Code–Guide for coordinate space spherical Hartree–Fock Solver

TALENT 4 Course: DFT

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Chapter 1

Numerical methods

1.1 Mesh choice

The choice of the mesh depends on the problem we need to treat. Given a function $f(x)$ defined on a given domain $\mathcal{D}$, the optimal choice of the mesh is related to the knowledge of the function $f(x)$ (irregularities? strong oscillations?) and on the domain (finite, infinite?).

For example we could adopt a uniform mesh for a finite domain as $\mathcal{D} = [0, R]$ so that $h = \frac{R}{N_{points}}$.[1].

On the contrary if we want to use an infinite domain $\mathcal{D} = [-\infty, +\infty]$, we could use as a mesh the zero of the Hermite polynomial of order N. This can be very well adapted to treat finite nuclei which are localised in space although the wavefunctions extend to infinity (exponential decay).

1.2 Numerical derivation methods

The derivative, if it exist, is defined as the limit of the Newton's difference quotient

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}, \tag{1.1}$$

thus the algorithms for numerical derivation are based on the calculation of finite differences coefficients for the approximation of this quotient.

Forward (or backward) differences

First order of convergence is just the definition of the Newton's quotient

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \tag{1.2}$$

where h is the mesh spacing. Precision is given by $\frac{f''(x)}{2}h$

Given a uniform mesh, the difference can be calculated with second order accuracy as

$$f'(x) \approx \frac{2f(x+h) - 3f(x)/2 - f(x+2h)/2}{2h}. \tag{1.3}$$

Symmetric differences

Symmetric differences are more precise for computational cost, however cannot be always applied (in proximity of the extremes or singularities). Second order is given by

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}, \tag{1.4}$$

[1] In some cases to avoid knowing the function at 0 one could shift the mesh of $\frac{h}{2}$

and precision is given by $\frac{f'''(x)}{6}h^2$.

Fourth order

$$f'(x) \approx \frac{f(x+2h)/12 - 2f(x+h)/3 + 2f(x-h)/3 - f(x-2h)/12}{4h}. \tag{1.5}$$

1.3 Numerical integration methods

There are several integration methods with different grades of efficiency and resiliency.

1.3.1 Newton–Cotes based algorithms

Newton–Cotes formulae are a class of numerical integration methods on the mesh that rely on the approximation of the function to be integrated with progressively higher degree of interpolation. Higher degree guarantee a faster convergence respect to the mesh size, however are potentially unstable for wildly oscillating functions.

Midpoint rule

Midpoint rule approximates the function's integral with a sum of rectangles calculated at midpoint within the mesh points.

$$\int_{x_0}^{x_n} f(x)\mathrm{d}x \approx \sum_{i=1}^{n}(x_i - x_{i-1})f\left(\frac{x_i + x_{i-1}}{2}\right) \tag{1.6}$$

Trapezoidal rule

The trapezoidal rule approximates the solution of a definite integral as the sum of trapezoid areas over the mesh points. Is usually the one of the most useful integration routines since it can be used with numerical functions on the defined mesh (n.b. that does not need to be made of equal step sizes!) without using the analytic representation.

$$\int_{x_0}^{x_n} f(x)\mathrm{d}x \approx \sum_{i=1}^{n}(x_i - x_{i-1})\left(\frac{f(x_i) + f(x_{i-1})}{2}\right) \tag{1.7}$$

Simpsons' (or Kepler or Cavalieri) rule

Is based on the third degree of Newton–Cotes formulae, making use of both midpoint and trapezoidal interpolations.

$$\int_{x_0}^{x_n} f(x)\mathrm{d}x \approx \sum_{i=1}^{n}\frac{x_i - x_{i-1}}{6}\left(f(x_i) + 4f\left(\frac{x_i + x_{i-1}}{2}\right) + f(x_{i-1})\right) \tag{1.8}$$

1.4 Zero Finding

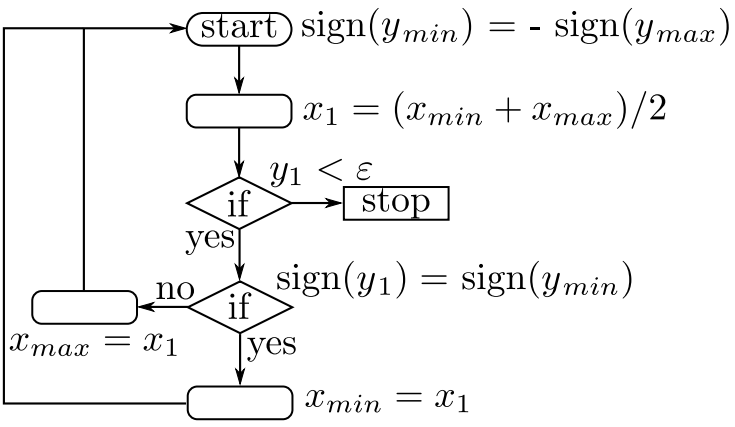
Most of the times we need to find the roots of an equation/ function.

1.4.1 Bisection

The bisection method although relatively slow in convergence is the one of the most robust since we make very few assumption on the zeros and the shape of the function.

Let's suppose we want to find the solution of $f(x) = 0$ within an interval $[x_{min}, x_{max}]$. The basic assumption of the method is that we have 1 zero within the interval (things can be saved for an odd

number of zeros). If $y_{min} = f(x_{min})$ and $y_{max} = f(x_{max})$ have a different sign than the zero must be in between. We take then the middle point $x_1 = (x_{min} + x_{max})/2$. If the function in the middle point $y_1 = f(x_1)$ has the same sign as y_{min} we take x_1 as the new x_{min}. If y_1 is already smaller than the cutoff value of precision ε, than we can stop the algorithm having found the zero. If it has the same sign as y_{max} we take it has the new x_{max}, and we iterate the procedure to the desired precision.



1.4.2 Newton Method

The Newton method could be very efficient if the derivative of the function can be calculated in advance, either analytically or numerically. The method assumes that the derivative is smoothly varying and can have problems in the proximity of flex points (where the second derivative cancels).

It is simply the iteration of the following equation,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{1.9}$$

starting from a reasonable x_0 and then iterating to find the root until the desired precision.

1.5 Differential Equations

1.5.1 Numerov

Numerov algorithm is a numerical solution of second order differential equations of the form

$$f''(x) + v(x)f(x) = 0, \tag{1.10}$$

with a precision of order 6, thus it is particularly suited to solve one dimensional Schrödinger equations. The above differential equation is soluble step by step considering a equidistant mesh, f at a particular point $x + h$ is related to the previous two mesh points in the following way,

$$\left(1 + \frac{h^2}{12}v(x+h)\right) f(x+h) = 2\left(1 - \frac{5h^2}{12}v(x)\right) f(x) - \left(1 + \frac{h^2}{12}v(x-h)\right) f(x-h). \tag{1.11}$$

Note that $f''(x) + v(x)f(x) = 0$ can admit more than one solution, thus $f(x)$ depends on boundary conditions. E.g. $f''(x)+f(x) = 0$ could notably be both $\sin(x)$ and $\cos(x)$. Moreover this equation might easily give as solution exponential–type functions if not properly constrained.

1.6 Schroedinger Equation

We consider here simple example of Schroedinger equation and how the previous method apply

1.6.1 Infinite Square Well

We consider as a starting point a simple 1D Schroedinger equation

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{elsewhere} \end{cases} \tag{1.12}$$

The Schroedinger equation (time independent) reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{1.13}$$

the solution of this equation is known $\psi_n = \sqrt{\frac{2}{a}} sin\left(\frac{n\pi}{a}x\right)$ $n = 1, 2, 3, \ldots$ and energy

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{1.14}$$

We can use such a simple example to start learning the numerical procedure used to solve more complex problems.

The Eq.1.13 is discretised on a uniform mesh h using the Numerov method. To start this method we need to know the behaviour of the solution at the edges. In this case we know

$$\psi_n(0) = \psi_n(a) = 0 \tag{1.15}$$

You have at least two ways to solve such an equation:

- You propagate a solution from the *left* and one from the *right* and you impose matching conditions on a given point inside the box

$$\psi_{left}(b) = \psi_{right}(b) \tag{1.16}$$
$$\psi'_{left}(b) = \psi'_{right}(b) \tag{1.17}$$

  This system of equation is satisfied only for a discretised set of energy values (the eigenvalues).

- We propagate only from the *left* and we count the number of nodes in the wave-function. We thus assume that the low eigenvalues correspond to low number of nodes and high energy one to high number of nodes.

In the present exercise we focus on the second method also known as *shooting*, but you are free to explore also the first one (see Ref. [2] for a more detailed explanation of the first method).

Let's solve the example numerically. We consider

$$\frac{\hbar^2}{2m} = 20.75 \tag{1.18}$$
$$a = 6\ fm \tag{1.19}$$
$$h = 0.1\ fm \tag{1.20}$$

These are simple value that are compatible with the nuclear case. The choice of the mesh is arbitrary! You need to check that your solution does not change dramatically when you change it. For $h \to 0$ you should get the *exact* solution, but in the realistic case for small values of h the Eqs presented in Sec.1.2 will be contaminated by numerical noise of your machine. The number of digits able to be stored in a

real mantissa is referred to as precision. High precision refers to the ability to store more information than low precision. In Fortran 90, this precision is referred to using the symbol p, which indicates the minimum number of decimal digits which can be stored. The exponent is also stored for a real number. In Fortran 90, the decimal size of a real number is referred to with the symbol, r, for the range of the number.

A single precision real number on most computers has a precision, p, of between 6 and 7 decimal digits, and a range, r, of 37. Thus, numbers as small as 10**(-37), and as large as 10**37 can be stored, with between 6 and 7 significant decimal digits.

We usually make use of *double* precision real numbers $p \approx 14$, but you can use higher precision as well. More precision you require more space on disk you will need and the execution time to perform numerical operation will also be affected.

Warning 1: each language has its own definition of precision so please figure out this element from the very beginning to avoid surprises!

Warning 2: attention to the conversion from one type of variable to another! Example: $a = 1.99$ defined as a real number. Let's assume that I define b as integer and I do the following operation $b = a$. The result will be $b = 1$! this is one of the most common mistakes in computer coding. This is quite common when using *implicit definition* of variables so please if you use Fortran start every code/subroutine with *implicit none* statement.

The main algorithm is the following

```
set Eup, Edown as extremes eigenvalues.
set epsilon convergence as desired precision.
set Node as the number of nodes you want in the wavefunction you're looking for

!(finds energy as zero with bisection rule)!
loop over tries until convergence
   Etrial=(Eup+Edown)/2
   trialwf(0)= 0.
   trialwf(1)= 1. !(arbitrarily initialize trial wavefunction)!

   !(Numerov Algorithm)!
   loop over meshmpoints ix

      vx=Etrial/(hbar^2/2m) !(setup Numerov Potential)!

      a1=2.*(1. - 5./12. * vx * mesh^2)
      a2=   (1. + 1./12. * vx * mesh^2)
      a3=   (1. + 1./12. * vx * mesh^2)

      trialwf(ix+1)= ( a1*trialwf(ix)- a2*trialwf(ix-1) ) / a3
   end loop over meshmpoints ix

   Nodecount=0  !(counting nodes)!
   loop over meshmpoints
      if(trialwf changes sign)Nodecount=Nodecount+1
   end loop over meshmpoints

   if(Nodecount > Node)then !(this determines if the wavefuction overshoots or undershoots)!
```

```
      Eup=Etrial
   else if(Nodecount < Node)then
      Edown=Etrial
   end if

   if( |Eup-Edown| < epsilon convergence ) exit loop
end loop over tries until convergence

!(renormalize the wavefuction)!
```

In Fig.1.1 we compare show the energy difference between the eigenvalues obtained numerically by employing the shooting method and the *exact* value extracted from Eq.1.14

We observe that till $h = 0.01$ fm we have a systematic gain in accuracy, then the trend gets more complicated and we observe that reducing the mesh h does not always increase the accuracy of the solution. It is finally worth reminding that here we deal only with numerical errors and not with other errors related to other approximations in the problem that lead to the differential equation we want to solve!

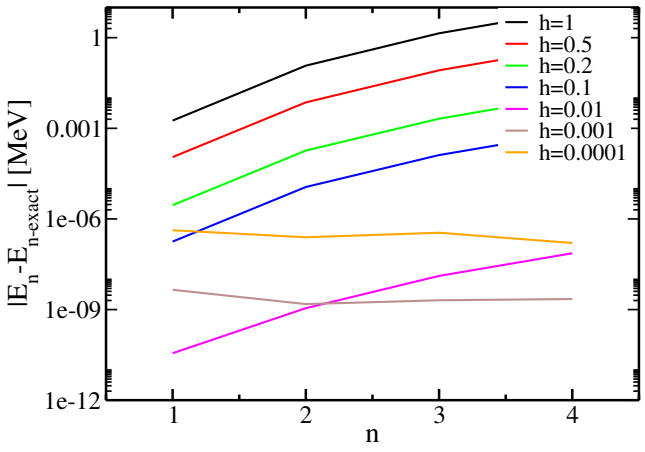


Figure 1.1: Accuracy of the first 4 eigenvalues of the 1D square well problem. The mesh h is expressed in fm..

In Fig.1.2 we show the eigenfunctions of the box for the first 4 eigenvalues.

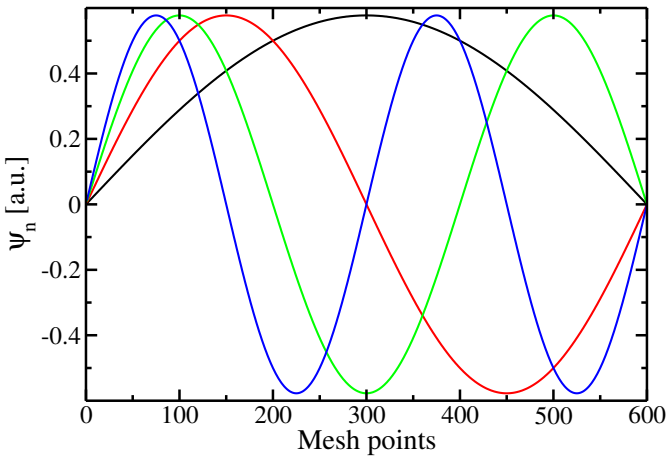


Figure 1.2: Wavefunctions in arbitrary units as a function of the number of mesh points (h=0.01) for the first 4 eigenvalues.

Chapter 2

Skyrme-Hartree-Fock equations in r-space

In this section we want to analyse in detail how to solve Hartree-Fock equations calculated with a Skyrme interaction in the case of spherical symmetry. Following the notation adopted in ref. [13], we define the single particle wavefunction as

$$\begin{aligned} \psi_\nu(\vec{r},\sigma,q) &= \frac{u^q_\nu(r)}{r} Y_{ljm}(\widehat{r},\sigma)\chi_q(\tau), \\ Y_{ljm}(\widehat{r},\sigma) &= \sum_{m_l m_s} \langle l \frac{1}{2} m_l m_s | jm \rangle Y_{lm_l}\chi_{m_s}(\sigma), \end{aligned} \tag{2.1}$$

where $\chi_q(\tau)$ is the isospin component. We used the following quantum numbers: the charge q (this is a label that is p for protons and n for neutrons), the principal quantum number n, the orbital angular momentum l, the total angular momentum j and the magnetic quantum number m, while we introduced a shorthand notation $\nu \equiv \{nlj\}$. Solving the Skyrme-Hartree-Fock equations in the case of spherical symmetry means to solve the following equation [13] for the radial part of the single particle wavefunction (cf. Eq.2.1). We omit for simplicity the isospin label for the wavefunction.

$$\begin{aligned} \frac{\hbar^2}{2m^*_q}\left[-u''_\nu(r) + \frac{l(l+1)}{r^2}u_\nu(r)\right] - \frac{d}{dr}\left(\frac{\hbar^2}{2m^*_q}\right)u'_\nu(r) + \\ \left\{U_q(r) + \frac{1}{r}\frac{d}{dr}\left(\frac{\hbar^2}{2m^*_q}\right) + \left[j(j+1) - l(l+1) - \frac{3}{4}\right]\frac{1}{r}W_q(r)\right\}u_\nu(r) = e_\nu u_\nu(r), \end{aligned} \tag{2.2}$$

where $W_q(r)$ is the spin-orbit potential and $U_q(r)$ is the central potential. This equation has to be solved in a spherical box with the appropriated boundary conditions,

$$u_\nu(0) = u_\nu(R_{box}) = 0. \tag{2.3}$$

This differential equation can be reduced to a general class of linear differential equations of the kind

$$y''(r) + g(r)y'(r) + f(r)y(r) = 0, \tag{2.4}$$

where we can define

$$
\begin{aligned}
g(r) &= \left[\frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right)\right] / \left[\frac{\hbar^2}{2m_q^*}\right], \\
g(r)' &= \left\{\frac{d^2}{dr^2}\left(\frac{\hbar^2}{2m_q^*}\right)\frac{\hbar^2}{2m_q^*} - \left[\frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right)\right]^2\right\} / \left[\frac{\hbar^2}{2m_q^*}\right]^2, \\
h(r) &= \left\{U_q(r) + \frac{1}{r}\frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right) + \left[j(j+1) - l(l+1) - \frac{3}{4}\right]\frac{1}{r}W_q(r)\right\}, \\
f(r) &= -\left[h(r) + \frac{\hbar^2}{2m_q^*}\frac{l(l+1)}{r^2} - e_\nu\right] / \left[\frac{\hbar^2}{2m_q^*}\right].
\end{aligned} \tag{2.5}
$$

An usual algorithm used to solve this type of equation is the Runge-Kutta, but in self-consistent solutions it is better to use different method to approximate the second derivative. This was proposed by B.V. Numerov in 1923 [7], and works only for differential equations of the kind

$$w''(r) + k(r)^2 w(r) = S(r), \tag{2.6}$$

the great advantage is the improved numerical accuracy using the same discrete mesh. Employing the following transformation we can recast Eq.2.4 in the more appropriate form of Eq.2.6. We define

$$y(r) = w(r)\exp\left(-\frac{1}{2}\int g(r)dr\right), \tag{2.7}$$

where $g(r)$ is defined in Eq.2.4-2.5, $y(r)$ is the solution of Eq.2.4, while $w(r)$ is a new function that will be the solution of a differential equation of the form Eq.2.6. To demonstrate the validity of the method let's now calculate the first and the second derivative of this function (cf .Eq. 2.7),

$$
\begin{aligned}
y(r)' &= w(r)'\exp\left(-\frac{1}{2}\int g(r)dr\right) + w(r)\exp\left(-\frac{1}{2}\int g(r)dr\right)\left(-\frac{1}{2}g(r)\right), \\
y(r)'' &= \left[w(r)'' - \frac{1}{2}g(r)'w(r) - \frac{1}{2}g(r)w(r)'\right]\exp\left(-\frac{1}{2}\int g(r)dr\right) \\
&\quad + \left[w(r)' - \frac{1}{2}g(r)w(r)\right]\left(-\frac{1}{2}g(r)\right)\exp\left(-\frac{1}{2}\int g(r)dr\right),
\end{aligned} \tag{2.8}
$$

and inserting in Eq.2.4, simplifying the common term $\left[\exp\left(-\frac{1}{2}\int g(r)dr\right)\right]$, we finally obtain,

$$w(r)'' - \frac{1}{2}g(r)'w(r) - g(r)w(r)' + \frac{1}{4}g(r)^2w(r) + g(r)w(r)' - \frac{1}{2}g(r)^2w(r) + f(r)w(r) = 0. \tag{2.9}$$

We see immediately that the terms containing the first derivative cancel, so we finally have

$$w(r)'' + w(r)\left(-\frac{1}{4}g(r)^2 + f(r) - \frac{1}{2}g(r)'\right) = 0, \tag{2.10}$$

to which we can apply the Numerov algorithm. We can now see in more detail the specific case of the Skyrme-Hartree-Fock equations. The transformation reads

$$
\begin{aligned}
u_\nu(r) &= \overline{u}_\nu(r)\exp\left(-\frac{1}{2}\int g(r)dr\right), \\
g(r) &= \left[\frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right)\right] / \left[\frac{\hbar^2}{2m_q^*}\right],
\end{aligned} \tag{2.11}
$$

we can calculate the integral obtaining

$$\begin{aligned} u_\nu(r) &= \overline{u}_\nu(r) \exp\left(-\frac{1}{2}\int g(r)dr\right) = \\ &= \overline{u}_\nu(r) \exp\left[-\frac{1}{2}\ln\left(\frac{\hbar^2}{2m_q^*}\right)\right] = \\ &= \overline{u}_\nu(r) \exp\left[\ln\left(\frac{\hbar^2}{2m_q^*}\right)^{-1/2}\right] = \\ &= \sqrt{\frac{2m_q^*}{\hbar^2}}\overline{u}_\nu(r). \end{aligned} \tag{2.12}$$

Our new Schröedinger equation will be

$$\overline{u}_\nu''(r) + \overline{u}_\nu(r)\left[-\frac{1}{4}g(r)^2 + f(r) - \frac{1}{2}g(r)'\right] = 0,$$

with the definitions of $g(r), g(r)'$ given in Eq.2.5. We will solve Eq.2.13 using the Numerov method and, automatically, we will find the solution of Eq.2.2, that is related to $\overline{u}_\nu(r)$ by the following relation

$$u_\nu(r) = \sqrt{\frac{2m_q^*}{\hbar^2}}\overline{u}_\nu(r).$$

2.1 Densities in spherical symmetry

In this section we write the three local densities used in the code. The scalar hartree-fock density

$$\rho(r)_q = \frac{1}{4\pi r^2}\sum_{(nlj)_{occ}}(2j+1)u_q^2(nlj,r) \tag{2.13}$$

where the sum is restricted to the occupied states. The kinetic density is

$$\tau(r)_q = \sum_{(nlj)_{occ}}\frac{2j+1}{4\pi r^2}\left[\left(u_q'(nlj,r) - \frac{u_q(nlj,r)}{r}\right)^2 + \frac{l(l+1)}{r^2}u_q^2(nlj,r)\right] \tag{2.14}$$

Finally the spin current vector density

$$J(r) = \frac{1}{4\pi r^3}\sum_{(nlj)_{occ}}(2j+1)\left[j(j+1) - l(l+1) - \frac{3}{4}\right]u_q^2(nlj,r) \tag{2.15}$$

For the case of HFB the previous equation have to be modified, the sum extend to all the quasiparticles and instead of using $u_q(nlj,r)$ we use the quasiparticle wavefunction $v_q(nlj,r)$.

2.2 Fields

In this section we discuss in detail the fields that appear in Eq.2.2, the solution of this set of equations we'll define the basis on which we will solve our HF problem.

2.2.1 Wood Saxon

We can use a not self consistent solution (*i.e.* Wood Saxon potential) so they have the shape [8]

$$
\begin{aligned}
U_q(r) &= -\left(51 - 33\frac{N-Z}{N+Z}\right) f(r) && (2.16)\\
W_q &= 0.44\frac{1}{r}\frac{dU_q(r)}{dr}\cdot r_0^2 && (2.17)\\
\frac{\hbar^2}{2m_q} &= 20.73553 && (2.18)
\end{aligned}
$$

where N, Z are the neutron and proton number, $f(r)$ is the Fermi function

$$f(r) = \frac{1}{1+\exp\left(\frac{r-R_q}{a_0}\right)} \tag{2.19}$$

and $a_0 = 0.67$ fm is the diffusivity and $r_0 = 1.27$ fm is a constant, and $R_q = r_0 \cdot (N+Z)^{1/3}$. For protons we have to add to the central potential the Coulomb potential that is approximated as

$$V_{Coul}(r) = \begin{cases} \frac{Ze^2}{R_p}\left(3 - \left(\frac{r}{R_p}\right)^2\right) & r \le R_p \\ \frac{Ze^2}{r} & r > R_p \end{cases} \tag{2.20}$$

2.2.2 Skyrme

The Skyrme interaction has the shape [4]

$$
\begin{aligned}
V(\mathbf{r}_1,\mathbf{r}_2) &= t_0(1+x_0P_\sigma)\delta(\mathbf{r})\\
&+ \frac{1}{2}t_1(1+x_1P_\sigma)\left[\mathbf{k}'^2\delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{k}^2\right]\\
&+ t_2(1+x_2P_\sigma)\mathbf{k}'\delta(\mathbf{r})\mathbf{k}\\
&+ \frac{1}{6}t_3(1+x_3P_\sigma)\left[\rho(\mathbf{R})\right]^\alpha\delta(\mathbf{r})\\
&+ iW_0\sigma\left[\mathbf{k}'\times\delta(\mathbf{r})\mathbf{k}\right] \qquad (2.21)
\end{aligned}
$$

with

$$
\begin{aligned}
\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad , \quad \mathbf{R} &= \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)\\
\mathbf{k} = \frac{1}{2i}\left(\nabla_1 - \nabla_2\right) \quad , \quad \mathbf{k}' &\text{ c.c. of } \mathbf{P}\\
\sigma = \sigma_1 + \sigma_2 \quad , \quad P_\sigma &= \frac{1}{2}\left(1 + \sigma_1\sigma_2\right)
\end{aligned}
$$

Following closely the derivation in ref.[2] we obtain the potentials

$$\begin{aligned} U_q(r) &= \rho\left[\frac{1}{2}t_0(2+x_0)+(2+\alpha)\frac{t_3}{24}(2+x_3)\rho^\alpha\right] \\ &+ \rho_q\left[-\frac{t_0}{2}(2x_0+1)-\frac{t_3}{12}(2x_3+1)\rho^\alpha\right] \\ &+ \alpha\rho^{\alpha-1}\left[-\frac{t_3}{24}(2x_3+1)\right](\rho_p^2+\rho_n^2) \\ &+ \tau\frac{1}{8}\left[t_1(2+x_1)+t_2(2+x_2)\right] \\ &- \frac{1}{16}\left[3t_1(2+x_1)-t_2(2+x_2)\right]\left(\rho''+2\frac{\rho'}{r}\right) \\ &- \frac{1}{8}\left[t_1(2x_1+1)-t_2(2x_2+1)\right]\tau_q \\ &- \frac{1}{8}\left[t_1x_1+t_2x_2\right]\left(\rho_q''+2\frac{\rho_q'}{r}\right) \end{aligned} \tag{2.22}$$

where the densities are given by Eq.2.13,2.14 and 2.15 the field mass read

$$\begin{aligned} M_q(r) &= \frac{\hbar^2}{2m}+\frac{t_1}{4}\left[\left(1+\frac{x_1}{2}\right)\rho-\left(x_1+\frac{1}{2}\right)\rho_q\right] \\ &+ \frac{t_2}{4}\left[\left(1+\frac{x_2}{2}\right)\rho-\left(x_2+\frac{1}{2}\right)\rho_q\right]. \end{aligned} \tag{2.23}$$

At the central potential because of the structure of Eq.2.2 (as it's implemented in the code) we have to had to the central potential the part

$$U_q(r) = U_q(r)+\frac{1}{r}\frac{d}{dr}M_q(r). \tag{2.24}$$

The spin-orbit potential reads

$$W_q(r) = -\frac{1}{8}(t_1x_1+t_2x_2)J(r)+\frac{1}{8}(t_1-t_2)J_q(r)+W_0\nabla(\rho+\rho_q). \tag{2.25}$$

2.2.3 Coulomb

For the protons we have to add the Coulomb potential

$$V_c(r) = \frac{e^2}{2}\int_0^{R_{box}} d^3r'\frac{\rho_q(r')}{|r-r'|}-e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_q^{1/3}(r) \tag{2.26}$$

where we treat the exchange with the Slater approximation, while the direct term is expanded in spherical harmonics following ref.[10]. This can not be treated directly due to the singularity for $r = r'$ Following Ref. [12], we can make a multipolar expansion of the term $1/r$ as

$$\frac{1}{|r_1-r_2|} = \frac{4\pi}{r_2}\sum_{l=0}\frac{1}{2l+1}\left(\frac{r_1}{r_2}\right)^l\sum_m Y_{lm}(\Omega_1)Y_{lm}^*(\Omega_2) \tag{2.27}$$

if $r_1 < r_2$, wheras $r_2 < r_1$ one has to exchange $r_1 \leftrightarrow r_2$. By performing the analytical integration over the angular part we get

$$V_c(r) = 4\pi e^2\left[\frac{1}{r}\int_0^r dr'\rho_q(r')r'^2-\int_0^r dr'\rho_q(r')r'+\int_0^\infty dr'\rho_q(r')r'\right] \tag{2.28}$$

The density apperaing in these formulas is the point-like proton density. It is also possible to include the charge-density in these expressions. See Ref. [1] for details.

2.3 Using different boundary conditions

In previous lectures we have seen that it is possible to select different boundary conditions at the edge of the box. In the following we give some highliths on these different boundary conditions

2.3.1 Dirichlet-Neumann mixed condition

Instead of imposing the condition $u_{nlj}(R_{box}) = 0$ we can use the Dirichlet-Neumann (DN) boundary conditions.

For example in Fig.2.1 we show the density profile $\rho(r)$ of several Wigner-Seitz cells in the inner crust calculated using Hartree-Fock-Bogoliubov equations into a box with DN boundary conditions. These condition read

- **BCE** even-parity wave function vanish at the edge of the box and the first derivative of odd-parity wave functions vanishes at the edge of the box
- **BCO** odd-parity wave function vanish at the edge of the box and the first derivative of even-parity wave functions vanishes at the edge of the box

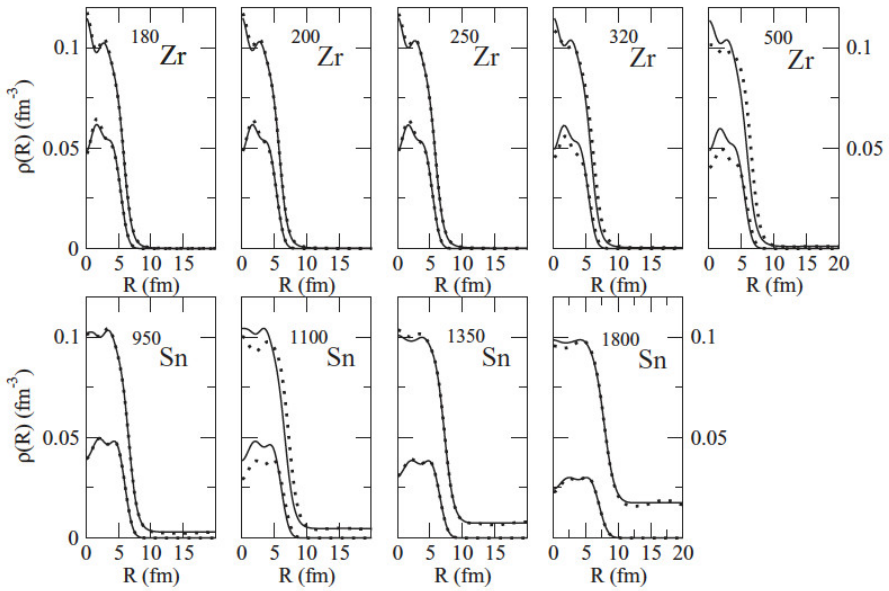


Figure 2.1: Density profile $\rho(r)$ of different Wigner-Seitz cells in the inner crust of a neutron star obtained with DN boundary conditions

Clearly a change in the boundary condition changes the way we discretize our continuum, but this simple trick allows us to get a flat behaviour of the density at the edge instead of a sharp drop. This is not relevant to describe well bound nuclei, but it can be important for more exotic systems as Wigner-Seitz cells where nuclei are in phase coexistance with a neutron gas.

2.3.2 Asymptotic boundary conditions

Instead imposing vanishing boundary conditions, we can consider the asymptotic behavior of the wave function at the edge.

Let's considder the Skyrme case for neutrons. We know that the nuclear potential as well as spin-orbit go to zero as $r \to R_{box}$ assuming that $R_{box} >> r_{nucleus}$. So the Schroedinger equation reads (very far way from the nucleus)

$$-\frac{\hbar^2}{2m}u''_\nu(r) = e_\nu u_\nu(r) \tag{2.29}$$

where the effective mass m^* goes back to its bare value in this limit (see Skyrme-HF equations and fields). According to the value of the energy (positive/negative) the wave function behaves either as an exponential or as an oscillating function. This is particular relevant to describe loosely bound states or to improve the description of the continuum and take into account resonant states in a proper way.

How to treat a real continuum? This requires the use of more sophisticated methods. See Refs. [6, 11] for more details.

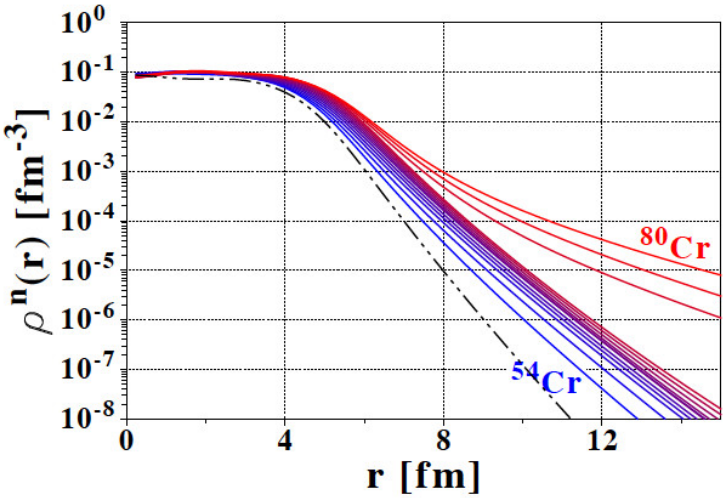


Figure 2.2: Neutron densities for even-even Cr isotpes from ^{54}Cr to ^{80}Cr. Taken from [9]

Chapter 3

Exercise

This section is devoted to the explanation of the computational project you need to deliver at the end of the TALENT school.

The project is organised in small steps you need to follow week by week.

In the last section, we give

3.1 Week 1

For the first exercise you will need to solve a 1D Schroedinger equation.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) = e_n\psi_n(x) \tag{3.1}$$

You need to solve this equation in a box R_{box} discretizing the second derivative on a unifrom grid. You need to use the Numerov alghoritm.

3.1.1 Infinite square well

As a starting point you can consider the infinite square well. The potential is thus defined

$$V(x) = \begin{cases} 0 & [0, R_{box}] \\ \infty & \text{elsewhere} \end{cases} \tag{3.2}$$

- Calculate the first eigenvalues in an interval [0-100] MeV
- Calculate the corresponding eigenfunctions

Important: Remember that the solution to this problem can be found analytically and it can be used as a test for your numerical code!

3.1.2 Finite square well

We considet a new potential

$$V(x) = \begin{cases} -V_0 & [-a, a] \\ 0 & \text{elsewhere} \end{cases} \tag{3.3}$$

into a box of radius R_{box} larger than a.

- Calculate the first eigenvalues in an interval $[-V_0 - 100]$ MeV
- Calculate the corresponding eigenfunctions

3.1.3 Optional

Compare numerically the position of the eigenstates of a Wood-Saxon (WS) potential and a finite square well with size equal to the radius R of the WS potential

3.2 Week 2

We now considet the other dimensions, by working in a 3-dimensional shperically symmetric problem. We work in spherical coordinates and the angular part can be treated analytically.

You can now treat a realistic nuclear case: consider a WS potential for ^{208}Pb.

$$V(r) = V_0 f(r) \tag{3.4}$$

$$f(r) = \frac{1}{1 + \exp\left[\frac{r-R}{a}\right]} \tag{3.5}$$

with parameters

$$R = r_0 A^{1/3} \text{ [fm]} \tag{3.6}$$

$$r_0 = 1.27 \text{ [fm]} \tag{3.7}$$

$$a = 0.67 \text{ [fm]} \tag{3.8}$$

$$V = \left(-51 + 33\frac{N-Z}{A}\right) \text{ [MeV]} \tag{3.9}$$

$$\tag{3.10}$$

Since this is a non self-consistent calculation you can start considering only neutrons. You have to consider the spin-orbit potential as

$$V_{so}(r) = V_{ls}(\mathbf{l}\cdot\mathbf{s})r_0^2\frac{1}{r}\frac{df(r)}{dr} \tag{3.11}$$

Calculate the eigenvalues and eigenfunction of the occupied neutron states.

In Fig.3.1 we show the evolution of neutron single particle states as a function of the mass number [3].

To include protons you have to consider a Coulomb potential. since you are dealing with a simple phenomenological potential you can use

$$V_c(r) = \begin{cases} \frac{Ze^2}{R}\sqrt{3 - \left(\frac{r}{R}\right)^2} & \text{if } r < R \\ \frac{Ze^2}{r} & \text{elsewhere} \end{cases} \tag{3.12}$$

- Make a plot of central potential for neutrons and protons. What do you notice?
- Calculate eigenvalues and eigenfunctions in ^{208}Pb
- Calculate the total matter density $\rho(r) = \rho_n(r) + \rho_p(r)$ for ^{208}Pb

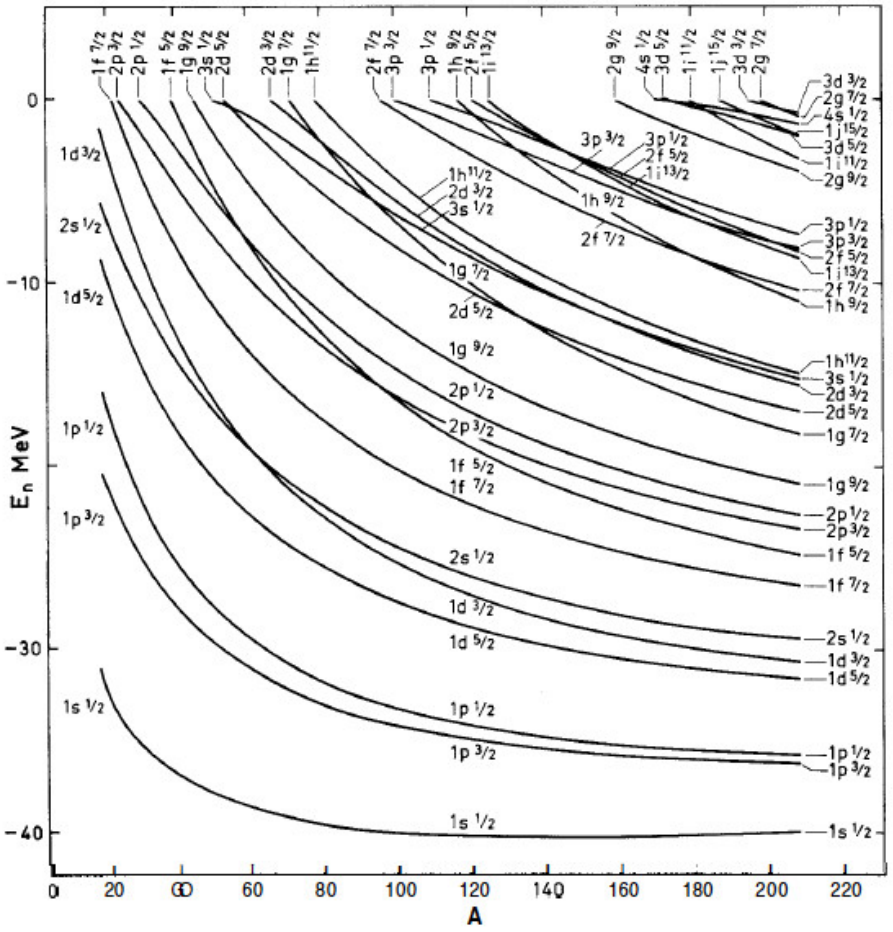


Figure 3.1: Neutron orbits as function of the mass number A.

Remeber that

$$\rho_{q=n,p}(r) = \sum_{nlj \in occupied} \frac{2j+1}{4\pi r^2} [u_{qnlj}(r)]^2 \tag{3.13}$$

as a check for your calculations

$$\int d^3 r \rho(r) = A \tag{3.14}$$

3.3 Week 3

We now include a realistic potential derived from an effective Skyrme interaction. The definitions of the fields in spherical symmetry can be found in Ref. [2] as well for the densities.

You can decide to implement a full Skyrme interaction. In this case we suggest you to use the interaction SLY5

```
t0 = -2483.4500
 x0 =      0.77600
 t1 =    484.2300
```

```
x1 =    -0.31700
t2 =  -556.6900
x2 =    -1
t3 = 13757
x3 =     1.2630
W0 =   125
alpha =   1 / 6
hb2m0 = 20.735530
```

notice that the parameter hb2m0 corresponds to $\frac{\hbar^2}{2m}$ the bare mass value. We use the same value for both protons and neutrons as prescribed by the authors of the interaction [4]. This value is not fixed and it changes interaction by interaction!

3.3.1 A simple t_0, t_3 system

If you think the previous step is too complicated you can use a much simpler Skyrme interaction. In this case the interaction has been tuned to work in the test case ^{16}O [14].

```
t0 = -1132.400
x0 = x3=0
t1 =   x1 =  0
t2 =  x2 =  0
t3 = 23610.40
w  =   0.0
alpha = 1
hb2m0 = 20.735530
```

In this way the non-zero fields are strongly reduced (essentially all derivative terms are zero) and you do not need to consider the current $J(r)$.

3.3.2 Center of mass correction

Due to the breaking of translational invariance we have to correct the binding energy. We need to subtract from the total kinetic energy K the contribution coming from center of mass motion [1]. This means

$$K - \frac{\mathbf{P}^2}{2mA} = K - \frac{\left(\sum_i \mathbf{p}_i\right)^2}{2mA} = K - \frac{1}{2mA}\left[\sum_i \mathbf{p}_i^2 + \sum_{i\neq j} \mathbf{p}_i\mathbf{p}_j\right] \tag{3.15}$$

traditionally only the one-body correction term is taken into accout. this yields to adding a term $-1/A$ to the kinetic energy term.

It is also include the second term (2-body center or mass correction), but this makes the calculations much longer. See Ref. [1].

3.4 Extra: pairing correlations

Solving Hartree-Fock-Bogoliubox equations in coordinate space.

For open shell nuclei we need to consider the following equations

$$\left[-\frac{d}{dr}\mathcal{M}\frac{d}{dr}+\mathcal{U}+\mathcal{M}\frac{l(l+1)}{r^2}+\frac{\mathcal{M}'}{r}+\mathcal{U}_{so}\right]\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = E\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{3.16}$$

where the defintions of the matrices $\mathcal{M},\mathcal{U},\dots$ can be found in Ref. [2]. In this case you need to solve a system of 2 coupled differential equations.

In this case a simple *shooting* method does not work anymore due to the particular structure of the two spinors u_1, u_2. See discussion in Ref. [5].

A possible method is expained in Ref. [2] and it is based on the propagation from the *left* side of the box and *right* side of the box

3.4.1 BCS

A possible simpler extension include the use of the BCS approximation.

In this case the main alghorithm is left unchanged and by using a simple pairing interaction of the form $v_{pair} = G$ we do not need to introduce major changes in the code. The allow the convergence we also restrict the appearence of pairing correlations within 1 major shell. The strength G is tuned in such a way that the resulting average pairing gap $\bar{\Delta}$ is equal to $\bar{\Delta} = \frac{12}{\sqrt{A}}$

Few key points

- Once the HF equations are quite well converged we can start adding pairing correlations. The BCS method is acceptable only for bound nuclei so that these correlations can be added on top of the man field in a *perturbative* way
- At BCS level the occupations number are changed and given by

$$v_k^2 = \frac{1}{2}\left(1-\frac{e_a-e_F}{E_a}\right) \qquad v_k^2+u_k^2=1 \tag{3.17}$$

  where e_F is the Fermi energy and $E_a = \sqrt{(e-e_F)^+\Delta^2}$
- the Δ_a is obtained by solving at each iteration the corresponding gap equation. See Ref. [8] for details
- at each step the average number of neutrons N and protons Z should be constrained ($[H_{pair}, \hat{N}] \neq 0$). The corresponding Lagrange multiplier we get is the Fermi energy e_F.

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