Computational Methods: Homework 2: Hartree-Fock

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Homework is due on 26 February.

I. THE SCIENCE PROBLEM

We will consider a slab of nuclear matter, infinite in the x-y direction, but of finite extent in the z-direction. We will use a density-dependent one-body potential (of Skyrme type), and we will solve the coupled nonlinear differential equations using lattice methods. A full exposition of this kind of calculation can be found in an excellent and seminal paper on nuclear collisions by Bonche, Koonin, and Negele, Phys. Rev. C13, 1226 (1976) from which we are working.

The HF equations are

$$\left[-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}} + W(z)\right]\psi_i(\vec{r}) = \varepsilon_i\psi_i(\vec{r}) \ . \tag{1}$$

This equation has separable solutions in $\vec{r}_\perp$ and z. The density-dependent potential is given by

$$W(z) = \frac{3}{4}t_0\rho(z) + \frac{3}{16}t_3\rho^2(z) + 2\pi a^2 V_0\int_{-\infty}^{\infty} dz'\rho(z')\exp\left(-\mid z - z'\mid /a\right) \tag{2}$$

where the parameters t_0, t_3, a, and aV_0 are chosen to reproduce properties of nuclear matter (saturation density and binding energy) and the measured skin thickness in nuclei (this is the Yukawa term). These parameters are $t_0 = -497.726$ MeV-fm^3, $t_3 = 17270$ MeV-fm^6, $aV_0 = -166.9239$ MeV-fm, and $a = 0.45979$ fm.

Equations 1 are separable, so that the energy $\varepsilon_i = \varepsilon_{nk_\perp}$ and the single-particle wave functions are given by

$$\psi_i(\vec{r}) = \psi_{nk_\perp}(\vec{r}) = \frac{1}{\sqrt{\Omega}}\exp\left(i\vec{k}_\perp \times \vec{r}_\perp\right)\phi_n^{HF}(z) \ , \tag{3}$$

with the normalization

$$\int_{-\infty}^{\infty} \mid \phi_n^{HF}(z)\mid^2 dz = 1 \ . \tag{4}$$

These wave functions are the solution of the one-dimensional equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + W(z)\right]\phi_n^{HF}(z) = \varepsilon_n\phi_n^{HF}(z) \ . \tag{5}$$

The single-particle energy from Eq. 1 is given by

$$\varepsilon_{nk_\perp} = e_n + \frac{\hbar^2}{2m}k_\perp^2 \le \varepsilon_F \ , \tag{6}$$

where ε_F is the Fermi energy of the system. Thus

$$\mid \vec{k}_\perp \mid < \left[\frac{2m}{\hbar^2}(\varepsilon_F - \varepsilon_n)\right]^{1/2} = k_{\max}(n) \ . \tag{7}$$

So, each ϕ_n is associated with the plane waves of transverse momentum within a circle in the $\vec{k}_\perp$ plane of radius $k_{\max}(n)$. The fermi energy is given implicitly by the size of the slab we want to construct.

The density is

$$\begin{aligned}
\rho(z) &= 4\sum_{n,k_\perp} \mid \psi_{nk_\perp}(\vec{r})\mid^2 & (8)\\
&= 4\sum_{n=\text{occupied}} \mid \phi_n^{HF}(z)\mid^2 \int_0^{k_{\max}(n)} \frac{d^2k_\perp}{(2\pi)^2} & (9)\\
&= \sum_{n=\text{occupied}} \mid \phi_n^{HF}(z)\mid^2 \frac{k^2_{\max}(n)}{\pi} & (10)\\
&= \sum_{n=\text{occupied}} \mathcal{A}_n \mid \phi_n^{HF}(z)\mid^2 \ . & (11)
\end{aligned}$$

We define $\mathcal{A}_n$ as

$$\mathcal{A}_n = \frac{k^2_{\max}(n)}{\pi} = \frac{2m}{\hbar^2}(\varepsilon_F - \varepsilon_n)\ , \tag{12}$$

and we note that

$$\mathcal{A} = \sum_{n=1}^{N} \mathcal{A}_n = \sum_{n=1}^{N} \frac{2m}{\pi\hbar^2}(\varepsilon_F - \varepsilon_n)\ . \tag{13}$$

By using the fact that $\varepsilon_{N+1} > \varepsilon_F$ we can solve Eqn. 13 implicitly. Thus, the solution of Eqn. 13 also yields the value of N.

The energy per unit area is given by

$$\begin{aligned} \frac{E}{\Omega} &= \frac{\hbar^2}{2m}\sum_{n=1}^{N}\mathcal{A}_n\int_{-\infty}^{\infty} \mid \frac{d\phi_n^{HF}(z)}{dz} \mid^2 + \sum_{n=1}^{N}\frac{\hbar^2}{4m}\pi\mathcal{A}_n^2 \\ &+ \frac{3}{8}\int_{-\infty}^{\infty} t_0\rho^2(z)dz + \frac{t_3}{16}\int_{-\infty}^{\infty}\rho^3(z)dz \\ &+ \pi a^2 V_0 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dzdz'\rho(z)\rho(z')\exp\left(\frac{-\mid z-z'\mid}{a}\right) \end{aligned} \tag{14}$$

II. BASIC CODE STRUCTURE

The code you will receive is set up in the following manner.

- *initialization* Here you read in some initial input, allocate arrays, and initialize several variables. For example, the initial density is

$$\rho_0(z) = \left[1 + \exp\left(\frac{\mid z\mid - L}{a_0}\right)\right]^{-1} \tag{15}$$

  where we choose $L = 5$ fm and $a_0 = 0.5$ fm. We normalize the density to the $\mathcal{A}$ that we input. Typical values of A range from 0.5 (for oxygen) to 2.5 (for lead).

- We then iterate the solutions.
  - Build from the initial density a solution to the Helmholtz equation. Call this term *yukawa*.
  - Once you have *yukawa* and ρ, build the hamiltonian matrix.
  - Diagonalize the hamiltonian matrix.
  - Reorder the eigenvalues (lowest to highest).
  - Make a new ρ.
  - Calculate the energy density (you have to develop this)
  - Test for convergence by comparing the present energy density with the previous one (you have to implement this).

III. YOUR MISSION

- Familiarize yourself with this code. You want to make a subroutine that calculates the energy (see Eq. 14) and include an iteration.
- Once you have a running code, you will want to try a few examples for $\mathcal{A} = 0.5, 1.0, 1.5, 2.0$. Make plots of the density for each case. What are the single-particle energies below the ε_F (put them into a table). What is the E/Ω for each case? Try to reproduce the features of Fig.2 in the BKN paper.

  STOP HERE

- We are going to implement time dependence into this code.You will need to review the notes on time-dependent evolution for this part. In order to obtain time-dependence you will need to do several things.
  - You need to set up a new vector that is a complex*16 variable and store in it the real*8 wave functions that were generated in the static case. You could call it psin_c or something like that.
  - You need to write a time-evolution subroutine. This subroutine will evolve the following equation

$$i\hbar \frac{d\phi_n(z,t)}{dt} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + W(z,t) \right) \phi_n(z,t) \ , \tag{16}$$

    with $\phi_n(z, t = 0) = \phi_n^{HF}(z)$ times a boost term (see below). $W(z,t)$ is given in Eq. 2 except now the densities in that equation are time dependent:

$$\rho(z,t) = \sum_{n=\text{occupied}} \mathcal{A}_n \mid \phi_n(z,t) \mid^2 \ , \tag{17}$$

  - You need to "boost" your static solution. This is done by introducing a common phase factor into all single-particle wave functions such that

$$\phi_n(z, t = 0) = \phi_n^{HF}(z) \exp(ikz) \ , \tag{18}$$

    which yields a total energy per particle of

$$\frac{E}{\Omega} = \frac{E^{HF}}{\Omega} + \mathcal{A}\frac{\hbar^2 k^2}{2m} \ . \tag{19}$$

    The total energy involves both the internal energy (E^{HF}) and the total kinetic energy (the second term above) in the lab frame of the nucleus. You need to make a subroutine that will boost your original slab to some velocity. You can test your time-dependent code by a) plotting the density as a function of time (it will move once boosted) b) calculating the internal energy, which should remain constant as a function of time.

- You are now in a position to begin a symmetric nuclear collision (with $\mathcal{A} = 1.4$ fm^{-1}, and moving toward each other with a speed corresponding to a kinetic energy of $E/A = 0.5$ MeV, and 3.5 MeV. You first perform a static calculation on a mesh that goes from $z = -30$ fm to $z = 30$ fm. You place two nuclei on that mesh separated by several fermi. (You can do this by setting up the appropriate initial condition.) Then you boost the nuclei so that they move toward eachother in time (boost one with $+k$ and the other with $-k$ momentum.

- You should choose $\Delta z = 0.2$ fm, and $\Delta t \leq \frac{\Delta z}{4 v_{\max}}$, where $v_{\max}$ can be calculated from equation 5.2 in the BKN paper.

- Can you reproduce Figs. 7 and 9 from the BKN paper?

- Can you find a range of kinetic energies for which the two nuclei don't appear to separate (this is called the fusion window)?

- What happens at higher collision energies (say $E/A = 50$ MeV)?