# CHAPTER 2

## Single-particle excitations in nuclei

*Pairing interaction in nuclei. Spin-orbit coupling. Parity. One-particle Hamiltonian in one dimension.Magnectic fields and magnetic moments. Dipole magnetic moments in nuclei. Schmidt values. Single-particle states.*

### Pairing interaction in nuclei

The nucleus is a many-body system which consists of $N$ neutrons and $Z$ protons. One denotes by ${}^{A}_{Z}X_N$ the nucleus $X$ with the total number of nucleons $A = N + Z$ (although the simpler notation ${}^{A}X$ is often used). It is very difficult to treat this system. On the one hand, the nucleon-nucleon interaction provided by fundamental theories, as Quantum Chromo Dynamics (QCD), is extremely difficult to apply. On the other hand the many-body problem itself is very difficult since the number of particles is large, but not large enough to be able to be treated in statistical terms, as it happens with other many-body systems like e. g. condensed matter. Therefore the main tasks in nuclear structure studies is first to find effective forces that explain the available experimental data and then to be able to perform this task within a manageable theoretical framework. In this course we will present the most important solutions that have been found to perfom those tasks.

Effective forces are introduced to explain in a treatable fashion nuclear properties. Thus, it is known that all nuclei with $N$ even and $Z$ even (even-even nuclei) have in the ground state spin and parity $0^+$. This indicates that nucleons of the same kind are arranged in pairs. The nucleons in each pair are coupled with the corresponding spins pointing in opposite directions, such that the pair is coupled to zero angular momentum. The force inducing this pairing of nucleons is called "pairing force".

Another important nuclear quantity is the binding energy per nucleon, which for some nucleon numbers $N$ and $Z$ is larger than the average. These numbers are called "magic numbers". They include the numbers 2, 8, 20, 28, 50, 82 and 126. A nucleus having magic N and Z, like e. g. ${}^{16}_{8}O_8$ (Oxigen 16), ${}^{48}_{20}Ca_{28}$ (Calcium 48) and ${}^{208}_{82}Pb_{126}$ (Lead 208) are very bound. It was found that a nucleon moving outside the nuclear field induced by a double magic nucleus does not influence appreciably the motion of the nucleons inside the nucleus. The double magic nucleus is as a "frozen core". The field induced by the core acts as a whole upon the odd nucleon moving outside the even-even core. In other words, the low-lying excitations of even-odd or odd-even nuclei outside a magic core can be considered as single-particle excitations. Below we will study them.

### Spin-orbit coupling

A Fermion moving outside a spherically symmetric central field carries an angular momentum $\boldsymbol{l}$ and a spin $\boldsymbol{s}$ ($s = 1/2$). The total angular momentum is $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$ and the angular-spin part of the wave function is

$$< \theta\varphi | l 1/2; jm >= \left[ Y_l(\theta\varphi)\chi_{1/2} \right]_{jm}$$

To this one has to include the radial part $R_{nlj}(r)$, where $n$ labels all quantum numbers associated to the radial part of the nucleon-core interaction. The total wave function thus is,

$$< r\theta\varphi|nljm >= \Psi_{nljm}(\boldsymbol{r}) = R_{nlj}(r) \left[Y_l(\theta\varphi)\chi_{1/2}\right]_{jm}$$

where we have dropped the obvious spin label 1/2 in the set of quantum numbers $\{nljm\}$, as it is usually done in nuclear studies.

**Parity**

Since we assume that the nucleon-core potential is sphericallly symmetric the quantum numbers $l.j,m$ are conserved (as discussed in the previous Chapter). This potential will also be assumed to be invariant under reflections, and therefore the parity $\pi$ of the state $|nljm>$ will also be conserved. To find the value of the parity one has to analzse the Spherical Harmonics $Y_{lm_l}(\theta\varphi)$ which, for $m_l \geqslant 0$, is given by

$$Y_{lm_l}(\theta\varphi) = \sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m_l)!}{(l+m_l)!}}(-1)^{m_l}\mathrm{e}^{\mathrm{i}m_l\varphi}P_l^{m_l}(\cos\theta)$$

where

$$P_l^{m_l}(\xi) = \frac{(-1)^{m_l}}{2^l l!}\frac{(l+m_l)!}{(l-m_l)!}(1-\xi^2)\frac{\mathrm{d}^{l-m_l}}{\mathrm{d}\xi^{l-m_l}}(\xi^2-1)^l$$

For $m_l < 0$ it is,

$$Y_{lm_l}(\theta\varphi) = (-1)^{m_l}Y^*_{l-m_l}(\theta\varphi)$$

The parity transformation corresponds to $\boldsymbol{r} \longrightarrow -\boldsymbol{r}$, that is $(r,\theta,\varphi) \longrightarrow (r,\pi-\theta,\varphi+\pi)$, and since for spherically simmetric potentials the value of $r$ is the same for all values of the angles, only the transformation of the Spherical Harmonics has to be considered. Therefore one finds,

$$\Psi_{nljm}(-\boldsymbol{r}) \quad\longrightarrow\quad (-1)^l\Psi_{nljm}(\boldsymbol{r})$$

The spin-orbit part of the wave function is as above independently of the spherically invariant potential, but the radial part has to be studied separately for each potential one has to deal with. We will start with the simple case of a one-dimesional potential.

**One-particle Hamiltonian in one dimension**

The one-dimension Hamiltonian is.

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\Phi_n(x) = E_n\Phi_n(x) \tag{1}$$

and we will consider the square well potential shown in Fig. 1. To solve the eigenvalue problem given by Eq. (1) we notice that there are two regions:

Region (1): $0 < x < a$; $V(x) = -V_0$
Region (2): $x \geqslant a$; $V(x) = 0$

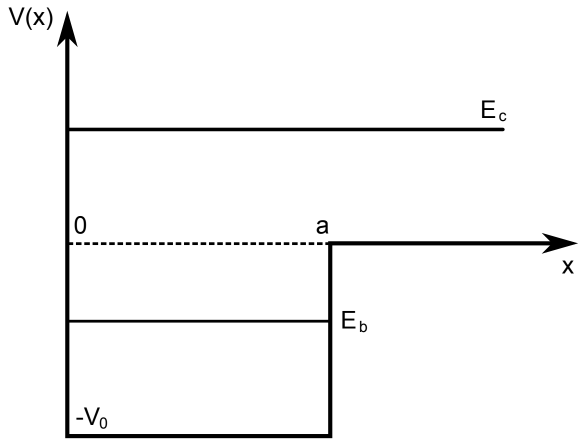


Figure 1: Square well potential in one-dimension. The range of the potential is $a$ and the depth is $-V_0$. For $x < 0$ the potential is infinite and, therefore, the wave function vanishes at $x = 0$. $E_b$ ($E_c$) is the energy of a bound (continuum) state.

There are also two possibilities for the energy: Continue ($E = E_c > 0$) and Bound ($E = -E_b < 0$)

$$\begin{aligned}
\text{Region (1):} \qquad \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - V_0\right]\Phi_n^{(1)}(x) &= E_n\Phi_n^{(1)}(x) \\
\text{Region (2):} \qquad \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right]\Phi_n^{(2)}(x) &= E_n\Phi_n^{(2)}(x)
\end{aligned}$$

with

$$q^2 = \frac{2\mu}{\hbar^2}(E_n + V_0); \quad k^2 = \frac{2\mu}{\hbar^2}E_n$$

the eigenvectors solution of the eigenvalue problem are

$$\begin{cases} \Phi_n^{(1)}(x) = A_n \mathrm{e}^{\mathrm{i}qx} + B_n \mathrm{e}^{-\mathrm{i}qx} \\ \Phi_n^{(2)}(x) = C_n \mathrm{e}^{\mathrm{i}kx} + D_n \mathrm{e}^{-\mathrm{i}kx} \end{cases}$$

To determine the constant $A_n$, $B_n$, $C_n$ and $D_n$, the boundary conditions of continuity of density and current have to be applied. In addition, since $V(x) = \infty$ for $x \leqslant 0$, one has

$$\Phi_n^{(1)}(x = 0) = 0 \Longrightarrow A_n + B_n = 0$$

I) Bound states

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 - E_b) > 0; \quad k^2 = -\frac{2\mu}{\hbar^2}E_b < 0$$

Notice that we assume $E_b > 0$ and, therefore, the energy of the bound state is $-E_b$.

$$k = \pm\mathrm{i}\chi; \quad \chi = \sqrt{\frac{2\mu E_b}{\hbar^2}}$$

$$\begin{cases} \Phi_n^{(1)}(a) = \Phi_n^{(2)}(a) \\ \dfrac{\mathrm{d}}{\mathrm{d}x}\Phi_n^{(1)}(x)\Big|_{x=a} = \dfrac{\mathrm{d}}{\mathrm{d}x}\Phi_n^{(2)}(x)\Big|_{x=a} \end{cases}$$

An additional condition in $\Phi_n^{(2)}(x) = C_n \mathrm{e}^{-\chi x} + D_n \mathrm{e}^{\chi x}$ is that since $\mathrm{e}^{\chi x}$ diverrges as $x \to \infty$ one has to impose $D_n = 0$. Besides there is the normalization condition. With the constants thus evaluated one obtains the possible energies as those for which the continuity relations are satisfied.

II) Continuum

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 + E_c) > 0; \quad k^2 = \frac{2\mu}{\hbar^2}E_c > 0$$

assuming that the system is confined in the region

$$0 < x < L \Longrightarrow \int_0^L |\Phi_n(x)|^2 \,\mathrm{d}x = 1$$

Notice that all energies $E_c > 0$ are allowed in the continuum, but only a discrete number of energies $-E_b < 0$ are allowed as bound states.

We will now study what happens when one applies a magnetic field to a nucleon moving in a single-particle state as the one we have analyzed here. As we will see, this has applications in many different fields, but particularly in Medicine.

**Magnectic fields and magnetic moments**

A nucleon moving in a single-particle state outside a central potential, as discussed above, will be affected by the presence of an external magnetic field. The corresponding Hamiltonian is,

$$H = -\frac{q}{2mc}\boldsymbol{\mu} \cdot \boldsymbol{B} \tag{2}$$

where $q$ is the effective charge of the nucleon, $\boldsymbol{B}$ is the magnetic field and $\boldsymbol{\mu}$ is the dimensionless nuclear dipole moment defined as,

$$\boldsymbol{\mu} = g_l \hat{l} + g_s \hat{s} \tag{3}$$

The effective charge should be $q = 1.0\ e$ ($e$ is the absolute value of the electron charge) for protons and 0 for neutrons. However, its value is taken to be about 1.5 $e$ for protons and about 1.0 $e$ for neutrons (these are illustrative values that can vary in different nuclear regions, i. e. for different values of $N$ and $Z$). The reason why the effective charge was introduced is that the odd nucleon affects the core and it has been shown that its influence can be taken into account by the effective charge.

The magnetic moments can be measured with great presicion, thus providing precise value for the g-factors also. These are given by,

$$g_l = \begin{cases} 1 & \text{proton} \\ 0 & \text{neutron} \end{cases} \qquad g_s = \begin{cases} 5.58 & \text{proton} \\ -3.82 & \text{neutron} \end{cases}$$

**Dipole magnetic moments in nuclei**

When the magnetic field is applied the energies observed experimentally are quantized according to the allowed angular momenta in Eq. (3). To measure the dipole magnetic moment $\mu$ one chooses the maximum splitting of the levels. One sees from Eq. (2) that the maximun effect of the magnetic field would be induced by the maximum alignment of $\boldsymbol{\mu}$ and $\boldsymbol{B}$. This is what one chooses experimentally. Classically this occurs when $j_z = j$ (since $\boldsymbol{B}$ is in the z-direction). In Quantum Mechanics one has to choose the projection $m$ of the total angular momentum such that $m = j$. Therefore one defines the dipole magnetic moment as

$$\mu = \langle jm = j | g_l \hat{l}_z + g_s \hat{s}_z | jj \rangle$$

notice that $\mu$ is just a number without dimensions.

Since $\boldsymbol{l} = \boldsymbol{j} - \boldsymbol{s}$ one can write

$$\mu = \langle jj | g_l \hat{j}_z + (g_s - g_l)\hat{s}_z | jj \rangle$$

To calculate the values obtained by the application of the operator $\hat{s}_z$ upon the state $|jj\rangle$, we expand this state in terms of the eigenvectors of $\hat{s}_z$, i. e.

$$|jm\rangle = \sum_{m_l m_s} \langle l m_l 1/2 m_s | jm \rangle | l m_l 1/2 m_s \rangle$$

and one obtains

$$\begin{aligned} \mu &= \langle jj | \sum_{m_l m_s} \langle l m_l 1/2 m_s | jj \rangle \left[ g_l j + (g_s - g_l) m_s \right] | l m_l 1/2 m_s \rangle \\ &= \sum_{m_l m_s} \langle l m_l 1/2 m_s | jj \rangle^2 \left[ g_l j + (g_s - g_l) m_s \right] \end{aligned}$$

It is $m_l = j - m_s$ and $m_s = \pm 1/2$, $m_l = j \mp 1/2$. Therefore

$$\begin{aligned} \mu &= \left\langle l, j - \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 \left[ g_l j + \frac{g_s - g_l}{2} \right] \\ &\quad + \left\langle l, j + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 \left[ g_l j - \frac{g_s - g_l}{2} \right] \end{aligned} \tag{4}$$

**Schmidt values. Single-particle states**

The general expression for the magnetic moments corresponding to a nucleon moving outside a central field is given by Eq. (4). There are two different possibilities, namely a) $l = j + 1/2$; b) $l = j - 1/2$.

a) $j = l - 1/2$

$$\begin{aligned} \left\langle j + \frac{1}{2}, j - \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 &= \frac{1}{2(j+1)} \\ \left\langle j + \frac{1}{2}, j + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 &= \frac{2j+1}{2(j+1)} \end{aligned}$$

$$\mu = g_l j - (g_s - g_l)\frac{j}{2(j+1)}$$

b) $j = l + 1/2$

$$\begin{aligned} \left\langle j-\frac{1}{2}, j-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 &= 1 \\ \left\langle j-\frac{1}{2}, j+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 &= 0 \end{aligned}$$

$$\mu = g_l j + (g_s - g_l)/2$$

Our assumption that the nucleon moves around the core without farther disturbances (for instance without exciting other nucleons in the core) is equivalent to assume that the nucleon moves in a single-particle state. If this is valid, then one can estimate probable values of the angular momenta $l$ and $j$ (we will perform this task in this Course). Since also the Schmidt values for the magnetic moment should be valid, then one can compare these magnetic moments with experiment to probe the models used to infere the angular momenta as well as the single-particle assumption that this implies. We will attest the success of this in the exercises.