Hartree-Fock Calculations of Neutron Drops
Phase 1: Development of a generic HF solver

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1   Introduction

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. Since Hartree-Fock theory is the starting point for most of these techniques (BCS, HFB, RPA, DME, etc.), the first phase of the computational project is to develop a computer program to solve the HF equations in a given s.p. basis (e.g., HO basis).

Rather than attacking the full neutron drop problem head-on, in the first phase we will solve a simplified, somewhat contrived version of the problem in order to get a working HF implementation as quickly as possible. As we will discuss below, a well-designed HF code is split into two components

1. A **Solver class** (or Fortran module) that solves the HF equations independent of the details of the physical system (e.g., neutron drops, nuclei, quantum dots, atoms, choice of s.p. basis, calculation of two-body matrix elements, etc.).

2. A **System class** (or Fortran module) that implements/administers all the details specific to the particular system.

Therefore, in the first phase we will work with a simplified picture of neutron drops in which only S-wave ($l = 0$) single particle basis states are considered. This will allow us to focus on developing the HF solver without getting bogged down with technical details (angular momentum recoupling, Talmi-Moshinsky transformation brackets, etc.) associated with generating the input two-body matrix elements for the general case.

2 Hartree Fock Equations

As shown in the lectures, the Hartree-Fock equations can be written as a matrix diagonalization problem in a given basis $|\alpha\rangle$ as

$$\sum_\beta h_{\alpha\beta} D_{\beta q} = \epsilon_q D_{\alpha q}\,. \tag{1}$$

The HF hamiltonian is defined as

$$h_{\alpha\beta} = t_{\alpha\beta} + \Gamma_{\alpha\beta}\,, \tag{2}$$

where the single-particle potential $\Gamma_{\alpha\beta}$ is

$$\Gamma_{\alpha\beta} \equiv \sum_{\mu\nu} v_{\alpha\nu\beta\mu} \rho_{\mu\nu}\,, \tag{3}$$

$v_{\alpha\beta\gamma\delta}$ are antisymmetrized two-body matrix elements (TBMEs),

$$v_{\alpha\beta\gamma\delta} = \langle\alpha\beta|V|\gamma\delta\rangle = (\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma)\,, \tag{4}$$

and the density matrix is given by

$$\rho_{\mu\nu} = \sum_{i=1}^{N} \langle\mu|i\rangle\langle i|\nu\rangle = \sum_{i=1}^{N} D_{\mu i} D_{\nu i}^{*}\,. \tag{5}$$

Note that $t_{\alpha\beta}$ denotes the matrix elements of the 1-body part of the starting hamiltonian. For self-bound nuclei $t_{\alpha\beta}$ is the kinetic energy, whereas for neutron drops, $t_{\alpha\beta}$ represents the harmonic oscillator hamiltonian since the system is confined in a harmonic trap. If we are working in a harmonic oscillator basis with the same ω as the trapping potential, then $t_{\alpha\beta}$ is diagonal.

The HF equations need to be solved iteratively, since $h_{\alpha\beta}$ depends on the eigenvectors $D_{\alpha q}$ via the density matrix. Therefore, one typically follows the following procedure

1. Start with an initial guess for $D_{\alpha q}^{(0)}$ and construct $\rho_{\nu\mu}^{(0)}$, $h_{\alpha\beta}^{(0)}$.

2. Diagonalize $h_{\alpha\beta}^{(0)}$ and use the lowest N eigenvectors $D_{\alpha i}^{(1)}$ to construct the next iteration for $\rho_{\nu\mu}^{(1)}$, $h_{\alpha\beta}^{(1)}$.

3. Continue the process until things don't change above some threshold from one iteration to the next. For instance, one could iterate until the change in the HF eigenvalues obeys

$$\frac{\sum_p |\epsilon_p^{(n)} - \epsilon_p^{(n-1)}|}{m} \leq \lambda,$$

   where λ is a user prefixed quantity ($\lambda \sim 10^{-8}$ or smaller) and p runs over all calculated single-particle energies and m is the number of single-particle states.

3 Code Example

An example of a function in C++ which performs the Hartree-Fock calculation is shown here. In setting up your code you will need to write a function which sets up the single-particle basis, the matrix elements $t_{\alpha\gamma}$ of the one-body operator (called $h0$ in the function below) and the antisymmetrized TBMEs (called *matrixElement* below) and the density matrix elements $\rho_{\beta\delta}$ (called *densityMatrix* below).

```cpp
void hartreeFock::run() {
    double spPot;
    // ———————————— Setting up the HF–hamiltonian using D = 1 as
        guess, Armadillo is used for vectors
    mat h;
    vec E = zeros(nStates, 1);
    vec ePrev = zeros(nStates, 1);
    mat D = eye(nStates, nStates);
    vec diff;

    // Hartree−Fock loop
    int hfIt = 0;
    while (hfIt < HFIterations) {
        cout << "iteration = " << hfIt << endl;

        h = zeros(nStates, nStates);
        for (int alpha = 0; alpha < nStates; alpha++) {
            for (int gamma = 0; gamma < nStates; gamma++) {
                spPot = 0;
                    for (int beta = 0; beta < nStates; beta++) {
                        for (int delta = 0; delta < nStates; delta++)
                        {
                            spPot += densityMatrix(beta, delta ,D) *
                                matrixElement(alpha, beta, gamma, delta
                                );
                        }
                    }

                h(alpha, gamma) = h(gamma, alpha) = h0(alpha, gamma) +
                    spPot;
            }
        }
        //Computing the HF one−body energies
        eig_sym(E, D, h);
        // Transposing the vectors
        D = trans(D);
```

```
        hfIt++;
        // Convergence test
        diff = E − ePrev;
        if (abs(diff.max()) < threshold)
            break;
        ePrev = E;
    }
    double E0 = calcEnergy(D);
    cout << "Final energy E = " << E0 << " after " << hfIt << "
        iterations, error < " << threshold << endl;
}
```

4 Project work plan

Each group should start discussing and working on the following tasks.

4.1 Statement of the model problem

To bypass complications associated with calculating the input $v_{\alpha\beta\gamma\delta}$ (angular momentum coupling, Talmi-Moshinsky transformation, etc.), we start with a simplified version of neutron drops in which our single-particle model space is comprised entirely of S-wave HO wave functions.

$$|\alpha\rangle = |n, l, m, \sigma\rangle \quad \Rightarrow \quad |n, 0, 0, \sigma\rangle. \tag{6}$$

In this restricted model space, we will start with the lightest "closed-shell" neutron drop, $N = 2$. (What are the other possible closed-shell drops in this model space?)

4.2 HF Solver

1. Write "pseudo-code" for your HF solver. Feel free to refer to the C++ listing above for guidance.

2. Translate your pseudo-code into an actual implementation.

4.3 System class/module

1. Before you tackle the Minnesota potential, with all the complications arising from it's spin-dependence and exchange character (i.e., the occurrence of terms like $V(r)P_r$, where P_r exchanges the spacial positions of particles 1 and 2.), consider a simple spin-independent local central potential. Evaluate the expression for the un-antisymmetrized matrix elements

$$(n_1 00\sigma_1, n_2 00\sigma_2 | V | n_3 00\sigma_3 n_4 00\sigma_4) \tag{7}$$

5 The Microscopic Neutron Drop Hamiltonian

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

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \sum_{i=1}^{N} \frac{1}{2} m\omega \boldsymbol{r}_i^2 + \sum_{i<j} \hat{V}_{ij}, \tag{8}$$

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

$$\hat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \left[\hat{V}_R(\boldsymbol{r}_1, \boldsymbol{r}_2) + \frac{1}{2}\left(1 + \hat{P}_\sigma\right) \hat{V}_t(\boldsymbol{r}_1, \boldsymbol{r}_2) + \frac{1}{2}\left(1 - \hat{P}_\sigma\right) \hat{V}_s(\boldsymbol{r}_1, \boldsymbol{r}_2) \right]$$
$$\times \frac{1}{2}\left(1 + \hat{P}_r\right), \quad (9)$$

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

$$\hat{V}_R(\boldsymbol{r}_1, \boldsymbol{r}_2) = +V_{0,R} e^{-\kappa_R(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}, \tag{10}$$
$$\hat{V}_t(\boldsymbol{r}_1, \boldsymbol{r}_2) = -V_{0,t} e^{-\kappa_t(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}, \tag{11}$$
$$\hat{V}_s(\boldsymbol{r}_1, \boldsymbol{r}_2) = -V_{0,s} e^{-\kappa_s(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}. \tag{12}$$

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

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

1. Ground-work

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}

(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.

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

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

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

    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 $\langle n_a\ell_aj_am_a, n_b\ell_bj_bm_b|\hat{v}|n_c\ell_aj_am_a, n_d\ell_bj_bm_b\rangle$]

(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).

$$[\langle n_an_b|\hat{v}|n_cn_d\rangle = \int r_1^2 dr_1 \int r_2^2 dr_2 \ R_{n_a0}(r_1)R_{n_b0}(r_2)e^{-(r_1-r_2)^2/\mu_2}R_{n_c0}(r_1)R_{n_d0}(r_2)]$$

(e) Compute the direct and exchange matrix elements of the Minnesota interaction. [Hint: Use the result that $\sum_{m_b}\langle n_aan_bb|\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2|n_can_db\rangle = 0$. If you want to have fun with angular momentum algebra, you can demonstrate this result...]

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