Hartree-Fock Calculations of Neutron Drops

Phase 3: Development of Extensions Beyond Hartree-Fock

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1 Introduction

The HF solver that you have developed is the starting point to study a number of different approximations to the many-body problem. In phase III of the computational projects, we propose that you try and implement one of the following extensions beyond HF.

- Implement the density matrix expansion of the Minnesota potential. The goal here is to benchmark the DME – which produces a functional of the local density – against the exact result.
- Solve the HFB equations in spherical symmetry. The level of difficulty should not be too high if you understand your HF solver well. In addition to doubling the size of the matrix to diagonalize and dealing with the pairing tensor, one technical difficulty is to determine the Fermi energy by solving a Newton-like method.
- Solve the RPA equations in spherical symmetry. It is also relatively simple, but you will need to pay attention to your implementation, since naive brute force could make your code very slow.
- Solve the deformed HF equations. This is probably the most ambitious project: you need to set up new quadrature rules and basis functions, and put up some significant work into designing your implementation, else your code will run for ever...

2 Building EDFs at the LDA and DME level

As discussed in the lectures, the density matrix expansion (DME) is a promising technique to build a quasi-local EDF starting from the underlying NN and NNN interactions, working

either at the Hartree-Fock (HF) or Brueckner-Hartree-Fock (BHF) level. In the following, we outline the basic steps to derive and implement quasi-local EDF approximations to the fully non-local HF calculations you implemented in the first two phases of the project.

Local Density Approximation to Hartree-Fock The LDA gives the simplest path for deriving a local EDF starting from a microscopic hamiltonian. In the most sophisticated implementation, one only applies the LDA to the non-local exchange (Fock) energy, treating the finite-range Hartree contribution exactly since it only probes the diagonal densities. With your HF code, it is no problem in principle to treat the Hartree term exactly. However, this requires that one treats the direct and exchange matrix elements of the anti-symmetrized NN potential separately. Unfortunately, the "black box" code used to generate the m-scheme and J-scheme matrix elements has the antisymmetry built in, making it hard to separate the direct and exchange contributions without digging deep into the workings of the code. Therefore, for the present problem you will apply the LDA to both the Hartree and Fock energy contributions to avoid this technicality.

At the heart of the LDA is a calculation of the energy/particle of the infinite homogenous system– pure neutron matter in the present problem. Here is an outline of the steps you need to do this.

1. Starting from the general expression for the HF interaction energy, show that one gets the following expression for the Minnesota potential for spin-saturated systems (i.e., systems with vanishing spin-vector density matrices)

$$\begin{aligned} E_{int}^{HF} &= E_H + E_F \qquad (1)\\ E_H &= \frac{1}{2}\int d\mathbf{R}\int d\mathbf{r}\, V_C(r)\rho(\mathbf{R}+\mathbf{r}/2)\rho(\mathbf{R}-\mathbf{r}/2)\\ E_F &= \frac{1}{2}\int d\mathbf{R}\int d\mathbf{r}\, V_C(r)\rho(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)\rho(\mathbf{R}-\mathbf{r}/2,\mathbf{R}+\mathbf{r}/2)\,, \end{aligned}$$

   where $V_C = \frac{1}{4}(V_R + V_S)$.

2. Now apply this to the system of infinite homogenous neutron matter ($A \to \infty$, $V \to \infty$, $\rho \to const$), remembering that $\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho\, \rho_{SL}(k_F r)$, where $\rho_{SL}(x) = 3j_1(x)/x$. This gives the following expression for the HF interaction energy per particle

$$\frac{E_{int}^{HF}}{A} \equiv e_{HF}(\rho) = \frac{1}{2}\rho\int d\mathbf{r} V_C(r) + \frac{1}{2}\rho\int d\mathbf{r}\rho_{SL}^2(k_F r)V_C(r)\,. \qquad (2)$$

3. Now that you have the HF energy for the infinite system, the LDA amounts to defining the interaction energy piece of the EDF as

$$E_{int}[\rho] \equiv \int d\mathbf{r}\rho(\mathbf{r})e_{HF}(\rho(\mathbf{r}))\,. \qquad (3)$$

The LDA approximation to the HF s.p. hamiltonian is then purely local, and is given by

$$h(\mathbf{r}) = h_0(\mathbf{r}) + \frac{\delta}{\delta\rho(\mathbf{r})}E_{int}[\rho] \equiv h_0(\mathbf{r}) + \Gamma_{LDA}(\mathbf{r})\,, \tag{4}$$

where h_0 is the HO hamiltonian and the s.p. field Γ_{LDA} is given by

$$\Gamma_{LDA}(\mathbf{r}) = \frac{\delta}{\delta\rho(\mathbf{r})}E_{int}[\rho] = e_{HF}(\rho(\mathbf{r})) + \rho(\mathbf{r})\frac{\partial}{\partial\rho}e_{HF}(\rho)|_{\rho(\mathbf{r})} \tag{5}$$

Note that $\Gamma_{LDA}(\mathbf{r})$ depends on the density, so the resulting s.p. equations need to be solved self-consistently as in the original HF calculations. You can use your existing HF code to do this, once you have implemented functions to calculate $e_{HF}(\rho)$ and $\Gamma_{LDA}(\mathbf{r})$, and to take matrix elements of $\Gamma_{LDA}(\mathbf{r})$ on the HO basis

$$\langle nljm|\Gamma_{LDA}|n'ljm\rangle = \int r^2 dr R_{nl}(r)\Gamma_{LDA}(r)R_{n'l}(r) \tag{6}$$

4. Once you have reached self-consistency, the LDA approximation to the HF energy is evaluated as

$$E^{HF}_{LDA} = \sum_{i=1}^{A}\langle\phi_i|h_0|\phi_i\rangle + E_{int}[\rho]\,, \tag{7}$$

where ϕ_i are the self-consistent HF-LDA orbitals and ρ is the self-consistent density

$$\rho(\mathbf{r}) = \sum_{i=1}^{A}\phi_i^*(\mathbf{r})\phi_i(\mathbf{r}) \tag{8}$$

Density Matrix Expansion - The DME approximation to HF looks very similar to the simple LDA outlined above, but now with explicit gradient corrections and dependence on the local kinetic energy density, $\tau(\mathbf{R}) = \nabla_1\cdot\nabla_2\rho(\mathbf{r}_1,\mathbf{r}_2)\big|_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{R}}$. As with the LDA calculation, we will not treat the full finite-range Hartree energy exactly. Rather, we will apply a naive Taylor expansion to map the Hartree energy into a Skyrme-like form. Here are the steps to implement the DME approximation to HF:

1. In the non-local Fock energy expression, plug in the DME expression for the density matrix

$$\rho(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2) \approx \pi_0(k_F r)\rho(\mathbf{R}) + \frac{r^2}{6}\pi_2(k_F r)\big[\frac{1}{4}\nabla^2\rho - \tau + \frac{3}{5}k_F^2\rho\big]\,, \tag{9}$$

keeping only terms to 2nd-order in small quantities (i.e., treat the terms involving π_2 as 2nd-order), so that

$$\rho^2(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2) \approx \pi_0^2\rho^2 + \frac{r^2\pi_0\pi_2}{3}\left[\frac{\rho\nabla^2\rho}{4} - \rho\tau + \frac{3}{5}k_F^2\rho^2\right] \tag{10}$$

2. Simplify your expression for $E_F[\rho, \tau, \nabla^2\rho]$ to get it into the form

$$E_F \approx \int d\mathbf{R}\Big\{ C^{\rho\rho}\rho^2 + C^{\rho\tau}\rho\tau + C^{\rho\nabla^2\rho}\rho\nabla^2\rho \Big\}. \tag{11}$$

Your expressions for the density-dependent couplings should take the form as integrals of the π-functions over the finite range NN potential. For example, you should find

$$C^{\rho\rho} = \int d\mathbf{r} V_C(r)\big[\pi_0^2(k_F r) + \frac{1}{5}(k_F r)^2\pi_0(k_F r)\pi_2(k_F r)\big] \tag{12}$$

In both Negele-Vautherin and PSA flavors of the DME, you should be able to get analytical expressions for all couplings. As a reminder, the PSA π-functions are all equal to ρ_{SL}, while the NV ones are given by $\pi_0(x) = \rho_{SL}(x)$, $\pi_2(x) = 105 j_3(x)/x^3$.

3 HFB equations in spherical symmetry

HFB equations - Remember that the most general form of the HFB equations is

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix} \tag{13}$$

In this expression, h and Δ are matrices of size $n \times n$, with n the size of the single-particle basis (i.e. the total number of states in the HO basis in our example). λ is a shorthand notation for λI, with I the $n \times n$ identity matrix; λ is the Fermi level introduced to constrain the average value of the particle number to its actual value. For each of the n eigenvectors of energy E_μ, there is one with eigenvector $-E_\mu$.

Bogoliubov transformation - In spherical symmetry, the conjugate single-particle states a and $\bar{a}$ are characterized by $|a\rangle \equiv |n_a l_a j_a m_a\rangle$ and $|\bar{a}\rangle \equiv |n_a l_a j_a - m_a\rangle$. As Peter discussed in this lecture on pairing, a and $\bar{a}$ are related by the time-reversal operator. Just as in the HF case, the U and V matrices are block diagonal, i.e., they take the generic form

$$U_{ab} \equiv \delta_{l_a l_b}\delta_{j_a j_b}U^{(l_a j_a)}, \quad V_{ab} \equiv \delta_{l_a l_b}\delta_{j_a j_b}V^{(l_a j_a)}. \tag{14}$$

The difference with the HF case is that things are not entirely independent of the projection m. Suppose we reorder the labelling of the $2j_a + 1$ m-projections in each (l_a, j_a) block according to

$$m = -j, -j+1, \ldots, +j \rightarrow m = +j, -j, +j-1, -j+1, \ldots, +1/2, -1/2. \tag{15}$$

In other words, we form pairs of states $(+m, -m)$; there are $j + 1/2$ such pairs in each block j. Spherical symmetry imposes that the U and V matrices are block diagonal in each

of these $j+1/2$ blocks. Denoting generically $U^{(lj)}_{|m|}$ and $V^{(lj)}_{|m|}$ such blocks, we find

$$U^{(lj)}_{|m|} = \begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix}, \qquad V^{(lj)}_{|m|} = \begin{pmatrix} 0 & v \\ \bar{v} & 0 \end{pmatrix}. \tag{16}$$

For each s.p. state a, we will note

$$u \equiv u^{(a)}, \quad v \equiv (-1)^{j_a - m_a} v^{(a)}, \quad \bar{v} \equiv (-1)^{j_a + m_a} v^{(a)}, \tag{17}$$

The dimension of the block matrices $u^{(a)}$ and $v^{(a)}$ is $(N_0 - l_a)/2$, where N_0 is the number of oscillator shells.

Densities - From these relations, it is straightforward to compute the density matrix ρ and pairing tensor κ. Remember the general definition,

$$\rho_{ab} = (V^* V^T)_{ab}, \qquad \kappa_{ab} = (V^* U^T)_{ab} \tag{18}$$

The density matrix and pairing tensor have a similar block structure as the U and V in the (reordered) s.p. basis. We find

$$\rho^{(lj)}_{|m|} = \begin{pmatrix} \rho & 0 \\ 0 & \rho \end{pmatrix}, \qquad \kappa^{(lj)}_{|m|} = \begin{pmatrix} 0 & \kappa \\ \bar{\kappa} & 0 \end{pmatrix}, \tag{19}$$

with

$$\rho \equiv v^{(a)} v^{(a)T}, \quad \kappa \equiv (-1)^{j_a - m_a} v^{(a)} u^{(a)T}, \quad \bar{\kappa} \equiv (-1)^{j_a + m_a} v^{(a)} u^{(a)T}, \tag{20}$$

HFB equations - Based on the previous remarks, one can show (i) first that the HFB equations can also be reduced to a block diagonal form in each of the $j+1/2$ blocks characterized by l, j and $|m|$, (ii) then that these new equations can be further reduced so that they also become block-diagonal in the subspace of $(+m, -m)$. The end result is that the HFB equations take the following form

$$\begin{pmatrix} h^{(a)} - \lambda & -\Delta^{(a)} \\ -\Delta^{(a)} & -h^{(a)} + \lambda \end{pmatrix} \begin{pmatrix} u^{(a)} \\ v^{(a)} \end{pmatrix} = E^{(a)} \begin{pmatrix} u^{(a)} \\ v^{(a)} \end{pmatrix} \tag{21}$$

where the $u^{(a)}$ and $v^{(a)}$ have been introduced before. Denoting

$$\rho^{(a)} = v^{(a)} v^{(a)T}, \quad \kappa^{(a)} = v^{(a)} u^{(a)T} \tag{22}$$

we find the mean-field,

$$h^{(a)}_{n_a n_c} = t^{(a)}_{n_a n_c} + \Gamma^{(a)}_{n_a n_c} \tag{23}$$

the HF potential,

$$\Gamma^{(a)}_{n_a n_c} = \sum_{n_b n_d} \langle n_a m_a n_b m_a | \bar{v} | n_c m_a n_d m_a \rangle \rho^{(a)}_{n_d n_a} \tag{24}$$

and the pairing field

$$\Delta^{(a)}_{n_a n_c} = \sum_{n_b n_d} \langle n_a m_a n_b - m_a | \bar{v} | n_c m_a n_d - m_a \rangle \kappa^{(a)}_{n_d n_a} \tag{25}$$

Practical implementation

1. In your HF code, you were already dealing with the blocks of the density matrix, which I denoted by $\rho^{(a)}$; you must now introduce another such object that will contain the pairing tensor $\kappa^{(a)}$. This object will also have to be initialized before to start the HFB iterations [See what happens if you initialize it with zeros only].

2. The number of particles is not conserved in HFB. You must, therefore, not forget to readjust λ at each iteration. This is done by requesting that

$$\mathrm{Tr}\rho = A \tag{26}$$

where A is your input particle number. The simplest way to do this is to use a BCS-like expression for quasiparticle occupations. At a given iteration, we thus define $\bar{\varepsilon}_n$ and $\bar{\Delta}_n$ according to

$$E_n = \sqrt{(\bar{\varepsilon}_n - \lambda)^2 + \bar{\Delta}_n^2} \tag{27}$$

$$N_n = \frac{1}{2}\left[1 - \frac{\bar{\varepsilon}_n - \lambda}{\sqrt{(\bar{\varepsilon}_n - \lambda)^2 + \bar{\Delta}_n^2}}\right] \tag{28}$$

where E_n is the energy of quasiparticle number n, $E_n \equiv E^{(l_a j_a)}$, and N_n is the norm of the V matrix for this q.p.

$$N_n \equiv N^{(l_a j_a)} = \sum_{n'} |v^{(a)}_{n'n}|^2 \tag{29}$$

[recall that you should get $\sum_{n'} |u^{(a)}_{n'n}|^2 + |v^{(a)}_{n'n}|^2 = 1$ from the diagonalization of the HFB matrix]. By computing the particle number as

$$A(\lambda) = \sum_{l_a j_a} (2j_a + 1) N^{(l_a j_a)} \tag{30}$$

we can set up a Newton-like method to obtain λ.

3. The corollary of the previous steps is that you do not need to impose that only the first n_{occ} occupied states are included when defining the density matrix.

4 RPA equations in spherical symmetry

RPA equations - Recall that the RPA equations for channel ν read

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} = E_\nu \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} \tag{31}$$

with

$$A_{mi,nj} = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \langle \overbrace{m\underbrace{j|\hat{V}^{\rm res}|i}_{J}n}^{J} \rangle \tag{32}$$

$$B_{mi,nj} = \langle \overbrace{m\underbrace{j|\hat{V}^{\rm res}|i}_{J}n}^{J} \rangle \tag{33}$$

where

- As before, labels $m, n, \ldots$ refer to particle states (above the Fermi level) and labels $i, j, \ldots$ refer to hole states (below the Fermi level)
- ϵ_i are the eigenvalues of the HF equations
- $\hat{V}_{\rm res}$ is the residual interaction; in your project, you will take the same interaction as for the HF equations, i.e., $\hat{V}^{\rm res}$ will be the Minnesota potential

Matrix elements - The notation for the matrix elements indicates that they are computed in the J-scheme; since the couping is between *particle and holes of the HF states*, you do not have access to these matrix elements: the ones that you obtain from Morten's code are matrix elements *in the HO basis*, and the coupling is between s.p. states of the bra and kets.

The simplest way to proceed is the brute force method (as usual). The coupled matrix elements for the RPA are defined from the uncoupled ones as

$$\langle \overbrace{m\underbrace{j|\hat{V}^{\rm res}|i}_{J}n}^{J} \rangle = \sum_{\text{all m}} (-1)^{j_b - m_b + j_c - m_c} (j_a j_c m_a - m_c | JM)(j_b j_d m_b - m_d | JM) \times \langle j_a m_a, j_b m_b | \hat{V}^{\rm res} | j_c m_c, j_d m_d \rangle \tag{34}$$

Now, the matrix elements $V^{\rm res}_{abcd} = \langle j_a m_a, j_b m_b | \hat{V}_{\rm res} | j_c m_c, j_d m_d \rangle$ are uncoupled (in terms of angular momentum), but the states are still HF states. However, from the diagonalization of the HF Hamiltonian, you get the expansion of these states as function of HO states,

$$|\bar{n} l j m\rangle_{HF} = \sum_{n'} D^{lj}_{n'\bar{n}} |n' l j m\rangle_{HO} \tag{35}$$

You can, therefore, express all the matrix elements $V^{\rm res}_{abcd}$ as a function of the original matrix elements of the potential in the HO basis.

Practical implementation

1. For a given J and parity π, define the basis of coupled particle-hole excitations, i.e., the states $|mi\rangle$ by taking all hole states below the Fermi level, and all the particle states up to a cut-off $E_{\rm cut}$ that should be an input of your code. Note that in the various expressions given above, I dropped the indices related to the n and l quantum numbers. In practice, the HF states coming out as eigenstates of the HF matrix are

$$\begin{aligned} k=0: &\quad |0,0,1/2\rangle \equiv 0s1/2 \\ k=1: &\quad |0,1,3/2\rangle \equiv 0p3/2 \\ k=2: &\quad |0,1,1/2\rangle \equiv 0p1/2 \\ k=3: &\quad |0,2,3/2\rangle \equiv 0d3/2 \\ k=4: &\quad |0,2,5/2\rangle \equiv 0d5/2 \\ k=5: &\quad |2,0,1/2\rangle \equiv 1s1/2 \\ &\vdots \qquad\qquad \vdots \end{aligned}$$

   The first step is, therefore, to set up some bookkeeping mechanism to keep track of your s.p. states and compute the p.h. two-body states.

2. Compute the JJ matrix elements according to Eq.(34)

3. Compute the matrix elements of your RPA matrix according to Eqs.(32)-(33)

4. Diagonalize the RPA matrix

5 Deformed HF equations

In principle, one could solve the deformed HF equations in the spherical basis by "simply" adding several loops over l_c, j_c, l_d, j_d instead of assuming a block diagonal structure of the HF matrix. However, since our neutrons are confined in a *spherical* trap, one would probably never be able to observe symmetry breaking and deformation for the HF potential and/or the density. To avoid this, we will introduce the Cartesian version of the HO oscillator basis functions and solve the HF functions in this basis. To make calculations doable, we also need to explicitly introduce the Moshinsky transformation, which, luckily, is simpler in Cartesian coordinates than it is in spherical coordinates.

In the following, we will see how to compute the matrix elements of a general Gaussian potential in the Cartesian deformed HO basis. The potential is defined as

$$\hat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{w=1}^{N_w} \alpha_w e^{-\beta_w(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2}, \tag{36}$$

where the dimensions are $[\alpha_w] = \text{MeV}$ and $[\beta_w] = \text{fm}^{-2}$.

Harmonic Oscillator Basis in Cartesian Coordinates - The eigenfunctions of a spin-less three-dimensional harmonic oscillator (HO) are given by

$$\varphi_{\boldsymbol{n}}^{(\boldsymbol{b})}(\boldsymbol{r}) = \langle \boldsymbol{r} | \boldsymbol{n} \rangle \tag{37}$$

with $\varphi_{\boldsymbol{n}}^{(\boldsymbol{b})}(\boldsymbol{r}) = \varphi_{\boldsymbol{n}}^{(\boldsymbol{b})}(x, y, z)$ and

$$\varphi_{\boldsymbol{n}}^{(\boldsymbol{b})}(x, y, z) = \left(\sqrt{b_x} e^{-\frac{1}{2}\xi_x^2} H_{n_x}^{(0)}(\xi_x)\right) \left(\sqrt{b_y} e^{-\frac{1}{2}\xi_y^2} H_{n_y}^{(0)}(\xi_y)\right) \left(\sqrt{b_z} e^{-\frac{1}{2}\xi_z^2} H_{n_z}^{(0)}(\xi_z)\right) \tag{38}$$

where

- The variables in the Hermite polynomials are dimensionless and are defined as

$$\xi_\mu = b_\mu x_\mu, \quad \mu = x, y, z \text{ and } x_\mu = x, y, z, \tag{39}$$

  with the oscillator scales $\boldsymbol{b} \equiv (b_x, b_y, b_z)$ given by

$$b_\mu = \sqrt{\frac{m\omega_\mu}{\hbar}}, \quad \mu = x, y, z. \tag{40}$$

  The oscillator scales have dimensions $[b_\mu] = [\text{fm}]^{-1}$.

- The Hermite polynomials are normalized

$$H_{n_\mu}^{(0)}(\xi_\mu) = \frac{1}{\left(\sqrt{\pi} 2^{n_\mu} n_\mu!\right)^{1/2}} H_{n_\mu}(\xi_\mu), \tag{41}$$

  and the $H_{n_\mu}(\xi_\mu)$ are the standard Hermite polynomials as can be found, e.g., in Abramovitz & Stegun, *Handbook of mathematical functions*, Chapter 22, Eq. 22.2.14.

- The spatial quantum numbers are $\boldsymbol{n} = (n_x, n_y, n_z)$, and the energy of the HO is given by

$$E_{\boldsymbol{n}}^{\text{HO}} = \hbar\omega_x \left(n_x + \frac{1}{2}\right) + \hbar\omega_y \left(n_y + \frac{1}{2}\right) + \hbar\omega_z \left(n_z + \frac{1}{2}\right) \tag{42}$$

Matrix Elements of the Potential - The matrix elements of the Gaussian potential in the HO basis are

$$\langle \boldsymbol{n}'\boldsymbol{m}'|\hat{V}|\boldsymbol{n}\boldsymbol{m}\rangle = \langle \boldsymbol{n}'\boldsymbol{m}'|\sum_w \alpha_w e^{-\beta_w(\boldsymbol{r}_1-\boldsymbol{r}_2)^2}|\boldsymbol{n}\boldsymbol{m}\rangle. \tag{43}$$

Explicitly, they read

$$\langle \boldsymbol{n}'\boldsymbol{m}'|\hat{V}|\boldsymbol{n}\boldsymbol{m}\rangle = \sum_w \prod_{\mu=x,y,z} \iint dx_\mu dx'_\mu \; \varphi^{(b_\mu)}_{n'_\mu}(x_\mu)\varphi^{(b_\mu)}_{m'_\mu}(x'_\mu)\alpha_w^{1/3} e^{-\beta_w(x_\mu-x'_\mu)^2}\varphi^{(b_\mu)}_{n_\mu}(x_\mu)\varphi^{(b_\mu)}_{m_\mu}(x'_\mu) \tag{44}$$

In the following, we will focus on the generic matrix elements

$$v^w_{n'm'nm} = \iint dxdx' \; \varphi^{(b)}_{n'}(x)\varphi^{(b)}_{m'}(x)\alpha_w^{1/3} e^{-\beta_w(x-x')^2}\varphi^{(b)}_{n}(x)\varphi^{(b)}_{m}(x') \tag{45}$$

Expansion of Hermite Polynomials - We search for an expansion of the product of two Hermite functions in the form

$$\varphi^{(b)}_{n'}(x)\varphi^{(b)}_{n}(x) = \sum_{A=0}^{n'+n} C^A_{n'n}\varphi^{(b')}_A(x). \tag{46}$$

After some not-so-lengthy algebra, we find

$$C^A_{n'n} = \sum_{i=1}^{N} w_i \varphi^{(b/\sqrt{\alpha})}_{n'}(x_i)\varphi^{(b/\sqrt{\alpha})}_{n}(x_i)\varphi^{(b'/\sqrt{\alpha})}_{A}(x_i)\alpha^{1/4}e^{x_i^2}. \tag{47}$$

At this point, we choose $b' = b\sqrt{2}$, hence $\alpha = 2b^2$ (and $b' = \sqrt{\alpha}$). Our coefficients read

$$C^A_{n'n} = \sum_{i=1}^{N} \left(b\sqrt{2}\right)^{1/2} w_i e^{x_i^2} \; \varphi^{(1/\sqrt{2})}_{n'}(x_i)\varphi^{(1/\sqrt{2})}_{n}(x_i)\varphi^{(1)}_{A}(x_i). \tag{48}$$

Let us then rescale the Gauss-Hermite nodes and weights in the following way:

$$w_i \to \omega_i = \frac{w_i}{b\sqrt{2}}e^{x_i^2}, \qquad x_i \to X_i = \frac{x_i}{b\sqrt{2}}. \tag{49}$$

We have

$$\begin{cases} \varphi^{(1/\sqrt{2})}_n(x_i) = \dfrac{1}{2^{1/4}}H^{(0)}_n\left(\dfrac{x_i}{\sqrt{2}}\right)e^{-\frac{1}{2}\left(\frac{x_i}{\sqrt{2}}\right)^2} = \dfrac{1}{\sqrt{b\sqrt{2}}}\varphi^{(b)}_n(X_i) \\ \varphi^{(1)}_B(x_i) = H^{(0)}_B(x_i)e^{-\frac{1}{2}x_i^2} = \dfrac{1}{\sqrt{b\sqrt{2}}}\varphi^{(b\sqrt{2})}_B(X_i) \end{cases} \tag{50}$$

After these simplifications, we find

$$C^A_{n'n} = \sum_{i=1}^{N} \omega_i \varphi^{(b)}_{n'}(X_i)\varphi^{(b)}_{n}(X_i)\varphi^{(b\sqrt{2})}_{A}(X_i). \tag{51}$$

Moshinsky Transformation - After introducing the expansion (46) of the two product of two Hermite functions in the matrix element (45), we arrive at

$$v^w_{n'm'nm} = \alpha_w^{1/3} \sum_{AB} C^A_{n'n} C^B_{m'm'} \iint dx dx' \; \varphi^{(b\sqrt{2})}_A(x) e^{-\beta_w (x-x')^2} \varphi^{(b\sqrt{2})}_B(x'). \tag{52}$$

The Moshinsky transformation consists in introducing the variables

$$\left\{ \begin{array}{l} U = \dfrac{1}{\sqrt{2}}(x + x') \\ \\ u = \dfrac{1}{\sqrt{2}}(x - x') \end{array} \right. \tag{53}$$

The Jacobian of this transformation is 1. Note that, in our case, since x and x' are in fermis, so are the U and u variables. In fact, the Moshinsky transformation below can be applied either on the normalized Hermite polynomials, $H^{(0)}_n$, or on the Hermite functions, φ_n, irrespective of whether the latter are properly normalized by the $\sqrt{b}$ scale, in exactly the same way. The new variables (U, u) have always the same units as the old one (x, x'). In our case, we apply the transformation on the fully normalized Hermite functions to find

$$\varphi^{(b\sqrt{2})}_A(x)\varphi^{(b\sqrt{2})}_B(x') = \sum_{N,n} D^{Nn}_{AB} \; \varphi^{(b\sqrt{2})}_N(U)\varphi^{(b\sqrt{2})}_n(u). \tag{54}$$

Hence, our matrix element becomes

$$v^w_{n'm'nm} = \alpha_w^{1/3} \sum_{AB} C^A_{n'n} C^B_{m'm'} \sum_{N,n} D^{Nn}_{AB} I_N J_n \tag{55}$$

with

$$\begin{aligned} I_N &= \int dU \; \varphi^{(b\sqrt{2})}_N(U) \\ J_n &= \int du \; e^{-2\beta_w u^2} \varphi^{(b\sqrt{2})}_n(u). \end{aligned} \tag{56}$$

Calculation of the integrals - We give below the analytical results for the integrals [You can calculate them yourselves as a very simple and very boring little exercise]. We have

$$I_N = (-1)^N \left(\frac{\sqrt{2}}{b}\right)^{1/2} \frac{\sqrt{N!}}{2^{N/2}(N/2)!}. \tag{57}$$

and

$$J_n = \frac{1}{\sqrt{\alpha}} \sum_{n'} D_{nn'} \left(\frac{1}{\alpha}\right) I_{n'} \tag{58}$$

where the $D_{nn'}$ matrices are defined by

$$H_n^{(0)}\left(\frac{x}{b}\right) = \sqrt{\frac{b}{b'}} \sum_{n'} D_{nn'} \left(\frac{b'}{b}\right) H_n^{(0)}\left(\frac{x}{b'}\right) \tag{59}$$

Summary - We define the auxiliary integral G_{AB} as

$$G_{AB}^w = \alpha_w^{1/3} \sum_{Nn} D_{AB}^{Nn} I_N J_n = \alpha_w^{1/3} \frac{1}{\sqrt{\alpha}} \sum_{Nn} D_{AB}^{Nn} I_N \sum_{n'} D_{nn'} \left(\frac{1}{\alpha}\right) I_{n'} \tag{60}$$

The matrix element of a single Gaussian w in one-dimension reads

$$v_{n'm'nm}^w = \sum_{AB} C_{n'n}^A C_{m'm'}^B G_{AB}^w \tag{61}$$

In three dimensions, we have

$$V_{\boldsymbol{n'm'nm}}^w = v_{n'_x m'_x n_x m_x}^w v_{n'_y m'_y n_y m_y}^w v_{n'_z m'_z n_z m_z}^w, \tag{62}$$

which expands into

$$V_{\boldsymbol{n'm'nm}}^w = \sum_{A_x B_x} C_{n'_x n_x}^{A_x} C_{m'_x m_x}^{B_x} G_{A_x B_x}^w \sum_{A_y B_y} C_{n'_y n_y}^{A_y} C_{m'_y m_y}^{B_y} G_{A_y B_y}^w \sum_{A_z B_z} C_{n'_z n_z}^{A_z} C_{m'_z m_z}^{B_z} G_{A_z B_z}^w \tag{63}$$

Practical implementation

1. Set up a new module/class/set of routines to compute Gauss-Hermite quadratures and the HO functions in Cartesian coordinates. Some unit tests to check the accuracy of GH quadratures would be welcome.

2. In the next step, you should compute the various coefficients appearing in Eqs.(60)-(63). The coefficients D_{AB}^{Nn} and $C_{n'n}^A$, and the integrals I_N and J_n can be precalculated once and for all.

3. In Cartesian coordinates, pre-computing all matrix elements and storing them on disk (or in memory) is *not a viable option.* There are 12 indices involved, the $n_\mu, \mu = x, y, z$ for each of the 4 s.p. states a, b, c and d, and both the CPU time and the disk space needed to store all matrix elements would be prohibitive. In current DFT solvers

implementing a finite-range force (such as Gogny) in the Cartesian HO basis, the *HF potential and two-body matrix elements are computed on the fly* at each iteration as

$$\Gamma_{ac} = \sum_{bd} \bar{v}_{abcd} \rho_{db} \tag{64}$$

Even then, you need to carefully think of how you will set up your loops in order to obtain a reasonable compute time.

4. The rest of the HF loop is no different from the spherical case. Note that each HF state is not characterized by any particular quantum number.