# Nilsson model

The program `nilsson.py` calculates the Nilsson single-particle levels in the space of selected harmonic oscillator shells. The Nilsson Hamiltonian is specified by the four parameters $\omega_0, \varepsilon_2, \kappa, \mu$ in the formula

$$H = \omega_z(a_z^\dagger a_z + \frac{1}{2}) + \omega_r(a_x^\dagger a_x + a_y^\dagger a_y + 1) + \omega_0 \kappa(\hat{L} \cdot \hat{\sigma} - \mu(\hat{L}^2 - \langle L^2 \rangle)) \quad (1)$$

where $a_i$ are the Cartesian harmonic oscillator annihilation operators and $\hat{\sigma}$ is twice the nucleon spin operator. The oscillator frequencies are given by

$$\omega_z = \omega_0(1 - \frac{2}{3}\varepsilon_2) \quad (2)$$

$$\omega_r = \omega_0(1 + \frac{1}{3}\varepsilon_2)$$

and $\omega_0$ is parameterized as usual by

$$\omega_0 = \frac{41}{A^{1/3}} \quad \text{MeV.} \quad (3)$$

This Hamiltonian is diagonalized within each major shell, approximating the matrix elements of the angular momentum operator $\hat{L}$ by the values for a spherically symmetric shell. The most convenient representation for calculating matrix elements is the cylindrical basis $|n_z n_+ n_- \sigma_z\rangle$ where $n_z$ is the number of oscillator quanta in the $z$-direction and $n_+, n_-$ are numbers of quanta corresponding to the annihilation operators $2^{-1/2}(a_x \pm i a_y)$ respectively.

The nonzero matrix elements of the Hamiltonian in this basis are

$$\langle n_z, n_+, n_-, \sigma_z|H|n_z, n_+, n_-, \sigma_z\rangle = \omega_z(n_z + 1/2) + \omega_r(n_+ + n_- + 1) + \quad (4)$$

$$+\omega_0\kappa\left(M\sigma_z - \mu(M^2 + (2n_z + 1)(n_+ + n_- + M) + 2n_z - \langle L^2 \rangle)\right);$$

$$\langle n_z + 2, n_+ - 1, n_- - 1, \sigma_z|H|n_z, n_+, n_-, \sigma_z\rangle = \quad (5)$$

$$2\omega_0\kappa\mu\sqrt{(n_z + 1)(n_z + 2)n_+ n_-};$$

$$\langle n_z + 1, n_+ - 1, n_-, +1|H|n_z, n_+, n_-, -1\rangle = \kappa\sqrt{2n_+(n_z + 1)}; \quad (6)$$

$$\langle n_z + 1, n_+, n_- - 1, -1|H|n_z, n_+, n_-, +1\rangle = \kappa\sqrt{2n_-(n_z + 1)} \quad (7)$$

together with the Hermitian conjugate formulas. Here we have written $M = n_+ - n_-$.

Following the construction of the eigenstates of Hamiltonian, the occupation numbers $v_i^2$ of the orbitals are computed by the BCS formula for a pairing Hamiltonian,

$$v_i^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_i - \lambda}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta^2)}}\right). \quad (8)$$

The calculation requires input of the chemical potential $\lambda$ and the BCS gap parameter $\Delta$; it is assumed that the latter quantities have been already computed

from some pairing Hamiltonian with $\lambda$ determined by the required (average) particle number.

The last part of the program computes a number of operator expectation values for the nucleus as a whole, given the single-particle matrix elements and the pairing occupation probabilities $v_i^2$. The quantities computed are the number of particles $N_p$, the total number of oscillator quanta $N_z$, $N_x + N_y$, $N_t = N_z + N_x + N_y$, the quadrupole moment $q_0 = z^2 - \frac{1}{2}(x^2 + y^2)$, and the mean square radius $\langle r^2 \rangle$, according to the formulas

$$N_p = 2 \sum_i v_i^2 \tag{9}$$

$$N_z = 2 \sum_i v_i^2 (n_z^i + \frac{1}{2}) \quad \text{etc.} \tag{10}$$

$$q_0 = 2 \sum_i v_i^2 \left( \frac{n_z^i + \frac{1}{2}}{M\omega_z} - \frac{n_x^i + n_y^i + 1}{2M\omega_r} \right) \tag{11}$$

$$\langle r^2 \rangle = \frac{2}{N_p} \sum_i v_i^2 \left( \frac{n_z^i + \frac{1}{2}}{M\omega_z} + \frac{n_x^i + n_y^i + 1}{M\omega_r} \right) \tag{12}$$

The sums over $i$ include only orbitals with $j_z > 0$.

The code in written in Python and requires the `numpy` library for matrix algebra. A test case can be run by typing on the command line $./gd154.sh. The input file for the test case corresponds to the proton wave function in the nucleus $^{154}$Gd at a deformation $\varepsilon_2 = 0.2$. Another test case can be run with the input file `zr80.in`, giving $N_p$ and $N_x$ etc. for wave function with completely filled shells up to $N_o sc = 3$.