ABOUT SYMETRIES AND MICROSCOPIC ORIGIN OF THE NUCLEAR MEAN FIELD

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INTRODUCTION & SPIRIT OF THE PRESENTATION

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- ★ Also, in the spirit of

$$\textbf{Workshop} = \frac{\textbf{School+Conference}}{\textbf{2}}$$

we would like to re-investigate a certain number of "old" technical questions solved with an approach adapted to our needs

QUESTION* : *IS THERE A WAY TO INVESTIGATE SYSTEMATICALLY THE ALLOWED TWO-BODY INTERACTIONS ?

ANSWER* : *YES, USE THE SPIN-TENSOR DECOMPOSITION !

THE SPIN-TENSOR DECOMPOSITION

★ In the fermionic spin-1/2 space, any operator can be expressed with the help of $\boldsymbol{\sigma_0} \equiv \mathbb{I}$ and the Pauli matrices $\boldsymbol{\sigma_x}$, $\boldsymbol{\sigma_y}$ and $\boldsymbol{\sigma_z}$

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- ★ Therefore, the space of two nucleons can be described by a set of $\mathbf{4 \times 4 = 16}$ operators composed of the tensor product of the corresponding operators for each particle, as e.g. $\boldsymbol{\sigma_i^a \sigma_j^b}$, with $\boldsymbol{i = 0, 1, 2, 3}$ and $\boldsymbol{j = 0, 1, 2, 3}$

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- ★ We require the interaction to be independent of the interchange between the two particles, and therefore we use the **6 irreducible tensors** :

$$S_1^{(0)} = 1, \qquad S_2^{(2)} = [\vec{\sigma}^a \times \vec{\sigma}^b]^{(0)}, \qquad S_3^{(1)} = \vec{\sigma}^a + \vec{\sigma}^b$$

$$S_4^{(2)} = [\vec{\sigma}^a \times \vec{\sigma}^b]^{(2)}, \qquad S_5^{(1)} = [\vec{\sigma}^a \times \vec{\sigma}^b]^{(1)}, \qquad S_6^{(1)} = \vec{\sigma}^a - \vec{\sigma}^b$$

THE SPIN-TENSOR DECOMPOSITION

★ **Advantage** : These 6 tensors $S_\mu^{(k)}$ of rank k can immediately be coupled with a tensor operator of the same rank in configuration space $X_\mu^{(k)}$ to a scalar and the so obtained scalar functions finally summed to the **general scalar** (i.e. invariant with respect to spatial rotations) two-particle interaction ($P_{T=0}$ and $P_{T=1}$ are projectors on the states $T = 0$ and $T = 1$) :

$$V(a,b) = \sum_{\mu=1}^{6} \left\{ [X_\mu^{(k)} \times S_\mu^{(k)}]^{(0)} P_{T=0} + [Y_\mu^{(k)} \times S_\mu^{(k)}]^{(0)} P_{T=1} \right\}$$

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- ★ The combinations S_5, S_6 are **anti-symmetric** with respect to the interchange of the spins of the particles, and therefore the corresponding tensors X_5, X_6 and Y_5, Y_6 will have to be **anti-symmetric**

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★ However, this is true for the **free interaction**, but not really necessary in **effective interactions**. For a recent example, see the article on shell evolution and nuclear forces by N.A. Smirnova et al., Phys. Lett. **B686** (2010) 109

RECALLING THE HF EQUATIONS ...

... JUST TO FIX THE NOTATIONS

HARTREE-FOCK EQUATIONS

★ With the notations of second quantization, the many-body hamiltonian reads :

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | \hat{t} | \beta \rangle a^{\dagger}_{\alpha} a_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{V} | \gamma\delta \rangle a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{\gamma}$$

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★ Hartree-Fock potential :

$$\langle \alpha | \hat{U}_{HF} | \beta \rangle \equiv \sum_{\mu=1}^{A} \langle \alpha\mu | \hat{V} | \widetilde{\beta\mu} \rangle = \sum_{\mu=1}^{A} \left[\langle \alpha\mu | \hat{V} | \beta\mu \rangle - \langle \alpha\mu | \hat{V} | \mu\beta \rangle \right]$$

THE HF EQUATIONS IN MATRIX FORM

★ Introduce a single-particle basis $|i\rangle$, $|j\rangle$, $|k\rangle$, $|l\rangle$ ..., and the coefficients $C_i^\alpha \equiv \langle i|\alpha\rangle$.

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★ and where the **density matrix** is given by :

$$\rho_{lj} \equiv \sum_{\mu \text{ occ.}} C_j^{\mu *} C_l^\mu$$

NEXT STEP ...

... CALCULATING TWO-BODY MATRIX ELEMENTS

TWO-BODY MATRIX ELEMENTS

★ We want to calculate the two-body matrix elements of a **central interaction**

$$V_{n_1,n_2;m_1,m_2} = \langle n_{x_1} n_{y_1} n_{z_1}; n_{x_2} n_{y_2} n_{z_2} | V(|r_1 - r_2|) | m_{x_1} m_{y_1} m_{z_1}; m_{x_2} m_{y_2} m_{z_2} \rangle$$

where

$$\varphi_{n_\mu}(x_\mu) = \mathcal{N}_{n_\mu} e^{-\frac{\beta_\mu^2 {x_\mu}^2}{2}} H_{n_\mu}(\beta_\mu x_\mu) = \beta_\mu^{1/2} e^{-\xi_\mu^2/2} H_{n_\mu}^{(0)}(\xi_\mu)$$

and the normalization constant

$$\mathcal{N}_{n_\mu} = \frac{\sqrt{\beta_\mu}}{\sqrt{2^{n_\mu} n_\mu! \sqrt{\pi}}}$$

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- Explicitely :

$$E_{n_1,n_2;m_1,m_2} = \iint d^3\vec{r}_1 d^3\vec{r}_2 \; \varphi_{n_{x_1}}(x_1)\varphi_{n_{y_1}}(y_1)\varphi_{n_{z_1}}(z_1)\varphi_{n_{x_2}}(x_2)\varphi_{n_{y_2}}(y_2)\varphi_{n_{z_2}}(z_2)$$
$$V(r) \; \varphi_{m_{x_1}}(x_1)\varphi_{m_{y_1}}(y_1)\varphi_{m_{z_1}}(z_1)\varphi_{m_{x_2}}(x_2)\varphi_{m_{y_2}}(y_2)\varphi_{m_{z_2}}(z_2)$$

A FEW EXAMPLES

★ Probably one of the most succesfull approch to the evaluation of such two-body matrix elements is the **Gogny separation method**. For a recent extension to gaussian matrix elements in the cylindrical harmonic oscillator basis, see W. Younes, Comp. Phys. Comm. **180** (2009) 1013.

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- ★ For very exotic nuclear systems, approaching for instance the drip lines, one can select other basist states than the usual harmonic oscillator states. As an example, one can use the **Kamimura-Gauss** sets which are adapted to systems with slowly decreasing density distributions. See for example H. Nakada and M. Sato, Nucl. Phys. **A699** (2002) 511.

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- The fundamental importance of **Yukawa** type forces has been recognized very early in Nuclear Physics, but is also very important in other branches of Physics. Few examples are the **screened Thomas-Fermi** potential in solid-states physics, or the **Debye-Hückel** potential in plasma physics; S.L. Garavelli and F.A. Oliveira, Phys. Rev. Lett. **66** (1991) 1310. Theories of **quantum gravity** predict also the existence of graviphotons (spin 1) and graviscalars (spin 0) for which phenomenological descriptions with the help of the Yukawa potential is important; M.M. Nieto et al., Phys. Rev. **D36** (1987) 3688.

MULTIPOLE DECOMPOSITION OF THE YUKAWA INTERACTION

★ The **Yukawa multipole analysis** is based on the relation (M. Abramowitz and I. Stegun, Handbook of Mathematical Functions) :

$$\frac{e^{-|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = \frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)i_l(r_L)k_l(r_G)P_l(\cos\theta)$$

where the modified Bessel Functions of the first and third kinds read

$$i_l(r_L) = \frac{1}{2r}\sum_{k=0}^{l}\frac{\Gamma(l+k+1)}{\Gamma(k+1)\Gamma(n-k+1)}\frac{1}{(2r)^k}\Big[(-)^k e^{z} - (-)^l e^{-z}\Big]$$

and

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★ **But how about practical realizations : highest multiplole order ... ?**

WHY DO WE NOT BENEFIT FROM TECHNIQUES ...

... USED FOR ONE-BODY MATRIX ELEMENTS ?

A FIRST NAIVE IDEA

★ It is known that the **one-body** matrix elements of a potential $\boldsymbol{V}$, evaluated in the cartesian basis of the harmonic oscillator, can be calculated by **recurrence** (U. Götz et al., Nucl. Phys. **A175** (1971) 481).
Indeed, using the recursion formulae for the Hermite polynomials

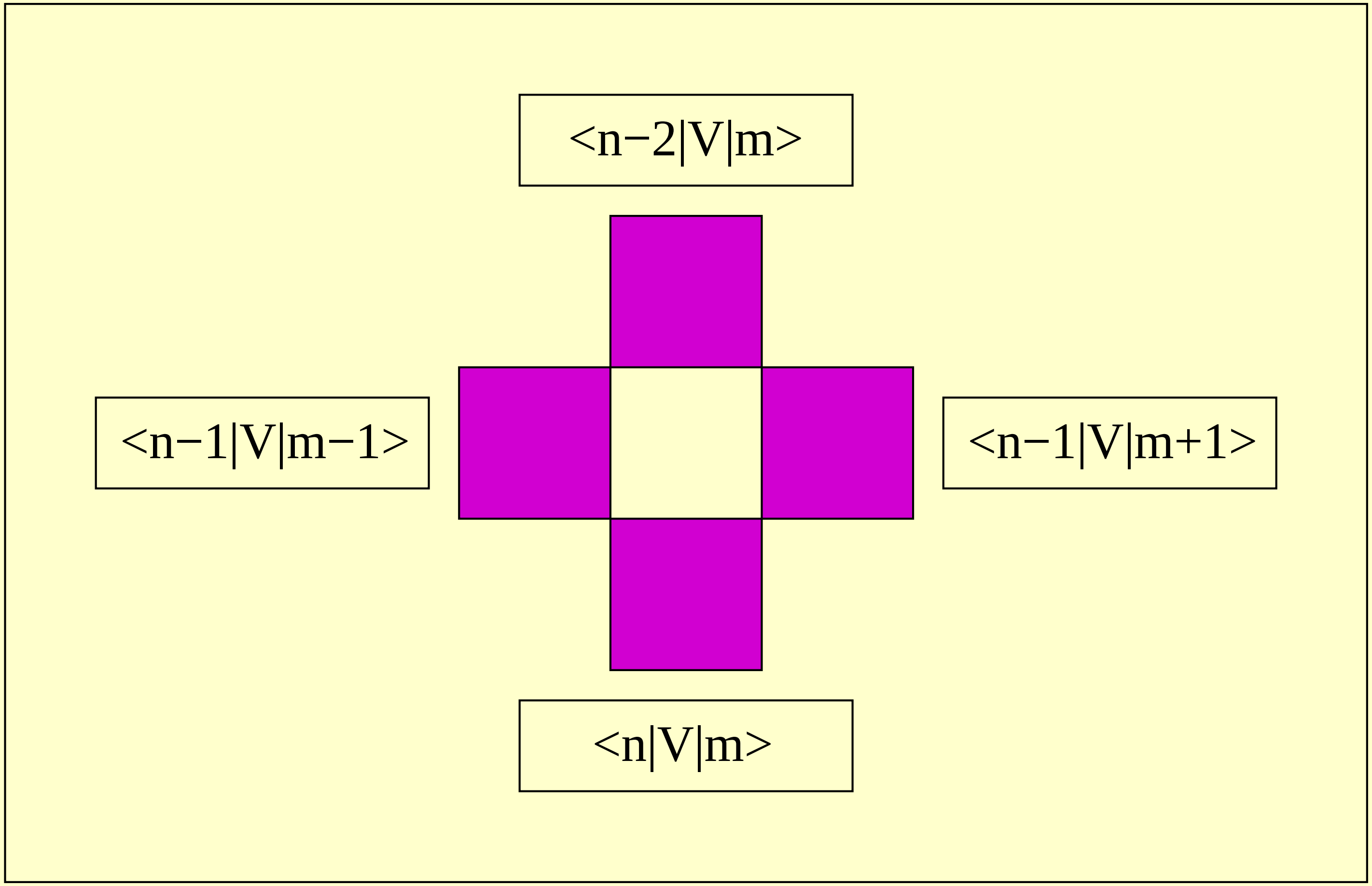
$$\boldsymbol{H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n\xi H_{n-1}(\xi)}$$

one shows easily that

$$\begin{aligned}
\langle n_x\ n_y\ n_z|V|m_x\ m_y\ m_z\rangle = &\quad \sqrt{\tfrac{m_x+1}{n_x}} \quad \langle n_x-1\ n_y\ n_z|V|m_x+1\ m_y\ m_z\rangle \\
+ &\quad \sqrt{\tfrac{m_x}{n_x}} \quad \langle n_x-1\ n_y\ n_z|V|m_x-1\ m_y\ m_z\rangle \\
- &\quad \sqrt{\tfrac{n_x-1}{n_x}} \quad \langle n_x-2\ n_y\ n_z|V|m_x\ m_y\ m_z\rangle
\end{aligned}$$

and with similar expressions in the "y" and "z" directions

★ One can illustrate this recursion relation schematically in the (n_x, m_x)-plane for fixed values of (n_y, n_z, m_y, m_z) :



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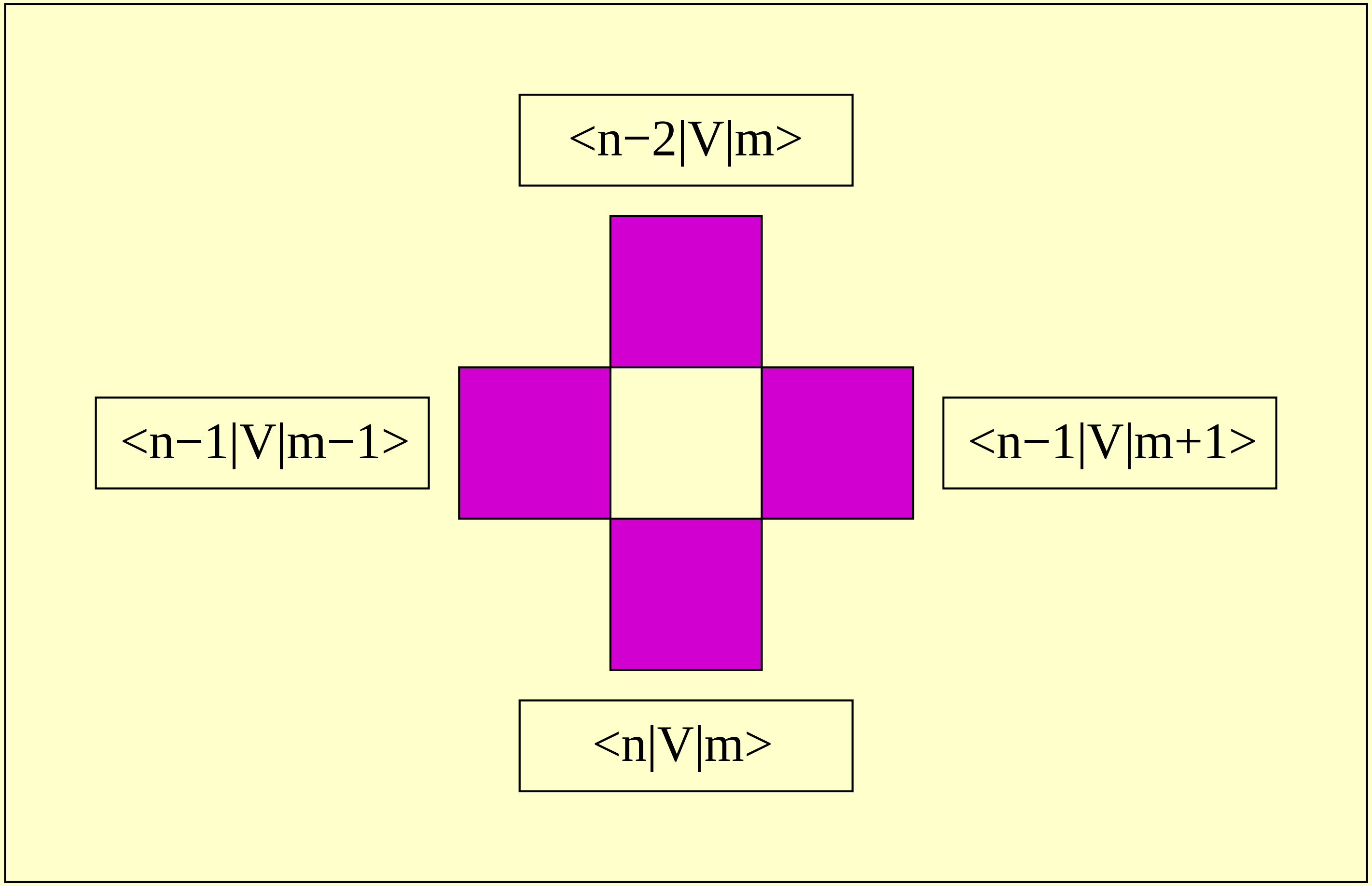

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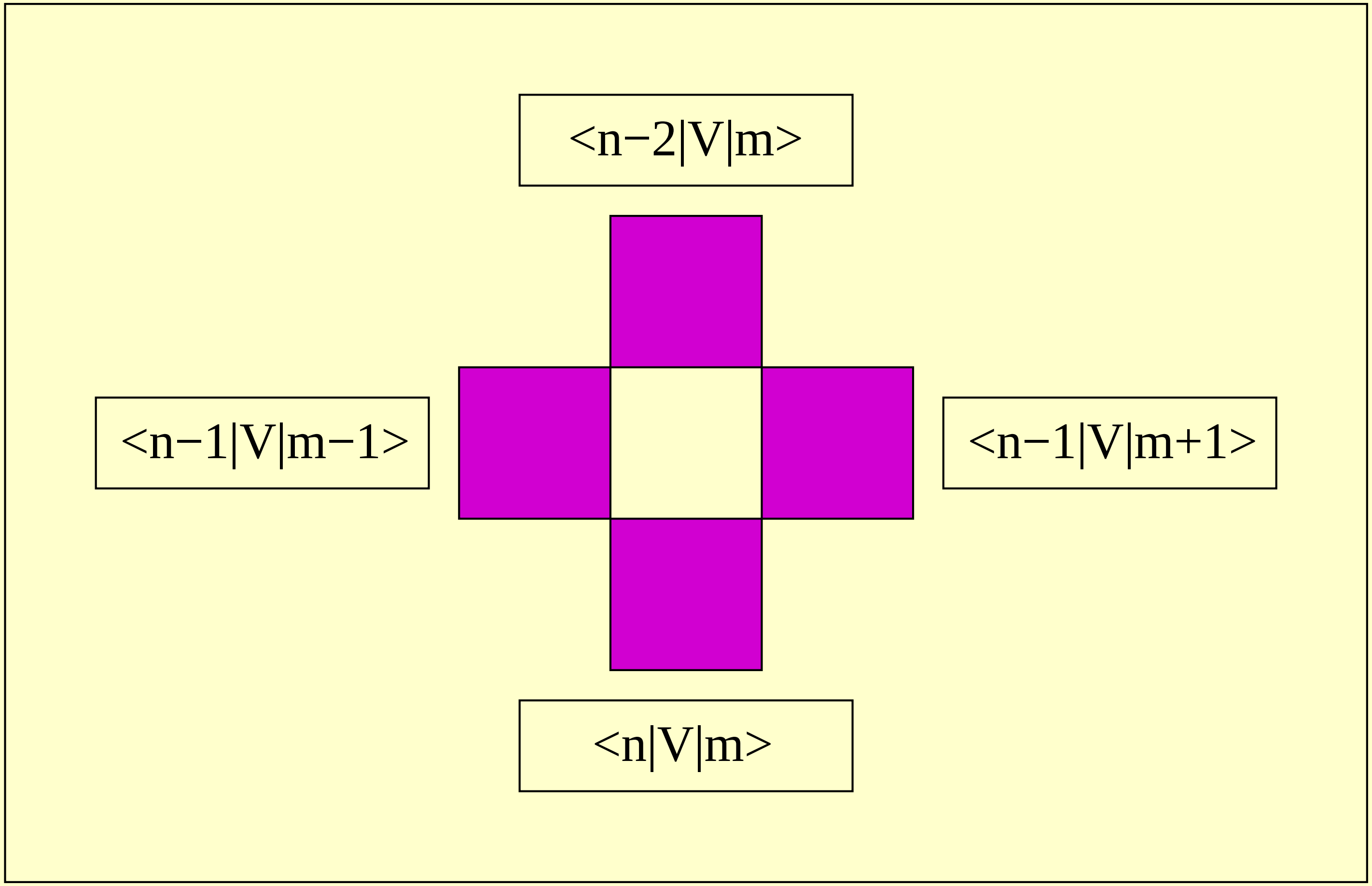

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★ Generalization to **two-body matrix elements** not straightforward

SO BACK TO BASICS ...

... THE MOSHINSKY TRANSFORMATION

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★ Consider the **products of harmonic oscillator wave functions** :

$$\varphi_{n_{x_1}}(x_1)\varphi_{n_{x_2}}(x_2) = \mathcal{N}_{n_{x_1}}\mathcal{N}_{n_{x_2}} e^{-\frac{\beta_x^2 {x_1}^2}{2}} e^{-\frac{\beta_x^2 {x_2}^2}{2}} H_{n_{x_1}}(\beta_x x_1) H_{n_{x_2}}(\beta_x x_2)$$
$$= \mathcal{N}_{n_{x_1}}\mathcal{N}_{n_{x_2}} e^{-\frac{\beta_x^2 X^2}{2}} e^{-\frac{\beta_x^2 x^2}{2}} H_{n_{x_1}}(\beta_x x_1) H_{n_{x_2}}(\beta_x x_2)$$

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★ Performing the **Moshinsky transformation** :

$$\vec{R} \equiv \frac{\vec{r}_1 + \vec{r}_2}{\sqrt{2}} \quad \text{and} \quad \vec{r} \equiv \frac{\vec{r}_1 - \vec{r}_2}{\sqrt{2}}$$

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★ We obtain :

$$\varphi_{n_{x_1}}(x_1)\varphi_{n_{x_2}}(x_2) = \varphi_{n_{x_1}}\Big(\frac{X + x}{\sqrt{2}}\Big)\varphi_{n_{x_2}}\Big(\frac{X - x}{\sqrt{2}}\Big)$$

$$= \mathcal{N}_{n_{x_1}}\mathcal{N}_{n_{x_2}} e^{-\frac{\beta_x^2 X^2}{2}} e^{-\frac{\beta_x^2 x^2}{2}} H_{n_{x_1}}\Big[\beta_x(\frac{X + x}{\sqrt{2}})\Big] H_{n_{x_2}}\Big[\beta_x(\frac{X - x}{\sqrt{2}})\Big]$$

★ This expression can further be transformed using :

$$H_n(a+b) = \sum_{k=0}^{n} \mathcal{C}_k^n H_k(a\sqrt{2}) H_{n-k}(b\sqrt{2})$$

where

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$$\left[H_{k_{x_1}}(\beta_x X) H_{k_{x_2}}(\beta_x X)\right]\left[H_{n_{x_1}-k_{x_1}}(\beta_x x) H_{n_{x_2}-k_{x_2}}(\beta_x x)\right]$$

OLD FRIENDS - PART 1 - ...

... THE TALMI-BRODY-MOSHINSKY (TBM) COEFFICIENTS !

TALMI-BRODY-MOSHINSKY (TBM) COEFFICIENTS

★ Now one can make use of the formula :

$$H_m^{(0)}(\xi) H_n^{(0)}(\xi) = \sum_{\mu=0}^{m+n} C_{mn}^{\mu}(00) H_\mu^{(0)}(\xi)$$

TALMI-BRODY-MOSHINSKY (TBM) COEFFICIENTS

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- Where the **Talmi-Brody-Moshinsky** coefficients are given by :

$$M_{n_{x_1}n_{x_2}}^{(N_X)n_x} = \delta_{n_{x_1}+n_{x_2},N_X+n_x}\,\beta_x\,\mathcal{N}_{n_{x_1}}\mathcal{N}_{n_{x_2}}$$

$$\times\sum_{k_{x_1}=0}^{n_{x_1}}\sum_{k_{x_2}=0}^{n_{x_2}}\delta_{N_X,k_{x_1}+k_{x_2}}(-)^{(n_{x_2}-k_{x_2})}\frac{c_{k_{x_1}}^{n_{x_1}}c_{k_{x_2}}^{n_{x_2}}\,C_{k_{x_1}k_{x_2}}^{N_X}(00)C_{n_{x_1}-k_{x_1},n_{x_2}-k_{x_2}}^{n_x}(00)}{\mathcal{N}_{k_{x_1}}\mathcal{N}_{k_{x_2}}\mathcal{N}_{n_{x_1}-k_{x_1}}\mathcal{N}_{n_{x_2}-k_{x_2}}}$$

COMPACT FORM OF THE TBM COEFFICIENTS

★ Using the following decomposition (see e.g. M. Girod and B. Grammaticos, Phys. Rev. C27 (1983) 2317 or W. Younes, Comp. Phys. Comm. 180 (2009) 1013) :

$$\varphi_m(x)\varphi_n(x) = e^{-\xi^2/2} \sum_{\mu=|m-n|,2}^{m+n} \mathcal{N}_\mu I^\mu_{mn} \varphi_\mu(x),$$

where

$$I^\mu_{mn} = \frac{\mu!(n_m!n_n!2^\mu)^{1/2}}{(\frac{n_m-n_n+\mu}{2})!(\frac{n_n-n_m+\mu}{2})!(\frac{n_m+n_n-\mu}{2})!}$$

one gets the more **compact form** :

$$M^{(N)n}_{n_1 n_2} = \delta_{n_1+n_2,N+n} \frac{1}{\sqrt{2^{n_1+n_2}}} \sqrt{\frac{n_1!n_2!}{N!n!}} \sum_k (-)^{(n-n_1+k)} \binom{N}{k} \binom{n}{n_1-k}$$

(see for example Y.F. Smirnov, Nucl. Phys. **39** (1962) 346, or R.R. Chasman and S. Wahlborn Nucl. Phys. **A90** (1967) 401, or more recently L. Robledo, Phys. Rev. C **81**, 044312 (2010) , who uses the properties of the harmonic oscillator generating function).

BACK TO THE TWO-BODY MATRIX ELEMENTS

★ We obtain the final expression for the central interaction

$$E_{n_1,n_2;m_1,m_2} = \sum_{n_x,n_y,n_z} \mathcal{D}^{n_1,n_2;m_1,m_2}_{n_x n_y n_z;m_x m_y m_z} \langle n_x n_y n_z | V(\sqrt{2}r) | m_x m_y m_z \rangle$$

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- ★ Note that, because of **orthonormality conditions**, one has $M_X = N_X$, $M_Y = N_Y$ and $M_Z = N_Z$.

- ★ Note also that, because of **energy conservation**, one has $n_{x_1} + n_{x_2} = N_X + n_x$. Thus, the sum over m_x, m_y and m_z disappears.

OLD FRIENDS - PART 2 - ...

... THE SMIRNOV BRACKETS !

USE OF SMIRNOV BRACKETS

★ We are lead to the evaluation of the cartesian matrix elements :

$$\langle n_x n_y n_z | V(\sqrt{2}r) | m_x m_y m_z \rangle = \sum_{nlm} \sum_{n'l'm'} \langle n_x n_y n_z | nlm \rangle \langle nlm | V(\sqrt{2}r) | n'l'm' \rangle \langle n'l'm' | m_x m_y m_z \rangle$$

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★ One has explicitely to calculate

$$\langle nlm | V(\sqrt{2} r) | n'l'm' \rangle = \delta_{ll'} \delta_{mm'} \int_0^\infty R_{nl}(r) V(\sqrt{2} r) R_{n'l}(r) dr$$

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  which are evaluated numerically via **Gauss-Laguerre quadrature**.

- Alternative suggestions may occur, as for instance the one proposed recently by L. Robledo, Phys. Rev. C **81**, 044312 (2010), who calculates **approximately** the matrix elements in the cartesian basis with the help of the theorem of **spectral decomposition** :

$$\langle n_x n_y n_z | V(\sqrt{2}r) | m_x m_y m_z \rangle \approx \sum_{L=0}^{L_C} D^*_{n_x,n_y,n_z} v_L D_{m_x,m_y,m_z}$$

FORMULAE FOR SMIRNOV COEFFICIENTS

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★ For direct numerical applications one can utilize the transformation brackets given explicitly by K.T.R. Davies and S.J. Krieger, Can. J. Phys. **69** (1991) 62 :

$$\langle nlm|n_x n_y n_z\rangle = \delta_{2n+l,n_x+n_y+n_z}(-)^{(2n+n_x+n_y-m)/2}\; i^{n_y}$$

$$\times \left[\frac{(2l+1)(l-m)!(n+l)!}{2^l(l+m)!n!(2n+2l+1)!}\right]^{1/2}$$

$$\times \left(\frac{n_x+n_y+m}{2}\right)!\left[n_x!n_y!n_z!\right]^{1/2}\left[\frac{1+(-)^{(n_x+n_y+m)}}{2}\right]$$

$$\times \sum_{s=s_{\min}}^{s_{\max}} \frac{(-)^s(2l-2s)!(n+s)!}{s!(l-s)!(l-2s-m)!(n+s-\frac{n_x+n_y-m}{2})!}$$

$$\times \sum_{p=p_{\min}}^{p_{\max}} \frac{(-)^p}{p!(n_x-p)!(p+\frac{n_x-n_y-m}{2})!(\frac{n_x+n_y+m}{2}-p)!}$$

AN ALTERNATIVE FORMULATION

★ Based on the same principles as in Davies and Krieger, we have derived the following **alternative formula** :

$$
\begin{aligned}
\langle nlm|n_x n_y n_z\rangle &= \delta_{2n+l,n_x+n_y+n_z}(-)^{(2n+n_x+n_y-m)/2}\, i^{n_y} \\
&\times \Big[\frac{2^l(2l+1)(n+l)!(l+m)!(l-m)!}{n!(2n+2l+1)!}\Big]^{1/2} \\
&\times \Big(\frac{n_x+n_y+m}{2}\Big)!\Big[n_x!n_y!\Big]^{-1/2}\Big[n_z!\Big]^{1/2}\Big[\frac{1+(-)^{(n_x+n_y+m)}}{2}\Big]\frac{1}{2^m}t_0! \\
&\times \sum_s \frac{(-)^s\binom{n}{t_0-s}}{2^{2s}s!(m+s)!(l-2s-m)!} \\
&\times \sum_p (-)^p\binom{n_x}{p}\binom{n_y}{q}
\end{aligned}
$$

where $t_0 = (n_x+n_y-m)/2$ and $q = (n_x+n_y+m)/2 - p$.

★ The technique utilized by Davies and Krieger starts from the expression of the spherical harmonic oscillator basis (see for instance the textbook M. Moshinsky and Y.F. Smirnov, *The Harmonic Oscillator in Modern Physics*, Harwood Academic Publishers, Amsterdam, 1996)) :

$$|nlm\rangle = (-)^n \left[\frac{4\pi 2^l (n+l)!}{n!(2n+2l+1)!} \right]^{1/2} (\vec{\eta} \cdot \vec{\eta})^n \mathcal{Y}_{lm}(\vec{\eta})|0\rangle$$

where

$$\vec{\eta} \equiv \vec{a}^\dagger = (\vec{r} - i\vec{p})/\sqrt{2} = (a_x^\dagger, a_y^\dagger, a_z^\dagger)$$

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★ Introduce the **spherical components** of the vector $\vec{\eta}$:

$$\begin{cases} \eta_+ = -\frac{1}{\sqrt{2}}(\eta_x + i\eta_y) \\ \eta_0 = \eta_z \\ \eta_- = +\frac{1}{\sqrt{2}}(\eta_x - i\eta_y) \end{cases}$$

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★ The **binomial expansion** allows to write (Davies and Krieger) :

$$(\vec{\eta}\cdot\vec{\eta})^n = (\eta_z^2 - 2\eta_+\eta_-)^n = \sum_t (-)^t 2^t \binom{n}{k} \eta_+^t \eta_-^t \eta_z^{2n-2t}$$

- ★ The **solid spherical harmonics** are expanded according to (see D.A. Varshalovich, A.N. Moskalev and V.K. Khersonskii, *Quantum Theory of Angular Momentum*, World Scientific, Singapore, 1988)) :

$$\mathcal{Y}_{lm}(\vec{\eta}) = \sqrt{\frac{2l+1}{4\pi}(l+m)!(l-m)!}\sum_{s}\frac{1}{2^{\frac{2s+m}{2}}s!(m+s)!(l-2s-m)!}\eta_{+}^{m+s}\eta_{-}^{s}\eta_{z}^{l-2s-m}$$

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★ The cartesian realization of the three-dimensional harmonic oscillator states reads, using again the **binomial expansion** (Davies and Krieger) :

$$\begin{aligned} |n_x n_y n_z\rangle &= \frac{1}{\sqrt{n_x! n_y! n_z!}} \eta_x^{n_x} \eta_y^{n_y} \eta_z^{n_z} |0\rangle \\ &= \frac{1}{\sqrt{n_x! n_y! n_z!}} \left(\frac{\eta_- - \eta_+}{\sqrt{2}} \right)^{n_x} \left(i \frac{\eta_- + \eta_+}{\sqrt{2}} \right)^{n_y} \eta_z^{n_z} |0\rangle \\ &= i^{n_y} \sqrt{\frac{n_x! n_y!}{2^{n_x+n_y} n_z!}} \sum_{p,q} \frac{(-)^p}{p!(n_x-p)!q!(n_y-q)!} \eta_+^{p+q} \eta_-^{n_x+n_y-p-q} \eta_z^{n_z} |0\rangle \end{aligned}$$

★ Comparing these two expressions, one sees that the **overlap** between the cartesian and spherical states vanishes, unless one has the conditions :

$$n_z = l - 2s - m + 2n - 2t = 2n + l - m - 2(s + t)$$

which fixes the value of $s + t \equiv t_0$. One also must have

$$s + t = n_x + n_y - p - q$$

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$$|nlm\rangle = (-)^n \Big[\frac{2^l (2l+1)(n+l)!(l+m)!(l-m)!}{n!(2n+2l+1)!}\Big]^{1/2}$$
$$\times \sum_s \frac{(-)^{t_0-s} 2^{t_0-s} \binom{n}{t_0-s}}{2^{\frac{2s+m}{2}} s!(m+s)!(l-2s-m)!} \eta_+^{m+t_0} \eta_-^{t_0} \eta_z^{2n+l-m-2t_0}$$

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★ The above expression terminates the final calculation of the Smirnov brackets $\langle nlm|n_x n_y n_z\rangle$ in the form given previously.

ANOTHER FANCY ...

... AND VERY EFFICIENT METHOD !

USE OF RECURRENCE FORMULEA

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- ★ Consider the following **generating function of the spherical harmonic oscillator basis** :

$$|G(z, \xi^0, r)\rangle = \sum_{nlm} \left(\frac{4\pi}{2l+1} \right)^{1/2} \frac{z^n}{N_{nl}} \Phi_{lm}(\xi^0) |nlm\rangle$$

where $\xi^0 = (\xi, \eta) \in \mathbb{C}^2$ and

$$\Phi_{lm}(\xi^0) = \frac{\xi^{l+m} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}}$$

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$$\Phi_{lm}(\xi^0) = \frac{\xi^{l+m}\eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}}$$

★ This can be transformed with the help of the **generating function of the solid spherical harmonics** (see J. Schwinger in *Quantum Theory of Angular Momentum*, ed. Biedenharn and Van Dam, Academic press, New York,1965, p.229) :

$$\left(\frac{4\pi}{2l+1}\right)^{1/2}\sum_{m}\Phi_{lm}(\xi^0)\mathcal{Y}_{lm}(\vec{a}^\dagger) = \frac{(\vec{b}^*\cdot\vec{a}^\dagger)^l}{2^l\, l!}$$

★ In the latter expression one has introduced the **null-length vector** $\vec{b} = (b_x, b_y, b_z)$, i.e. such that $\vec{b}^* \cdot \vec{b} = 0$:

$$\begin{cases} b_x = -\xi^2 + \eta^2 \\ b_y = -i(\xi^2 + \eta^2) \\ b_z = 2\xi\eta \end{cases}$$

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$$\vec{a}^\dagger = (\vec{r} - i\vec{p})/\sqrt{2} = (a_x^\dagger, a_y^\dagger, a_z^\dagger)$$

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★ The three-dimensional spherical harmonic oscillator basis can be expressed as :

$$|nlm\rangle = (-)^n \frac{1}{n!2^{n+l/2}} N_{nl} \rho^{2n} \mathcal{Y}_{lm}(\vec{a}^\dagger)|000\rangle$$

with

$$N_{nl} = \sqrt{\frac{2\pi^{3/2}\Gamma(n+1)}{\Gamma(n+l+3/2)}}$$

★ And therefore one gets

$$
\begin{aligned}
|G(z,\xi^0,r)\rangle &= \sum_{nlm} \left(\frac{4\pi}{2l+1}\right)^{1/2} \frac{z^n}{N_{nl}} \Phi_{lm}(\xi^0)|nlm\rangle \\
&= \sum_{nl} (-)^n \frac{1}{n!2^{n+l/2}} \frac{z^n \rho^{2n}}{2^l l!} (\vec{b}^* \cdot \vec{a}^\dagger)^l |000\rangle \\
&= e^{\left(-\frac{z\rho^2}{2} + \frac{\vec{b}^* \cdot \vec{a}^\dagger}{2\sqrt{2}}\right)} |000\rangle
\end{aligned}
$$

★ And therefore one gets

$$|G(z,\xi^0,r)\rangle = \sum_{nlm}\left(\frac{4\pi}{2l+1}\right)^{1/2}\frac{z^n}{N_{nl}}\Phi_{lm}(\xi^0)|nlm\rangle$$
$$= \sum_{nl}(-)^n\frac{1}{n!2^{n+l/2}}\frac{z^n\rho^{2n}}{2^l l!}(\vec{b}^*\cdot\vec{a}^\dagger)^l|000\rangle$$
$$= e^{(-\frac{z\rho^2}{2}+\frac{\vec{b}^*\cdot\vec{a}^\dagger}{2\sqrt{2}})}|000\rangle$$

★ On the other hand, one knows that the **generating function of the three-dimensional harmonic oscillator** can be writte as (here $\vec{t} = (z_x, z_y, z_z)$) :

$$|\Phi(\vec{r},\vec{t})\rangle = e^{\vec{t}^*\cdot\vec{a}^\dagger}|000\rangle = \sum_{n_x n_y n_z}\frac{{z_x^*}^{n_x}{z_y^*}^{n_y}{z_z^*}^{n_z}}{\sqrt{n_x!n_y!n_z!}}\frac{{a_x^\dagger}^{n_x}{a_y^\dagger}^{n_y}{a_z^\dagger}^{n_z}}{\sqrt{n_x!n_y!n_z!}}|000\rangle$$

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$$

★ One is now in the position to evaluate the **generating function for changing from the cartesian to the spherical basis** : $G(s,\vec{b},\vec{t}) = \langle\Phi(\vec{r},\vec{t})|G(s,\xi^0,r)\rangle$

★ One obtains two expressions :

$$G(s,\vec{b},\vec{t}) = e^{(-\frac{s\vec{t}^2}{2}+\frac{\vec{b}^*\cdot\vec{t}}{2\sqrt{2}})} = e^Q$$

with

$$Q = -\frac{s\vec{t}^2}{2} + \frac{\vec{b}^*\cdot\vec{t}}{2\sqrt{2}}$$

and

$$G(s,\vec{b},\vec{t}) = \sum_{nlm}\sum_{n_x n_y n_z} \frac{{z_x}^{n_x}{z_y}^{n_y}{z_z}^{n_z}}{\sqrt{n_x!n_y!n_z!}}\left(\frac{4\pi}{2l+1}\right)^{1/2}\frac{s^n}{N_{nl}} \times \frac{\xi^{l+m}\eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}}\langle n_x n_y n_z|nlm\rangle$$

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★ Then **partial derivatives** with respect to ξ, η and s are taken :

$$\begin{cases} \frac{\partial Q}{\partial \xi}G = \frac{\partial G}{\partial \xi} \\ \frac{\partial Q}{\partial \eta}G = \frac{\partial G}{\partial \eta} \\ \frac{\partial Q}{\partial s}G = \frac{\partial G}{\partial s} \end{cases}$$

★ **Let us illustrate the procedure on the case of ξ** :

On one hand one can derive that

$$\frac{\partial Q}{\partial \xi} = \frac{1}{\sqrt{2}}[-\xi z_x - i\xi z_y + \eta z_z]$$

wherefrom

$$\frac{\partial Q}{\partial \xi}\, G = T_x + T_y + T_z$$

with

$$T_x = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \Big(-\frac{\xi}{\sqrt{2}} z_x \Big) \Big(\frac{4\pi}{2l+1} \Big)^{1/2} \frac{s^n}{N_{nl}} \frac{\xi^{l+m} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x n_y n_z | nlm \rangle$$

$$T_y = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \Big(-i \frac{\xi}{\sqrt{2}} z_y \Big) \Big(\frac{4\pi}{2l+1} \Big)^{1/2} \frac{s^n}{N_{nl}} \frac{\xi^{l+m} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x n_y n_z | nlm \rangle$$

$$T_z = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \Big(+\frac{\eta}{\sqrt{2}} z_z \Big) \Big(\frac{4\pi}{2l+1} \Big)^{1/2} \frac{s^n}{N_{nl}} \frac{\xi^{l+m} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x n_y n_z | nlm \rangle$$

★ On the other hand one has :

$$\frac{\partial G}{\partial \xi} = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \left(\frac{4\pi}{2l+1} \right)^{1/2} \frac{s^n}{N_{nl}} (l+m) \frac{\xi^{l+m-1} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x n_y n_z | nlm \rangle$$

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★ The idea is to identify in both expressions the terms with equal powers. This is done separately for T_x, T_y **and** T_z.

★ The **term** T_x can also be expressed in the form :

$$T_x = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x+1} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \Big(-\frac{1}{\sqrt{2}}\Big) \Big(\frac{4\pi}{2l+1}\Big)^{1/2} \frac{s^n}{N_{nl}} \frac{\xi^{l+m+1} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x n_y n_z | nlm \rangle$$

By posing the change of variables $\lambda = l+1$, $\nu_x = n_x + 1$ and $\mu = m+1$ and coming finally back again to n_x, l and m (mute variables) one finds

$$T_x = \sum_{\substack{nlm \\ n_x n_y n_z}} \frac{{z_x}^{n_x} {z_y}^{n_y} {z_z}^{n_z}}{\sqrt{n_x! n_y! n_z!}} \Big(-\frac{n_x^{1/2}}{2^{1/2}}\Big) \Big(\frac{4\pi}{2l-1}\Big)^{1/2} \frac{s^n}{N_{nl}}$$

$$\times \; [(l+m)(l+m-1)]^{1/2} \frac{\xi^{l+m-1} \eta^{l-m}}{[(l+m)!(l-m)!]^{1/2}} \langle n_x - 1 \; n_y \; n_z | n \; l-1 \; m-1 \rangle$$

★ Equating terms of equal powers for the **contribution T_x** gives :

$$\sqrt{l+m}\,\langle n_x n_y n_z | nlm\rangle \rightsquigarrow -\frac{1}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$
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★ In the same way, equating terms of equal powers for the **contribution T_y** gives :

$$\sqrt{l+m}\,\langle n_x n_y n_z | nlm\rangle \rightsquigarrow -\frac{i}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$
$$\sqrt{n_y(l+m-1)}\langle n_x\; n_y-1\; n_z | n\; l-1\; m-1\rangle$$

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★ And finally equating terms of equal powers for the **contribution T_z** gives :

$$\sqrt{l+m}\,\langle n_x n_y n_z | nlm\rangle \rightsquigarrow \frac{1}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$
$$\sqrt{n_z(l-m)}\langle n_x\, n_y\, n_z-1 | n\, l-1\, m\rangle$$

★ Bringing now the contributions of T_x, T_y and T_z together leads to the desired **recurrence relations** :

$$\sqrt{l+m}\,\langle n_x n_y n_z | nlm\rangle = -\frac{1}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$
$$\Big[\sqrt{n_x(l+m-1)}\langle n_x-1\; n_y\; n_z | n\; l-1\; m-1\rangle$$
$$+\, i\,\sqrt{n_y(l+m-1)}\langle n_x\; n_y-1\; n_z | n\; l-1\; m-1\rangle$$
$$-\,\sqrt{n_z(l-m)}\langle n_x\; n_y\; n_z-1 | n\; l-1\; m\rangle\Big]$$

with

$$\frac{N_{nl}}{N_{nl-1}} = \frac{1}{\sqrt{n+l+1/2}}$$

★ In the same way, by **derivating with respect to η** :

$$\sqrt{l-m}\,\langle n_x n_y n_z | nlm\rangle = +\frac{1}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$

$$\Big[\sqrt{n_x(l-m-1)}\langle n_x-1\; n_y\; n_z | n\; l-1\; m+1\rangle$$

$$-\,i\,\sqrt{n_y(l-m-1)}\langle n_x\; n_y-1\; n_z | n\; l-1\; m+1\rangle$$

$$+\,\sqrt{n_z(l+m)}\langle n_x\; n_y\; n_z-1 | n\; l-1\; m\rangle\Big]$$

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$$\sqrt{l-m}\,\langle n_x n_y n_z|nlm\rangle = +\frac{1}{\sqrt{2}}\frac{N_{nl}}{N_{nl-1}}\sqrt{\frac{2l+1}{2l-1}}$$
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★ And finally by **derivating with respect to s**:

$$n\,\langle n_x n_y n_z|nlm\rangle = -\frac{1}{2}\frac{N_{nl}}{N_{nl-1}}$$
$$\Big[\sqrt{n_x(n_x-1)}\langle n_x-2\; n_y\; n_z|n-1\; l\; m\rangle$$
$$-\,i\,\sqrt{n_y(n_y-1)}\langle n_x\; n_y-2\; n_z|n-1\; l\; m\rangle$$
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REMARK ON GENERATING FUNCTIONS

★ In **Quantum Chemistry**, the issue of constructing **common generating functions** of harmonic oscillator wave functions, for cartesian, circular and spherical coordinates, and transformation brackets in D dimensions, has been given explicitely by L. Chaos-Cador and E. Ley-Koo, International Journal of Quantum Chemistry **97** (2004) 844

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- 5 - A natural extension to **non-central forces** is of course needed

- 6 - The formalism is also well suited for **HFB** type calculations (pairing field)

THANK YOU FOR YOUR ATTENTION !