Hartree-Fock Calculations of Neutron Drops

Neutron drops are a powerful theoretical laboratory for testing, validating and improving nuclear structure models. Indeed, all approaches to nuclear structure, from ab initio theory to shell model to density functional theory are applicable in such systems. We will, therefore, use neutron drops to analyze some of the techniques that will be presented in this course. The starting point of nearly all quantum many-body techniques is the Hartree-Fock equations (HF). We will, therefore, develop a computer program to solve the HF equations by expanding the solutions in the Harmonic Oscillator basis.

1 The Microscopic Neutron Drop Hamiltonian

The Hamiltonian for a system of N neutron drops confined in a harmonic potential reads

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \sum_{i=1}^{N} \frac{1}{2} m\omega \boldsymbol{r}_i^2 + \sum_{i<j} \hat{V}_{ij}, \tag{1}$$

with $\hbar^2/2m = 20.73$ fm^2, $mc^2 = 938.90590$ MeV, and $\hat{V}_{ij}$ is the two-body, local, finite-range Minnesota interaction potential

$$\hat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \left[\hat{V}_R(\boldsymbol{r}_1, \boldsymbol{r}_2) + \frac{1}{2}\left(1 + \hat{P}_\sigma\right) \hat{V}_t(\boldsymbol{r}_1, \boldsymbol{r}_2) + \frac{1}{2}\left(1 - \hat{P}_\sigma\right) \hat{V}_s(\boldsymbol{r}_1, \boldsymbol{r}_2) \right] \times \frac{1}{2}\left(1 + \hat{P}_r\right), \tag{2}$$

with $\hat{P}_\sigma$ the spin-exchange operator, and $\hat{P}_r$ the space-exchange operator. The spatial form-factors are

$$\hat{V}_R(\boldsymbol{r}_1, \boldsymbol{r}_2) = +V_{0,R} e^{-\kappa_R (\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}, \tag{3}$$

$$\hat{V}_t(\boldsymbol{r}_1, \boldsymbol{r}_2) = -V_{0,t} e^{-\kappa_t (\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}, \tag{4}$$

$$\hat{V}_s(\boldsymbol{r}_1, \boldsymbol{r}_2) = -V_{0,s} e^{-\kappa_s (\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}. \tag{5}$$

The numerical parameters for the range of the Gaussians and the energy scales are listed in the table below.

Table 1: Parameters defining the Minnesota potential

V	Value	κ	Value
$V_{0,R}$	200.00 MeV	κ_R	1.487 fm^{-2}
$V_{0,t}$	178.00 MeV	κ_t	0.639 fm^{-2}
$V_{0,t}$	91.85 MeV	κ_s	0.465 fm^{-2}

2 Hartree-Fock Equations in the s-wave Model Space

1. Ground-work
   (a) Write the Hamiltonian in second quantization form
   (b) We will assume spherical symmetry is conserved. Hence the basis states $|a\rangle$ are eigenstates of the $\hat{J}^2$ and $\hat{J}_z$ operators, $|a\rangle \equiv |n_a, \ell_a, j_a, m_a\rangle$.
      i. Give the generic expression of the basis states $\langle \boldsymbol{r}\sigma|a\rangle \equiv \langle \boldsymbol{r}\sigma|n_a, \ell_a, j_a, m_a\rangle$ using spherical coordinate, radial wave functions, spherical harmonics, spin functions, etc.
      ii. The local density matrix in r-space is denoted by $\rho(\boldsymbol{r}, \sigma)$, and ρ_{ac} in configuration space. Use the relations between the two representations to obtain conditions on the labels n_a, ℓ_a, j_a, m_a and n_c, ℓ_c, j_c, m_c.
      iii. Does the density matrix depend on the quantum number m_a?
2. One-body potential
   (a) Write down the matrix elements of the one-body term of the Hamiltonian in the HO basis.
3. Minnesota Potential
   (a) Write the antisymmetrized Minnesota potential in the form $\hat{V}^D + \hat{V}^E \hat{P}_r$
   (b) Recall the definition of the Hartree-Fock potential Γ_{ac} and the total HF potential energy as a function of the antisymmetrized two-body matrix elements (TBME) and the density matrix.
   (c) Based on the symmetry properties of the density matrix derived in 1.b.ii and 1.b.iii, what TBME do you need to compute?
   (d) Now and in the following, we will only take $\ell = 0$ states in our basis. Compute the (non-antisymmetrized) matrix elements of a generic Gaussian $e^{-(r_1-r_2)^2/\mu^2}$ (compute only the matrix elements needed based on the results of the previous question).
   (e) Optional: the radial integrals that you obtained in the previous step can be computed directly by numerical quadrature, but they may also be simplified before. We have not checked if it is possible and what is the gain, so we leave it to you to do it if you are interested...
   (f) Compute the direct and exchange matrix elements of the Minnesota interaction. [Hint: Use the result that $\sum_{m_b} \langle n_a a n_b b|\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2|n_c a n_d b\rangle = 0$. If you want to have fun with angular momentum algebra, you can demonstrate this result...]

After these exercises, you should be able to set up the fully Hartree-Fock matrix, and, therefore, proceed with the iterative HF procedure: initialize the density, compute the HF field, form the HF matrix, diagonalize it, calculate a new iteration of the density, etc., until convergence is achieved.