Lecture 6. The Nuclear Shell Model. One-Particle Problem

1 Basic principles of the nuclear shell model

The basic assumption of the nuclear shell model is that to a first approximation each nucleon moves independently in a potential that represents the average interaction with the other nucleons in a nucleus. This independent motion can be understood qualitatively from a combination of the weakness of the long-range nuclear attraction and the Pauli exclusion principle.

The complete Schrödinger equation for A nucleons reads as

$$\hat{H}\Psi(1,2,\ldots,A) = E\Psi(1,2,\ldots,A) \tag{1}$$

where $\hat{H}$ contains single nucleon kinetic energies and two-body interactions

$$\hat{H} = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\Delta_i\right) + \sum_{i<j=1}^{A} W(i,j)\,, \tag{2}$$

and $\Psi(1,2,\ldots,A)$ is a totally antisymmetric wave function, while i denotes all coordinates $\vec{r}_i, \vec{s}_i, \vec{t}_i$ of a given particle ($i = 1,2,\ldots,A$).

We can always formally re-write the Hamiltonian (2), adding and subtracting a potential of the form $\sum_{i=1}^{A} U(i)$:

$$\begin{gathered}\hat{H} = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\Delta_i\right) + \sum_{i=1}^{A} U(i) + \sum_{i<j=1}^{A} W(i,j) - \sum_{i=1}^{A} U(i) = \\ \sum_{i=1}^{A}\left[-\frac{\hbar^2}{2m}\Delta_i + U(i)\right] + \sum_{i<j=1}^{A} W(i,j) - \sum_{i=1}^{A} U(i) = \hat{H}^{(0)} + \hat{H}^{(1)}\,,\end{gathered} \tag{3}$$

where we denoted a sum of single-particle Hamiltonians as $\hat{H}^{(0)}$,

$$\hat{H}^{(0)} = \sum_{i=1}^{A}\left[-\frac{\hbar^2}{2m}\Delta_i + U(i)\right] \equiv \sum_{i=1}^{A}\hat{h}(i)\,, \tag{4}$$

and $H^{(1)}$ is called a *residual interaction*. The assumption of the existence of a nuclear average potential allows to hope that there exists such a potential $\sum_{i=1}^{A} U(i)$, that the residual interaction $H^{(1)}$ is small.

There exist a few approaches to deal with this many-body problem.

1. *Naive shell model* We suppose that $U(i)$ is a known suitable potential (e.g., the harmonic oscillator potential, or the Woods-Saxon potential, or the square-well), solve the Schrödinger equation for $\hat{H}^{(0)}$,

$$\hat{H}^{(0)}|\Phi_k\rangle = E_k^{(0)}|\Phi_k\rangle\,, \tag{5}$$

and neglect the residual interaction $\hat{H}^{(1)}$.

2. *Realistic shell model* First, we repeat the procedure indicated in the previous item. Then we take into account the residual interaction $\hat{H}^{(1)}$, diagonalizing it in the basis of functions $|\Phi_k\rangle$. The standard shell model codes acts in this way, using the harmonic oscillator potential.

3. We can try to construct a one-body potential $\sum_{i=1}^{A} U(i)$ which would be the best approximation to the two-body potential $\sum_{i<j=1}^{A} W(i,j)$, such that $\hat{H}^{(1)} \approx 0$. This can be reached by the so-called *Hartree-Fock* procedure.

In Sections 2 and 3 we consider a single-particle problem with the harmonic oscillator and the Woods-Saxon potentials, respectively. In Section 4 we discuss the basic principles of the naive and realistic shell models. Section 5 is devoted to the Hartree-Fock method. The problems are given in Section 6.

2 Harmonic Oscillator Potential

Let us suppose that each particles move in a harmonic oscillator potential, i.e.

$$\hat{h} = -\frac{\hbar^2}{2m}\Delta + \frac{m\omega^2 r^2}{2} \,. \tag{6}$$

Then the Schrödinger equation

$$\hat{h}\phi(\vec{r}) = \epsilon\phi(\vec{r}) \tag{7}$$

is separable in radial and angular coordinates. The eigenfunctions are given by the products

$$\phi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta,\phi) \,, \tag{8}$$

where $Y_{lm}(\theta,\phi)$ are spherical harmonics (they always appear for a spherically symmetric potential).

The radial wave functions for the harmonic oscillator potential are given by

$$R_{nl}(r) = N_{nl}\, r^l \, \exp\left(-\frac{r^2}{2b^2}\right) L_{n-1}^{l+1/2}\left(\frac{r^2}{b^2}\right) \,, \tag{9}$$

where $b = \sqrt{\frac{\hbar}{m\omega}}$ and $L_{n-1}^{l+1/2}\left(\frac{r^2}{b^2}\right)$ are Laguerre polynomials (they are tabulated for given n and l, see e.g. [1]). The normalization factor N_{nl} is defined by the condition

$$\int_0^\infty r^2 R_{nl}^2(r) dr = 1 \,. \tag{10}$$

The energy eigenvalues are given by

$$\epsilon_N = \hbar\omega\left(2n + l - \frac{1}{2}\right) = \hbar\omega\left(N + \frac{3}{2}\right) \,, \tag{11}$$

with

$$\begin{aligned} &N = 0, 1, 2, \ldots, \\ &l = N, N-2, \ldots, 1 \text{ or } 0 \\ &n = (N - l + 2)/2 \,. \end{aligned} \tag{12}$$

The energy level with a given N is called an *oscillator shell*.

The resulting levels can be denoted as

$N = 0$ $1s$
$N = 1$ $1p$
$N = 2$ $1d$, $2s$
$N = 3$ $1f$, $2p$,
$N = 4$ $1g$, $2d$, $3s$
...

(here the numbers refer to n and the letters denote l).

Each oscillator shell contains orbitals with either even or odd l and it is either even or odd with respect to the parity operation $\hat{P}\,(\vec{r} \to -\vec{r})$:

$$\hat{P}\phi_{nlm}(\vec{r}) = \hat{P}(R_{nl}(r)Y_{lm}(\theta,\phi)) = R_{nl}(r)\hat{P}Y_{lm}(\theta,\phi)) = \\ R_{nl}(r)(-1)^l Y_{lm}(\theta,\phi)) = (-1)^l \phi_{nlm}(\vec{r})\ . \tag{13}$$

The total degeneracy of the Nth oscillator shell is

$$\Omega = 2\sum_{l=0\text{ or }1}^{N} 2(2l+1) = 2(N+1)(N+2)\,, \tag{14}$$

where we take into account the intrinsic spin $s = 1/2$ and isospin $t = 1/2$ of nucleons.

The distance between two different shells is estimated as

$$\hbar\omega = 41A^{-1/3}\text{MeV}\,. \tag{15}$$

The degeneracy of the oscillator shells can be removed by adding the spin-orbit coupling term:

$$\hat{h} = -\frac{\hbar^2}{2m}\Delta + \frac{m\omega^2 r^2}{2} + f(r)(\vec{l}\cdot\vec{s})\ . \tag{16}$$

Taking into account the intrinsic spin of the nucleons, we can write down the single-particle wave functions as

$$\phi_{nlsjm}(\vec{r},\vec{s}) = R_{nl}(r)\left[Y_l(\theta,\phi)\times\chi_{1/2}(\vec{s})\right]^{(j)}_m\ , \tag{17}$$

where the orbital and the spin angular momenta are coupled to a total angular momentum j. These wave functions are eigenfunctions of the Hamiltonian (16). Taking into account the isospin of the nucleons, the final single-particle wave functions are

$$\phi_{nlsjm,tm_t}(\vec{r},\vec{s},\vec{t}) = R_{nl}(r)\left[Y_l(\theta,\phi)\times\chi_{1/2}(\vec{s})\right]^{(j)}_m \theta_{1/2}(\vec{t})\ . \tag{18}$$

The wave function (18) is a coordinate-spin-isospin representation of a state vector $|nlsjm,tm_t\rangle$, i.e.

$$\langle\vec{r},\,\vec{s},\,\vec{t}\,|nlsjm;tm_t\rangle \equiv \phi_{nlsjm,tm_t}(\vec{r},\vec{s},\vec{t}) \tag{19}$$

In future we will use the notations of state vectors. Since always $s = 1/2$ and $t = 1/2$, we will often suppress the indices s and t. Moreover, we will use only space-spin part $|nlsjm\rangle$,

while calculating isoscalar operators. To get the value of the spin-orbit splitting we will calculate the matrix elements

$$\Delta\epsilon_{nlsjm} = \langle nlsjm|f(r)(\vec{l}\cdot\vec{s})|nlsjm\rangle = \begin{cases} +\frac{1}{2}l\langle f(r)\rangle_{nl} \text{ for } j = l+\frac{1}{2} \\ -\frac{1}{2}(l+1)\langle f(r)\rangle_{nl} \text{ for } j = l-\frac{1}{2} \end{cases} \tag{20}$$

Here

$$\langle f(r)\rangle_{nl} = \langle nl|f(r)|nl\rangle = \int R^*_{nl}R_{nl}f(r)r^2dr \ . \tag{21}$$

Each oscillator shell splits into orbitals:

$N = 0$ $1s_{1/2}$
$N = 1$ $1p_{1/2}$; $1p_{3/2}$
$N = 2$ $1d_{5/2}$; $1d_{3/2}$; $2s_{1/2}$
$N = 3$ $1f_{7/2}$; $1f_{5/2}$; $2p_{3/2}$; $2p_{1/2}$
$N = 4$ $1g_{9/2}$; $1g_{7/2}$; $2d_{5/2}$; $2d_{3/2}$; $3s_{1/2}$
... ...
(here the half-integer values refer to the total angular momentum j).

3 Woods-Saxon Potential

The more realistic representation of the nuclear mean field is given by the Woods-Saxon potential:

$$\hat{h} = -\frac{\hbar^2}{2m}\Delta + \frac{U_0}{1+\exp\left(\frac{r-R_0}{a}\right)} \ . \tag{22}$$

Usually $U_0 \approx -50$ MeV, $R_0 = r_0A^{1/3}$ with $r_0 \approx 1.2$ fm and a diffuseness $a \approx 0.5$ fm.

The wave functions have a form (8), but the radial wave functions $R_{nl}(r)$ as well as the eigenvalues ϵ can be found only numerically. Each eigenvalue is characterized by a certain n and l, and the eigenvalues with different n and l are non-degenerate. The resulting levels can be labelled by nl.

The total degeneracy of the orbital with a given l is

$$\Omega = 4(2l+1) \ , \tag{23}$$

if we take into account spin and isospin of nucleons.

Addition of the spin-orbit interaction to the Hamiltonian (22),

$$\hat{h} = -\frac{\hbar^2}{2m}\Delta + \frac{U_0}{1+\exp\left(\frac{r-R_0}{a}\right)} + f(r)(\vec{l}\cdot\vec{s}) \, , \tag{24}$$

leads to the splitting of the $2(2l+1)$-fold degenerate levels into $(2j+1)$-fold degenerate levels. The resulting levels can be denoted as $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, etc.

In order to estimate the value of this splitting we have calculate the matrix elements

$$\Delta\epsilon_{nlsjm} = \langle nlsjm|f(r)(\vec{l}\cdot\vec{s})|nlsjm\rangle = \begin{cases} +\frac{1}{2}l\langle f(r)\rangle_{nl} \text{ for } j = l+\frac{1}{2} \\ -\frac{1}{2}(l+1)\langle f(r)\rangle_{nl} \text{ for } j = l-\frac{1}{2} \end{cases} \tag{25}$$

Here the values $\langle f(r)\rangle_{nl}$ differ from those which were calculated with the harmonic oscillator wave functions in the previous section.

4 Applications of the harmonic oscillator and the Woods-Saxon potentials

4.1 Shell model with pure configurations

In the naive shell model we neglect the residual interaction $H^{(1)}$. The solution of the Schrödinger equation with a Hamiltonian $H^{(0)}$ (4) can be given by any product of single-particle wave functions

$$\phi_{k_1}(1)\phi_{k_2}(2)\ldots\phi_{k_A}(A)\ . \tag{26}$$

Here each k_i labels the single-particle state $|nlsjm, tm_t\rangle$, while (i) refers to all coordinates of a nucleon, $i \equiv (\vec{r}_i, \vec{s}_i, \vec{t}_i)$. The single-particle wave functions are solutions of the corresponding Schrödinger equations

$$\hat{h}(i)\phi_k(i) = \epsilon_k\phi_k(i)\,. \tag{27}$$

This can be a single-particle equation with a harmonic oscillator potential, (16), or with Woods-Saxon potential, (24), or anything else.

However, since we are dealing with the fermions of two sorts, protons and neutrons, *the correct shell model wave function should be antisymmetric under permutation of any two nucleons with respect to its space, spin and isospin coordinates and it should possess definite values of the total angular momentum J and the total isospin T.* So, we can construct the final shell model wave functions as certain linear combinations of functions (26), totally antisymmetric and coupled to certain J and T. We will denote them as

$$\Phi_\Gamma(1, 2, \ldots, A) \tag{28}$$

where $\Gamma = (J, T)$, i.e.

$$\hat{H}^{(0)}\Phi_\Gamma(1, 2, \ldots, A) = E^{(0)}_\Gamma\Phi_\Gamma(1, 2, \ldots, A)\ . \tag{29}$$

In this section we will think of Φ_Γ as of the solution of the problem. The total energy is thus given by

$$E^{(0)}_\Gamma = \sum_{i=1}^{A}\epsilon_{k_i}\ . \tag{30}$$

Such a model is useful to get simple single-particle estimations of different physical observables, assuming that the properties are determined only by the last nucleon. Here we consider the operators of electric and magnetic multipole transitions in the proton–neutron

formalism, i.e. we explicitly imply that the valence particle is either proton or neutron (the isospin formalism will be considered later).

The single-particle electric multipole operator reads

$$\hat{T}(\mathcal{E}, LM) = er^L Y_{LM}(\theta, \phi)\,, \tag{31}$$

where e refers to either free ($e(p) = e$, $e(n) = 0$) or effective nucleon charges.

The reduced probability of the $\mathcal{E}L$-transition from the initial to the final state is

$$B(\mathcal{E}L; J_i \to J_f) = \frac{1}{2J_i + 1} |\langle J_f || T(\mathcal{E}, L) || J_i \rangle|^2\,. \tag{32}$$

In a single-particle model $J_i = j_i$ and $J_f = j_f$. Thus we have

$$\begin{aligned} B(\mathcal{E}L; j_i \to j_f) = \; & \tfrac{1}{2j_i+1} |\langle n_f l_f s_f j_f || T(\mathcal{E}, L) || n_i l_i s_i j_i \rangle|^2 = \\ & \tfrac{1}{2j_i+1} |\langle n_f l_f s_f j_f || e r^L Y_L(\theta, \phi) || n_i l_i s_i j_i \rangle|^2 = \\ & e^2 \tfrac{1}{2j_i+1} \langle r^L \rangle^2 |\langle l_f s_f j_f || Y_L(\theta, \phi) || l_i s_i j_i \rangle|^2\,. \end{aligned} \tag{33}$$

Here we employed the fact that the total single-particle wave functions $|nlsj\rangle$ is a product of the radial part $|nl\rangle$ and the angular part $|lsj\rangle$ and we introduced a notation

$$\langle r^L \rangle = \int R^*_{n_f l_f}(r) r^{L+2} R_{n_i l_i}(r) dr \tag{34}$$

(an additional r^2 arises from the normalization (10)).

Using formula (60) from Lecture 5 with $U^{(k_1)} = Y_L(\theta, \phi)$ and $V^{(k_2)} = 1$, and the reduced matrix element of the spherical functions (see Problem 4 of Lecture 5), we obtain from (33):

$$\begin{aligned} B(\mathcal{E}L; j_i \to j_f) = e^2 \tfrac{1}{4\pi} \langle r^L \rangle^2 (2j_f + 1)(2l_i + 1)(2L + 1)(l_i 0 L 0 | l_f 0)^2 \begin{Bmatrix} \frac{1}{2} & l_f & j_f \\ L & j_i & l_i \end{Bmatrix}^2 = \\ e^2 \tfrac{1}{4\pi} \langle r^L \rangle^2 (2j_f + 1)(2L + 1) \begin{pmatrix} j_i & j_f & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^2\,. \end{aligned} \tag{35}$$

The only unknown ingredient in this expression if the matrix element (34), which can be calculated using the explicit radial wave functions.

The same can be done to estimate the static electric multipole moments in a single-particle state. For example, the electric quadrupole operator of a single particle reads

$$\hat{Q} = \sqrt{\frac{16\pi}{5}} e r^2 Y_{20}\,. \tag{36}$$

The electric quadrupole moment is defined as

$$Q = \langle JM = J | \hat{Q} | JM = J \rangle\,. \tag{37}$$

For a single-particle state we have

$$Q = \sqrt{\frac{16\pi}{5}} \langle nlsjj | e r^2 Y_{20} | nlsjj \rangle = -\frac{2j - 1}{2j + 2} e \langle r^2 \rangle\,. \tag{38}$$

Similarly, we can estimate the magnetic multipole transitions. The single-particle magnetic multipole operator has a form

$$\hat{T}(\mathcal{M}, LM) = \nabla \left(r^L Y_{LM}(\theta, \phi) \right) \left(\frac{2g_l}{L+1} \vec{l} + g_s \vec{s} \right) \mu_N \ , \tag{39}$$

where the g-factors of free nucleons are $g_l(p) = 1$, $g_l(n) = 0$, $g_s(p) = 5.58$ and $g_s(n) = -3.82$, and $\mu_N = \frac{e\hbar}{2mc}$.

The reduced probability of the ML-transition from the initial to the final state is

$$B(\mathcal{M}L; J_i \to J_f) = \frac{1}{2J_i + 1} |\langle J_f || T(\mathcal{M}, L) || J_i \rangle|^2 \, . \tag{40}$$

In a single-particle model $J_i = j_i$ and $J_f = j_f$:

$$\begin{gathered} B(\mathcal{M}L; j_i \to j_f) = \frac{1}{2j_i + 1} \langle n_f l_f s_f j_f || T(\mathcal{M}, L) || n_i l_i s_i j_i \rangle|^2 = \\ \langle r^{L-1} \rangle^2 \langle l_f || Y_{L-1}(\theta, \phi) || l_i \rangle^2 (2j_f + 1)(2L + 1) \frac{2}{L} \\ \left[(-1)^{j_f + l_f + 1/2} 2g_l \frac{L}{L+1} \sqrt{j_i(j_i+1)(2j_i+1)} \left\{ \begin{array}{ccc} \frac{1}{2} & l_f & j_f \\ L-1 & j_i & l_i \end{array} \right\} \left\{ \begin{array}{ccc} j_f & L & j_i \\ 1 & j_i & L-1 \end{array} \right\} + \right. \\ \left. \sqrt{\frac{3}{2}} \left(g_s L - 2g_l \frac{L}{L+1} \right) \left\{ \begin{array}{ccc} l_f & \frac{1}{2} & j_f \\ l_i & \frac{1}{2} & j_i \\ L-1 & 1 & L \end{array} \right\} \right]^2 \mu_N^2 \, . \end{gathered} \tag{41}$$

Similarly, we can estimate the static magnetic multipole moments. For example, the magnetic dipole operator of a single nucleon is given by

$$\hat{\mu} = \left(g_l \vec{l} + g_s \vec{s} \right) \mu_N \tag{42}$$

(note that the radial dependence disappears because $r^{L-1} = 1$ for $L = 1$). The magnetic dipole moment is defined as

$$\mu = \langle JM = J | \hat{\mu} | JM = J \rangle \ . \tag{43}$$

In order to estimate it in a single-particle state we calculate

$$\mu = \langle nlsjj | \left(g_l \vec{l} + g_s \vec{s} \right) \mu_N | nlsjj \rangle \ , \tag{44}$$

getting the Schmidt values (see Problem 2).

4.2 Shell model with configuration mixing

In the realistic shell model, we have to take into account $\hat{H}^{(1)}$, i.e. we solve the eigenvalue problem

$$\hat{H} |\Psi_p\rangle = E_p |\Psi_p\rangle \, . \tag{45}$$

In this case, we use the solutions of $\hat{H}^{(0)}$, functions Φ_Γ (28), only as a *basis* of the diagonalization of the full Hamiltonian $\hat{H}$.

This means that we are looking for the wave function of the system in the form

$$|\Psi_p\rangle = \sum_{k=1}^{g} a_{kp}|\Phi_k\rangle\,, \tag{46}$$

where g denotes the number of pure configurations $|\Phi_k\rangle$ considered, i.e. it is related to the model space used. Usually, the model space incorporates all possible configurations of N_π valence protons and N_ν valence neutrons in the partially filled orbitals, while the rest is considered as an inert core. Since the Hamiltonian $\hat{H}$ is invariant in the space and isospace, its eigenstates are characterized by good values of the total angular momentum J and isospin T. In other words, the functions $(\Psi_\Gamma)_p$ and $(\Phi_\Gamma)_k$ have the same labels Γ which we suppressed in the equation (46) for the simplicity.

Substituting (46) into equation (45), we get

$$(\hat{H}^{(0)} + \hat{H}^{(1)}) \sum_{k=1}^{g} a_{kp}|\Phi_k\rangle = E_p \sum_{k=1}^{g} a_{kp}|\Phi_k\rangle\,. \tag{47}$$

Since

$$\hat{H}^{(0)}|\Phi_k\rangle = E_k^{(0)}|\Phi_k\rangle\,, \tag{48}$$

the matrix elements of the Hamiltonian $\hat{H}$ are given by

$$H_{lk} \equiv \langle\Phi_l|\hat{H}|\Phi_k\rangle = E_k^{(0)}\delta_{lk} + H_{lk}^{(1)}\,, \tag{49}$$

where

$$H_{lk}^{(1)} = \langle\Phi_l|H^{(1)}|\Phi_k\rangle\,. \tag{50}$$

Thus we have to solve a system of equations

$$\sum_{k=1}^{g} H_{lk}a_{kp} = E_p a_{lp}\,, \tag{51}$$

that means to diagonalize the matrix H_{lk} and to find the eigenvalues E_p and the coefficients a_{kp}. Since the basis is orthogonal and normalized, the eigenvectors belonging to different eigenvalues are necessarily orthogonal and can be normalized such that

$$\sum_{k=1}^{g} a_{kp}a_{kp'} = \delta_{pp'} \text{ for } E_p \neq E_p\,. \tag{52}$$

Equation (51) can be re-written as

$$\sum_{l,k=1}^{g} a_{lp'}H_{lk}a_{kp} = E_p\delta_{pp'}\,, \tag{53}$$

or in a matrix form

$$A^{-1}HA = E\,, \tag{54}$$

where on the right-hand side is a diagonal matrix.

The diagonalization can be performed even by hand for small matrices, such as (2×2) or (3×3). For higher dimensions there exist different numerical algorithms: the Jacobi method $g \leq 50$, the Householder method $50 \leq g \leq 200$, the Lanczos method $200 \geq g$ and for giant matrices.

We can estimate the dimension of the configuration space for N_π protons in the (nlj) orbital and N_ν neutrons in the $(n'l'j')$ orbital, i.e. just to count all possible configurations taking into account $2j+1$ and $2j'+1$ degeneracies. It is given by binomial coefficients

$$\left(\begin{array}{c} 2j+1 \\ N_\pi \end{array} \right) \left(\begin{array}{c} 2j'+1 \\ N_\nu \end{array} \right) \tag{55}$$

This is the total dimension of the space. We can reduce it taking into account invariance of the Hamiltonian with respect to the total angular momentum J and isospin T, i.e. we can diagonalize the operators J^2 and T^2, in order to construct from all possible basis functions, the number of which is given by (55), those which possess certain J and T.

The only ingredient which was not discussed here is the residual interaction, or the Hamiltonian $\hat{H}^{(1)}$. This will be the subject of the next lecture.

Comment

There exist one particular case when we do not need the residual interaction in a realistic shell model. This is the case when we have only one particle above the inert core. Such nuclei are very important since they provide information about the relative single-particle energies.

^{17}O can be considered as a core of ^{16}O plus an additional neutron in the *sd* shell model space. Their binding energies are $E_B(^{17}\mathrm{O}) = -131.77$ MeV and ^{16}O is $E_B(^{16}\mathrm{O}) = -127.62$ MeV. Since the ground state of ^{17}O has the spin and parity $5/2^+$, then

$$\epsilon_{1d_{5/2}} = E_B(^{17}\mathrm{O}) - E_B(^{16}\mathrm{O}) = (-131.77 + 127.66)\ \mathrm{MeV} = -4.15\ \mathrm{MeV}\,. \tag{56}$$

^{17}O has an excited state of spin and parity $1/2^+$ at the energy $E_x = 0.87$ MeV. Thus, the single-particle energy of a neutron in $2s_{1/2}$ is

$$\epsilon_{2s_{1/2}} = E_B(^{17}\mathrm{O}) - E_B(^{16}\mathrm{O}) + E_x = (-131.77 + 127.66 + 0.87)\ \mathrm{MeV} = -3.28\ \mathrm{MeV}\,. \tag{57}$$

5 Hartree-Fock approximation

The Hartree-Fock method is a tool to find the average potential $\sum_{i=1}^{A} U(i)$ which is the best approximation to the two-body potential $\sum_{i<j=1}^{A} W(i,j)$.

Let us search for a wave function in the form

$$\Phi(1,2,\ldots,A) = \frac{1}{\sqrt{A!}} \left| \begin{array}{cccc} \phi_{k_1}(1) & \phi_{k_1}(2) & \ldots & \phi_{k_1}(A) \\ \phi_{k_2}(1) & \phi_{k_2}(2) & \ldots & \phi_{k_2}(A) \\ & \ldots & & \\ \phi_{k_A}(1) & \phi_{k_A}(2) & \ldots & \phi_{k_A}(A) \end{array} \right| \tag{58}$$

and require that the eigenvalue of the Hamiltonian (2) in the state (58) is minimal:

$$\langle\Phi|H|\Phi\rangle = \min \ , \tag{59}$$

on in other words the variation

$$\delta\langle\Phi|H|\Phi\rangle = 0 \ . \tag{60}$$

Let us assume that the two-body interaction is local and does not depend on spin or isospin. The condition (60) can be reduced to the system of equations called the *Hartree-Fock* equations, which in the coordinate representation has a form:

$$-\frac{\hbar^2}{2m}\Delta\phi_k(\vec{r}) + U_H(\vec{r})\phi_k(\vec{r}) - \int U_F(\vec{r},\vec{r}\,')\phi_k(\vec{r}\,')d\vec{r}\,' = \epsilon_k\phi_k(\vec{r}) \ . \tag{61}$$

In this equation we get two terms as a potential energy:

$$U_H(\vec{r}) = \sum_{j=1}^{A}\int \phi_j^*(\vec{r}\,')V(\vec{r},\vec{r}\,')\phi_j(\vec{r}\,')d\vec{r}\,' \tag{62}$$

which is called a *direct*, or *Hartree* term, and

$$U_F(\vec{r},\vec{r}\,') = \sum_{j=1}^{A}\phi_j^*(\vec{r}\,')V(\vec{r},\vec{r}\,')\phi_j(\vec{r}) \ , \tag{63}$$

which is called an *exchange*, or *Fock* term, since it appears when we take into account that our wave functions should be antisymmetrized.

The Hartree-Fock equations (61) are solved by iterations. First, we take a set of trial wave functions, e.g. the harmonic oscillator eigenfunctions $\phi(\vec{r})$, and calculate the direct (62) and exchange (63) potentials. Then we input the calculated potentials to the equations (61) and solve them, getting thus the wave functions $\phi_k^{(0)}(\vec{r})$ and the single-particle energies $\epsilon_k^{(0)}$ after the first iteration. These wave functions will be different from the trial ones. The wave functions $\phi_k^{(0)}(\vec{r})$ are now used in order to get the new values of the potentials (62) and (63), which then are input again in Hartree-Fock equations and we get the set of the wave functions $\phi_k^{(1)}(\vec{r})$ and the single-particle energies $\epsilon_k^{(1)}$ after the second iteration. Continuing in this way, we will obtain that after a large number of iterations, the wave functions used in calculating the potentials coincide with the solutions of the Hartree-Fock equations. Thus, the problem is solved self-consistently.

References

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