

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

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

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

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

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

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

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

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

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}
$V_{0,s}$	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 $\langle \mathbf{r}\sigma | a \rangle \equiv \langle \mathbf{r}\sigma | n_a, \ell_a, j_a, m_a \rangle$ using spherical coordinate, radial wave functions, spherical harmonics, spin functions, etc.

$$[\langle \mathbf{r}\sigma | a \rangle = R_{n_a \ell_a}(r) \mathfrak{Y}_{j_a m_a}(\theta, \varphi) = R_{n_a \ell_a}(r) \sum_{m_s=\pm 1/2} Y_{\ell_a m_{\ell, a}}(\theta, \varphi) \chi_{s_a m_{s, a}}]$$

- ii. The local density matrix in r -space is denoted by $\rho(\mathbf{r}, \sigma)$, 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 .

$$[\rho_{ac} = \rho_{n_a n_c}^{\ell_a j_a m_a} \delta_{\ell_a \ell_c} \delta_{j_a j_c} \delta_{m_a m_c}]$$

- iii. Does the density matrix depend on the quantum number m_a ? [No, because of spherical symmetry]

2. One-body potential

- (a) Write down the matrix elements of the one-body term of the Hamiltonian in the HO basis.

$$[\langle n_a, \ell_a, j_a, m_a | \hat{h}_0 | n_c, \ell_c, j_c, m_c \rangle = \hbar\omega \left(2n_a + \ell_a + \frac{3}{2} \right) \delta_{n_a n_c} \delta_{\ell_a \ell_c} \delta_{j_a j_c} \delta_{m_a m_c}]$$

3. Minnesota Potential

- (a) Write the antisymmetrized Minnesota potential in the form $\hat{V}^D + \hat{V}^E \hat{P}_r$

$$[\hat{V}^D = \hat{V}^E = \frac{1}{2}(V_R + V_S)(1 - \hat{P}_\sigma)]$$

- (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.

$$[\Gamma_{ac} = \sum_{bd} \bar{v}_{abcd} \rho_{db}, \quad E = \frac{1}{2} \sum_{ac} \Gamma_{ac} \rho_{ca}]$$

- (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? [Only $\langle n_a \ell_a j_a m_a, n_b \ell_b j_b m_b | \hat{v} | n_c \ell_c j_c m_c, n_d \ell_d j_d m_d \rangle$]

- (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).

$$[(n_a n_b | \hat{v} | n_c n_d) = \int r_1^2 dr_1 \int r_2^2 dr_2 R_{n_a 0}(r_1) R_{n_b 0}(r_2) e^{-(r_1-r_2)^2/\mu^2} R_{n_c 0}(r_1) R_{n_d 0}(r_2)]$$

- (e) 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...]

$$[\langle \hat{V}^D \rangle = \langle \hat{V}^E \rangle = \frac{1}{4} \langle V_R + V_S \rangle]$$