Nuclear Structure Program

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1 cNucleus class

In order to caracterize the different nuclei I take advantage of the object-orienting programming of C++. The cNucleus object represent a nucleus where the main features are the atomic number(Z) and the neutronic number(N).

Moreover the mass excess of the nucleus is the tabuled data that characterizes its mass. So we use a txt file with this data for a lot of nuclei.

1.1 Mass excess

Let's recall the definition of mass excess Δ. This is an atomic value, not directly a nucleus value:

$$\Delta = M_{atm} - A[u] \cdot 931.493614838475 MeV/u \tag{1.1}$$

where M_{atm} is the atomic mass with neutral charge. And the atomic mass is:

$$M_{atm} = M_{nuc} + Z \cdot m_e - B_e(Z) \tag{1.2}$$

where is B_e the total biding energy of the electrons.

An approximation that one could make in order to get an approximate value of the nucleus mass is:

$$M_{nuc} \approx M_{atm} - Z \cdot m_e \tag{1.3}$$

Every time a cNucleus object variable is declared the method Getmassexcess() is called and the massexcess is well defined in the variable. The values are stored in .txt file (they are given in keV. If there's no data available for the specified nucleus then this value is not assigned.

1.2 Alpha desintegration

$$^{A}_{Z}\mathrm{X}_{N} - - - > ^{A-4}_{Z-2}\mathrm{Y}_{N-2} + \alpha \ . \tag{1.4}$$

This process is due to Coulombian repulsion between the protons, therefore it is more important in heavy nuclei. Spontaneous process due to the aparition of kinetic energy in the sytem caused by a decrease in its mass. Alpha particle, its mass is relatively small compared to its elements alone, that's why it has a tendency to get formed inside the nucleus.

$$Q = m({}^{A}_{Z}\mathrm{X}_{N}) - m({}^{A-4}_{Z-2}\mathrm{Y}_{N-2}) - m_{\alpha} \ , \tag{1.5}$$

where m are nuclear masses. To transform them into atomic masses m_a we have to use eq.[1.1]. Then we have:

$$Q = m_a({}^{A}_{Z}\mathrm{X}_{N}) - m_a({}^{A-4}_{Z-2}\mathrm{Y}_{N-2}) - m_a({}^{4}\mathrm{He}) + B_e(Z) - B_e(Z-2) - B_e(2) \ , \tag{1.6}$$

we neglect the $B_e(Z) - B_e(Z-2) - B_e(2)$ part which is absolutely correct and using the definition of mass excess we have:

$$Q \approx \Delta(X) - \Delta(Y) - \Delta(\alpha) \ , \tag{1.7}$$

In a non-relativistic system and using energy and momentum conservation we have:

$$T_{\alpha} = Q\left(1 + \frac{m_{\alpha}}{m_Y}\right)^{-1} \approx Q\left(1 + \frac{4}{A}\right)^{-1} \ . \tag{1.8}$$

And the daughter kinetic energy is:

$$T_Y = Q - T_{\alpha} \ . \tag{1.9}$$

1.2.1 AlphaEnergy method

A vector of three coordinates as the argument, in it will be the returns. First is the reaction energy provided by eq.[1.7], second is the alpha kinetic energy eq.[1.8] and the third is the eq.[1.9]. All this quantities are returned in MeV.

1.3 Beta- desintegration

$${}^{A}_{Z}\mathrm{X}_{N} - - - > {}^{A}_{Z+1}\mathrm{Y}_{N-1} + e - + \vec{\mu}_e \ . \tag{1.10}$$

In this case neglecting electronic binding energy terms as we did in eq.[1.7] and neglecting the antineutrino mass we have:

$$Q_{\beta-} \approx \Delta(Z,N) - \Delta(Z+1, N-1) \ . \tag{1.11}$$

NBetaEnergy method provides this value in MeV using eq.[1.11].

1.4 Beta+ desintegration

$${}^{A}_{Z}\mathrm{X}_{N} - - - > {}^{A}_{Z-1}\mathrm{Y}_{N+1} + e + + \mu_e \ . \tag{1.12}$$

In this case neglecting electronic binding energy terms as we did in eq.[1.7] and neglecting the neutrino mass we have:

$$Q_{\beta+} \approx \Delta(Z,N) - \Delta(Z-1, N+1) - 2m_e \ . \tag{1.13}$$

PBetaEnergy method provides this value in MeV using eq.[1.13].

1.4.1 Neutronic separation energy

$$ {}^{A}_{Z}\mathrm{X}_{N} - - - > {}^{A}_{Z}\mathrm{Y}_{N-1} + n \ . \tag{1.14} $$

Neglecting electronic binding energy terms as we did in eq.[1.7] we have:

$$ Q_n \approx \Delta(Z,N) - \Delta(Z,N-1) - \Delta_n \ . \tag{1.15} $$

We define the neutronic separation energy S_n as:

$$ S_n = -Q_n \ . \tag{1.16} $$

$Neutronic_Sep_Energy$ method provides this energy.

1.4.2 Protonic separation energy

$$ {}^{A}_{Z}\mathrm{X}_{N} - - - > {}^{A}_{Z-1}\mathrm{Y}_{N} + p \ . \tag{1.17} $$

Neglecting electronic binding energy terms as we did in eq.[1.7] we have:

$$ Q_p \approx \Delta(Z,N) - \Delta(Z-1,N) - \Delta_p \ . \tag{1.18} $$

We define the neutronic separation energy S_n as:

$$ S_n = -Q_p \ . \tag{1.19} $$

$Proton_Sep_Energy$ method provides this energy.

2 Deuteron.cpp

2.1 Finite Square Function To Solve function

The porpuse of this function is to construct the function associated with the finite square well problem in three dimensions in quantum mechanics. In nuclear physics this is associated to the deuteron problem. The function to be solved is:

$$ f(\alpha,\beta,a) = \alpha\frac{j_{l+1}(\alpha a)}{j_l(\alpha a)} - i\beta\frac{h_{l+1}(i\beta a)}{h_l(i\beta a)} \ . \tag{2.1} $$

where h is the hinkel function and j is the spherical Bessel function of first kind.

The actual arguments of the function are not the α and β values. They are e, normalized energy, V, depth potential(MeV), a radius of the nucleus(fm),m reduced mass of the system(MeV) and l the quantum oribtal angular number.

We have $\alpha = \alpha(e,V)$ and $\beta = \beta(e)$. This function provides the value for the function described in eq.[2.1].

2.2 Bisection Finite Square function

It solves the following equation:

$$f(\alpha, \beta, a) = 0 \ , \tag{2.2}$$

where f is described in eq.[2.1], using the bisection method. You have to introduce the energy value E, the radius value R, the angular momentum of the system l,a range for the potential depth V_min and V_max, and the absolute error you wish for. It provides a solution between the range if there is any.

3 Nuclear.cpp

3.1 $\hbar\omega$ function

From [2] we have the isotropic harmonic oscillator $\hbar\omega$ as:

$$\hbar\omega[N, Z] = 41 \cdot A^{-1/3} \left(1 \pm \frac{1}{3}\frac{N-Z}{A}\right) MeV \ , \tag{3.1}$$

is correct within $1 - 2percentage$ for all nuclei with exception of the very lightest ones. The plus sign is for neutrons and minus sigh for protons.

3.2 α parameter

From [3] we have that the α parameter for the harmonic isotropic oscillator is:

$$\alpha = \sqrt{\frac{\mu\omega_0}{\hbar}} = \frac{\sqrt{\mu c^2 \hbar\omega_0}}{\hbar c} \ , \tag{3.2}$$

It is dimensionless.

3.3 Isotropic harmonic oscillator normalization constant N_{nl}

From [3] we have that the N_{nl} normalization parameter for the harmonic isotropic oscillator is:

$$N_{nl} = \left[\frac{2\alpha^{2l+3}\Gamma(l + \frac{3}{2} + n - 1)}{!(n-1)\Gamma^2(l + \frac{3}{2})}\right]^{1/2} \ , \tag{3.3}$$

where Γ is the gamma function. It is dimensionless.

3.4 Radial wave function

From [3] the solution for the IHO problem is:

$$R_{nlm}(r) = N_{nl} r^l e^{-\frac{\alpha^2 r^2}{2}} M(-n+1, l+\frac{3}{2}, \alpha^2 r^2) \ , \tag{3.4}$$

3.5 μ and κ functions

We get the constants μ and κ as shown in [2]. It just depends on the nucleon and on the shell n.

3.6 Monoparticle energies function

In the Mono-Energy-NoCou function we get the mono-particle energies for IHO problem withouth the coulombian term. That is:

$$E_{Nlj} = \hbar\omega_0 \left[N + \frac{3}{2} - \mu \left(l(l+1) - \frac{N(N+3)}{2} \right) - \kappa \begin{cases} l & \text{if } j = l + \frac{1}{2} \ , \\ -(l+1) & \text{if } j = l - \frac{1}{2} \ . \end{cases} \right] \tag{3.5}$$

with $N = 2(n-1) + l$.

3.7 Coulomb potential

In the Spherical-Coulomb-Potential we have [2]:

$$V_C(r) = \begin{cases} \dfrac{Ze^2}{4\pi\epsilon_0 R \left(\frac{1}{2}\frac{r^2}{R^2} - \frac{3}{2} \right)}; & r < R \\ -\dfrac{Ze^2}{4\pi\epsilon_0 r}; & r > R \end{cases} \tag{3.6}$$

3.8 Total potential

In the Potential-MSO function we have the total potential for the IHO problem:

$$V(r) = V_o + \frac{1}{2}\hbar\omega(Z, N, nucleon)r^2 + V_C(r) \tag{3.7}$$

3.9 MO-EigenRadial-to-Integration function

Preparing the integration. This function represents the following one:

$$f(r) = |R_{nl}(r)|^2 r^2 \tag{3.8}$$

3.10 MO-Exp-Vc-f-to-Integration function

Preparing the integration. This function represents the following one:

$$f(r) = R_{nl}(r) V_C(r) R_{n'l}(r) r^2 \tag{3.9}$$

3.11 Sor-Mono-Energy-MSO function

This function calculates the single-particle energies for a lot of subshells given a nucleus. Create a vector with state tags. Then sort these vectors from maximum energy to minimum energy.

3.12 Occupied-Levels-GS

Given a nucleus it provides the occupied levels in the Ground State. It is sorted based on energy values

3.13 V-o-MSO

Gives a possible depth potential for the MSO. This depth is calculated to make match the $S_n(S_p)$ with the energy of the last ocuppied subshell (in the GS).

3.14 MO-EigenRadial-to-Integration-r

This function concatenates the function described in eq.[] to a function only dependent on r. We have to clarify that function is not only dependent on r, it is dependent on other variables as Z,N, kind of nucleon and more.

3.15 I-Normalization

Check the normalization of the MSO radial eigenfunction. It should return 1 It returns:

$$\int_{r=0}^{R} |R_{nl}(r)|^2 r^2\, dr + \int_{R}^{\infty} |R_{nl}(r)|^2 r^2\, dr \tag{3.10}$$

3.16 MO-Exp-Vc-f-to-Integration-r function

Function described in eq. [3.9] to be only dependent on r.

3.17 I-MSO-Exp-Vc function

$$< nl|V_C|n'l >= \int_{r=0}^{R} R_{nl}(r) V_C(r) R_{n'l}(r) r^2\, dr + \int_{R}^{\infty} R_{nl}(r) V_C(r) R_{n'l}(r) r^2\, dr \tag{3.11}$$

3.18 n-Vc-nprim-MSO function

This function fill the matrix $V_c[n][n']$ for a number of values of n and a fixed l using the former function.

3.19 n-H-nprim-MSO function

This function fill the matrix $H[n][n']$ for a number of values of n and a fixed l as:

$$< nl|H|n'l >= \delta_{n,n'} E_{nlj} + < nl|V_C|n'l > \tag{3.12}$$

3.20 $\hbar\omega_0(\delta)$ function

We use the following term for the deformed case:

$$\hbar\omega_0(\delta) = \hbar\omega_0 \left[\frac{1}{1 - \frac{4}{3}\delta^2 - \frac{16}{27}\delta^3} \right]^{\frac{1}{6}} \tag{3.13}$$

3.21 $\hbar\omega_z$

$$\hbar\omega_z = \hbar\omega_0(\delta) \left(1 - \frac{4}{3}\right)^{\frac{1}{2}} \tag{3.14}$$

3.22 $\hbar\omega_\rho$

$$\hbar\omega_\rho = \hbar\omega_0(\delta) \left(1 + \frac{2}{3}\right)^{\frac{1}{2}} \tag{3.15}$$

3.23 Deformed monoparticle energies

$$E_{Nlj}(\delta) = \hbar\omega_0(\delta) \left[N + \frac{3}{2} - \mu \left(l(l+1) - \frac{N(N+3)}{2} \right) - \kappa \begin{cases} l & \text{if } j = l + \frac{1}{2} \ , \\ -(l+1) & \text{if } j = l - \frac{1}{2} \ . \end{cases} \right] \tag{3.16}$$

with $N = 2(n-1) + l$.

3.24 $\alpha(\delta)$

$$\alpha(\delta) = \frac{[\hbar\omega(\delta)m]^{\frac{1}{2}}}{\hbar c} \tag{3.17}$$

3.25 MO-r2exp-to-I

It returns the function:

$$R_{n'l'}(r) r^4 R_{nl}(r) \tag{3.18}$$

3.26 MO-r2exp-to-I-r

It just resturns the previous function as a function only depending on r.

3.27 I-MSOdef-Exp-r2

$$I = \int_{r=0}^{r=\infty} R_{n'l'}(r) r^4 R_{nl}(r) dr \tag{3.19}$$

which it's the term for the operator r^2.

3.28 nljmj-r2Y20-exp

It returns:

$$\langle n'l'j'm'|r^2Y_{20}|nljm\rangle = \langle l'j'm'|Y_{20}|ljm\rangle I \tag{3.20}$$

where I is the previous function.

3.29 nljmj-Hdef-exp

Elements of the hamiltonian $H = H_0 - \beta r^2 Y_{20}$ in the basis $|nljm\rangle$:

$$H_0(\delta) = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m\omega_0^2(\delta)}{2}r^2 + C\vec{l}\vec{s} + D(\vec{l}^2 - <\vec{l}^2>_N) \ . \tag{3.21}$$

$$\langle nljm(\delta)|H(\delta)|n'l'j'm'(\delta)\rangle = \delta_{n,n'}\delta_{l,l'}\delta_{j,j'}\delta_{m,m'_j}E_{nlj}(\delta) - \beta(\delta)\langle nl(\delta)|r^2|n'l'(\delta)\rangle\langle ljm|Y_{20}|l'j'm'\rangle \tag{3.22}$$

3.30 n-and-l

Given $N = 2(n-1) + l$ it provides the (n, l) possible quantum numbers.

3.31 Ω_N

Given N quantum number it provides all the possible $\Omega = |m|$ quantum numbers

3.32 States-N-and-Omega

Given N and Ω quantum numbers provides all the possible states with n, l, j (zero deformation).

3.33 Hdef

Given NN and Omega quantum numbers, create the matrix of the deformed hamiltonian (MSO) for all the possible states identified by n, l and j. Blocks with fixed N and Ω.

3.34 All-Def-States

Given the N quantum number calculated all the possible states (Ω, n, l, j).

Referencias

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