Exercise: ground state of the deuteron

In this exercise we will solve for the ground state of the deuteron nucleus using a suitable expansion in a complete basis set. The system is composed of two particles, a neutron and a proton, characterized by a 3D coordinate $\vec{r}$, a spin and an isospin. The wave-function of the system can be separated into a center-of-mass component and a relative component

$$\Psi(\vec{r}_1, \vec{r}_1, \sigma_1, \tau_1, \sigma_2, \tau_2) = \Psi_{CM}(\vec{r}_{CM}, \sigma_1, \tau_1, \sigma_2, \tau_2)\Psi_{rel}(\vec{r}_{rel}, \sigma_p, \tau_1, \sigma_2, \tau_2) \ .$$

The CM component is trivial and we can simply focus on the relative one. If we consider only states in an s-wave state in the relative coordinates (which is a reasonably good approximation for our problem) we can express the relative state in the form

$$\Psi(\vec{r}, \sigma_1, \tau_1, \sigma_2, \tau_2) = \sum_j \psi_j(r)\Phi_j(\sigma_1, \tau_1, \sigma_2, \tau_2) \ , \tag{1}$$

where we dropped the subscript *rel* in both the state and the coordinate for ease of notation. For this state to be anti-symmetric we need the spin-isospin part to be odd under a permutation $n \leftrightarrow p$. There are only 4 such states which we can take to be (NOTE: might not be consistent with names given in class)

$$\begin{aligned}
|\Phi_A\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle\right) \\
|\Phi_B\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle\right) \\
|\Phi_C\rangle &= \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\downarrow\uparrow\rangle\right) \\
|\Phi_D\rangle &= \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle\right) \ .
\end{aligned} \tag{2}$$

The wavefunctions are then obtained from the overlap

$$\Phi_j(\sigma_1, \tau_1, \sigma_2, \tau_2) = \langle\sigma_1, \tau_1, \sigma_2, \tau_2|\Phi_j\rangle \ . \tag{3}$$

For the radial wave-function we can use a basis spanned by eigenstates of the 3D harmonic oscillator

$$R_n(r) = N_n e^{-\nu r^2} L_n^{1/2}(2\nu r^2) \ , \tag{4}$$

where $\nu = \mu\omega/(2\hbar)$, μ the reduced mass and ω the oscillator frequency. In the expression above N_n is a normalization constant while $L_n^\alpha(x)$ is a generalized Laguerre polynomial. For $\alpha = 1/2$ these can be expressed as

$$L_n^{1/2}(x^2) = \frac{(-1)^n}{2^{2n+1}n!x} H_{2n+1}(x) \ , \tag{5}$$

where $H_n(x)$ are Hermite polynomials. The latter are defined through the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \ , \tag{6}$$

starting from $H_0(x) = 1$ and $H_1(x) = 2x$. These polynomials are orthogonal under a Gaussian measure, that is

$$\int_{-\infty}^{\infty} dx H_m(x) H_n(x) e^{-x^2} = \sqrt{\pi} 2^n n! \delta_{nm} \ . \tag{7}$$

The radial basis can then be expressed as

$$R_n(r) = \widetilde{N}_n(\nu) \frac{e^{-\nu r^2}}{r} H_{2n+1}(\sqrt{2\nu} r) \ , \tag{8}$$

with the normalization constant determined using Eq. (7). Putting everything together, the relative state can be approximated as

$$\Psi_M(\vec{r}, \sigma_1, \tau_1, \sigma_2, \tau_2) = \sum_{m=0}^{M} \sum_{j=\{A,B,C,D\}} c_{mj} R_m(r) \Phi_j(\sigma_1, \tau_1, \sigma_2, \tau_2) \ , \tag{9}$$

with M determining the size of the basis. The $4M$ coefficients c_{mj} can then be obtained by solving for the lowest energy state of the $4M \times 4M$ matrix

$$\langle mj | \hat{H} | nk \rangle \ , \tag{10}$$

with $\hat{H}$ the Hamiltonian of the system containing a kinetic energy

$$\hat{K} = -\frac{\hbar^2}{2\mu} \nabla^2 \ , \tag{11}$$

as well as a spin-dependent interaction

$$\hat{V} = V_R(r) + \frac{1}{2}\left(1 + \hat{P}^\sigma\right) V_t(r) + \frac{1}{2}\left(1 - \hat{P}^\sigma\right) V_s(r) \tag{12}$$

with $\hat{P}^\sigma$ the permutation operator over the spins acting as

$$\hat{P}^\sigma |\sigma_1, \sigma_2\rangle = |\sigma_2, \sigma_1\rangle \ . \tag{13}$$

The radial functions are instead given by

$$\begin{aligned} VR(r) &= v_{0r} \exp(-k_R r^2) \\ Vt(r) &= -v_{0t} \exp(-k_T r^2) \\ Vs(r) &= -v_{0s} \exp(-k_S r^2) \end{aligned} \tag{14}$$

where the constants are the following

$$\begin{aligned} v_{0r} = 200MeV \quad v_{0t} = 178MeV \quad v_{0s} = 91.85MeV \\ k_R = 1.487fm^{-2} \quad k_T = 0.639fm^{-2} \quad k_S = 0.465fm^{-2} \end{aligned} \tag{15}$$

This nuclear interaction is called the Minnesota potential.

For the exercise you'll need to do the following

1. find the correct expression of the normalization constant in Eq. (8)
2. calculate the expression for the matrix elements of the Hamiltonian in our basis. Note that
   - for the kinetic energy you can use the expression for the derivative of an Hermite polynomial

     $$H_n'(x) = 2nH_{n-1}(x) \tag{16}$$

   - for the potential energy you can perform the required integral in two ways
     (a) using Gauss-Hermite quadrature with enough points so that the value is exact (FYI: with K points you can integrate exactly a polynomial of order $2K-1$ times a gaussian)
     (b) using the orthogonality from Eq. (7) together with the following property

     $$H_{2n+1}(\eta x) = \sum_{i=0}^{n} \eta^{2(n-i)+1}(\eta^2-1)^i \binom{2n+1}{2i} \frac{(2i)!}{i!} H_{2(n-i)+1}(x) \; . \tag{17}$$

     If you choose this way make sure to evaluate ratios and product of factorials in a stable way (ie. take logarithms and add/subtract them before exponentiating the result)
   - the spin-isospin part of the Hamiltonian will be block-diagonal. Try to exploit this fact
3. start with a reasonable value of ν obtained by requiring that the width of the Gaussian defining the radial basis is about the same size of the deuteron. Solve for the ground state energy for different values of M until you reach convergence
   - what is the value of the total spin and total isospin in the ground state?
4. try to repeat the same procedure with other values of ν and check that you obtain the same converged result if you take M large enough (try at least a couple values lower and a couple higher than what you used in the previous point)