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 Solving the Hartree-Fock Equations

1. Ground-work
   (a) Write the Hamiltonian in second quantization form
   (b) We will assume spherical symmetry is conserved. Hence the basis states $\psi_{n\ell jm}$ are eigenstates of the $\hat{J}^2$ and $\hat{J}_z$ operators.
      i. What is the consequence for matrix elements of the type $\langle\psi_{n\ell jm}|\hat{H}|\psi_{n'\ell'j'm'}\rangle$ [Hint: If spherical symmetry is conserved, then the relevant angular momentum operator commutes with the Hamiltonian.]
      ii. If the general definition of the density matrix is $\rho(\boldsymbol{r}) = \sum_{ab}\rho_{ab}\phi_a^*(\boldsymbol{r})\phi_b(\boldsymbol{r})$, obtain a reduced expression for $\rho(\boldsymbol{r})$ depending only on n_a, ℓ_a, j_a, n_b and the radial wave-functions
   (c) Write down the antisymmetrized matrix elements of the Hamiltonian as a function of the HO basis functions $\psi_{n\ell jm}$
   (d) Derive the expression of the matrix elements of the oscillator term, one-body component of the Hamiltonian in the spherical HO basis. [We will give you the matrix elements of the kinetic energy term]
   (e) Derive the expression of the matrix elements of the two-body term in the spherical HO basis
2. Setting up the HF Equations
   (a) Derive the expression for the matrix elements of the HF mean-field Γ_{ij} in the HO basis
   (b) Wrapping up: Define the HF equations to be solved