

Definitions

For axially deformed nuclei, the spinors solutions of the Hartree-Fock equations can be expanded into an axially-deformed harmonic oscillator basis. Which in cylindrical coordinates takes the form:

$$\Psi_i(\mathbf{r}) = \begin{pmatrix} f_i^+(r_\perp, z)e^{i(m-\frac{1}{2})\theta} \\ f_i^-(r_\perp, z)e^{i(m+\frac{1}{2})\theta} \end{pmatrix} = \sum_\alpha f_\alpha^{(i)} \phi_\alpha(\mathbf{r}, \sigma) \quad (1)$$

Where $\alpha = \{n_r, m_l, n_z, m_s\}$ labels an eigenstate of the harmonic oscillator, f^\pm is the spinor expansion coefficient in the THO basis, and m is the total angular momentum projection. And $\phi_\alpha(\mathbf{r}, \sigma)$ represent the HO eigenstate, which may be explicitly written:

$$\phi_{n_r, m_l, n_z, m_s}(\mathbf{r}, \sigma) = \psi_{n_r, m_l}(r) \psi_{n_z}(z) \frac{e^{i\theta m_l}}{\sqrt{2\pi}} \chi_{m_s}(\sigma) \quad (2)$$

Where

$$\psi_{n_r, m_l}(r) = \frac{\mathcal{N}_{n_r, m_l}}{b_r} \sqrt{2\eta} \eta^{\frac{m_l}{2}} e^{-\frac{\eta}{2}} L_{n_r, m_l}(\eta) \quad (3)$$

$$\psi_{n_z}(z) = \frac{\mathcal{N}_{n_z}}{\sqrt{b_z}} e^{-\frac{\xi^2}{2}} H_{n_z}(\xi) \quad (4)$$

With $\{b_r, b_z\}$ the oscillators lengths, the dimensionless variables

$$\eta = \frac{r^2}{b_r^2}, \xi = \frac{z}{b_z} \quad (5)$$

And the normalisation constants

$$\mathcal{N}_{n_r, m_l} = \sqrt{\frac{n_r!}{(n_r + m_l)!}}, \mathcal{N}_{n_z} = \sqrt{\frac{1}{\sqrt{\pi} 2^{n_z} n_z!}} \quad (6)$$

The derivatives of (3) and (4) can be computed in cylindrical coordinates using,

$$\nabla = \begin{pmatrix} \frac{\partial_r}{r} \\ \frac{\partial_\theta}{r} \\ \frac{\partial_z}{b_z} \end{pmatrix} \quad (7)$$

Which gives,

$$\partial_r \psi_{n_r, m_l}(r) = \frac{\mathcal{N}_{n_r, m_l}}{b_r^2} \sqrt{2\eta} \eta^{\frac{m_l-1}{2}} e^{-\frac{\eta}{2}} L'_{n_r, m_l}(\eta) \quad (8)$$

$$L'_{n_r, m_l}(\eta) = [2(n_r + 1)L_{n_r+1, m_l}(\eta) - (2n_r + m_l + 2 - \eta)L_{n_r, m_l}(\eta)]$$

And

$$\partial_z \psi_{n_r, m_l}(r) = \frac{\mathcal{N}_{n_z}}{b_z^{\frac{3}{2}}} e^{-\frac{\xi^2}{2}} H_{n_z}(\xi)' \quad (9)$$

$$H'_{n_z}(\xi) = [\xi H_{n_z}(\xi) - H_{n_z+1}(\xi)]$$

For a cylindrical basis, one might be more efficient by defining the set of operators in spherical representation $\{p^+, p^-, p^3\}$.

$$p^+ = -\frac{1}{\sqrt{2}}(P_x + iP_y); p^- = \frac{1}{\sqrt{2}}(P_x - iP_y); p^3 = P_z \quad (10)$$

Defined by the derivatives:

$$\partial^+ = -\frac{1}{\sqrt{2}}e^{i\theta} \left(\partial_\perp + \frac{i}{r_\perp} \partial_\theta \right); \partial^- = \frac{1}{\sqrt{2}}e^{-i\theta} \left(\partial_\perp - \frac{i}{r_\perp} \partial_\theta \right); \partial^3 = \partial_z \quad (11)$$

Correction energy

The center-of-mass correction energy can be written:

$$E_{cm}^{corr} = \frac{\langle \Phi_{HFB} | \mathbf{P}^2 | \Phi_{HFB} \rangle}{2mA} \quad (12)$$

Thus one shall compute the expectation value of a two-body operator for an HFB vacuum. [?]

$$\frac{\langle \Phi | \mathbf{P}^2 | \Phi \rangle}{\langle \Phi | \Phi \rangle} = [Tr(P\rho)]^2 + Tr(P^2\rho) - Tr(P\rho P\rho) - Tr[P\kappa(P\kappa)^*] \quad (13)$$

Thus one must compute the matrix elements $P_{i,j} = \langle i | \hat{p} | j \rangle$. Where $\hat{p} = -i\hbar\nabla$. The components of the momentum operator are in the spherical representation.

$$\mathbf{i} \frac{\langle i_1 | p^3 | i \rangle}{\hbar} = \frac{1}{b_z} \sum_{\alpha, \alpha_1} \delta_{n_r, m_l, m_s}^{n_{r1}, m_{l1}, m_{s1}} f_{\alpha}^{(i)} f_{\alpha_1}^{(i_1)} \int d\xi \psi_{n_z}(\xi) \partial_{\xi} \psi_{n_{z1}}(\xi) \quad (14)$$

$$\frac{\langle i_1 | p^{\pm} | i \rangle}{\hbar} = \pm \frac{\mathbf{i}}{b_r \sqrt{2}} \sum_{\alpha, \alpha_1} \delta_{n_z, m_l+1, m_s}^{n_{z1}, m_{l1}, m_{s1}} \int d\eta \psi_{n_r, m_l}(\eta) \left[2\sqrt{\eta} \partial_{\eta} \psi_{n_{r1}, m_{l1}}(\eta) \mp \frac{m_{l1}}{\sqrt{\eta}} \psi_{n_{r1}, m_{l1}}(\eta) \right] \quad (15)$$

Then the average value of the one-body operator can be expressed in spherical representation according to (13):

$$\begin{aligned} \langle \hat{P}^2 \rangle = & -2Tr(P^+\rho)Tr(P^-\rho) + [Tr(P^z\rho)]^2 - 2Tr(P^+P^-\rho) + Tr((P^z)^2\rho) + Tr(P^+\rho P^-\rho) \\ & + Tr(P^-\rho P^+\rho) - Tr(P^z\rho P^z\rho) + Tr(P^+\kappa(P^-\kappa)^*) + Tr(P^-\kappa(P^+\kappa)^*) - Tr(P^z\kappa(P^z\kappa)^*) \end{aligned} \quad (16)$$

Corrective Fields

Following [?] one can construct the corrective terms which modify the Hartree-Fock-Bogoliubov hamiltonian

$$\mathcal{H}_{corr} = \mathcal{H} + kC_2 \quad (17)$$

Where

$$C_2 = \begin{pmatrix} 2\langle \hat{P} \rangle P + P^2 - 2P\rho P & 2P\kappa^t P \\ -(2P\kappa^t P)^* & -(2\langle \hat{P} \rangle P + P^2 - 2P\rho P)^* \end{pmatrix} \quad (18)$$

Where

$$2\langle \hat{P} \rangle P = -2Tr(P^+\rho)P^- - 2Tr(P^-\rho)P^+ + 2Tr(P^z\rho)P^z \quad (19)$$

$$P^2 = -2P^+P^- + (P^z)^2 \quad (20)$$

$$-2P\rho P = 2P^+\rho P^- + 2P^-\rho P^+ - 2P^z\rho P^z \quad (21)$$

$$2P\kappa^t P = -2P^+\kappa^t P^- - 2P^-\kappa^t P^+ + 2P^z\kappa^t P^z \quad (22)$$

This term shall be computed and calculated at each iteration of the Hartree-Fock-Bogoliubov procedure.

Bibliography

- [1] *Uncertainty analysis and symmetry restoration in nuclear self-consistent methods* Yuan Gao.(2014)