigma} \\ (-1)^{\sigma+\frac{1}{2}(|m|-\alpha)} (\tan\delta)^{\alpha+2\rho} &\binom{N}{\frac{N-\lambda+\gamma}{2}, \frac{N-\lambda-\gamma}{2}, \lambda} \binom{n}{\frac{n-\sigma+\rho}{2}, \frac{n-\sigma-\rho}{2}, \sigma} \binom{|M|}{\frac{|M|+\beta}{2}} \binom{|m|}{\frac{|m|+\alpha}{2}} \binom{\sigma+\lambda}{\frac{s}{4}} \end{aligned} \tag{19}$$

where $\rho = n_1 - n_2 - \gamma + \frac{1}{2}(|m_1| - |m_2| - \alpha - \beta)$, $s = 2(\sigma+\lambda) + \mathrm{sgn}(m)\alpha + \mathrm{sgn}(M)\beta + m_2 - m_1$. The summation is restricted by requiring all arguments in the multinomial coefficients being non-negative integers.

FORTRAN subroutine `double precision function TMC(nn, mm, n, m, n1, m1, n2, m2, r)` computes TMC $C(nn, mm, n, m; n1, m1, n2, m2, r)$. The code has been tested for various $N_{\max} = 2n_1 + |m_1| + 2n_2 + |m_2|$.



(a) The number of nonzero TMCs as a function of $N_{\max}$ (b) The evaluation time as a function of $N_{\max}$

Figure 2: $r = 1$

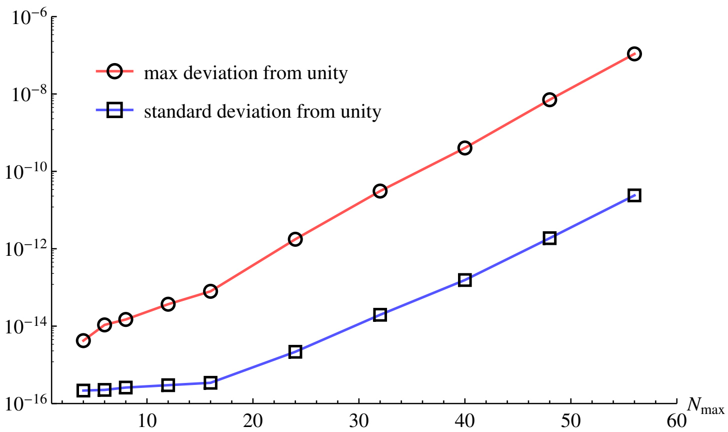


Figure 3: The standard and maximum derivation from unity for different $N_{\max}$ and $r = 1$. The intermediate numbers are represented in `double precision`.

Higher Dimensions The exponential generating function can be generalized to higher dimensional HO functions.

References

[1] M. Abramowitz and I. Stegun, eds. (1972), Handbook of Mathematical Functions, with Formulas, Graphs and Tables, **9.6**, p.376, New York: Dover Publication, ISBN 978-0-486-61272-0

[2] M. Abramowitz and I. Stegun, eds. (1972), Handbook of Mathematical Functions, with Formulas, Graphs and Tables, **22.9**, p.784, New York: Dover Publication, ISBN 978-0-486-61272-0