QNuclei Software 3.0

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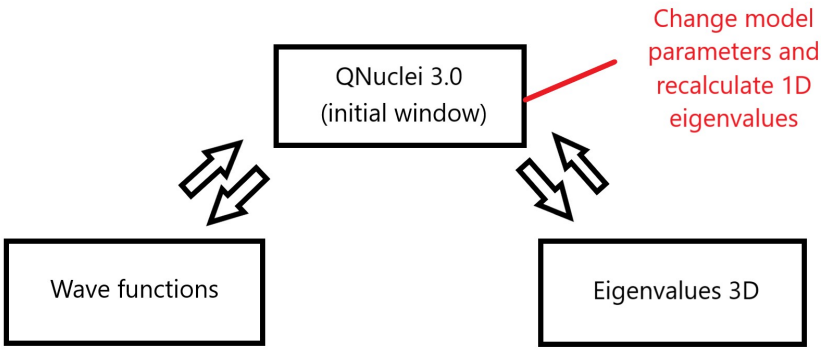
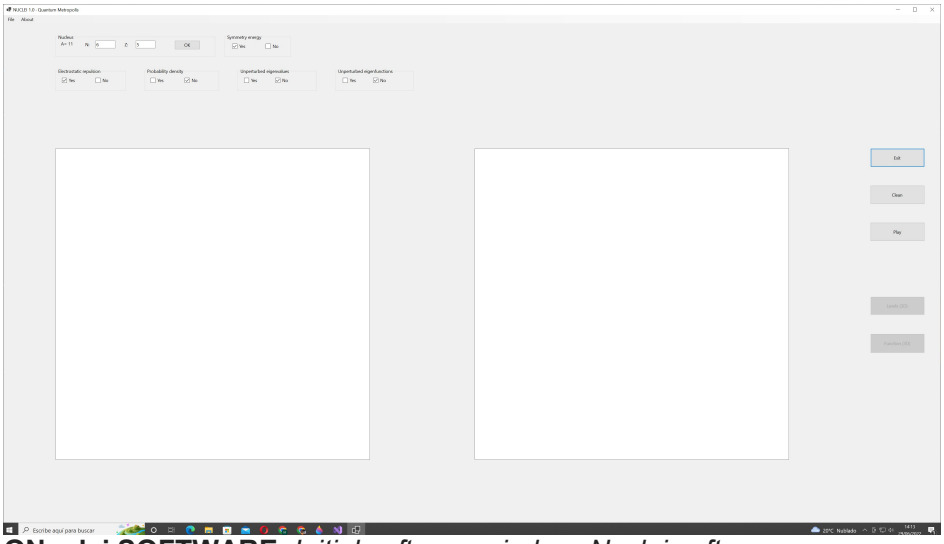
User's Manual

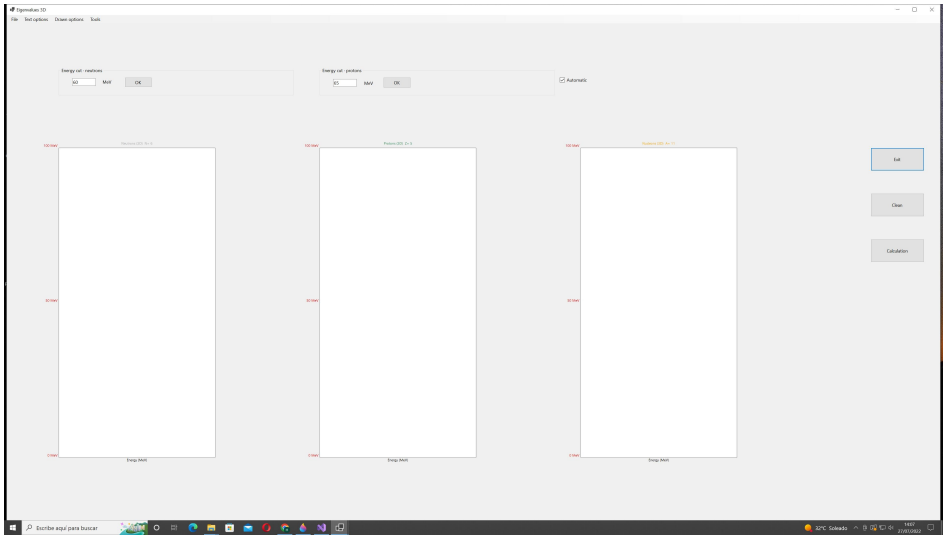
We can calculate the nuclear structure of all the elements in the periodic table. The software allows obtaining the Fermi level without the continuum hypothesis, considering only discretized eigenvalues. In addition, the wave function of all the protons and neutrons in a nucleus can be represented.



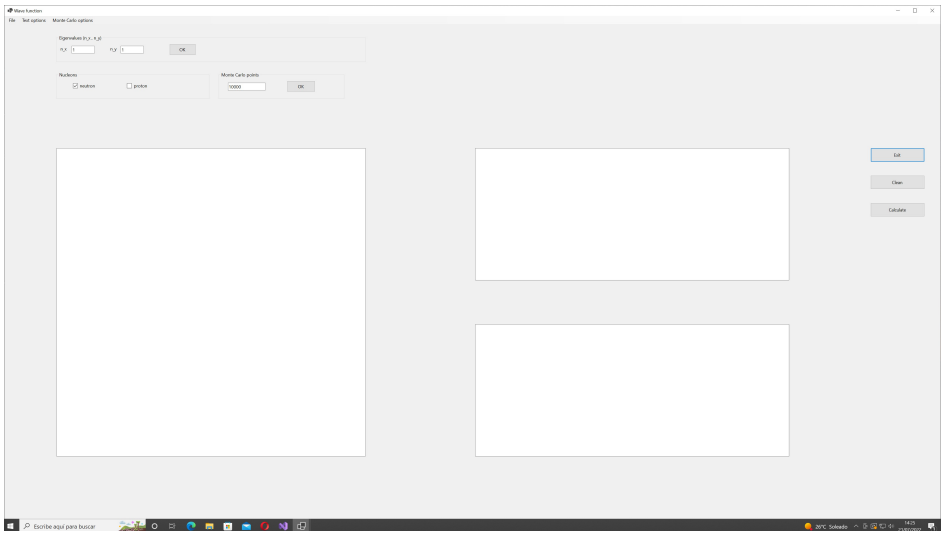
QNuclei SOFTWARE. *The software has three different windows.In the initial window, 1D (one-dimensional) eigenvalues and eigenfunctions can be calculated. In addition, the model parameters can be changed in the initial window. The other windows are the Eigenfunctions (3D) window and the Eigenvalues (3D) window. Every time model parameters or input data are changed, the 1D eigenvalues in the initial window must be recalculated.*



QNuclei SOFTWARE. *Initial software window. Nuclei software.*



QNuclei SOFTWARE · nuclear isotopes. *Initial window for Level (3D) calculation.*



QNuclei SOFTWARE · nuclear isotopes. *Initial window for Wave Function calculation.*

The algorithm for counting nucleons, which the program has, takes into account the degeneracy of quantum levels and allows us to see how the symmetrical energy acts in the nuclei. QNuclei is ab initio (from first principles) software. That is, you only have to enter the values of N (number of neutrons) and Z (number of protons) to perform the calculations. The program allows to see how the symmetrical energy acts in the nuclei.

The procedure that we are going to carry out will be the following.

1) Find a stable nucleus and get N and Z.
2) Adjust the value of c_sym (symmetry energy) with the following condition, Fermi level (neutrons)= Fermi level (protons).
3) We study the nucleus.

Characteristics

1. Easy to use. A few clicks are enough to obtain results (see DEMO version).
2. You can calculate the nuclear structure of all the elements in the periodic table.
3. QNuclei is an *ab initio* (from first principles) software. You only have to enter the values of N (number of neutrons) and Z (number of protons) to perform the calculations.
4. The wave function of all the protons and neutrons in a nucleus can be represented.
5. Export image files in GIF, JPG and NPG format.
6. You can calculate the Fermi level of any nucleus in the periodic table.

Advantages

1. It tells us the energy from which there are no nucleons at 0K temperature.
2. It allows to compare the energy of the nucleons and their rest mass to know the relativistic effects in the nuclei.
3. It allows obtaining the Fermi level without the continuum hypothesis, considering only discretized eigenvalues.
4. The algorithm for counting nucleons, which the program has, takes into account the degeneracy of quantum levels.
5. It allows to see how the symmetry energy acts in the nuclei. The symmetry energy cancels the electrostatic repulsion of the protons.
6. It allows studying hypothetical nuclei that are not found in nature due to their great instability, for example, nuclei with Z>N.
7. You can modify the thickness of the lines, the font sizes, the background colors,...
8. It allows knowing the Fermi temperature of a nucleus, from which the thermal effects are comparable to the quantum ones.
9. It allows scale changes in the energy axis of the nucleons.

Applications

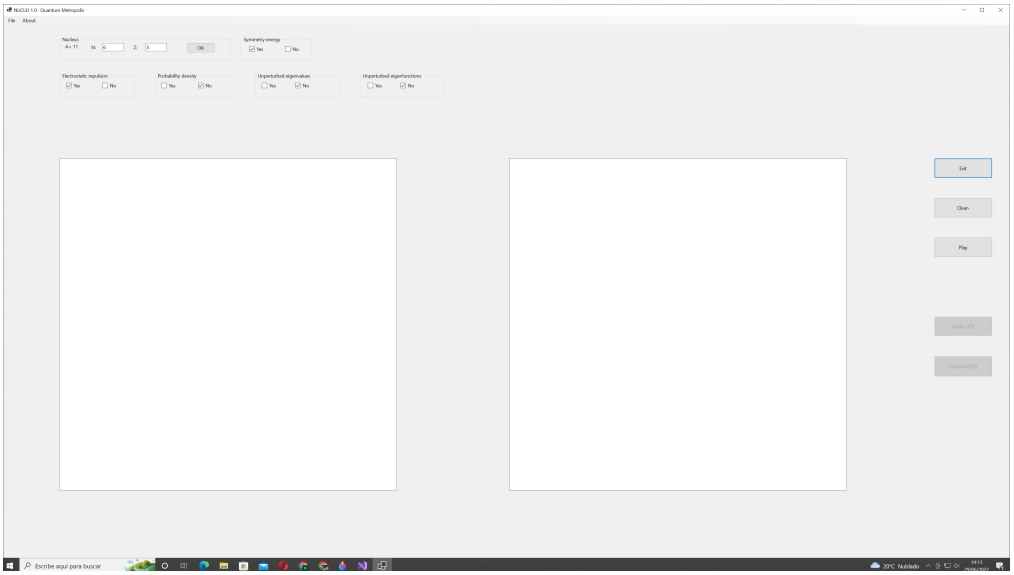
1. By not using the continuum hypothesis, we can obtain the individualized wave function of each of the nucleons.
2. It allows to estimate the symmetrical energy in the nuclei.
3. It allows evaluating the stability of a nucleus.

4. The algorithm allows to calculate the exact energy of the Fermi level, since it does not make use of the continuum hypothesis.
5. Relativistic effects on nucleons can be evaluated.
6. The number of holes for protons and neutrons in the last Fermi level can be obtained.

Input Data

Nuclei software is an *ab initio* program (since first principles) which simulates atomic nuclei. When starting the Nuclei software, we find the following window of the Program.

Initial Window



QNuclei SOFTWARE. *Initial software window. Nuclei software.*

This window corresponds to the Fermi Gas model for atomic nuclei.

N and Z numbers

In the upper left part of the window, we have the following controls.

QNuclei SOFTWARE. *Input data for nuclei.*

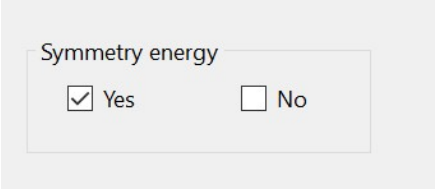
Here we write the number of protons (Z) and the number of neutrons (N) from the nucleus. Let us remember that A=Z+N where A is the number of nucleons. The number of nucleons (A) is the nearest integer to its atomic weight. The number of neutrons is N=A-Z. To get N and Z we do the following.

$_{Z}X^{A}$, element X.

For example, $_{11}Na^{23}$, (or $_{11}{}^{23}Na$), Z=11 and N=23-11=12.

After typing Z and N, you have to click on the "OK" button. Then, the program incorporates the new values for N and Z.

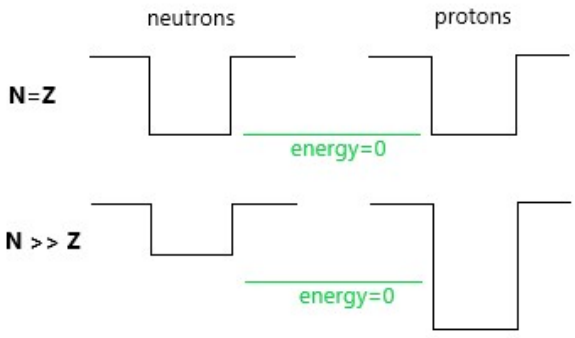
Symmetry energy



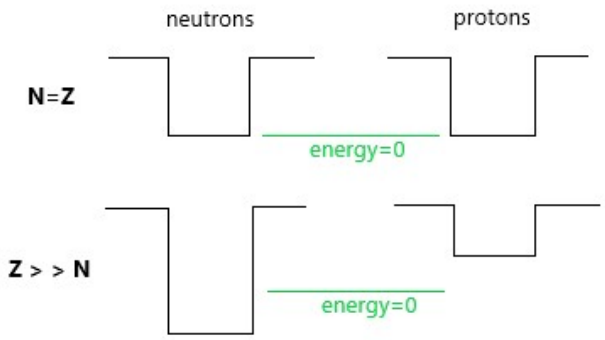
It is an important correction to the V (potential) value. The correction is known as symmetry energy, which arises from unequal numbers of neutrons and protons in the nucleus. A proton and a neutron can interact in more ways than two neutrons or two protons because in the latter cases, many of the interactions are forbidden by the Pauli exclusion principle. The effective force between a neutron and a proton is thus stronger than the others. Therefore, if a nucleus has more neutrons than protons, V is stronger for a proton, and weaker for a neutron, since its interaction is mostly with other neutrons. The shift in V, due to the symmetry energy (ΔV) , has been determined,

$\Delta V = \pm c\_sym \cdot (N-Z)/A$ (MeV)

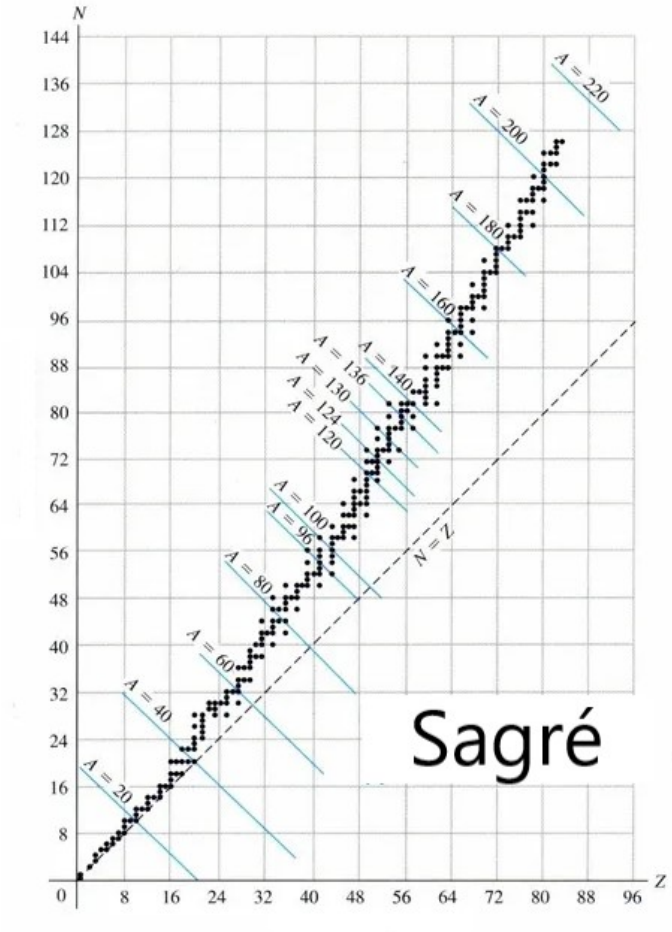
where (+) for protons and (-) for neutrons. c_sym is the symmetry energy coefficient. Its default value in QNuclei is 20 MeV.



QNuclei SOFTWARE · symmetry energy. *If N=Z, symmetry energy vanishes. If N>Z, symmetry potential is attractive for protons and repulsive for neutrons.*



QNuclei SOFTWARE · symmetry energy. *If N=Z, symmetry energy vanishes. If N>Z, symmetry potential is attractive for neutrons and repulsive for protons.*

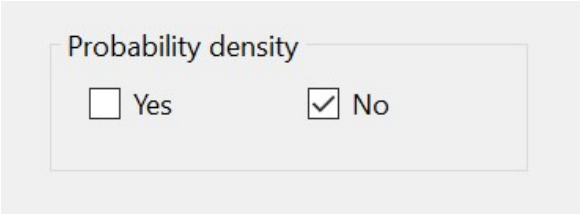


QNuclei SOFTWARE · symmetry energy. *Segre graph. Stable nuclei in nature.*

Several c_sym values (symmetry energy) for stable nuclei.

Z	N	A	c_sym (MeV)
8	10	18	20
16	20	36	30
20	24	44	37
32	40	72	43
40	52	92	49
56	80	136	45
64	93	157	47
80	120	200	50
88	132	220	54
103	159	262	56

Probability density



QNuclei SOFTWARE. *Probability density option.*

If [Yes] is chosen, the program will show the probability density $|\Psi|^2$ instead of the wave function Ψ.

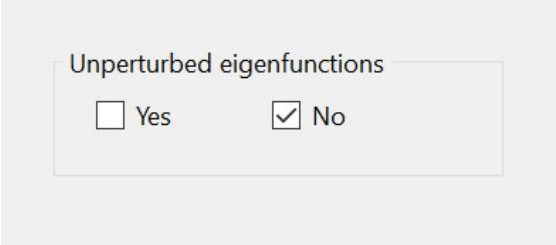
Unperturbed eigenvalues

In the upper left part of the window, we have the following controls.

QNuclei SOFTWARE. *Unperturbed eigenvalues option.*

If [Yes] is chosen, the program will also show the unperturbed eigenvalues. Unperturbed eigenvalues are calculation parameters in Perturbation Theory.

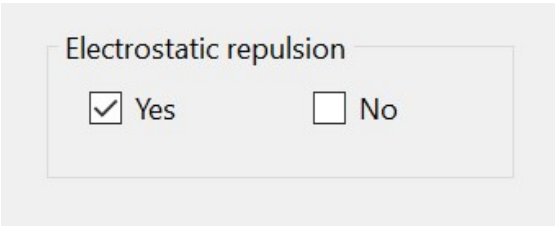
Unperturbed eigenfunctions



QNuclei SOFTWARE. *Unperturbed eigenfunctions option.*

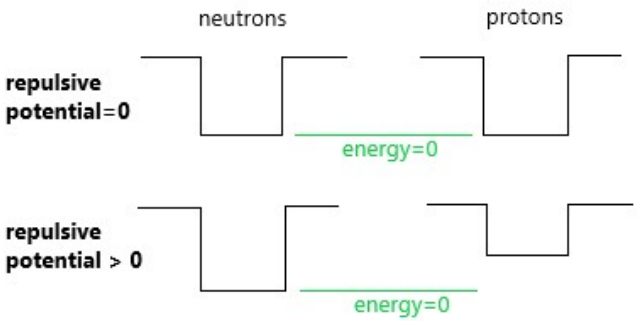
If [Yes] is chosen, the program will also show the unperturbed eigenfunctions. Unperturbed eigenfunctions are calculation parameters in Perturbation Theory.

Electrostatic repulsion



QNuclei SOFTWARE. *Electrostatic repulsion option.*

If [Yes] is chosen, the program will show the probability density $|\Psi|^2$ or the wave function Ψ considering electrostatic repulsion between protons.

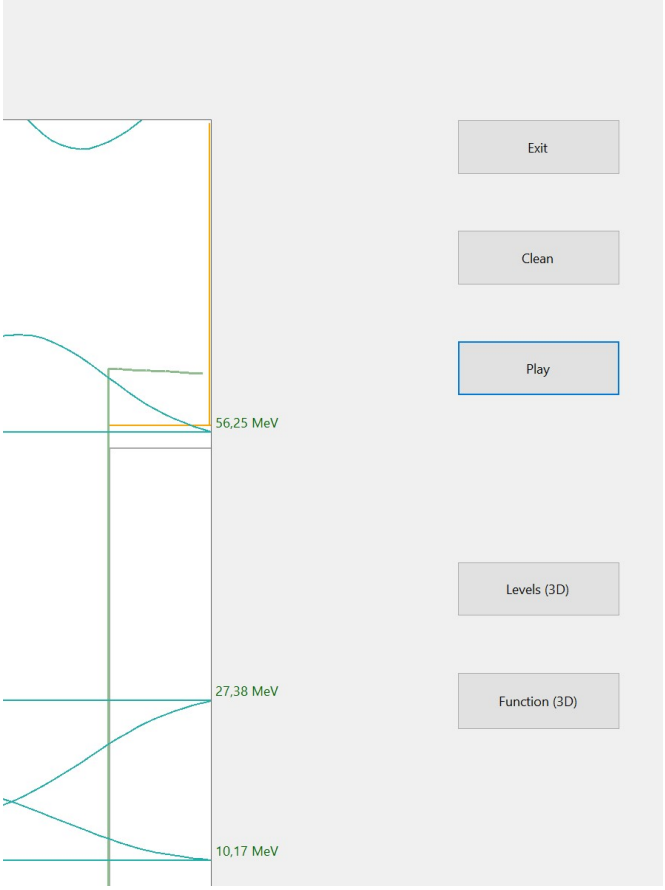


QNuclei SOFTWARE · electrostatic repulsion. *Without electrostatic repulsion, the potential is identical for neutrons and protons. With electrostatic repulsion, the potential is repulsive for protons.*

In nature, N>Z for stable nuclei. That is, the electrostatic potential and the potential due to symmetry energy cancel. When this happens, the protons and neutrons fill up to the same energy. In this way, the Fermi level for protons and neutrons coincide.

Buttons on the right side

On the right side of the window, we have the following controls.



QNuclei SOFTWARE. *Buttons on the right side of the window.*

Exit Exit the program.

Clear Clear the window.

Play or **Calculate** Compute to get results.

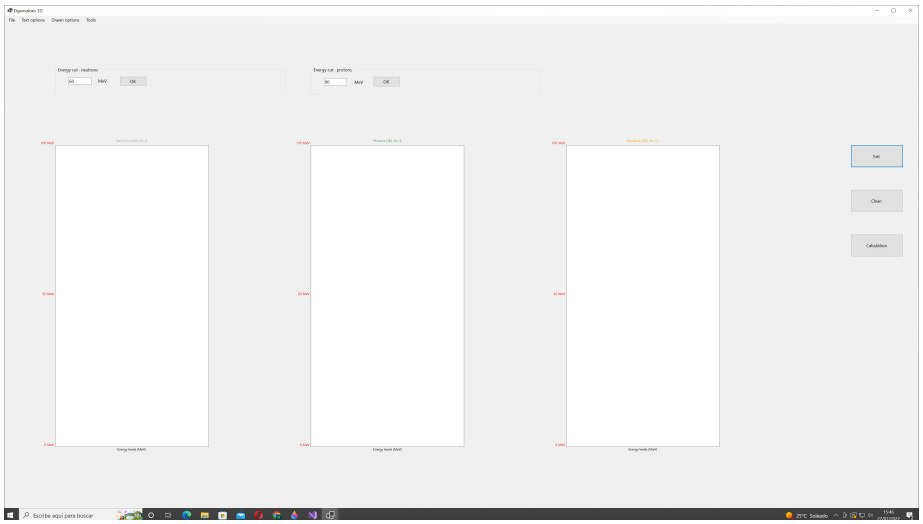
Levels (3D) This button is initially disabled. The button will be enabled after doing a calculation (Calculate button). A new program window will be displayed: Levels (3D) window.

Function (3D) This button is initially disabled. The button will be enabled after doing a calculation (Calculate button). A new program window will be displayed: Function (3D) window.

The procedure that we are going to carry out will be the following.

1) Find a stable nucleus and get N and Z.
2) Adjust the value of c_sym (symmetry energy) with the following condition, Fermi level (neutrons)= Fermi level (protons).
3) We study the nucleus.

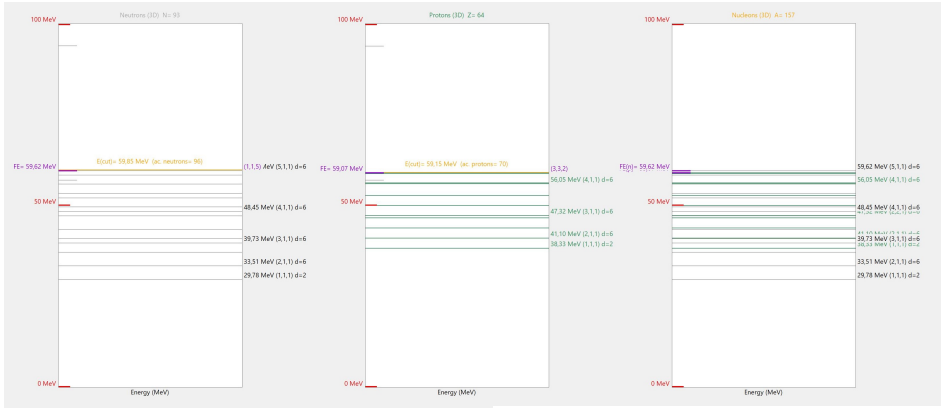
Eigenvalues (3D) Window



QNuclei SOFTWARE · nuclear fission. *Initial window for eigenvalues (3D) calculation.*

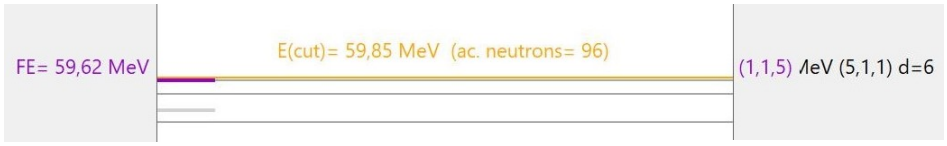
We can calculate nucleon energies considering 3D wave functions. Firstly, it is necessary to calculate (or recalculate) the 1D wave functions in the Main window of QNuclei.

For example, we obtain the next image.



QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels).*

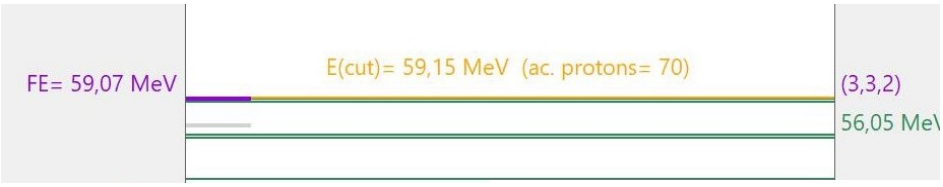
We now see that the Fermi level for protons and neutrons are practically identical. Now we look at the Fermi level for neutrons (see next image).



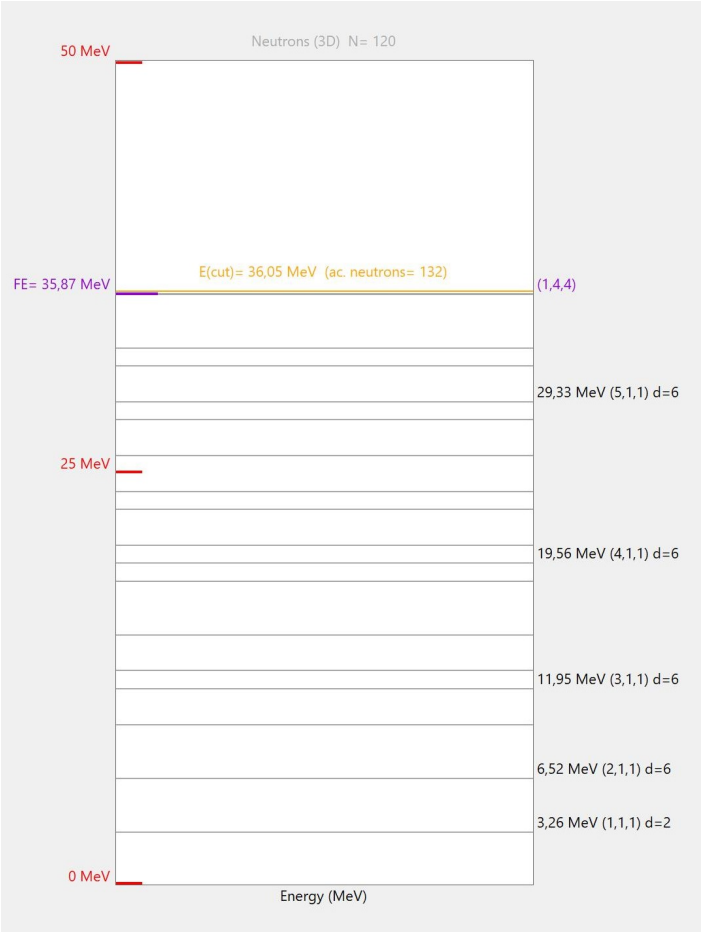
QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels). Neutrons (left column). The wave function at Fermi level is (1,1,5). Violet color. The software counts the possible states*

(nucleons) that are below an energy value 'E(cut)'. Accumulated neutrons= 96 and N=93. So that, we have 3 holes in the last eigenstate (3 unoccupied states).

Now we look at the Fermi level of the protons (see next image).



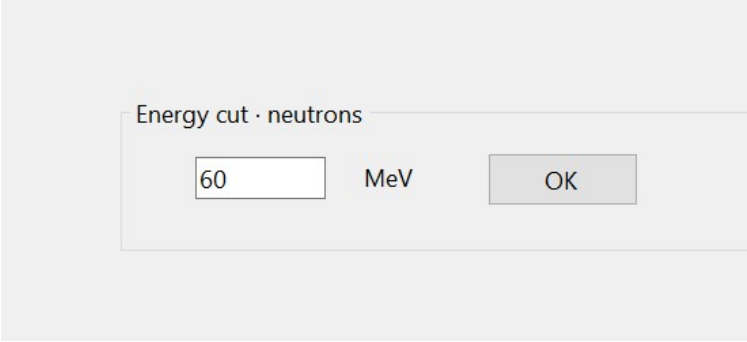
QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels). Protons (center column). The wave function at Fermi level is (3,3,2). Violet color. The software counts the possible states (nucleons) that are below an energy value 'E(cut)'. Accumulated protons= 70 and Z=64. So that, we have 6 holes in the last eigenstate (6 unoccupied states).*



QNuclei SOFTWARE · nuclear plant. *In the upper part of the figure (gray) we see that we are studying a nucleus with 120 neutrons (N=120). The cutoff energy has been calculated automatically (orange) and there are 132 states up to the Fermi level. So that, there are 12 holes (132-120) in the last level (Fermi level). On the right side (black), the levels of the type (X,1,1) are indicated, which are those of minimum energy with a value of n=X on one of their axes. The quantum degeneracy of the level is also indicated (d).*

Energy cut-off for neutrons

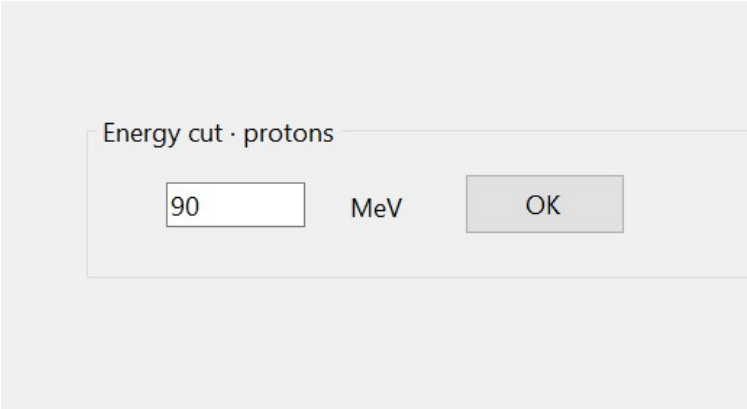
In the upper left part of the window, we have the following controls.



QNuclei SOFTWARE · nuclear fission. *Input data for QNuclei.*

You can write the energy cut-off value by hand. Otherwise, the energy cut-off value will be automatically obtained by the software.

Energy cut-off value for protons

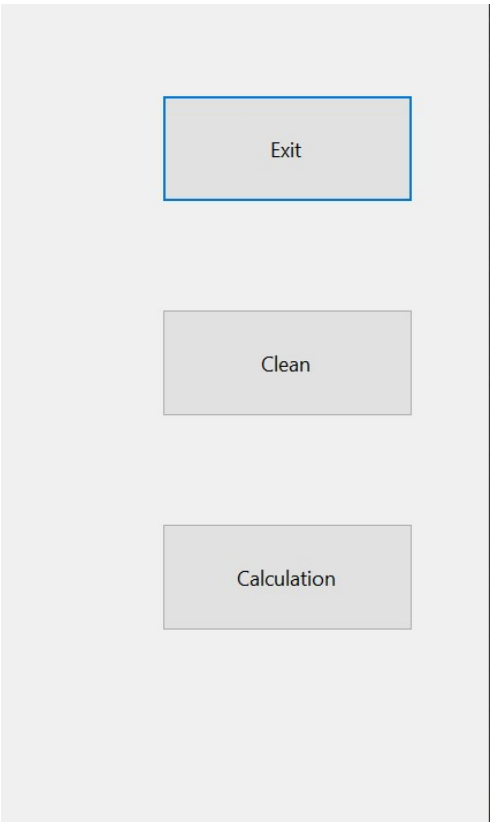


QNuclei SOFTWARE · nuclear fusion. *Electrostatic repulsion option.*

You can write the energy cut-off value by hand. Otherwise, the energy cut-off value will be automatically obtained by the software.

Buttons on the right side

On the right side of the window, we have the following controls.



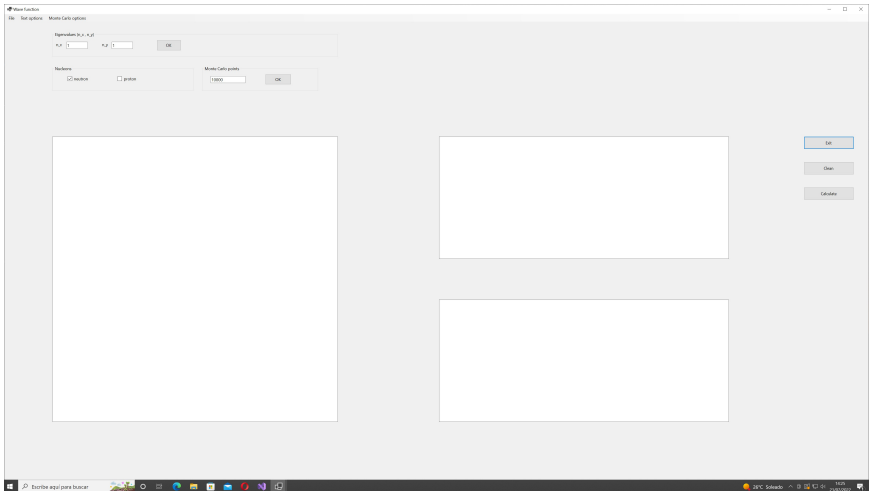
QNuclei SOFTWARE · nuclear fusion. *Buttons on the right side of the window.*

Exit Exit the program.

Clean Clean the window.

Play or **Calculate** Compute to get results.

Eigenfunctions Window



QNuclei SOFTWARE · nuclear isotopes. *Initial window for eigenfunctions calculation.*

This window corresponds to the Fermi Gas model for atomic nuclei. The 3D wave functions will be calculated through the Monte Carlo method of calculation and using the Metropolis algorithm.

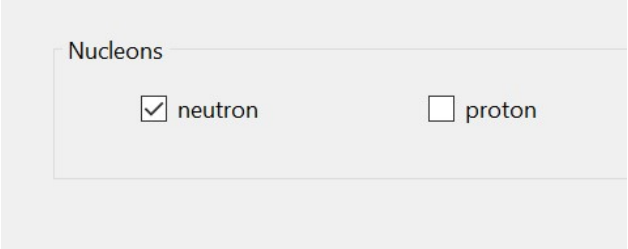
n_x and n_y numbers

In the upper left part of the window, we have the following controls.

QNuclei SOFTWARE · nuclear isotopes. *Input data for nuclei.*

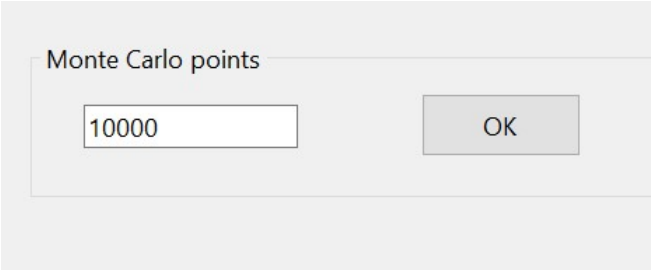
Here we write the n_x and n_y values. The 3D eigenfunction will be represented in a 2D plane. In our case, the probability in the z-axis will be taken to be equal to 1.

Neutron or proton



We can choose if the particle is a proton or a neutron. The 1D wave function will be taken to obtain a 3D eigenfunction through the Monte Carlo method of calculation and the Metropolis algorithm.

Number of Monte Carlo points

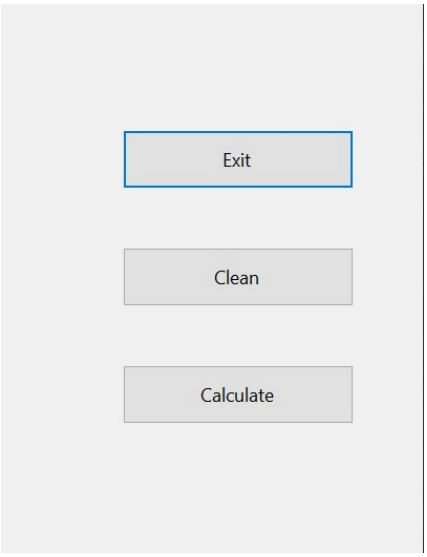


QNuclei SOFTWARE · nuclear industry. *Number of Monte Carlo points in the calculation.*

The number of Monte Carlo points will be used through the Metropolis algorithm.

Buttons on the right side

On the right side of the window, we have the following controls.



QNuclei SOFTWARE · nuclear industry. *Buttons on the right side of the window.*

Exit Exit the program.

Clear Clear the window.

Play or **Calculate** Compute to get results.

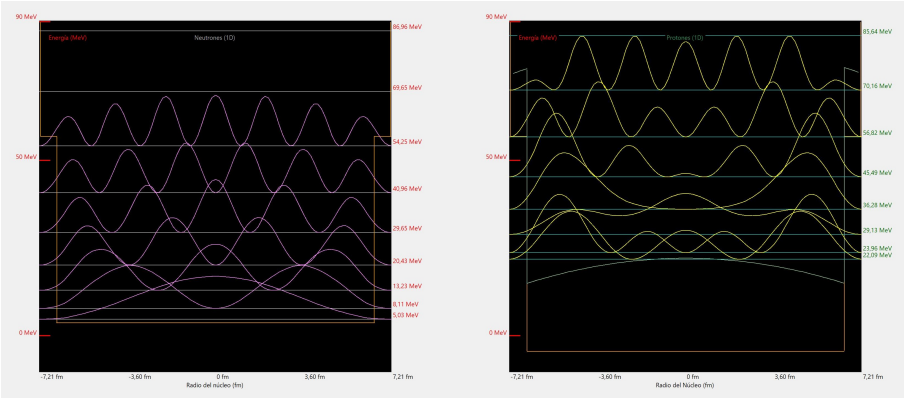
Exercises

Exercise 1.- Obtain the Fermi level for a barium nucleus Radium nucleus Ra (A=220, Z=88).

The number of protons is Z=88 and the number of neutrons is N=220-88=132. Then we start the program. We write the values of N and Z in the initial window of the program..

Start QNuclei Software >> Initial window >> button [Calculation]

Then we obtain the 1D eigenvalues and eigenfunctions (see next image)



QNuclei SOFTWARE · Fermi level · kinetic energy and potential energy. *1D probability density for a Radium nucleus.*

On the right side of the image we see that the electrical repulsion of the protons increases the energy of the protons. Next, in the initial window of the program we look for the options:

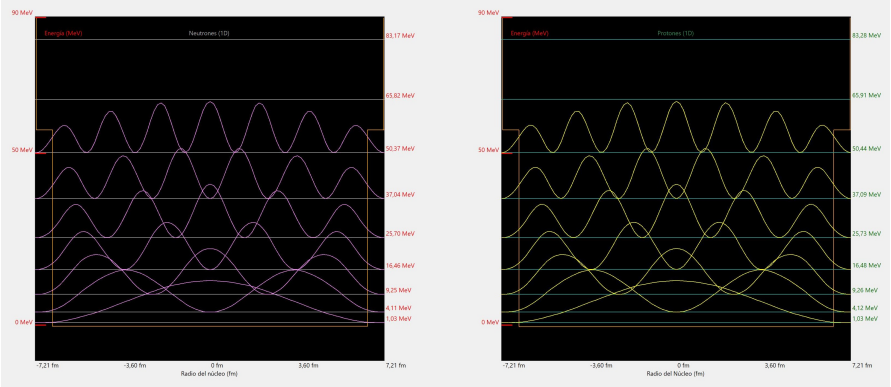
Initial window >> Symmetry energy >> [No]

Initial window >> Electrostatic repulsion >> [No]

We calculate again the 1D eigenvalues and eigenfunctions

Initial window >> button [Calculation]

We obtain the next image.

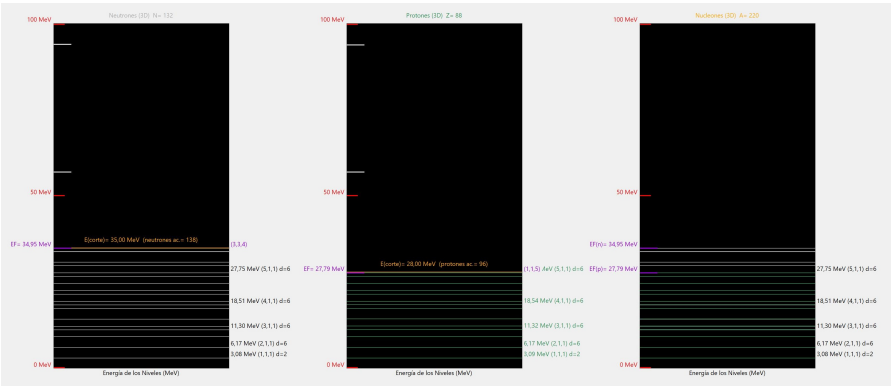


QNuclei SOFTWARE · Fermi level · nuclear kinetic energy and potential energy. *1D probability density for a Radium nucleus without electrostatic repulsion and without symmetry energy.*

We now see that the eigenvalues and wavefunctions for protons and neutrons are practically identical. Then in the initial window

Initial window >> button [Eigenvalues (3D)]

We obtain the following image in the Eigenvalues (3D) window



QNuclei SOFTWARE · Fermi level · nuclear kinetic energy and potential energy. *1D eigenvalues for a Radium nucleus without electrostatic repulsion and without symmetry energy.*

In the left column we have the levels of the neutrons without symmetric energy. At the top left we have a mark that indicates the value of the height of the 1D barrier (near 50MeV) and the value of 10% of the rest mass of the neutron (at almost 100 MeV). If we include the symmetric energy and the energy of the nucleon reaches such a value, relativistic effects will start to be important.

In the left column we have that the **Fermi level** of the neutrons is **34.95 MeV**. This will be the value of the Fermi level of a Barium nucleus. If the nucleus is stable and in equilibrium, the Fermi level for protons and neutrons coincide, that is, they are the same.

FE (Fermi Energy) = 34,95 MeV

Alternative method (Exercise 2).- To have the same Fermi value for neutrons and protons, we need to include both symmetric energy and electrostatic repulsion, which act in opposite directions. In such a case, we will adjust the value of the coefficient used by the model for the symmetric energy by trial (testing) . It is adjusted until both Fermi levels (protons and neutrons) coincide. Then, we calculate the difference between the Fermi energy and the

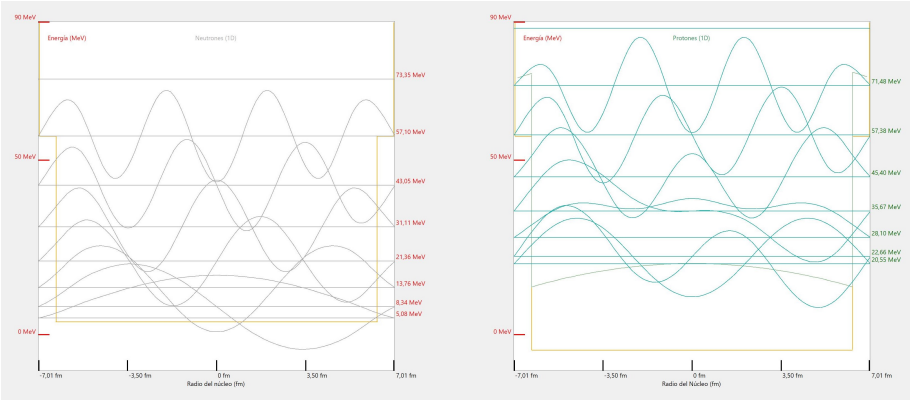
first energy value, which is approximately equal to FE= 34.95 MeV. The method, we have seen in this exercise, is easier.

<u>Exercise 2</u>.- Obtain the Fermi energy for a mercury nucleus Hg (A=200, Z=80) considering the symmetry energy and the electrostatic repulsion between protons.

The number of protons is Z=80 and the number of neutrons is N=200-80=120. Then we start the program. We write the values of N and Z in the initial window of the program..

Start *QNuclei Software >> Initial window >> button [Calculation]*

Then we obtain the 1D eigenvalues and eigenfunctions (see next image)

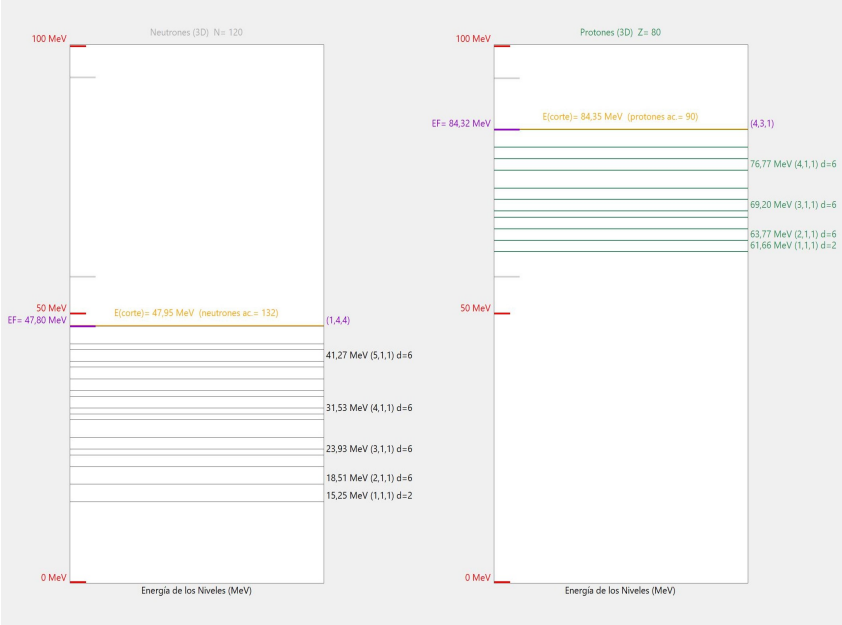


QNuclei SOFTWARE · nuclear reactor. *1D eigenfunctions for a Mercury nucleus in the initial window. The symmetry energy coefficient that we have used is 20 MeV (default value).*

On the right side of the image we see that the electrical repulsion of the protons increases the energy of the protons. Next, in the initial window of the program we look for the options:

Initial window >> button [Eigenvalues (3D)]

We obtain the next image.



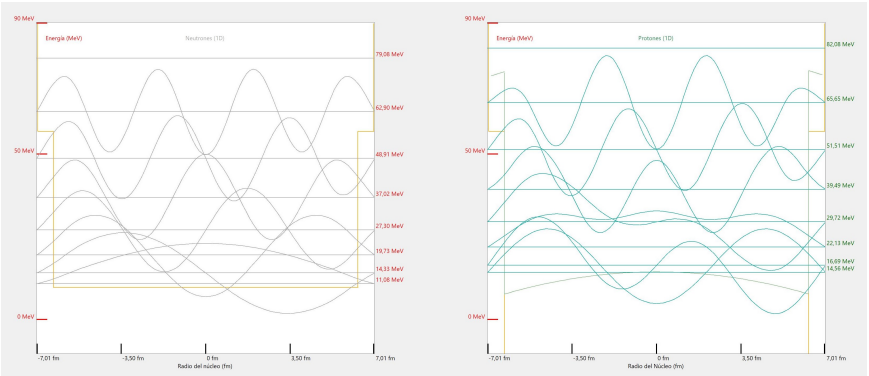
QNuclei SOFTWARE · nuclear reactor. *3D eigenvalues for a Mercury nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 20 MeV (default value).*

We now see that the Fermi levels for protons and neutrons are different. Therefore, WE CANNOT DEFINE a Fermi level. We have to go back to the initial window of the program, change the symmetry energy coefficient, recalculate the 1D levels, and recalculate the Eigenvalues (3D) again. It will have to be done, over and over again, until the Fermi levels of protons and neutrons match. We will define the Fermi level if, and only if, the values of the Fermi level for protons and neutrons are equal.

Initial window >> Menu >> Model options >> Model parameters >> Coefficient (MeV), symmetry energy >> 20MeV->50MeV. That is, c_sym=50MeV.

Initial window >> button [Calculation]

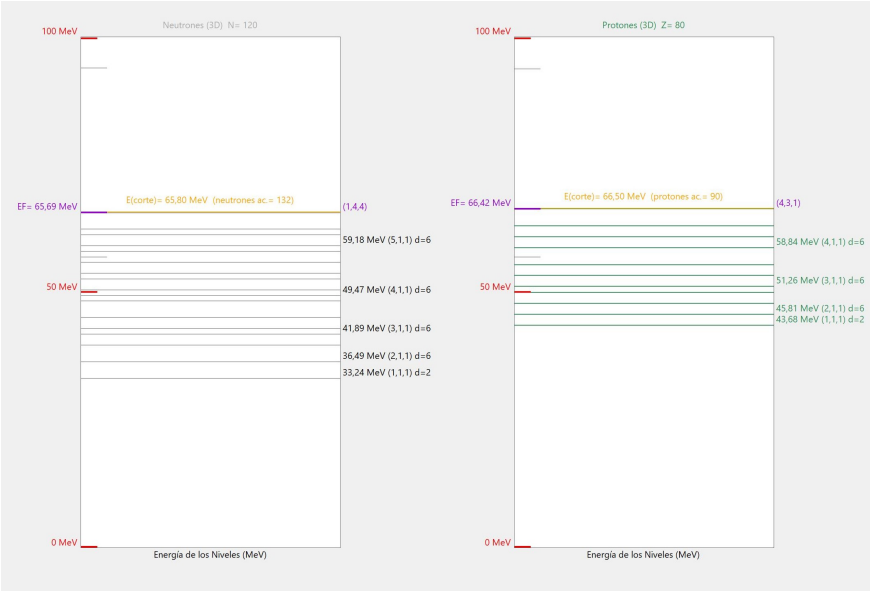
We obtain the following image in the initial window,



QNuclei SOFTWARE · nuclear reactor. *1D eigenfunctions for a Mercury nucleus in the initial window. The symmetry energy coefficient that we have used is 50 MeV.*

Next, in the initial window of the program we look for the options:
Initial window >> button [Eigenvalues (3D)]

We obtain the following image in the initial window,



QNuclei SOFTWARE · nuclear reactor. *3D eigenvalues for a Mercury nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 50 MeV (Such a value equals both Fermi levels).*

We have that the **Fermi level** of neutrons and protons is approximately equal and is worth about **66 MeV**. In the left column, we calculate the difference between the Fermi level (65.69 MeV) and the first level (33.24 MeV) which will be the Fermi energy of the nucleus.

EF= 65.69 - 33.24 MeV = 32.35 MeV

Most nuclei have a Fermi energy of 30 and few MeV.

Exercise 3.- Obtain the symmetry energy (c_sym value) for a Radium nucleus Ra (A=220, Z=88), which is stable.

The number of protons is Z=88 and the number of neutrons is N=220-88=132. Then we start the program. We write the values of N and Z in the initial window of the program.

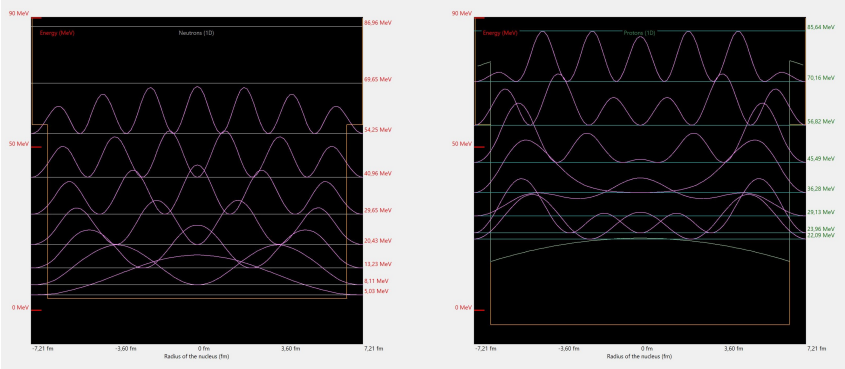
We remember that the effective force between a neutron and a proton is thus stronger than the others. Therefore, if a nucleus has more neutrons than protons, V is stronger for a proton, and weaker for a neutron, since its interaction is mostly with other neutrons. The shift in V, due to the symmetry energy (ΔV) , has been determined,

$\Delta V = \pm c\_sym \cdot (N-Z)/A$ (MeV)

where (+) for protons and (-) for neutrons. c_sym is the symmetry energy coefficient. Its default value in QNuclei is c_sym=20 MeV.

Start *QNuclei Software >> Initial window >> button [Calculation]*

Then we obtain the 1D eigenvalues and eigenfunctions (see next image)



QNuclei SOFTWARE · nuclear unit. *1D eigenfunctions for a Radium nucleus Ra (A=220, Z=88). Left: neutrons. Right: protons.* c_sym=20MeV.

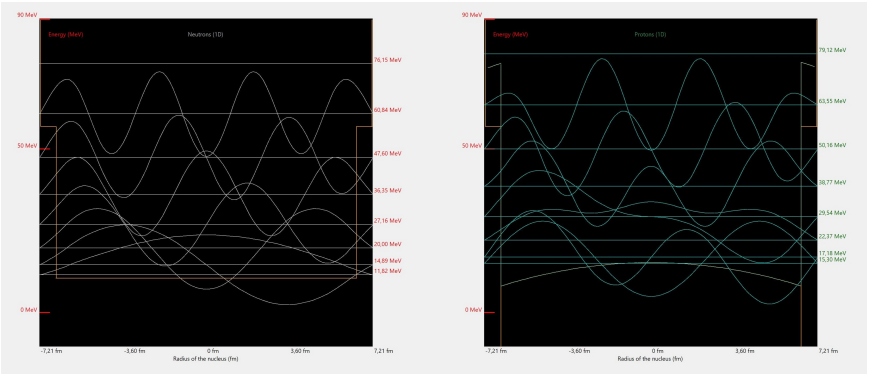
On the right side of the image we see that the electrical repulsion of the protons increases the energy of the protons.

We have to change the symmetry energy coefficient, recalculate the 1D levels, and recalculate the Eigenvalues again. It will have to be done, over and over again, until the energy levels of protons and neutrons match (as the same manner as in exercise 2). We will define the Fermi level if, and only if, the values of the Fermi level for protons and neutrons are equal.

Initial window >> Menu >> Model options >> Model parameters >> Coefficient (MeV), symmetry energy >> 20MeV->50MeV. That is, c_sym=50MeV.

Initial window >> button [Calculation]

We obtain the next image.

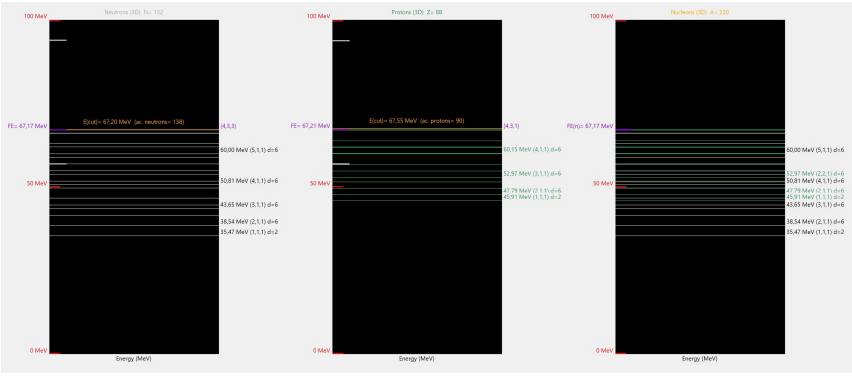


QNuclei SOFTWARE · nuclear unit. *1D eigenfunctions for a Radium nucleus Ra (A=220, Z=88). Left: neutrons. Right: protoes. c_sym=50MeV.*

We now see that the eigenvalues for protons and neutrons are practically identical. Then in the initial window

Initial window >> button [Eigenvalues (3D)]

We obtain the following image in the Eigenvalues (3D) window



QNuclei SOFTWARE · nuclear unit. *3D eigenvalues for a Radium nucleus (A=220, Z=88). Left: neutrons. Center: protons. Right: protons y neutrons. c_sym=50MeV.*

The Fermi level for protons and neutrons coincide, that is, they are the same.Then **c_sym=50MeV.**

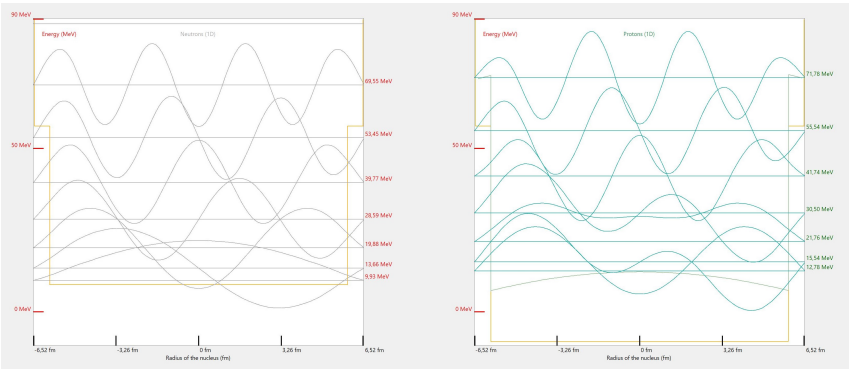
<u>Exercise 4</u>.- Obtain the wave functions at the Fermi level in a Gadolinium nucleus Gd (A=157, Z=64).

The number of protons is Z=64 and the number of neutrons is N=157-64=93. Then we start the program. We write the values of N and Z in the initial window of the program.

Initial window >> Menu >> Model options >> Model parameters >> Coefficient (MeV), symmetry energy >> 20MeV -> 47MeV. That is, c_sym=47MeV (such a c_sym value has been obtained as the same manner as exercise 3). Then,

Initial window >> button [Calculation]

Then we obtain the 1D eigenvalues and eigenfunctions (see next image)

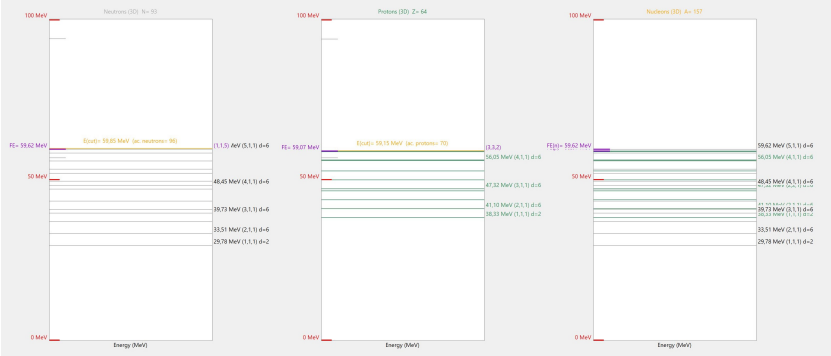


QNuclei SOFTWARE · nuclear plant. *1D eigenfunctions for a Gadolinium nucleus Ga (A=157, Z=64). Left: neutrons. Right: protons.* c_sym=47MeV.

On the right side of the image we see that the electrical repulsion of the protons increases the energy of the protons. Both neutron and proton levels are aligned.

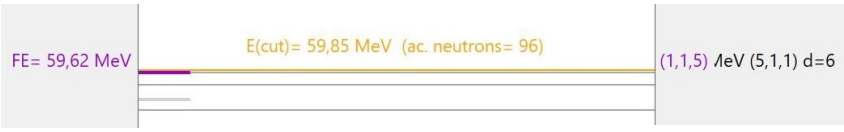
Initial window >> [Levels (3D)]

We obtain the next image.



QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels).*

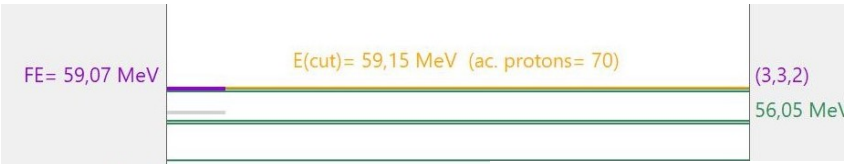
We now see that the Fermi level for protons and neutrons are practically identical. Now we look at the Fermi level for neutrons (see next image).



QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels). Neutrons (left column). The wave function at Fermi level is (1,1,5). Violet color.*

The wave function at the Fermi level for neutrons is (1,1,5). In a 2D representation, we have two possibilities (1,1) y (1,5) for the neutrons. A third axis with probability equal to 1 can be supposed in our 2D representation. (1,5) refers to n_x=1 and n_y=5 in our current notation.

Now we look at the Fermi level of the protons (see next image).



QNuclei SOFTWARE · nuclear plant. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV (Such a value equals both Fermi levels). Protons (center column). The wave function at Fermi level is (3,3,2). Violet color.*

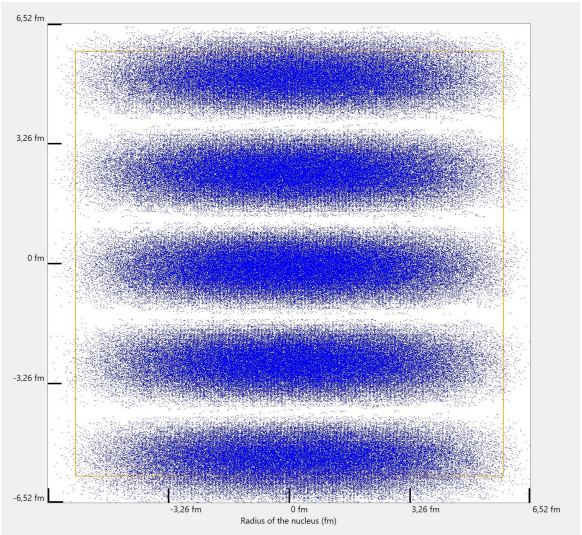
The wave function at the Fermi level for neutrons is (3,3,2). In a 2D representation, we have two possibilities (3,3) y (3,2) for the protons. A third axis with probability equal to 1 can be supposed in our 2D representation. (3,2) refers to n_x=3 and n_y=2 in our current notation.

Then in the initial window

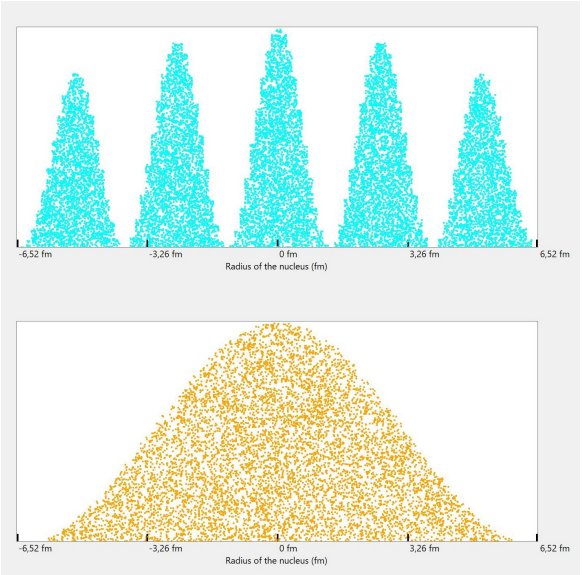
Initial window >> button [Function (3D)]
Function (3D) window >> Nucleon -> neutron

Function (3D) window >> n_x -> 1 , n_y -> 5
Function (3D) window >> button [Calculation]

We obtain the following image in the Function (3D) window



QNuclei SOFTWARE · nuclear plant. *3D probability density for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Neutron eigenfunction. The wave function at Fermi level is (n_x=1 , n_y=5).*



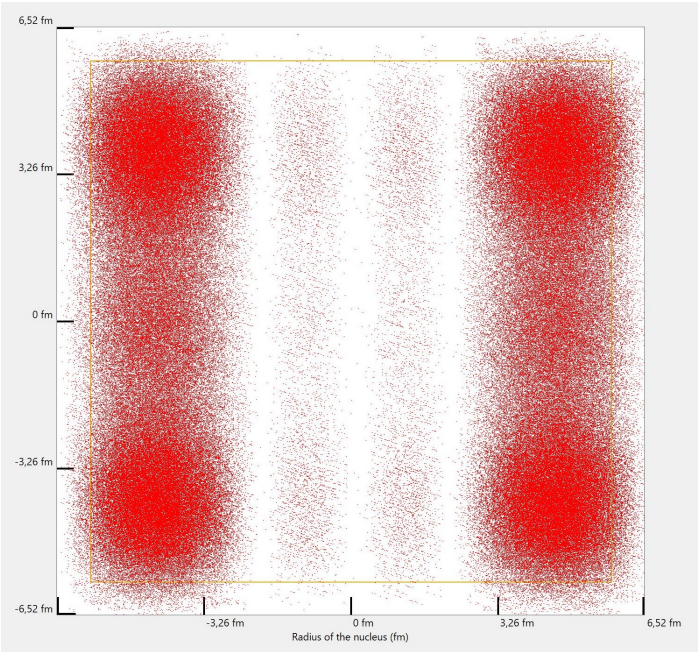
QNuclei SOFTWARE · nuclear plant. *Metropolis algorithm has been applied to obtain a 3D probability density for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Neutron eigenfunction. The wave function at Fermi level is (n_x=1 , n_y=5).*

Then in the initial window

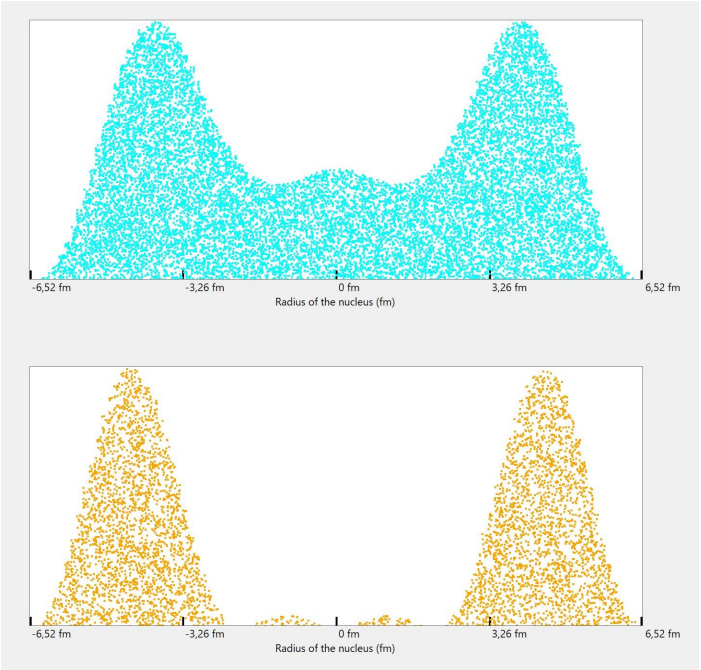
Initial window >> button [Function (3D)]
Function (3D) window >> Nucleon -> proton

Function (3D) window >> n_x -> 3 , n_y -> 2
Function (3D) window >> button [Calculation]

We obtain the following image in the Function (3D) window



QNuclei SOFTWARE · nuclear plant. *3D probability density for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Proton eigenfunction. The wave function at Fermi level is (n_x=3 , n_y=2).*



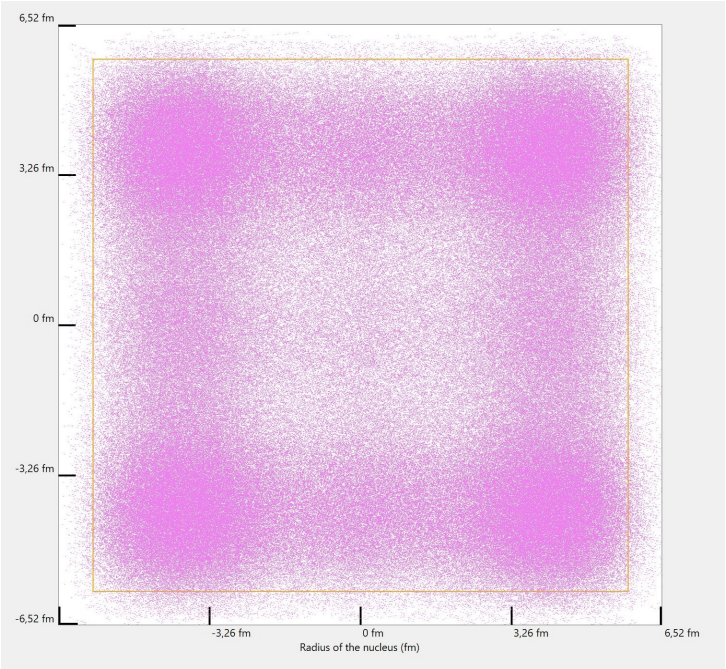
QNuclei SOFTWARE · nuclear plant. *Metropolis algorithm has been applied to obtain a 3D probability density for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Proton eigenfunction. The wave function at Fermi level is (n_x=3 , n_y=2).*

Then in the initial window

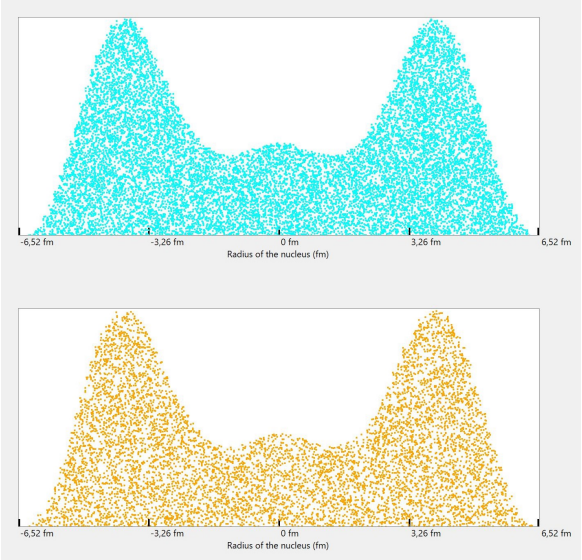
Initial window >> button [Function (3D)]
Function (3D) window >> Nucleon -> proton

Function (3D) window >> n_x -> 3 , n_y -> 3
Function (3D) window >> button [Calculation]

We obtain the following image in the Function (3D) window



QNuclei SOFTWARE · nuclear plant. *3D probability density for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Proton eigenfunction. The wave function at Fermi level is (n_x=3 , n_y=3).*



QNuclei SOFTWARE · nuclear plant. *Metropolis algorithm has been applied to obtain a 3D probability density for a Gadolinium nucleus with electrostatic repulsion and with*

symmetry energy. The symmetry energy coefficient that we have used is 47 MeV. Proton eigenfunction. The wave function at Fermi level is (n_x=3 , n_y=3).

Model

The nucleus is made up of neutrons and protons, two particles which are 1840 times more massive than electrons. Number of protons (p+) in a nucleus is Z (atomic number). The number of nucleons (A) is the integer closest to its atomic weight. Number of neutrons N=A-Z.

$_ZX^A$, element X.

For example, $_{11}Na^{23}$, (or $_{11}{}^{23}Na$), Z=11 and N=23-11=12.

All these phenomenological investigations have provided a remarkably simple relation for the radial size of the nucleus as a function of its nucleon number A R = r_0 A^(1/3) = 1.2 A^(1/3) fm. All results can be approximately explained by a charge distribution ρ given by

$$\rho(r) = \frac{\rho_0}{1 + \exp\left[\frac{r - R}{a}\right]}$$

(Equation 4)

where the nucleon density ρ_0 is 1.65·10^(44) nucleons/m^3 = 0.165 nucleons/fm^3.

$R \sim 1.07 \cdot A^{1/3}$ fm

a~0.55 fm

$1fm = 10^{-15}m$

(Equation 5)

$1\ eV = 1.6 \cdot 10^{-19}\ J$

$1MeV = 1.6 \cdot 10^{-13}\ J$

(Equation 3)

The energies of beta rays and gamma rays emitted from nuclei are of the order of 1 MeV. We calculate the electrostatic energy Ec required to insert a proton into a nucleus. This is approximately

$$E_c = \frac{Ze^2}{4\pi\epsilon_0}$$

(Equation 6)

This much coulomb energy would be released if the proton were allowed to come out of the nucleus, but still it does not ordinarily come out. This means that it is bound in the nucleus by even more energy. Since the velocity of a 10 MeV nucleon is only about 15 percent of

the speed of light (c), this means that relativistic effects are not important in considering the motion of nucleons in the nucleus.

Since the potential well is caused by the forces between nucleons, it seems reasonable to assume

that the depth of the well should be proportional to the density of nucleons. The potential is therefore

taken as,

$V= -V_0/ \{1+ \exp[(r- R)/ a]\}$.

The constants are V_0=57 MeV + corrections

$R = r_0 A^{(1/3)} = 1.2 A^{(1/3)}$ fm

a= 0.65 fm

Symmetry energy

The potential for a nucleus is therefore taken as,

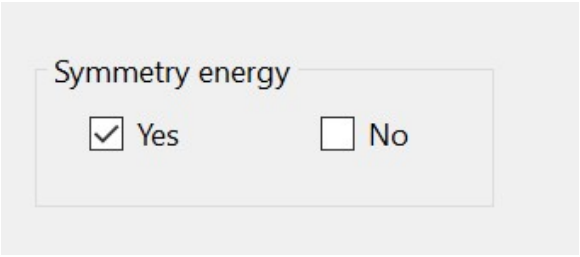
$V= -V_0/ \{1+ \exp[(r- R)/ a]\}$.

The constants are V_0=57 MeV + corrections

$R = r_0 A^{(1/3)} = 1.2 A^{(1/3)}$ fm

a= 0.65 fm

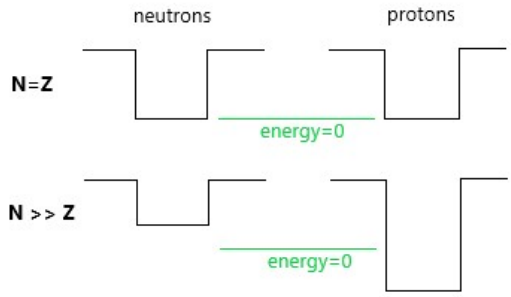
The most important correction to the value of V_0 is due to what is known as symmetry energy.
In the initial window, we can include symmetry energy effects on the results.



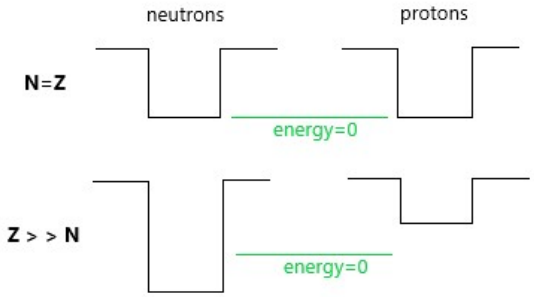
The correction is known as symmetry energy, which arises from unequal numbers of neutrons and protons in the nucleus. A proton and a neutron can interact in more ways than two neutrons or two protons because in the latter cases, many of the interactions are forbidden by the Pauli exclusion principle. The effective force between a neutron and a proton is thus stronger than the others. Therefore, if a nucleus has more neutrons than protons, V is stronger for a proton, and weaker for a neutron, since its interaction is mostly with other neutrons. The shift in V, due to the symmetry energy (ΔV), has been determined,

$\Delta V= \pm c_{sym} \cdot (N-Z)/A$ (MeV)

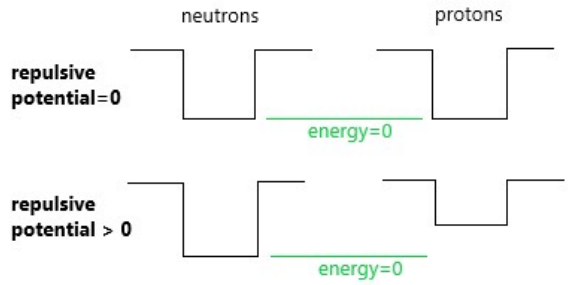
where (+) for protons and (-) for neutrons. c_{sym} is the symmetry energy coefficient. Its default value in QNuclei is c_{sym}=20 MeV.



QNuclei SOFTWARE · symmetry energy. *If N=Z, symmetry energy vanishes. If N>Z, symmetry potential is attractive for protons and repulsive for neutrons.*



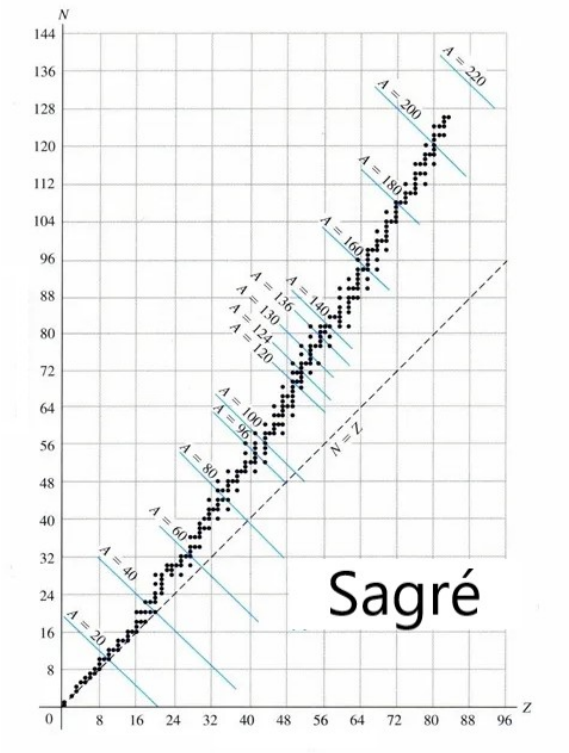
QNuclei SOFTWARE · symmetry energy. *If N=Z, symmetry energy vanishes. If N>Z, symmetry potential is attractive for neutrons and repulsive for protons.*



QNuclei SOFTWARE · electrostatic repulsion. *Without electrostatic repulsion, the potential is identical for neutrons and protons. With electrostatic repulsion, the potential is repulsive for protons.*

In nature, N>Z for stable nuclei. That is, the electrostatic potential and the potential due to symmetry energy cancel. When this happens, the protons and neutrons fill up to the same energy. In this way, the Fermi level for protons and neutrons coincide. The procedure that we are going to carry out will be the following.

1) Find a stable nucleus and get N and Z.
2) Adjust the value of c_sym (symmetry energy) with the following condition, Fermi level (neutrons)= Fermi level (protons).
3) We study the nucleus.



QNuclei SOFTWARE · symmetry energy. *Segre graph. Stable nuclei in nature.*

Several c_sym values (symmetry energy) for stable nuclei.

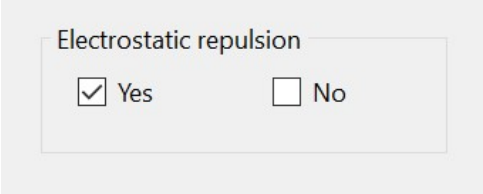
Z	N	A	c_sym (MeV)
8	10	18	20
16	20	36	30
20	24	44	37
32	40	72	43
40	52	92	49
56	80	136	45
64	93	157	47
80	120	200	50
88	132	220	54
103	159	262	56

Electrostatic repulsion between protons

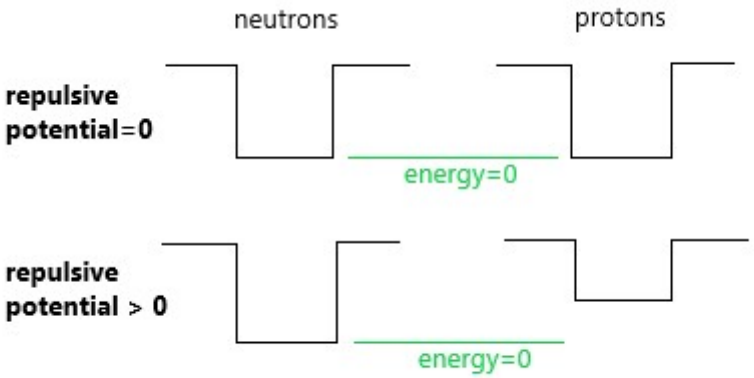
The potential energy is defined in electrostatics as,

$V(r)= (k Z e^2/ r^2) \{ 1+ ½ [1- (r/ R)^2] \}$.

This potential is therefore 1½ times larger at the center of the nucleus than at the edge. An spherically symmetric charge distribution has been considered in our model [COHEN].



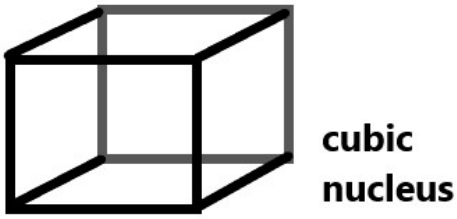
QNuclei SOFTWARE · nuclear data. *Electrostatic repulsion option. Initial window.*



QNuclei SOFTWARE · nuclear data. *If N=Z, symmetry energy vanishes. If N>Z, symmetry potential is attractive for neutrons and repulsive for protons.*

Model symmetry

To simplify, and without loss of generality, a cubic nucleus will be considered in this model.



QNuclei SOFTWARE · nuclear data. *A cubic nucleus.*

Then, we can simplify the electrostatic potential and the nuclear potential,

V(r)= V(x)+ V(y)+ V(y) [electrostatic potential]

for the electrostatic potential and for the nuclear potential,

V(r)= V(x)+ V(y)+ V(y) [nuclear potential].

Inside the cube, the nuclear potential is zero V_0=0MeV. Outside the cube, the nuclear potential is V_0=57MeV [COHEN]. This is the Fermi Gas model. To solve the Fermi gas model, we need Quantum Mechanics.

The infinite quantum well

The infinite quantum well V(x) is

V(x)=infinity, if x < 0 or x > L

V(x)=0, if 0 < x < L

So the particle is trapped between x=0 and x=L. The walls at x=0 and x=L are absolutely impenetrable. The particle is never outside the well and Ψ(x)=0 for x=0 or x=L. Inside the well, the Schrödinger equation has a simple form and we can solve it. Then,

$\Psi = A \sin(kx) + B \cos(kx)$

The continuity condition on Ψ at x=0 gives Ψ(0)=0, which is true only for B=0. At x=L, the continuity condition on Ψ gives

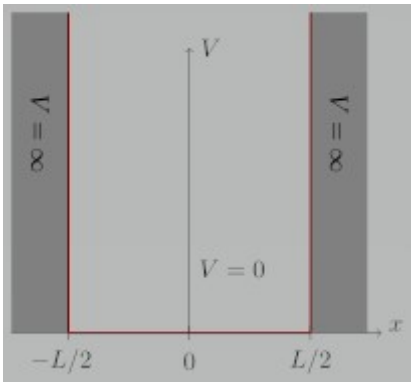
$A \sin(kL)=0$

Thus, $kL = n\pi$, n=1, 2, 3,... and then,

$E_n = \hbar^2 k^2 /2m = \hbar^2 \pi^2 n^2 /(2mL^2)$

Here the energy is quantized, i.e., only certain values of the energy are permitted. These states are bound states and the corresponding wave functions are

$\Psi_n = (2/L)^{1/2} \sin(n\pi x / L)$.



Infinite quantum well potential.

The finite quantum well

For this case, we assume the well has depth V_0 between -L/2 and L/2.

$V(x) = V_0$, if |x| > L/2

V(x)=0, if |x| < L/2

Now we look for bound-state solutions, with $E<V_0$. The solutions are

$\Psi_1(x) = A \exp(k_1 x) + B \exp(-k_1 x)$, if x < L/2

$\Psi_2(x) = C \exp(i k_2 x) + D \exp(-i k_2 x)$, if -L/2 < x < L/2

$\Psi_3(x) = F \exp(k_1 x) + G \exp(-k_1 x)$, if x > L/2

where $k_1 = [2m(V_0 - E)/\hbar^2]^{1/2}$ and $k_2 = [2mE/\hbar^2]^{1/2}$. To keep the wave function finite in region I, when x -> infinity, we require F = 0.

Applying the continuity conditions at x=-L/2 and at x=L/2, we find the following two relationships.

$k_2 \tan(k_2 L/2) = k_1$

$-k_2 \cot(k_2 L/2) = k_1$

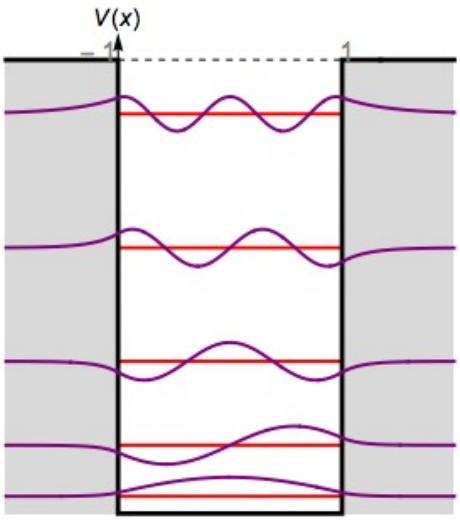
These transcendental equations cannot be solved directly. They can be solved numerically on a computer, or graphically. We rewrite the equations in the following form:

$\alpha \tan(\alpha) = (P^2 - \alpha^2)^{1/2}$

$-\alpha \cot(\alpha) = (P^2 - \alpha^2)^{1/2}$

where $\alpha = k_2 L/2$ and $P = (mV_0 L^2/2\hbar^2)^{1/2}$.

The right side of these equations defines a circle of radius P. The solutions are determined by the points where the circle intersects the tangent function, as shown in figure. Therefore, the number of solutions is determined by the radius P, and thus by the depth V_0 of the well.



Finite quantum well potential.

The infinite quantum well in 3D

We begin with a 3D potential in cartesian coordinates,

V(x, y, z) = 0, if 0 < x < L, 0 < y < L, 0 < z < L

V(x, y, z) = infinity, if L < x or x < 0, L < y or y < 0, L < z or z < 0.

The particle is then confined to a cubical box of dimension L. Beyond the impenetrable walls of the wells, Ψ=0 as before. Inside the well, the Schrödinger equation is

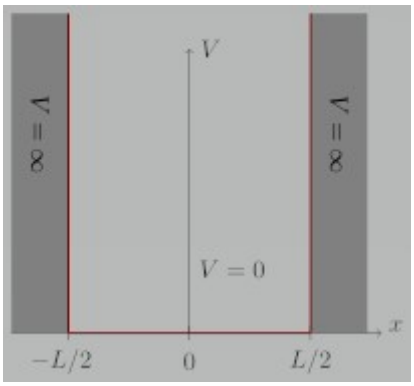
$-(\hbar^2/2m)[\,\partial^2/\partial x^2 + \partial^2/\partial x^2 + \partial^2/\partial x^2\,]\Psi(x, y, z) = E\,\Psi(x, y, z)$

The usual procedure for solving partial differential equations is to try to find a separable solution, with $\Psi(x, y, z)=X(x)\cdot Y(y)\cdot Z(z)$, where X, Y and Z are each functions for a single variable. We will skip the mathematical details and give only the result of the calculation.

$\Psi(n_1, n_2, n_3)=(2/L)^{3/2}\sin(n_1\pi x/L)\sin(n_2\pi y/L)\sin(n_3\pi z/L)$

$E(n_1, n_2, n_3)=(\hbar^2\pi^2/2mL)(n_1^2+n_2^2+n_3^2)$

where n_1, n_2 and n_3 are independent integers greater then zero and refer to x, y and z axis, respectively. The lowest state has quantum numbers (1, 1, 1). Its probability distribution would show a maximum at the center of the box. (x=y=z=L/2).



Infinite quantum well potential.

Quantum degenerancy

The Pauli exclusion principle in quantum mechanics tells us that two nucleons cannot have the same quantum numbers. For example, two protons can occupy the (1,1,1) state because they have different spins, +1/2 and -1/2. In such a case, the system is degenerated in energy. The energy of both +1/2 and -1/2 protons is the same.

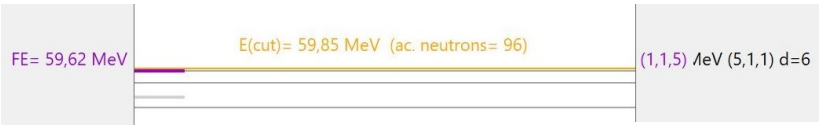
The first excited state has three possible sets of quantum numbers, (2, 1, 1), (1, 2, 1) and (1, 1, 2). In addition, we have two different possibilities for each quantum state due to the nucleon spin. It is a quantum degenerated state. The degenerancy is equal to 6, i.e., d=6.

Quantum State (example)	Degenerancy (d)
(1,1,1)	2
(2,1,1)	6
(1,2,3)	12

The (3,3,3) quantum state has the same energy than the (5,1,1) eigenstate, i.e., $3^2+3^2+3^2=5^2+1^2+1^2$. In such a case, the quantum degenerancy is d=2+6=8.

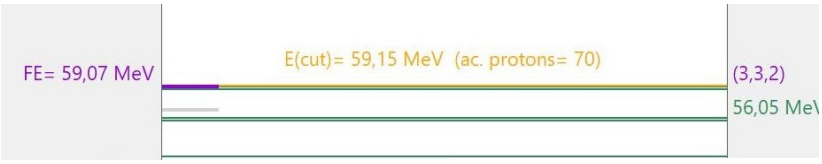
The nucleons occupy the possible states from the lowest energy to the last. The difference in energy between the last and the first state is the Fermi energy. We are zero temperature.

In the Level (3D) window



QNuclei SOFTWARE · Fermi gas. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. N=93. The software counts the possible states (nucleons) that are below an energy value 'E(cut)'. Accumulated neutrons= 96 and N=93. So that, we have 3 holes in the last eigenstate (3 unoccupied states).*

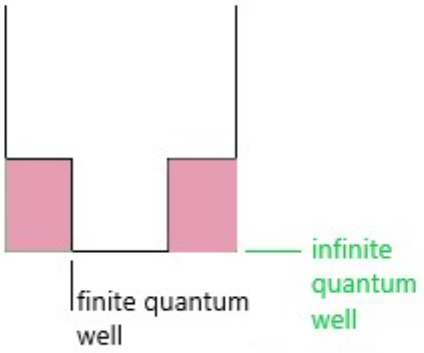
Now we look at the Fermi level of the protons (see next image).



QNuclei SOFTWARE · Fermi gas. *3D eigenvalues for a Gadolinium nucleus with electrostatic repulsion and with symmetry energy. Z=64. The software counts the possible states (nucleons) that are below an energy value 'E(cut)'. Accumulated protons= 70 and Z=64. So that, we have 6 holes in the last eigenstate (6 unoccupied states).*

Calculations

The software considers the nucleus as a finite quantum well, but in order to solve it we will use the infinite well solutions. In the graph below we have the well with infinite walls and the finite well. In order to solve the finite well, it is necessary to use the perturbation theory of quantum mechanics.



The pink part of the potential can be treated by perturbation theory.

Nondegenerate time-independent perturbation theory:

Suppose we have solved the time-independent Schrödinger equation for some potential.

$H_0 \Psi_n^{(0)} = E_n \Psi_n^{(0)}$

Obtaining a complete set of othonormal eigenfunctions, $\{ | \Psi_n^{(0)} > \}$ and the corresponding eigenvalues $\{ E_n^{(0)} \}$.
Now we perturb the potential slightly. Perturbation theory is a systematic procedure for obtaining approximate

solutions to the perturbed problem by building on the exact solutions to the unperturbed case.
We write the new Hamiltonian as the sum of two terms

$H = H_0 + \lambda H'$

and then

$H |\Psi_n\rangle = E_n |\Psi_n\rangle$

writing $|\Psi_n\rangle$ and E_n as power series in lambda.