Mean Field Approximations of ^{11}Be

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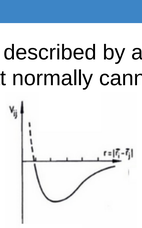
Introduction

The nucleus ^{11}Be is an interesting one because the neutronproton asymmetry (N-Z)/A=3/11 is relatively large and experimental data suggests that in its ground state the valence neutron is in the $1S_{1/2}$ orbit rather than the $0P_{1/2}$ orbit as the independent particle model predicts. We have carried out Hartree-Fock calculations for ^{11}Be, using six Skyrme type nucleon-nucleon interactions, with varying valence nucleon orbit. For each interaction, Skyrme parameters t_0 or t_3 were adjusted such that $1S_{1/2}$ orbit single particle energy would match the experimental values of -0.50 MeV.

Mean Field

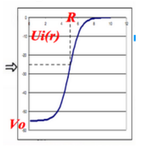
The wave equation of a many-body system is described by a non-linear system of differential equations that normally cannot be solved analytically

$$\widehat{H}_{total} = T + V \qquad V = \sum_{i<j} V(\vec{r_i}, \vec{r_j})$$
$$T = \sum_i \frac{p_i^2}{2m_i} \qquad \widehat{H}_{total}\Psi = E\Psi$$



In the Mean field approximation particles in the system interact individually with a single particle potential approximating the collective contributions from other particles

$$H = \sum_i h_i + H_{res} \qquad H_{res} = \sum_{i<j} V_i(\vec{r_i}, \vec{r_j}) - \sum_i U_i(\vec{r_i})$$
$$h_i \equiv \frac{p_i^2}{2m_i} + U_i(r) \qquad h_i\phi_i = \varepsilon_i\phi_i$$
$$\Phi = \mathfrak{A}\prod_{i=1}^{A}\phi_i(r_i) \text{ where } \mathfrak{A} \text{ is the asymmetry operato for fermions}$$



In the mean field approximation the anti-symmetric wave-function of the many nucleon system can be written as a slater determinant, the determinant of a matrix with single particle wave functions in columns and input particle coordinates in rows

$$\Phi_{SD} = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_1(\vec{r_1},\sigma_1,\tau_1) & \phi_2(\vec{r_1},\sigma_1,\tau_1) & \rightarrow & \phi_A(\vec{r_1},\sigma_1,\tau_1) \\ \phi_1(\vec{r_2},\sigma_2,\tau_2) & \phi_2(\vec{r_2},\sigma_2,\tau_2) & \rightarrow & \phi_A(\vec{r_2},\sigma_2,\tau_2) \\ \downarrow & \downarrow & \searrow & \downarrow \\ \phi_1(\vec{r_A},\sigma_A,\tau_A) & \phi_2(\vec{r_A},\sigma_A,\tau_A) & \rightarrow & \phi_A(r_A,\vec{\sigma_A},\tau_A) \end{vmatrix}$$

Each single-particle wave function is determined by a mean field that approximates its interactions with the other particles in the system. Through spherical symmetry of the nucleus, the solution becomes separable between its radial component and angular components

$$\phi_i(\vec{r_i},\sigma_i,\tau_i) = \frac{R_\alpha(r)}{r}Y_{jlm}(\vec{r_i},\sigma_i)\chi_i(\tau_i)$$

Hartree-Fock Method

the hamiltonian operator is the sum of both the kinetic and potential energy operators.

$$\widehat{H}_{total} = T + V \qquad T = \sum_i \frac{p_i^2}{2m_i} \qquad V = \sum_{i<j} V(\vec{r_i}, \vec{r_j})$$

total energy of the system is the expectation of the hamiltonian operator

$$E = \langle \Phi_{SD} \left| \widehat{H}_{total} \right| \Phi_{SD} \rangle$$

to find the wave functions, we desire the minimum energy possible with the condition that the sum of the density integral over all space equals A so as to conserve the number of nucleons in the system

$$\sum_{i=1}^{A}\int |\phi_i(\vec{r})|^2 d\vec{r} = \sum_{\sigma,\tau}\int \rho_{\sigma,\tau}(\vec{r})d^3\vec{r} = A$$

$$\delta(E - \sum_i \varepsilon_i \int \phi_i^*(\vec{r})\phi_i(\vec{r})d\vec{r}) = 0$$

&

and thus the Hartree-Fock Equation is derived

$$-\frac{\hbar^2}{2m}\Delta\phi_i(\vec{r}) + \sum_{j=1}^{A}\int \phi_j^*(\vec{r'})V(\vec{r},\vec{r'})(\phi_i(\vec{r})\phi_j(\vec{r'}) - \phi_i(\vec{r'})\phi_j(\vec{r}))d\vec{r'} = \varepsilon_i\phi_i(\vec{r})$$

Hartree-Fock with Skyrme Interaction

Skyrme nucleon-nucleon two-body potential

$$V_{ij}^{NN} = t_o(1 + x_oP_{ij}^\sigma)\delta(\vec{r_i} - \vec{r_j}) + \frac{1}{2}t_1(1 + x_1P_{ij}^\sigma)[\overleftarrow{k_{ij}^2}\delta(\vec{r_i} - \vec{r_j}) + \delta(\vec{r_i} - \vec{r_j})\overrightarrow{k_{ij}^2}] +$$
$$t_2(1 + x_2P_{ij}^\sigma)\overleftarrow{k_{ij}} + \frac{1}{6}t_3(1 + x_3P_{ij}^\sigma)\rho^\alpha(\frac{\vec{r_i} + \vec{r_i}}{2})\delta(\vec{r_i} - \vec{r_j}) + iW_o\overleftarrow{k_{ij}}\delta(\vec{r_i} - \vec{r_j})(\vec{\sigma_i} - \vec{\sigma_j}) \times \overrightarrow{k_{ij}}$$

where t0, t1, t2, t3, x0, x1, x2, x3, Wo, α, are the ten Skyrme parameters

$$\overrightarrow{k_{ij}^2} = -\frac{i}{2}(\overrightarrow{\nabla_i} - \overrightarrow{\nabla_j}) \text{ operates on the right side}$$
$$\overleftarrow{k_{ij}^2} = -\frac{i}{2}(\overleftarrow{\nabla_i} - \overleftarrow{\nabla_j}) \text{ operates on the left side}$$
$$P_{ij}^\sigma \text{ is the spin exchange operator}$$

the previous Hartree-Fock equation once all substitutions are done and all coefficients of all variations are made equal to zero then becomes

$$\frac{\hbar^2}{2m_\tau^*}\left[-\frac{\partial^2 R_\alpha}{\partial r^2} + \frac{l_\alpha(l_\alpha+1)}{r^2}R_\alpha(r)\right] - \frac{\partial}{\partial r}\left(\frac{\hbar^2}{2m_\tau^*(r)}\right)\frac{\partial R_\alpha}{\partial r} +$$
$$\left[U_\tau(r) + \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\hbar^2}{2m_\tau^*(r)}\right) + \frac{j_\alpha(j_\alpha+1) - l_\alpha(l_\alpha+1) - \frac{3}{4}}{r}W_\tau(r)\right]R_\alpha(r) = \varepsilon_\alpha(r)R_\alpha(r)$$

where $m_\tau^*(r), U_\tau$, and $W_\tau(r)$ are given in terms of the Skyrme parameters and nucleon densities

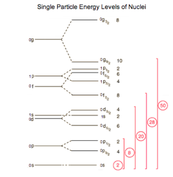
m_τ^*, U_τ^*, and W_τ^* can be determined with an appropriate initial guess for the single particle wave-functions and the Hartree-Fock equations are solved through iteration

^{11}Be

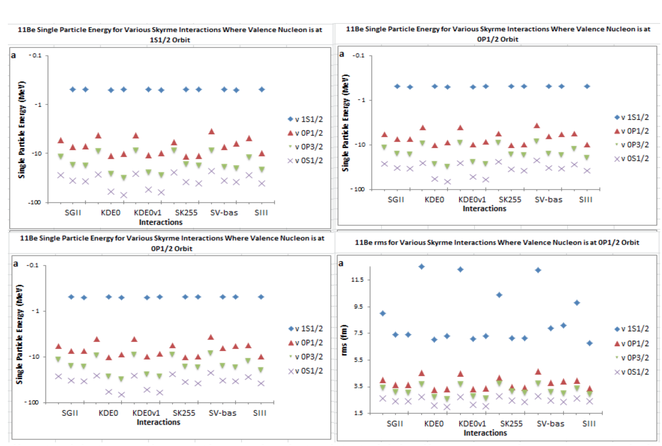
^{11}Be is an interesting nucleus because experimental data suggests that the valence neutron is in the $1S_{1/2}$ orbit rather than the $0P_{1/2}$ orbit as the independent particle model predicts.

KDE0 Results For 11Be Where Valence Nucleon is at 1S1/2 orbit

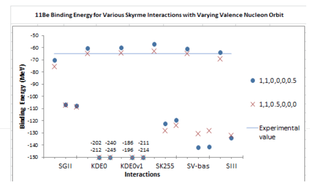
11Be	exp	KDE0	t0=-2849.5	t3=11295.5	KDE0	t0=-2849.5	t3=11295.5
total E	-65.48	-60.36	-201.92	-240.26	-60.36	-201.92	-240.26
			neutron			proton	
ε(1S1/2)	-0.50	0.05	-0.50	-0.50	0.29	-6.81	-9.35
0P1/2	-0.18	-4.20	-11.08	-10.10	-7.58	-22.86	-25.81
0P3/2		-9.12	-27.01	-32.32	-14.01	-43.16	-54.92
0S1/2		-26.98	-58.97	-71.10	-30.74	-71.79	-90.24
r(1S1/2)	6.40	34.75	11.48	11.50	33.33	4.14	3.70
0P1/2		4.37	3.15	3.14	3.76	2.80	2.65
0P3/2		3.57	2.58	2.41	3.26	2.42	2.23
0S1/2		2.60	2.02	1.88	2.60	2.02	1.86



We have carried out Hartree-Fock calculations for ^{11}Be, using six Skyrme type nucleon-nucleon interactions, with varying valence nucleon orbit. In all the original interactions the $1S_{1/2}$ orbit is not bound. None of the interactions predicted that the single particle energy of the particle in $1S_{1/2}$ orbit is lower than $0P_{1/2}$. The $1S_{1/2}$ radius orbit is unbound in original unadjusted interactions, and still much too large for modified values (~7.5 and ~11.5 fm, compared with the experimental value 6.4 fm)



For the adjusted interactions, the calculated total binding energies are much larger in magnitude than experimental values by factors of 2-3 when t0 and t3 values are calibrated.



Conclusions

Hartree-Fock calculations for ^{11}Be, using six skyrme type nucleon-nucleon interactions, fail to appropriately reproduce the single particle structure of the ^{11}Be nucleus. For all original Interactions $1S_{1/2}$ orbit is unbound. For all interactions the $0P_{1/2}$ single particle energy is lower than that of $1S_{1/2}$. predictions fail whether the valence neutron is placed in the $1S_{1/2}$ orbit or the $0P_{1/2}$ orbit and for both original Skyrme parameters and calibrated parameters for proper $1S_{1/2}$ orbit single particle energy. Further research is needed to carry out deformed HF calculations, improve the predictability of the Skyrme interactions, and go beyond the mean-field approximation (i.e. including correlations)