THE CHANGING MEAN FIELD IN EXOTIC NUCLEI: A SHELL-MODEL POINT OF VIEW

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“Se non è vero, è ben trovato.”
Abstract

Some of the intriguing questions related to the properties of exotic nuclei are how their shell structure is changing with respect to that of nuclei close to the line of $\beta$-stability, and which mechanisms are responsible for these (sometimes) experimentally observed changes. We discuss the variations of the nuclear mean field, in particular the single-particle energies, in series of isotopes and isotones within the framework of the nuclear shell model. We derive an approximate expression for the shell-model energy centroids of the single-particle states and in order to explore the evolution of these single-particle energies, we apply it in the series of Cu ($Z = 29$) and Bi ($Z = 83$) isotopes, and the $N = 51$ isotones. The approximation of using only the monopole Hamiltonian, corrected for pairing correlations amongst the identical nucleons (neutrons or protons, respectively), allows us to treat rather heavy nuclei far from stability, which at present cannot be handled by exact diagonalization. The changes of the single-particle energies are indeed shown to be mainly due to the monopole part of the effective two-body interaction. A detailed comparison between realistic forces and different types of schematic forces is carried out in an attempt to understand the role played by the specific nucleon-nucleon force components in the single-particle monopole shift.
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Part I

The Changing Mean Field
1 Introduction

The atomic nucleus turns out to be a complicated interacting many-body system, governed by the nucleon-nucleon interaction active inside the nucleus. The nucleus consists of a few up to two hundred nucleons. Compared to the relatively familiar environment of the atom in which the atomic nucleus is at the origin of the Coulomb field generating the motion of electrons in single-particle orbitals, the nucleus does not exhibit a natural central ‘field’.

It is possible to describe the nuclear bulk properties such as the mass, radius and shape via macroscopic theories like the Liquid Drop Model, exhibiting the saturation of the nuclear interaction inside the atomic nucleus, and pointing towards the existence of an average mean field \[1\]. On the other hand, one can obtain a nuclear mean field in a microscopic approach starting from the nucleon-nucleon force, which is short-ranged and charge independent, and gives rise to the observed saturation properties like \(BE(\frac{4}{3}X_N) \propto A\) (see figure 1.1), and the nuclear radius varying as \(R = r_0A^{1/3}\). Hartree-Fock (HF) theory essentially derives a one-body potential starting from a nucleon-nucleon two-body force \(V(\vec{r}, \vec{r}')\) according to:

\[U(\vec{r}) = \int V(\vec{r}, \vec{r}')\rho(\vec{r}')d\vec{r}',\]  

(1.1)

with the nuclear density \(\rho(\vec{r}')\) given by:

\[\rho(\vec{r}') = \sum_{j(\text{occ})}\left|\psi_j(\vec{r}')\right|^2,\]  

(1.2)

the sum running over all occupied orbitals \(j\) inside the atomic nucleus.

This is an iterative procedure: one starts from a good guess for the density and the two-body interaction, computes the mean field potential, derives the wave functions, and uses these wave functions to obtain a better approximation for the density. This self-consistent procedure works fine when one can make a good initial choice for the two-body interaction, such that the two-body interaction is well-behaved. This is mostly the case for nuclei at or near the valley of \(\beta\)-stability (see figure 1.2), since there is plenty of experimental data to constrain the two-body interaction in such a way as to describe the experimental data as accurately as possible.

A convincingly large amount of experimental data on odd-mass nuclei in the region of \(\beta\)-stable nuclei has given rise to the concept of largely independent particle motion, as indicated by the specific single-particle energy spectra giving rise to extra stability and corresponding closed shells characterized by a set of so-called magic numbers (see figure 1.3).
As such, a nuclear shell-model structure results, which, in a non-relativistic approach, starts from an $A$-nucleon problem: the nucleons each have their kinetic energy $T_i$ and interact through a two-body potential $V_{ij}$:

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i,j=1}^{A} V_{ij}. \quad (1.3)$$

One can formally introduce a one-body potential $U_i$ and rewrite the Hamiltonian of (1.3) as:

$$H = \sum_{i=1}^{A} \{ T_i + U_i \} + \left\{ \frac{1}{2} \sum_{i,j=1}^{A} V_{ij} - \sum_{i=1}^{A} U_i \right\}$$

$$= \sum_{i=1}^{A} h_{0,i} + H_{\text{res}}$$

$$= H_0 + H_{\text{res}}, \quad (1.4)$$

with $h_{0,i} \equiv T_i + U_i$. 

Figure 1.1: Binding energy per nucleon $B/A$ as a function of the nuclear mass number $A$. Figure taken from [2].
In most shell-model calculations, the separation of an average potential is not done in a self-consistent way (as prescribed in equation (1.1)), but by choosing an appropriate potential that allows for detailed analytical results. The original choice by Mayer and Jensen [5, 6] started from a harmonic oscillator, with the necessary introduction of both (a) a strong spin-orbit interaction $\alpha \vec{I} \cdot \vec{s}$ and (b) a term $\beta \vec{I} \cdot \vec{l}$ that provides residual energy lowering of the $l=0$ orbitals, in order to obtain good agreement with the experimental data, as shown in figure 1.3. The resulting single-particle Hamiltonian has the form:

$$h_{0,t} = \frac{p_t^2}{2m} + \frac{m \omega^2 r_t^2}{2} + \alpha (\vec{l}_t \cdot \vec{s}_t) + \beta (\vec{l}_t \cdot \vec{l}_t).$$  \hspace{1cm} (1.5)$$

The last term, $\beta (\vec{l}_t \cdot \vec{l}_t)$, breaks the remaining $l$-degeneracy within a given major harmonic oscillator shell. This breaking appears automatically in e.g. a square well or Woods-Saxon type of central potential (see figure 1.4).

With appropriate strengths, such an independent particle model explains the known shell gaps that give rise to additional stability at $N, Z = 2, 8, 20, 28$, (40), 50, 82, 126, and the spin and parity assignments of the ground states of most stable odd-$A$ nuclei. However, this shell structure of the single-particle energy spectra will change for nuclei situated far from the region of $\beta$-stability (neutron-rich and proton-rich nuclei).

The phenomenological potentials are certainly not applicable for carrying out extrapolations to nuclear systems at extreme values of isospin, because its parameters have been
Figure 1.3: Sequence of single-particle orbits and corresponding magic numbers. On the left most side, the splitting of the orbitals, induced by a harmonic oscillator potential, is given, in the absence of the spin-orbit coupling term $\hat{l} \cdot \hat{s}$. On the right side, the characteristic magic numbers show up, and the degeneracy of the levels is resolved by adding the spin-orbit term. Figure taken from [4].

Figure 1.4: Splitting of the $l$-degeneracy within a given major harmonic oscillator shell. The harmonic oscillator potential ($\alpha = \beta = 0$ in equation (1.5)) gives a single level, characterized by $N = 4$, while the square well potential (full line) or the Woods-Saxon potential [7] (dotted line) intrinsically lift the $l$-degeneracy, resulting in the levels $s$, $d$ and $g$. 
determined starting from the limited path of stable and almost stable nuclei. Using the Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) method, and starting from well-tested Skyrme functionals, it has been shown [8] that the local part of the mean field exhibits a more diffuse surface region in neutron-rich nuclei as compared to that in nuclei near stability (more like the shape of a Woods-Saxon potential). It has also been noted [8] that one can actually simulate this more uniform structure of the single-particle spectrum rather well by gradually turning off the $\sim \mathbf{l}_i \cdot \mathbf{l}_i$ term in the one-body potential (1.5). In figure 1.5, we present the levels originating from the $N = 4$ major harmonic oscillator shell, i.e. $3s_{1/2}$, $2d_{3/2}$, $2d_{5/2}$, $1g_{7/2}$ and $1g_{9/2}$. On the left side, the levels are depicted for the region near $\beta$-stability, and on the right side, we give the extreme situation where the splitting of the orbital degeneracy ($\beta (\hat{\mathbf{L}}_i \cdot \hat{\mathbf{L}}_i)$ term) has been turned off, with a remaining strong spin-orbit interaction. It is expected that in nuclei with a diffuse surface region (very neutron-rich nuclei), this situation could show up and the shell gaps may be quenched, or even disappear, at least for light nuclei [8].

Using effective two-body forces that allow to determine the nuclear average potential through HF(B) theory, one runs into problems when moving far away from the region of stable nuclei. Within self-consistent calculations, one needs a two-body force, which in turn generates the mean field and the energy spectra. Since there is no good ab-initio knowledge of how the nucleon-nucleon force changes with $N$ and/or $Z$ (isospin dependence), the applications to the regions very far from stability are still limited, and
various studies of nuclei with extreme ratios of neutrons to protons can be very helpful [8, 9, 10, 11, 12].

Present-day experimental research in nuclear structure has made extensive use of radioactive beams (RIB - Radioactive Ion Beams) in order to study nuclear properties further away from the region of $\beta$-stability. In particular, at a number of facilities such as ISOLDE at CERN [13], GSI in Darmstadt [14], GANIL in Caen [15], NSCL at Michigan State University [16], RIBF at RIKEN in Japan [17], HRIBF at Oak Ridge [18], ISAC at TRIUMF, Vancouver [19], researchers have obtained detailed information on the low-lying excited states in very unstable nuclei with an extreme $N/Z$ ratio (proton-rich or neutron-rich nuclei), also called exotic nuclei.

It is the aim of the present study to understand a number of the experimentally observed variations in the single-particle structure of nuclei using the nuclear shell model, this under the condition that the single-particle structure has been well determined experimentally for regions where the $Z$ or $N$ number is adjacent to a ‘closed’ core. We also explore the mechanisms behind these changes in single-particle structure, and make predictions for nuclei further towards instability.

In the first part, we lay out the theoretical foundations. In chapter 2, we present how one can calculate the change in the monopole part of the nuclear potential by focusing on the major contribution for nuclei containing a single nucleon outside a closed shell, or nuclei that are just one nucleon short of a closed shell.

This contribution mainly results from the proton-neutron interaction. Starting from the diagonal part of the monopole Hamiltonian, and using normal filling of the orbitals, the evolution of the single-particle energies as a function of neutron (proton) number can be investigated. Besides the monopole part, one also has to take into account the pairing correlations amongst the identical nucleons, which results in a modification of the generally used shell-model approach, and is discussed in chapter 2.

In order to test the validity of our proposed method to approximately calculate the changing mean field properties, we carry out a detailed comparison with large-scale shell-model calculations, in particular for the $Z = 28$ mass region. This allows us to reconstruct the full single-particle energy centroids, and thus also their variation with $N$ or $Z$.

Since most calculations will be carried out with realistic interactions, mainly based on the $G$-matrix [20, 21], we also intend to test what the various schematic nucleon-nucleon force components give as a result. By doing so, we can gain insight in which particular effective two-body force components are mainly responsible for the experimentally observed effects. Therefore, we give a succinct overview of the major properties of nucleon-nucleon forces and their interaction matrix elements in chapter 3.

In the second part, we concentrate on a number of applications, and we carry out a detailed study of the methods outlined in chapters 2 and 3 in various mass regions. In each case we (a) present the salient experimental features concerning changes in the single-particle energies, (b) carry out detailed calculations using realistic forces, (c) study the different contributions using simple schematic forces, and (d) formulate some conclusions. We also develop a method to study the neighbouring odd-odd nuclei. We study subsequently the Cu-nuclei ($Z = 29$) in chapter 4, the Bi-nuclei ($Z = 83$) in chapter 5 and the $N = 51$ isotones in chapter 6. Chapter 7 is devoted to the comparison of effects produced by realistic and schematic effective interactions. In chapter 8, we present our conclusions and an outlook.
2 Shell-Model Description of the Changing Mean Field

2.1 Introduction

One of the major successes of the nuclear shell model, even in its most simple version when the average one-body potential is approximated by a harmonic oscillator potential including the strong spin-orbit ($\vec{l} \cdot \vec{s}$) and centrifugal ($\vec{l} \cdot \vec{l}$) terms, has been the understanding of why, at certain proton and neutron numbers, additional stability shows up in the nucleus. Further incorporation of the residual interaction amongst the nucleons outside such closed shells has allowed to obtain a robust, yet very rich model that is able to describe a large number of correlations within the nuclear many-body system. However, the shell structure of nuclei with large proton or neutron excess seems to be quite different from that in the $\beta$-stable nuclei. The important role played by the proton-neutron interaction has long been recognized, see e.g. [22, 23, 24].

It has been demonstrated by mean field HFB calculations [8] that the neutrons in the very neutron-rich nuclei experience an average potential with a much more diffuse boundary due to the close-lying continuum and the increased importance of pair scattering into unbound states. Thus, resulting single-particle energies tend to be distributed more uniformly.

In section 2.2 we study a nuclear Hamiltonian describing such systems and we use the shell model to extract that part describing the variation of the single-particle energy of the odd particle (proton or neutron) as a function of changing number of nucleons of the other type (neutrons or protons), which is also called the monopole energy shift.

In section 2.3 we discuss what the effect of introducing lowest-order pairing correlations amongst the identical nucleons has on the monopole energy shift.

In section 2.4 we compare the procedure to calculate single-particle energy variations from the monopole part of the Hamiltonian with the result that would be obtained from a full diagonalization followed by the construction of the corresponding energy centroids. We conclude this chapter with some more general remarks about the monopole part of the nuclear Hamiltonian in section 2.5.

2.2 The Monopole Energy Shift

In this section, we will derive an analytical expression for the monopole energy shift. We will use the notations and conventions defined in appendix A, section A.1.
2.2.1 Multipole Decomposition

In the atomic nucleus, a number of valence proton particles outside a closed shell, moving in the proton orbitals \( j_\pi \), interact with a number of valence neutron particles filling a set of neutron orbitals \( j_\nu \). The Hamiltonian can be written as:

\[
H = \sum_{j_\pi} \epsilon_{j_\pi} n_{j_\pi} + \sum_{j_\nu} \epsilon_{j_\nu} n_{j_\nu} + V_{\pi\pi} + V_{\pi\nu} + V_{\nu\nu}.
\]  

(2.1)

Here, \( \epsilon_{j_\pi} \) and \( \epsilon_{j_\nu} \) denote the single-particle energies corresponding to the orbitals \( j_\pi \) and \( j_\nu \), respectively; \( n_{j_\pi} \) and \( n_{j_\nu} \) denote the number operators for protons and neutrons occupying orbitals \( j_\pi \) and \( j_\nu \), respectively. \( V_{\pi\pi}, V_{\pi\nu} \), and \( V_{\nu\nu} \) represent the residual two-body interaction between protons, protons and neutrons, and neutrons, respectively.

Using the notations defined in detail in section A.1 of appendix A, the general form of the two-body terms can be written as:

\[
V = -\frac{1}{4} \sum_{j_a,j_b,j_c,j_d} \sqrt{(1 + \delta_{ab})(1 + \delta_{cd})} \times \sum_j \hat{J}(j_a,j_b;JM|V|j_c,j_d;JM)_{\text{n.a.s.}} \left[ A^\dagger(j_a,j_b,J) \tilde{A}(j_c,j_d,J) \right]^{(0)}_0. 
\]

(2.2)

The subscript ‘n.a.s.’ means that the two-body matrix element is evaluated for normalized and antisymmetrized two-particle wave functions. From now on, we drop that subscript in order to simplify the notation, even though we always consider two-body matrix elements using normalized and antisymmetrized states.

First, we focus on the proton-neutron part of the Hamiltonian, \( V_{\pi\nu} \). Based on (2.2), we can write this part as:

\[
V_{\pi\nu} = -\sum_{j_\pi,j_\nu,j_\nu',j_\nu''} \sum_j \hat{J}(j_\pi,j_\nu;JM|V|j_\nu',j_\nu'';JM) \left[ A^\dagger(j_\pi,j_\nu,J) \tilde{A}(j_\nu',j_\nu'',J) \right]^{(0)}_0. 
\]

(2.3)

Now, we can recouple from the particle–particle (proton–neutron) basis to the particle–hole (proton–proton and neutron–neutron) basis:

\[
V_{\pi\nu} = \sum_{j_\pi,j_\nu,j_\nu',j_\nu''} \sum_j (2J + 1) \langle j_\pi,j_\nu,J|V_{\pi\nu}|j_\nu',j_\nu'',J \rangle 
\times \sum_{\lambda} \sqrt{2\lambda + 1} (-1)^{j_\nu' + j_\nu + \lambda + J} \left\{ \begin{array}{ccc} j_\pi & j_\nu' & \lambda \\ j_\nu & j_\nu'' & J \end{array} \right\} 
\times [U(j_\pi,j_\nu,J)U(j_\nu',j_\nu'',\lambda)]^{(0)}_0. 
\]

(2.4)

This recoupling gives rise to the so-called multipole decomposition. Hereby we have obtained a representation of the proton-neutron interaction which allows to study the effect of the various multipole contributions to the energy of the interacting system.

First, we study the specific case of \( \lambda = 0 \) (\( j_\pi = j_\nu' \) and \( j_\nu = j_\nu'' \)), or the monopole part extracted from the residual proton-neutron interaction. In this particular case, the more
general result of equation (2.4) reduces to:

\[ V_{\pi\nu}(\lambda=0) = \sum_{j_\pi, j_\nu} \sum_J (2J + 1) \langle j_\pi j_\nu, J | V_{\pi\nu} | j_\pi j_\nu, J \rangle \]

\[ \times (-1)^{j_\pi + j_\nu + J} \left\{ \begin{array}{ccc} j_\pi & j_\nu & 0 \\ j_\nu & j_\nu & J \end{array} \right\} [U(j_\pi, 0, J)U(j_\nu, 0, J)]_0^{(0)} . \]  

(2.5)

Since the \( U(j_\rho, 0, 0) \) operator is proportional to the number operator (see equation (A.11)), or:

\[ U(j_\rho, 0, 0) = \frac{1}{\sqrt{2j_\rho + 1}} n_{j_\rho} , \]  

(2.6)

and using the specific value of the Wigner 6\( j \)-symbol, we obtain the very simple result:

\[ V_{\pi\nu}(\lambda=0) = \sum_{j_\pi, j_\nu} \sum_J (2J + 1) \langle j_\pi j_\nu, J | V_{\pi\nu} | j_\pi j_\nu, J \rangle \frac{n_{j_\pi} n_{j_\nu}}{\sum_J (2J + 1)} . \]  

(2.7)

The factor multiplying the \( n_{j_\pi} n_{j_\nu} \) operator is just the centroid of a single proton particle in the orbital \( j_\pi \) interacting with a single neutron particle in the orbital \( j_\nu \) [25]. Since it is an angular momentum averaged interaction energy, this term contributes to a shift in the spherical single-particle energy. We bring in the notation:

\[ \tilde{E}(j_\pi j_\nu) = \frac{\sum_J (2J + 1) \langle j_\pi j_\nu, J | V_{\pi\nu} | j_\pi j_\nu, J \rangle}{\sum_J (2J + 1)} , \]  

(2.8)

with \( \tilde{E}(j_\pi j_\nu) \) denoting the average matrix element. Finally, the original Hamiltonian of equation (2.1) becomes (neglecting at this stage all interactions \( V_{\nu\nu} \) within the valence neutron space and all interactions \( V_{\pi\pi} \) within the valence proton space and retaining only proton-neutron interactions):

\[ H = \sum_{j_\pi} \epsilon_{j_\pi} n_{j_\pi} + \sum_{j_\nu} \epsilon_{j_\nu} n_{j_\nu} + \sum_{j_\pi, j_\nu} \tilde{E}(j_\pi j_\nu) n_{j_\pi} n_{j_\nu} + \text{higher } \lambda \text{ multipoles of } \pi\nu\text{-interaction} , \]  

(2.9)

or:

\[ H = H_{\lambda=0} + \text{higher } \lambda \text{ multipoles of } \pi\nu\text{-interaction} , \]  

(2.10)

where the monopole Hamiltonian \( H_{\lambda=0} \) is given by:

\[ H_{\lambda=0} = \sum_{j_\pi} \tilde{\epsilon}_{j_\pi} n_{j_\pi} + \sum_{j_\nu} \epsilon_{j_\nu} n_{j_\nu} , \]  

(2.11)

and \( \tilde{\epsilon}_{j_\pi} \) is the monopole-corrected single-particle proton energy:

\[ \tilde{\epsilon}_{j_\pi} = \epsilon_{j_\pi} + \sum_{j_\nu} \tilde{E}(j_\pi j_\nu) n_{j_\nu} . \]  

(2.12)

In (2.12), the operator \( n_{j_\nu} \) is replaced by its expectation value \( \langle n_{j_\nu} \rangle = n_{j_\nu} \) with respect to the wave function describing the neutrons outside of the closed core.
In this work, we focus on a single proton in the proton valence space, so that the
operator \( n_{j\nu} \) has the expectation value \( n_{j\nu} = 1 \).

The modified single-particle energies obtained in equation \((2.12)\) (\( \epsilon_{j\nu} \) or the analogously defined \( \tilde{\epsilon}_{j\nu} \)) are also called the ‘effective single-particle energies’ (ESPE) \([26]\).
The ESPE of an occupied orbital is defined as the corresponding separation energy of a
nucleon in that orbital, but with the opposite sign. This separation energy is calculated
starting from the bare energy to which the monopole shift has been added. For an unoc-
cupied orbital, the ESPE is obtained from the additional binding energy that results after
putting a nucleon in that particular orbital, again with the opposite sign. By construction
of the monopole Hamiltonian, these ESPE correspond to the spherical shell structure.

The starting or bare single-particle energies are taken from the experimentally ob-
served single-particle energies of a doubly-magic nucleus plus or minus one nucleon,
since one has (with CS a closed shell configuration):

\[
\langle \text{CS} \pm 1 | H | \text{CS} \pm 1 \rangle = \langle \text{CS} \pm 1 | H_{\lambda=0} | \text{CS} \pm 1 \rangle. \tag{2.13}
\]

These states normally carry the major part of the single-particle strength. They are ob-
tained for nuclei near stability through one-nucleon transfer reactions (pick-up or strip-
ping of a proton or a neutron).

The model space spans the available single-particle orbitals outside the doubly-magic
core, so the evolution of the single-particle levels within one or even two major shells can
be studied. Hole states are studied by selecting the relevant orbitals inside the core.

In writing down expression \((2.12)\), we have weighted the average matrix element for
each individual neutron orbital \( j\nu \) with the number of neutrons occupying that particu-
lar orbital. This is consistent with a HF approach in which either an orbital is empty
(\( n_{\rho} = 0 \)) or filled with a given occupation (\( n_{\rho} = 2j_{\rho} + 1 \)). The neutron operator \( n_{j\nu} \)
has been replaced by its expectation value \( n_{j\nu} = \langle n_{j\nu} \rangle \). The energy \( \tilde{\epsilon}_{j\nu} \) is the lowest-
order self-energy of the proton due to the proton-neutron interaction. It can be depicted
schematically in figure \(2.1\).

Therefore, the monopole Hamiltonian of \((2.11)\) is the natural tool to study the mean
field through the varying single-particle energies connected to the mean field. The higher-
order multipoles \((\lambda \neq 0)\) should be treated in order to determine the correlations not
present in the spherical mean field, or:

\[
H = H_{\text{monopole}} + H_{\text{multipole}(\lambda \neq 0)}. \tag{2.14}
\]

The proton monopole energy shift in equation \((2.12)\) is defined for the case where
the single-particle energy of one proton in orbit \( j\nu \) is modified when neutron particles are
being added to the valence orbital \( j\nu \) just outside the core. Likewise, the monopole shift
can be defined for the case where particles are being subtracted from the core, i.e. with
increasing hole number. The particle-particle matrix elements in expression \((2.8)\) for the
average matrix element need to be replaced by the corresponding particle-hole matrix
elements:

\[
\langle j\pi j\nu^{-1} | J | V_{\pi\nu} | j\pi j\nu^{-1} , J \rangle. \tag{2.15}
\]

The particle-hole matrix element and the particle-particle matrix element are linked via
2.3 Effect of Pair Correlations

In the discussion so far, we have not taken care of the fact that the neutrons filling the set of orbitals $j_{\nu_1}, j_{\nu_2}, \ldots, j_{\nu_n}$, with a total of $n_\nu$ neutrons, are affected by the strong pairing correlations. Coming back to the definition (2.12) of the monopole shift, it should be noted that in a shell-model calculation, the neutrons are usually spread over the various orbitals with a certain occupation probability $v_{\nu_\nu'}$.

The mechanism behind this spreading over various orbitals is the pairing force: it scatters pairs of nucleons from occupied orbitals into unoccupied orbitals. The occupation
Figure 2.2: Schematic distribution of nucleon pairs. On the left, the closed shell is represented by the nucleons filling the lowest energy levels up to the Fermi level. On the right, the pairing interaction spreads the nucleon pairs over the various orbitals. Figure taken from [29].

probabilities $v^2_{j, j'}$ are obtained by solving the BCS equations for a pairing Hamiltonian. In this work, we assume a pairing Hamiltonian with constant pairing strength [28, 29]:

$$H = -G \sum_{j, j', m, m' > 0} (-1)^{j+m}(-1)^{j'+m'} a^+_j a^+_m a^-_{j', -m} a^-_{j, m'},$$

with $G$ the constant pairing strength. So instead of the particles occupying the lowest energy levels up to the Fermi level, they are now spread over the various orbitals, as illustrated in figure 2.2.

The BCS transformation involves a canonical transformation from the particle creation and annihilation operators to the new ‘quasi-particle’ operators [28]:

$$c^\dagger_\alpha = u_\alpha a^\dagger_\alpha + v_\alpha \tilde{a}^\dagger_\alpha,$$

$$c_\alpha = u_\alpha a_\alpha + v_\alpha \tilde{a}_\alpha,$$

and the inverse transformation:

$$a^\dagger_\alpha = u_\alpha c^\dagger_\alpha - v_\alpha \tilde{c}^\dagger_\alpha,$$

$$a_\alpha = u_\alpha c_\alpha - v_\alpha \tilde{c}_\alpha.$$

The new operators still obey the anticommutation relation $\{c^\dagger_\alpha, c_\beta\} = \delta_{\alpha\beta}$, which leads to the condition:

$$u^2_\alpha + v^2_\alpha = 1.$$

$v^2_\alpha$ can be interpreted as the probability that the state $\alpha$ is occupied.

14
The HF vacuum state $|0\rangle$ is replaced with the BCS reference vacuum state $|\tilde{0}\rangle$, defined as [28]:

$$|\tilde{0}\rangle \equiv \prod_{j_2, m_2 > 0} \left( u_a + v_a a_{j_2, m_2} (-1)^{j_2 + m_2} a_{j_2, m_2}^\dagger \right) |0\rangle, \quad (2.26)$$

with $|0\rangle$ the ground state corresponding to the operators $a_{j_2}^\dagger$ and $a_{m_2}$. The quantities $v_a$ and $u_a$ are determined by performing a variational calculation by minimizing the Hamiltonian:

$$\mathcal{H} = \tilde{H} - \lambda n$$

$$= \sum_{j_2, m_2} (\epsilon_a - \lambda) a_{j_2, m_2} a_{j_2, m_2}^\dagger - G \sum_{j_2, j_3, m_2, m_3 > 0, m_3' > 0} (-1)^{j_2 + m_2} (-1)^{j_3' + m_3'} a_{j_2, m_2} a_{j_3, m_3}^\dagger a_{j_2, m_2}^\dagger a_{j_3', m_3'}^\dagger. \quad (2.28)$$

$\lambda$ is a Lagrange multiplier, chosen such that the average number of particles agrees with the actual number of valence nucleons $n$:

$$\langle \tilde{0} | n | \tilde{0} \rangle = n. \quad (2.29)$$

Minimizing the Hamiltonian of (2.28) with respect to $n$ results in:

$$\frac{\partial}{\partial n} \langle \tilde{0} | \tilde{H} | \tilde{0} \rangle = 0. \quad (2.30)$$

Inserting the expression (2.28) for the Hamiltonian in equation (2.30) yields the BCS equations:

$$\frac{2}{G} = \sum_{j_2, m_2 > 0} \frac{1}{\sqrt{(\epsilon_a' - \lambda)^2 + \Delta^2}}, \quad (2.31)$$

$$n = \sum_{j_2, m_2 > 0} \left( 1 - \frac{\epsilon_a' - \lambda}{\sqrt{(\epsilon_a' - \lambda)^2 + \Delta^2}} \right). \quad (2.32)$$

$\epsilon_a'$ is defined by:

$$\epsilon_a' \equiv \epsilon_a - G v_a^2, \quad (2.33)$$

and $\Delta$ is defined as:

$$\Delta \equiv G \sum_{j_2, m_2 > 0} u_a v_a. \quad (2.34)$$

$\lambda$ describes the Fermi energy, and $\Delta$ the pairing gap. The occupation probabilities $v_a^2$ and $u_a^2$ are then given by:

$$u_a^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_a' - \lambda}{\sqrt{(\epsilon_a' - \lambda)^2 + \Delta^2}} \right), \quad (2.35)$$

$$v_a^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_a' - \lambda}{\sqrt{(\epsilon_a' - \lambda)^2 + \Delta^2}} \right). \quad (2.36)$$

Without going into further detail, because our main interest is the single-particle monopole shift, we mention the two important changes to be incorporated in the description:
Because of the pair correlations, the neutron single-particle energy $\epsilon_{j_\nu}$ has to be replaced by the neutron one-quasi-particle energy $E_{j_\nu}$ [28]:

$$E_{j_\nu} = \sqrt{(\epsilon_{j_\nu} - \lambda)^2 + \Delta^2}. \quad (2.37)$$

The pair correlations make up for a distribution in the occupation of the various neutron orbitals $j_\nu$, expressed by the occupation probability $v_{j_\nu}^2$, with $\sum_{j_\nu} (2j_\nu + 1)v_{j_\nu}^2 = n_{j_\nu}$. The expectation value of $n_{j_\nu}$, appearing in the monopole part of equation (2.12), is evaluated for a single quasi-particle-configuration and gives as a result:

$$\langle n_{j_\nu} \rangle_{1qp} = (2j_\nu + 1)v_{j_\nu}^2. \quad (2.38)$$

The final expression for the proton monopole shift, to be used in the following chapters, becomes:

$$\bar{\epsilon}_{j_\nu} = \epsilon_{j_\nu} + \sum_{j_\nu} E_{j_\nu}(2j_\nu + 1)v_{j_\nu}^2, \quad (2.39)$$

which takes into account the fact that the actual filling of neutron orbitals is not following a sharp filling of single-particle levels but takes the BCS corrections in lowest order into account (see figure 2.3 for a schematic illustration).

### 2.4 Energy Centroids

We have separated the Hamiltonian in a diagonal part of the monopole Hamiltonian plus a sum of higher multipole parts as:

$$H = H_{\lambda=0} + \sum_{\lambda \neq 0} H_{\lambda \neq 0}, \quad (2.40)$$

and we thus have derived a procedure to study the changes in the single-particle energies caused by all kinds of self-energy corrections. However, the whole procedure still remains on a lowest-order scheme of dressing the single-particle motion with correlations.

It is not clear from the very start how well this procedure will describe the fully interacting system. In order to draw some conclusions, we can perform a direct comparison between:

(i) a calculation using a given two-body effective interaction in order to determine the monopole variation for the appropriate single-particle orbital $j_\pi$, and

(ii) a full diagonalization within the same model space but now considering all possible configurations with angular momentum quantum numbers equal to those of the single-particle configuration i.e. $J^\pi = j^\pi$ on equal footing.

The resulting full wave function $\psi^{(i)}(J)$ will contain a very large number of quite complicated configurations $\varphi_k(J)$, $k$ denoting a rank number of that specific configuration for fixed $J$, with amplitudes $a^{(i)}_k(J)$:

$$\psi^{(i)}(J) = \sum_k a^{(i)}_k(J) \varphi_k(J), \quad (2.41)$$
Figure 2.3: Upper panel: Self-energy correction for the proton in orbital $j_\pi$ as a function of changing neutron number $n_{j_\nu}$, with the neutrons being spread over the orbitals $j_{\nu_1}, \ldots, j_{\nu_n}$. Lower panel: The lowest-order BCS correction to the proton single-particle energy $\epsilon_{j_\pi}$ involves the neutrons being spread over the various neutron orbitals with an occupation probability $v_{j_\nu}^2$ because of the pairing interaction. This results in the corrected self-energy, or effective proton single-particle energy $\bar{\epsilon}_{j_\pi}$. 

$$\bar{\epsilon}_{j_\pi} = \epsilon_{j_\pi} + \sum_{j_{\nu_1}}^n \frac{\bar{E}_{j_\pi j_{\nu_1}}}{2} (2j_{\nu_1} + 1)v_{j_\nu}^2$$
such that:

$$H \sum_k a_k^{(i)}(J) \varphi_k(J) = E^{(i)}(J) \sum_k a_k^{(i)}(J) \varphi_k(J). \quad (2.42)$$

We define the overlap factor $S(J^{(i)}; j)$ or strength of the single-particle configuration in a given state $\psi^{(i)}(J)$ as:

$$S(J^{(i)}; j) = |\langle \varphi_{s.p.}(j = J) | \psi^{(i)}(J) \rangle|^2$$

$$= |a_k^{(i)}|_j = s.p. \text{ configuration } j = j(J)|^2. \quad (2.44)$$

It follows naturally that the centroid energy $\bar{\epsilon}_j$ is defined as:

$$\bar{\epsilon}_j \equiv \frac{\sum_i E^{(i)}(J) S(J^{(i)}; j)}{\sum_i S(J^{(i)}; j)}. \quad (2.45)$$

In comparing the results of (i) and (ii), or: $\bar{\epsilon}_j$ and $\bar{\epsilon}_j$, one will have a quantitative measure of ‘missing’ correlations, and, at the same time, a way to judge the quality of the monopole energy shift to determine the changing energy centroids (see figure 2.4).

This has been extensively studied, in particular in the Cu-region ($Z = 29$), and yields interesting results that will be discussed in chapter 4 and beyond.

2.5 A Final Remark on the Monopole Hamiltonian

The idea of ‘dressing’ a single particle moving inside the complicated nucleus is a generic procedure to single out the main degrees of freedom that appear in given mass regions. In the discussion above, we could show that by taking into account the strongly attractive proton-neutron interaction, and separating the monopole part from the higher multipoles, we obtain an elegant method to calculate and study ESPE. On top of that, it was possible to include pairing correlations in lowest order for the changing number of nucleons filling a set of orbitals, introducing a modified form including occupation probabilities.

Only via diagonalizing the full Hamiltonian $H = H_{\lambda=0} + \sum_{\lambda} H_{\lambda \neq 0}$ in the corresponding large model spaces, using the same effective two-body interaction, can one appreciate the quality of the above separation. It is exactly this what will be studied in the following chapters where applications to nuclei with configurations of a closed shell plus or minus one nucleon (CS $\pm 1$) are carried out.

There exist quite a number of papers studying the most general separation of the monopole Hamiltonian for a nucleon in orbit $i$, and the other nucleon in orbit $j$ ($i$, $j$ stand for all quantum numbers, including isospin). They all go back to the early work of Bansal and French [30], and the in-depth study by Zuker et al. [31]. The expression for the diagonal part of the monopole Hamiltonian takes on the following form [31]:

$$H_T = \sum_{i \leq j} \left( a_{ij} \frac{n_i (n_j - \delta_{ij})}{1 + \delta_{ij}} + b_{ij} \frac{T_i \cdot T_j - \frac{3}{2} n_i \delta_{ij}}{1 + \delta_{ij}} \right), \quad (2.46)$$

with $n_i$ and $T_i$ the number and isospin operator for orbital $i$, respectively, and the weights $a_{ij}$ and $b_{ij}$ are given by:

$$a_{ij} = \frac{1}{4} \left( 3V_{ij}^{T=1} + V_{ij}^{T=0} \right), \quad (2.47)$$

$$b_{ij} = V_{ij}^{T=1} - V_{ij}^{T=0}. \quad (2.48)$$
Figure 2.4: A schematic illustration of the extra correlation energy $\Delta \varepsilon$, obtained as the difference between the energy centroid $\bar{\varepsilon}_j$ (using (2.45)) and the monopole shifted single-particle energy $\tilde{\varepsilon}_j$ (using (2.39)). The solid curve, drawn as a guide for the eye, indicates the spectroscopic strength.
$V^T_{ij}$ is given by:

$$V^T_{ij} = \frac{\sum_J (2J + 1) \langle ij, JT | V | ij, JT \rangle}{\sum_J (2J + 1)},$$  

(2.49)

for $T = 0, 1$. It can be shown that it is also possible to work in the proton-neutron basis, which is what we did in the present chapter. Both descriptions can be proven to be equivalent, starting from the same original Hamiltonian (2.1) [32].
3 Nucleon-Nucleon Forces

3.1 Introduction

Since our basic assumption in using the shell-model to approximate the complicated nuclear many-body problem of $A$ nucleons interacting inside the atomic nucleus is the use of an effective ‘in-medium’ interaction, we will start by giving some general discussion of those forces used throughout the present study.

Although the effective nucleon-nucleon interaction (active in some limited part of the full Hilbert space and within a nuclear medium) will be largely different from the form of the free nucleon-nucleon interaction \[25\], we will start considering the properties of the bare force. To a good approximation, and incorporating one-pion exchange (OPEP), this latter force leads to a form of the type \[1, 33\]:

$$V_{\pi}\text{OPEP} = \frac{1}{3}\frac{f^2}{\hbar c}m_\pi c^2\{\tilde{\sigma}_1 \cdot \tilde{\sigma}_2 + \left(1 + \frac{3}{\mu r} + \frac{3}{(\mu r)^2}\right)S_{12}\} \frac{e^{-\mu r}}{\mu r} (\tilde{r}_1 \cdot \tilde{r}_2), \quad (3.1)$$

with $c$ the speed of light, $m_\pi$ the pion mass, $\mu \equiv \frac{m_\pi c}{\hbar} = 0.70$ fm$^{-1}$ the reduced pion mass, and $\frac{f^2}{\hbar c} = 0.081 \pm 0.002$ the pion-nucleon coupling constant. The factor $S_{12}$:

$$S_{12} = 3\left(\tilde{\sigma}_1 \cdot \tilde{r}\right)\left(\tilde{\sigma}_2 \cdot \tilde{r}\right) - \tilde{\sigma}_1 \cdot \tilde{\sigma}_2, \quad (3.2)$$

is the tensor operator. Expression (3.1) holds typically for a separation distance $r = |\tilde{r}_1 - \tilde{r}_2| \simeq 1.5 - 2$ fm, but the actual interaction becomes repulsive (in coordinate space) at distances $r \lesssim 0.5$ fm.

It is standard to determine a general form by imposing certain symmetry constraints (see further in the text), and the strength of this general form is fitted to experimental phase-shift data describing free nucleon-nucleon scattering up to $\simeq 350$ MeV laboratory energy [25]. One may then use many-body perturbation theory [34] in order to construct a $G$-matrix which is well-behaved, even at short distances. In chapters 4, 5, 6 and 7, where applications to specific mass regions are carried out, we most often start from such a $G$-matrix approach, e.g. the interaction of Hjorth-Jensen and co-workers [34] in the $fp$ shell-model space, or of Kuo and Herling in the Pb-region.

On the other hand, effective interaction matrix elements may be determined in a limited model space ($p, sd, pf(1g_9/2)$) by fitting the energy eigenvalues of the corresponding Schrödinger eigenvalue equation to an experimental data set of specific nuclear properties (excitation energies and binding energies). Since these effective interactions have been constructed, emphasizing past and present knowledge of nuclear structure properties, it
may well be interesting to explore the possibilities but also the limitations in moving away from the region near \( \beta \)-stability.

We also give some attention to those simple (often called schematic) forces which may highlight certain generic properties of a given nucleon-nucleon force, and the way this propagates in nuclei when moving away from stability. Results when using both simple zero-range forces (\( \delta \)-interaction with spin exchange), Yukawa forces, and multipole forces will be presented in the chapters which apply to the various mass regions.

### 3.2 The Bare Nucleon-Nucleon Force

The bare nucleon-nucleon force describes the interaction between two free nucleons. It is understood that the effect of the Coulomb-interaction is treated separately, so we focus entirely on the effect of the strong interaction between the nucleons.

The derivation of the interaction between free nucleons is based on some important assumptions \[28\]:

- we consider no substructure in the nucleon, and consider nucleons to describe the essential degrees of freedom,
- the \( A \) nucleons interact via a potential,
- relativistic effects are negligible,
- only two-body forces are considered.

The first assumption states that the interaction between two nucleons goes via a potential. The potential depends only on those two nucleons, and the dependence on their coordinates can be expressed in the most general way as:

\[
V(1, 2) = V(\vec{r}_1, \vec{p}_1, \vec{\sigma}_1, \vec{r}_2, \vec{p}_2, \vec{\sigma}_2, \vec{\tau}_2),
\]  

(3.3)

where \( \vec{r}_i \) denotes the spatial coordinate of nucleon \( i = 1, 2 \); \( \vec{p}_i \) the momentum; \( \vec{\sigma}_i \) the spin, and \( \vec{\tau}_i \) the isospin coordinates.

#### 3.2.1 Symmetry Properties and General Structure

The potential \( V(1, 2) \) has to fulfill a number of symmetry properties, imposed by the nature of the strong interaction between free nucleons:

- **hermiticity**

- **invariance under an exchange of the coordinates**

\[
V(1, 2) = V(2, 1).
\]  

(3.4)

- **translational invariance**

\[
V(1, 2) = V(\vec{r}, \vec{p}_1, \vec{\sigma}_1, \vec{r}_2, \vec{p}_2, \vec{\sigma}_2, \vec{\tau}_2),
\]  

(3.5)

with \( \vec{r} = \vec{r}_1 - \vec{r}_2 \) the relative spatial coordinate.
3.2 The Bare Nucleon-Nucleon Force

- **Galilean invariance**

\[ V(1, 2) = V(\vec{r}, \vec{p}, \vec{sr}_1, \vec{sr}_2), \quad (3.6) \]

with \( \vec{p} = \frac{1}{2}(\vec{p}_1 - \vec{p}_2) \) the relative momentum.

- **invariance under space reflection (parity conservation)**

\[ V(\vec{r}, \vec{p}, \vec{sr}_1, \vec{sr}_2) = V(-\vec{r}, -\vec{p}, \vec{sr}_1, \vec{sr}_2). \quad (3.7) \]

- **invariance under time reversal**

\[ V(\vec{r}, \vec{p}, \vec{sr}_1, \vec{sr}_2) = V(\vec{r}, -\vec{p}, -\vec{sr}_1, -\vec{sr}_2). \quad (3.8) \]

- **rotational invariance in coordinate space**

Also introducing the orbital angular momentum \( \vec{L} = \vec{r} \times \vec{p} \), only terms of the form \( \vec{sr}_1 \cdot \vec{sr}_2, (\vec{r} \cdot \vec{sr}_1)(\vec{r} \cdot \vec{sr}_2), (\vec{p} \cdot \vec{sr}_1)(\vec{p} \cdot \vec{sr}_2), (\vec{L} \cdot \vec{sr}_1)(\vec{L} \cdot \vec{sr}_2) + (\vec{L} \cdot \vec{sr}_2)(\vec{L} \cdot \vec{sr}_1) \) are possible. Multiplication with an arbitrary function of \( r^2, p^2 \) and \( \vec{L} \cdot \vec{L} \) does not affect this symmetry constraint.

- **rotational invariance in isospin space**

Only terms of the form:

\[ V_0 + V_\tau \vec{sr}_1 \cdot \vec{sr}_2, \quad (3.9) \]

are allowed.

A more elaborate discussion of the symmetry properties is given by Ring and Schuck [28].

One can make several combinations with good symmetry, but we present those combinations that have been used mainly in order to construct a realistic bare two-body nucleon interaction.

### 3.2.1.1 Central Force Component

The central forces are local forces since they do not depend on the velocity, and contain only scalar products of the major nucleon variables \( \vec{sr} \) and \( \vec{sr} \):

\[ V_C(1, 2) = V_0(r) + V_\sigma(r)\vec{sr}_1 \cdot \vec{sr}_2 + V_\tau(r)\vec{sr}_1 \cdot \vec{sr}_2 + V_{\sigma\tau}(r)\vec{sr}_1 \cdot \vec{sr}_2 \quad (3.10) \]

This form can be rewritten using certain exchange operators. One defines the spin exchange operator \( \vec{P}_\sigma \):

\[ \vec{P}_\sigma = \frac{1}{2}(1 + \vec{sr}_1 \cdot \vec{sr}_2); \quad (3.11) \]

and, likewise, the isospin exchange operator \( \vec{P}_\tau \):

\[ \vec{P}_\tau = \frac{1}{2}(1 + \vec{sr}_1 \cdot \vec{sr}_2). \quad (3.12) \]
The expectation value of $\hat{P}_\sigma$ becomes:

$$
\langle SM_S | \hat{P}_\sigma | SM_S \rangle = \langle SM_S | \frac{1}{2} \left( 1 + 2(\hat{S}_1^2 - \hat{s}_1^2 - \hat{s}_2^2) \right) | SM_S \rangle \\
= S(S + 1) - 1 \\
= \begin{cases} 
1 & \text{for } S = 1 \\
-1 & \text{for } S = 0.
\end{cases}
$$

(3.13)

The expectation value of $\hat{P}_\tau$ becomes:

$$
\langle SM_S | \hat{P}_\tau | SM_S \rangle = \langle SM_S | \frac{1}{2} \left( 1 + 2(\hat{S}_1^2 - \hat{s}_1^2 - \hat{s}_2^2) \right) | SM_S \rangle \\
= S(S + 1) - 1 \\
= \begin{cases} 
1 & \text{for } S = 1 \\
-1 & \text{for } S = 0.
\end{cases}
$$

(3.13)

If $\hat{P}_\sigma$ would act on a two-particle state with spin $S = 1$ (spin-triplet state or spin-symmetric state), there is no change of sign for the spin wave function; if it would act on a $S = 0$ state (spin-singlet or spin-antisymmetric), it produces an extra minus sign, to be interpreted as the interchange of the individual spin coordinates. Similar relations hold for $\hat{P}_\tau$. The exchange operator $\hat{P}_r$ for the spatial coordinate can be defined through the relation:

$$
\hat{P}_r \hat{P}_\sigma \hat{P}_r = -1,
$$

(3.14)

since the wave function has to be antisymmetric under the interchange of all coordinates of particles 1 and 2. Using (3.14), $\hat{P}_r$ can be rewritten as:

$$
\hat{P}_r = -\hat{P}_r \hat{P}_\sigma,
$$

(3.15)

and the general central force becomes:

$$
V_C = V_W(r) + V_M(r) \hat{P}_r + V_B(r) \hat{P}_\sigma + V_H(r) \hat{P}_r \hat{P}_\sigma.
$$

(3.16)

The coefficients of the different terms in (3.10) and (3.16) fulfill the following relation:

$$
V_W = V_0 - V_\sigma - V_\tau + V_{\sigma\tau}, \\
V_M = -4V_{\sigma\tau}, \\
V_B = 2V_\sigma - 2V_{\sigma\tau}, \\
V_H = -2V_\tau + 2V_{\sigma\tau}.
$$

(3.17) - (3.20)

Yet another way of writing down the central interaction makes use of projection operators:

$$
\hat{\Pi}_s = \frac{1}{2} (1 - \hat{P}_\sigma), \\
\hat{\Pi}_\tau = \frac{1}{2} (1 + \hat{P}_\sigma);
$$

(3.21)

$$
\hat{\Pi}_s = \frac{1}{2} (1 - \hat{P}_\tau), \\
\hat{\Pi}_\tau = \frac{1}{2} (1 + \hat{P}_\tau).
$$

(3.22)

Since table 3.1 indicates that it is sufficient to know the spin and isospin symmetry in order to establish the correct antisymmetry of the wave function, one can write the central force in terms of the operators $ij \hat{\Pi}$, defined as:

$$
\hat{\Pi} = (2T+1)(2S+1) \hat{\Pi} \equiv 2T+1 \hat{\Pi} 2S+1 \hat{\Pi},
$$

(3.23)

$$
2T+1 \hat{\Pi} = \frac{1}{2} \left[ 1 - (-1)^T \hat{P}_\tau \right],
$$

(3.24)

$$
2S+1 \hat{\Pi} = \frac{1}{2} \left[ 1 - (-1)^S \hat{P}_\sigma \right].
$$

(3.25)

The expression for the central force then becomes:

$$
V_C = V_C(r) \sum_{i,j=(1,3)} a_{ij} \hat{\Pi}.
$$

(3.26)

The relationship between the various representations of the central force is summarized in table 3.2.
Table 3.1: Different combinations giving rise to a totally antisymmetric two-body nuclear wave function. The notation $\langle \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rangle$ is a shorthand notation for the expectation value of the operator in a given two-particle state with total spin $S$: $\langle \frac{1}{2} \frac{1}{2} \rangle S M_S | \vec{\sigma}_1 \cdot \vec{\sigma}_2 | \langle \frac{1}{2} \frac{1}{2} \rangle S M_S \rangle$. Likewise, $\langle \vec{\tau}_1 \cdot \vec{\tau}_2 \rangle$ is a shorthand notation for $\langle (\frac{1}{2} \frac{1}{2}) T T_z | \vec{\tau}_1 \cdot \vec{\tau}_2 | (\frac{1}{2} \frac{1}{2}) T T_z \rangle$.

<table>
<thead>
<tr>
<th>$\langle \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rangle$</th>
<th>$\langle \vec{\tau}_1 \cdot \vec{\tau}_2 \rangle$</th>
<th>$S$</th>
<th>$T$</th>
<th>spatial</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3</td>
<td>-3</td>
<td>0</td>
<td>0</td>
<td>odd</td>
</tr>
<tr>
<td>-3</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>even</td>
</tr>
<tr>
<td>1</td>
<td>-3</td>
<td>1</td>
<td>0</td>
<td>even</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>odd</td>
</tr>
</tbody>
</table>

Table 3.2: Relation between the coefficients of the various representations (equations (3.10), (3.16) and (3.26)) of the central force.

<table>
<thead>
<tr>
<th>$\langle \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rangle$</th>
<th>$\langle \vec{\tau}_1 \cdot \vec{\tau}_2 \rangle$</th>
<th>$V(\vec{\sigma}_1 \cdot \vec{\sigma}_2, \vec{\tau}_1 \cdot \vec{\tau}_2)$</th>
<th>$V(P^r, P^r)$</th>
<th>$ij\Pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-3</td>
<td>$V_0 + V_{\sigma} - 3V_\tau - 3V_{\sigma\tau}$</td>
<td>$V_W + V_M + V_B + V_H$</td>
<td>$a_{13}$</td>
</tr>
<tr>
<td>-3</td>
<td>1</td>
<td>$V_0 - 3V_\sigma + V_\tau - 3V_{\sigma\tau}$</td>
<td>$V_W + V_M - V_B - V_H$</td>
<td>$a_{31}$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$V_0 + V_\sigma + V_\tau + V_{\sigma\tau}$</td>
<td>$V_W - V_M + V_B - V_H$</td>
<td>$a_{33}$</td>
</tr>
<tr>
<td>-3</td>
<td>-3</td>
<td>$V_0 - 3V_\sigma - 3V_\tau + 9V_{\sigma\tau}$</td>
<td>$V_W - V_M - V_B + V_H$</td>
<td>$a_{11}$</td>
</tr>
</tbody>
</table>

3.2.1.2 Two-Body Tensor Force Component

The two-body tensor force also has a local character, and has the form:

$$V_T(1, 2) = V_T(r) (v_{t0} + v_{t1} \vec{\tau}_1 \cdot \vec{\tau}_2) \frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2),$$

(3.27)

$$= V_T(r) (v_{t0} + v_{t1} \vec{\tau}_1 \cdot \vec{\tau}_2) S_{12},$$

(3.28)

and $S_{12}$ is the tensor operator defined in (3.2). The tensor force is particularly important since it causes orbital angular momentum mixing. Its presence in the nuclear force is shown by the non-vanishing quadrupole moment of the deuteron, which cannot be proven by a pure central forces alone [28].

3.2.1.3 Two-Body Spin-Orbit Force Component

The two-body spin-orbit force has a non-local structure:

$$V_{ls}(1, 2) = V_{ls}(r) \vec{t} \cdot \vec{S},$$

(3.29)

with $\vec{S}$ the total spin of the two-body system, and $\vec{t}$ the relative orbital angular momentum operator for the two-body system. The velocity dependence, or non-local character, enters the expression through the orbital angular momentum.
3.2.1.4 Radial Dependence

The radial dependence of the various contributions can be parameterized using simple central potentials. Various forms are often used:

- Yukawa potential: \( V(r) = -V_0 \frac{e^{-mr}}{mr} \),
- Gaussian potential: \( V(r) = -V_0 e^{-r^2/r_0^2} \),
- exponential potential: \( V(r) = -V_0 e^{-r/r_0} \),
- square well: \( V(r) = \begin{cases} V_0 & \text{if } r \leq r_0 \\ 0 & \text{if } r > r_0 \end{cases} \).

The strength \( V_0 \) and range \( r_0 \) are fitted to the experimental data.

The Yukawa potential [33], however, is based on field theory: the long-distance attractive tail of the nuclear force is mediated by the exchange of one pion between the interacting nucleons. The simplest form is derived from the exchange of a single pion. In this case, \( 1/\mu = \frac{\hbar}{m_\pi c} \) is the Compton wavelength of the pion, and is given by \( \mu = 0.70 \text{ fm}^{-1} \).

The potentials mentioned above are drawn schematically in figure 3.1.

3.2.2 Constructing the Bare Nucleon-Nucleon Interaction

Once a general analytical functional form of the two-body potential has been laid out, the parameters of the various contributions have to be determined. One can accomplish this by analyzing the scattering properties in the various two-body nucleon-nucleon systems, as well as the proton-neutron bound state, i.e. the deuteron. Scattering experiments are performed below the pion-production threshold (~350 MeV). This guarantees the appropriateness of the non-relativistic approach, and the nucleons involved can be treated as point-like particles (justifying the assumed existence of a potential) [35].

The parameters are obtained from an extensive fitting program to the experimental
3.2 The Bare Nucleon-Nucleon Force

Figure 3.2: The nuclear phase parameters for the $T = 1$ channels with $L \leq 2$, up to a laboratory energy of $E_{\text{lab}} = 400$ MeV. The phase shifts are given in radians. Positive phase shifts indicate attraction between the nucleons, negative phase shifts repulsion. Figure taken from [1].

Phase shifts between the waves describing the incoming and the outgoing scattered nucleon. These phase shifts contain the information about the shape, the strength, and the energy dependence of the potential. The relation between the phase shift and the potential (for an overview, see [1]) is illustrated schematically in figure 3.2. It shows that the bare nucleon-nucleon potential contains a short-range repulsive part, and a longer-ranged attractive part. The repulsive character of the potential increases rapidly with decreasing distance between the nucleons, and has quite often been approximated by means of a hard core.

There exist a number of potentials that are fitted to nucleon-nucleon scattering data and the deuteron binding energy. Some of the most famous are listed here: the Hamada-Johnston potential [36, 37], the Reid soft-core potential [38], the Nijmegen potential [39], the Paris potential [40, 41], the Bonn potential [42, 43], the CD-Bonn potential [44] and the Argonne potential [45, 46].

The Argonne potential consists of 8 (or 18) terms:

$$V_{ij} = \sum_{p=1,8(18)} v_p(r_{ij}) O_{ij}^p,$$  \hspace{1cm} (3.30)

with the operators $O_{ij}^p$ given by:

$$O_{ij}^p = \{ 1, \vec{\sigma}_i \cdot \vec{\sigma}_j, \vec{S}_{ij}, \vec{l} \cdot \vec{S}, \ldots \} \otimes \{ 1, \vec{r}_i \cdot \vec{r}_j \}.$$  \hspace{1cm} (3.31)
3 Nucleon-Nucleon Forces

The potentials have been fitted to 4300 nucleon-nucleon scattering data, and describe the bare scattering process very well over the energy range (up to 350 MeV laboratory scattering energy) [47]. They are phenomenological but describe the essential physics: Coulomb forces, one-pion exchange at the larger nuclear separation distance \( r \approx 1.5 - 2 \text{ fm} \), but also the intermediate and short-range parts.

The parameters of the potentials are fitted to the scattering data. The more data are included, the better the agreement; so it is crucial to fit to proton-proton, neutron-neutron, proton-neutron and deuteron data. Potentials that lack one of these sets in their parameter fit, provide a worse description for that particular set, as demonstrated in [48] for various potential models applied to the proton-proton scattering data.

Even though these potentials provide a precise description of the free nucleon-nucleon scattering, they are still subject to corrections when proceeding towards light nuclei. Usually, the potentials fitted to scattering data tend to underbind light nuclei. The correct binding energy is expected to be found by adding three-nucleon forces [47, 49, 50, 51, 52].

An approach different from the ones mentioned above involves writing the nucleon-nucleon potential as a sum over one-boson exchange potentials [53, 54, 55, 56, 57, 58, 59, 60].
3.3 Effective Interactions

Moreover, the inclusion of relativistic effects may prove to be important too: given the rather small distance scales, it might be necessary to go beyond the meson picture and to include quark-antiquark pair exchange, as depicted in figure 3.4. However, calculations become intractable because of the strong coupling $\alpha_s$ that is too large to allow a perturbative approach [35].

3.3 Effective Interactions

The bare nucleon-nucleon interaction is a starting point to derive an effective interaction to be used in nuclear calculations.

3.3.1 Microscopic Effective Interactions

One of the most successful approaches for the effective nuclear interaction is based on Brueckner’s $G$-matrix [20, 21]. It treats two nucleons in the nuclear medium in a way analogous to the scattering of two nucleons in vacuum. The problem of the hard core that arises in the scattering of free nucleons is solved by performing an infinite summation of the scattering processes of two nucleons in the nuclear medium. The resulting effective interaction is well-behaved at short distances. At the same time, more many-body effects are consistently treated than when just applying the bare force.

The $G$-matrix is obtained by solving the Bethe-Goldstone equation [61]:

$$G(\omega) = V + V \frac{Q_{2p}}{\omega - H_0} G(\omega).$$

(3.32)

Here, $\omega$ is the ‘starting energy’ at which $G$ is computed. $H_0$ is the unperturbed Hamiltonian for the intermediate two-particle state. $V$ is the bare interaction between the two
nucleons, unmodified for the nuclear medium. $Q_{2p}$ is a two-particle projection operator that guarantees that the scattered particles obey the Pauli exclusion principle: the two nucleons can only be scattered to unoccupied states, hence, states that lie above the Fermi energy. The effective interaction derived from this $G$-matrix can be expressed as:

$$V_{\text{eff}} = G + G \frac{Q'}{E_{0\nu} - H_0^V} V_{\text{eff}}, \quad (3.33)$$

where $H_0^V$ is describing the single-particle Hamiltonian for the valence space, and $E_{0\nu}$ is the corresponding single-particle energy. The prime on the projection operator $Q'$ indicates that the expansion of $V_{\text{eff}}$ does not sum over two-particle ladder diagrams already included in $G$, in order to avoid double-counting.

The first such derived effective interaction is the one of Kuo and Brown in the $sd$-shell [62]. Another example of an often-used effective interaction based on the $G$-matrix is the interaction derived by Hjorth-Jensen and collaborators [34], developed for the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, $1g_{9/2}$ space. Based on the method outlined in [63], monopole corrections have been incorporated [64] in order to account for correct saturation properties of the interaction. The resulting interaction gives a very good description of many spectroscopic properties of Ni- and Cu-isotopes, and will be used in chapter 4.

An effective interaction for the full $pf$-shell has been constructed by Honma et al., resulting in the GXPF1-interaction and various adjusted and updated versions [65, 66, 67]. This interaction is actually based on a microscopic approach ($G$-matrix), and fitted to the experimental data in the mass range $47 \leq A \leq 66$. It gives a good description of nuclei in the mass region $A \approx 50$. Kuo and Brown developed a good interaction for the lower $pf$-shell ($A \leq 52$) [68]; KB1 [69], KB3 (monopole modifications) [63] and KB3G [70] (shell gap adjusted) are modified and improved versions. Yet another interaction is the FPD6-interaction [71], an analytical potential whose parameters are fitted to the experimental data in the mass region $A = 41 \sim 49$.

### 3.3.2 Phenomenological Effective Interactions

It is also possible to obtain an effective nuclear interaction by using the single-particle energies and two-body matrix elements as parameters in a fit for a particular mass region [25]. The energy levels calculated with these parameters are compared to the experimental energy levels, and the parameter values are adjusted by means of a least-squares fitting procedure. A very good interaction for the $p$-shell is obtained by Cohen and Kurath [72].

The $sd$-shell region is covered by various interactions of the Utrecht group [25, 73, 74] and of Brown and Wildenthal and collaborators [75, 76, 77]. For a more detailed discussion, see [25].

### 3.3.3 Schematic Effective Interactions

The aim to cover large intervals of nuclei ($p$-shell, $sd$-shell, $fp$-shell, ... ) using detailed phenomenological interactions, is hindered by the fact that one just parameterizes the residual nuclear interaction properties with a set of two-body matrix elements of the form $\langle j_a j_b, JT | V | j_c j_d, JT \rangle$, which are just numbers. On the other hand, the construction of the bare nucleon-nucleon interaction started from a limited set of simple invariants, functions
of $\vec{r}$, $\vec{\sigma}$, $\vec{\tau}$, $\vec{l}$, $\vec{S}$ operators, given some simple radial factors. When brought inside the nucleus, its matrix elements do not exhibit any strong tendency to form $J^\pi = 0^+$ coupled pairs, a tendency commonly displayed by nucleons inside the atomic nucleus.

Therefore, we also use the properties of some of the simple forces, such as multipole forces, zero-range or delta-forces (sometimes with spin-exchange possibilities), to study their generic characteristics with respect to the description of nuclear structure properties (characteristics of odd-odd nuclei, variations of single-particle energies).

Here, we consider in particular the zero-range interaction $\delta(\vec{r}_i - \vec{r}_j)$ and the quadrupole-quadrupole force. They very clearly exhibit both properties for nuclei where only one type of nucleons is active (pairing properties — including the correct saturation of nuclear binding energies), and the tendency to develop collective effects when both protons and neutrons play an active role (open proton-neutron shells).

### 3.3.3.1 Zero-Range Interaction

The delta-interaction is defined as:

$$V_\delta(1, 2) = -V(r)\delta(\vec{r}_1 - \vec{r}_2),$$

and as such, is a zero-range interaction, the simplest approximation for the short-range character of the nuclear force. Its attractive character is ensured by the minus sign. Moreover, the $\delta$-force can be extended by including a spin-exchange component:

$$V_\delta(1, 2) = -V_0(1 - \alpha + \alpha\vec{\sigma}_1 \cdot \vec{\sigma}_2)\delta(\vec{r}_1 - \vec{r}_2),$$

with $\alpha$ the degree of spin-exchange, varying between 0 and 1, and $V_0$ the strength of the interaction and given in units MeV-fm$^3$.

### 3.3.3.2 Quadrupole-Quadrupole Interaction

The quadrupole-quadrupole interaction has a simple analytical form:

$$V_{QQ}(1, 2) = \chi \left( \sqrt{\frac{m \omega}{\hbar}} r_\pi \right)^2 \left( \sqrt{\frac{m \omega}{\hbar}} r_\nu \right)^2 Y_2^*(\Omega_\pi) \cdot \bar{Y}_2(\Omega_\nu).$$

The strength $\chi$ (in units MeV) is fitted to experimental data.
Part II

Applications in Various Mass Regions
4 Copper Isotopes

4.1 Experimental Status and Motivation

The copper isotopes form an interesting region to study the validity of the nuclear shell model in modeling the available nuclear data: they span a wide range of the nuclear chart, going from magic neutron number \( N = 28 \), thereby passing the questioned magic number \( N = 40 \), up to the next magic number \( N = 50 \), deep into the exotic region. Studying the nuclei around the (semi)magic nucleus \(^{68}\text{Ni}\) sheds light on the neutron shell closure at \( N = 40 \), and if it will hold when going towards the more neutron-rich nuclei.

The nucleus \(^{68}\text{Ni}\) exhibits some features of a doubly-magic nucleus, such as a higher excitation energy of the \( 2^+ \) state [78, 79] (see figure 4.1) compared to the surrounding \(^{66,70}\text{Ni}\)-nuclei, but it doesn’t hold up to its doubly-magic status when looking at other observables such as two-neutron separation energies [80] (see figure 4.2). Favorable arguments for the doubly-magic status of \(^{68}\text{Ni}\) are given by the single-particle gap at \( N = 40 \) and the occurrence of a change in parity between the \( pf \) orbitals (negative parity) and the higher-lying \( 1g_{9/2} \) orbital (positive parity) across the \( N = 40 \) gap. This leads to a reduced \( B(E2 : 0^+_1 \rightarrow 2^+_1) \) value, comparable to the low \( B(E2) \) values found in ‘real’ doubly-magic nuclei [81], and the above parity change provides an explanation for this [82]. However, recent work [83] suggests that this \( B(E2) \) strength forms only a part of the low-lying \( B(E2) \) strength, and thus this small experimental \( B(E2) \) value is not convincing enough to establish the double magicity of \(^{68}\text{Ni}\).

Figure 4.1: Systematic behaviour of the excitation energy of the first \( 2^+ \) state in the even Ni (\( Z = 28 \)), Zn (\( Z = 30 \)) and Fe (\( Z = 26 \)) isotopes. The neutron shell- and subshell-closures at \( N = 28 \) and \( N = 40 \) are indicated. Figure taken from [80].
The study of nuclei around $^{68}_{28}$Ni does not only provide valuable information about the neutron magic numbers; they also provide excellent input for a study of the evolution of the proton magic number $Z = 28$ when going towards the exotic neutron-rich nuclei. Franchoo et al. [84, 85] have reported a change in proton single-particle energy levels in $^{69,71,73}$Cu, and have interpreted it as due to a monopole shift in the proton energies at $Z = 29$, $N = 40$.

It is clear that the nuclei in the vicinity of $^{68}$Ni provide very interesting information about nuclear shell structure of exotic nuclei. Moreover, they are of astrophysical interest, particularly in stellar collapse models [86]. There, the $r$-process, or rapid neutron capture, occurs. Doubly-magic nuclei such as $^{78}$Ni feature as bottlenecks or so-called waiting-points, halting the $r$-process. The exact appearance or disappearance of magic numbers is of paramount importance for the evolution of these stellar collapse models and the abundance of the elements.

In this chapter, we intend to investigate the evolution of the proton mean-field from nuclei situated around the valley of $\beta$-stability towards very neutron-rich systems.

In the present study we apply this approach to neutron-rich Cu-isotopes. We choose two types of the effective interaction: a schematic zero-range force and a realistic effective interaction, based on the $G$-matrix [34, 64, 87], in order to test the sensitivity to the use of various (schematic versus realistic) types of forces. Finally, a comparison of the monopole shifts with the results of the large-scale shell-model diagonalization is carried out.

Figure 4.2: (a) Differential two-neutron separation energies in the Ni-isotopes, $S_{2n}(A) - S_{2n}(A + 2)$. (b) Similar for the two-proton separation energies in the $N = 50$ isotones. Figure taken from [80].
4.2 Spectroscopy of $^{70}$Cu

4.2.1 Experimental Situation

$^{70}$Cu$_{41}$ is an interesting nucleus to start the shell-model study. It differs from the proton magic number $Z = 28$ by one extra proton, and from the neutron semi-magic number $N = 40$ by one extra neutron. Based on the work of [80], $^{70}$Cu can be interpreted as an inert $^{68}$Ni-core, plus two valence particles: $^{70}$Cu = $^{68}$Ni$\otimes$1$\pi$ $\otimes$ 1$\nu$. This makes the nucleus an excellent tool to study the residual proton-neutron interaction.

Recent experimental work on the nucleus $^{70}$Cu [88, 89, 90] has yielded very interesting results: the level structure has been determined, a new isomer and two new isomeric transitions have been identified, and the absolute ordering of the resulting three isomers has been established (see the right frame in figure 4.3, and figure 4.4). The isomeric levels have been determined by their $\beta$-decay to the Zn-daughter nucleus.

The proton single-particle energies of $^{70}$Cu are determined by the lowest excited levels of $^{69}$Cu = $^{68}$Ni$\otimes$1$\pi$. The neutron single-particle energies are determined in the same way from the spectrum of $^{69}$Ni = $^{68}$Ni$\otimes$1$\nu$. The resulting energies are shown in figure 4.3.
4 Copper Isotopes

Figure 4.4: The deduced relative placement of the $^{70}$Cu isomers and their decay properties. The branching ratios for the isomeric transitions contain an internal conversion correction [91]. Figure taken from [89].

In the shell-model picture of Klingenerger [92], the single-particle states are ordered as depicted in figure 4.5. The experimental spectrum as in the left frame of figure 4.3 shows a different level ordering. The reason for this different ordering is that the single-particle energies are influenced by the precise numbers of protons and neutrons active in the nucleus: the relative surplus of neutrons influences the proton states, and changes their unperturbed ordering. Not only the proton states are influenced by the surplus of neutrons; the neutrons too display a different behaviour compared to the unperturbed single-particle structure (a single valence nucleon outside the inert core). Here, it is the subshell at $N = 40$ that affects the neutron behaviour: it is energetically more favorable to excite a neutron out of the $pf$-shell into the $1g_{9/2}$ orbital and to form a neutron pair in the $1g_{9/2}$-orbital, than to excite that neutron over the $N = 50$ shell gap; the energy gain is due to the pairing energy of the extra neutron pair in $1g_{9/2}$.

4.2.2 Shell-Model Study: Determining the Forces

In the extreme shell-model picture, $^{70}_{29}$Cu$_{41}$ can be viewed as having one valence proton outside the $Z = 28$ closed shell and one valence neutron outside the closed $N = 40$ subshell. The experimental quasi-particle energies in the vicinity of the $^{68}_{28}$Ni$_{40}$ semi-doubly-magic nucleus can be determined from the energy levels of the $^{69}_{29}$Cu$_{40} = ^{68}_{28}$Ni$_{40} \otimes 1\pi$ and $^{60}_{28}$Ni$_{41} = ^{68}_{28}$Ni$_{40} \otimes 1\nu$ nuclei, as shown in the left panel of figure 4.3. The order of the excited states in $^{69}_{29}$Cu is in agreement with the shell-model predictions for the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, and $1g_{9/2}$ proton orbitals. The $1g_{9/2}$ orbital lies high up in energy, at 2553 keV, indicating the existence of the $Z = 40$ subshell. The $^{60}_{28}$Ni case is similar and the excited states correspond to holes in the neutron $pf$ shell.
In $^{70}$Cu, the valence proton and neutron will couple giving rise to a multiplet of states with spin values ranging from \( J = j_1^\pi + j_2^\nu \) down to \( J = |j_1^\pi - j_2^\nu| \) with \( j_i \) being the total angular momentum of orbital \( i \). If the residual interaction is approximated by a quadrupole-quadrupole interaction, these states will split up in energy \([93, 94]\), and exhibit a quadratic dependence on \( J(J + 1) \), with \( J \) being the total spin, and thus:

\[
E_J = aJ^2(J + 1)^2 + bJ(J + 1) + c, \tag{4.1}
\]

i.e. the energy values lie on a parabola as a function of \( J(J + 1) \). Since it concerns both particles in $^{70}$Cu, the parabola will be faced down, having one maximum for an intermediate spin value. The most important $\pi$-$\nu$-coupling schemes are schematically drawn in the middle frame of figure 4.3.

A careful comparison with the levels observed in the beta decay of $^{70}$Ni (see figure 6 of [89]) shows that the six lowest levels can be readily explained using this simple approach (see also figure 2 of [90]). The $^{70}$Cu ground state and its first excited isomeric state at 101.1 keV were already attributed to the $6^-$ and $3^-$ members of the $\pi 2p_{3/2}\nu 1g_{9/2}$ multiplet. The other members are most probably the states at 226(6) and 506(6) keV according to Sherman et al. [95]. The 226(6) keV state was already associated with the $(4^-)$ state at 228.5 keV observed in the $^{70}$Ni decay. Hence the 506(6) keV state is most probably the $(5^-)$ state. The $\pi 2p_{3/2}\nu 1g_{9/2}$ configuration is indeed expected to determine the lowest energy states in $^{70}$Cu since it is made by coupling the two orbitals that are lowest in energy. The $(1^+)$ isomeric state at 242.4 keV and the $(2^+)$ state at 320.7 keV were already proposed to be members of the $(1,2)^+$ doublet having the $\pi 2p_{3/2}\nu (2p_{1/2}^{-1}2g_{9/2}^{+2})$ configuration. This configuration is indeed the second lowest in energy and is thus expected at energies of a few hundred keV.
Figure 4.6: Experimental and theoretical spectrum of $^{70}_{29}$Cu$_{41}$. The left panel shows the available experimental data, the middle panel the results obtained via a large-scale shell-model calculation with the realistic interaction [34], and the right panel the spectrum obtained with the $\delta$-interaction.

To check the degree of purity of the lowest multiplets, we have performed shell-model calculations using $^{68}$Ni as a core and the delta-interaction:

$$V = -V_0(1 - \alpha + \alpha \vec{\sigma}_\pi \cdot \vec{\sigma}_\nu)\delta(\vec{r}_\pi - \vec{r}_\nu),$$

(4.2)

acting between the valence proton and valence neutron with the strength $V_0 = 400$ MeV·fm$^3$ and $\alpha = 0.1$. These values of the parameters result in two-body matrix elements that come closest to those of the realistic interaction which will be described below, and they give a reasonable description of the spectrum of $^{58}$Cu. The eigenvalues of $^{70}$Cu are shown in figure 4.6 and are compared with the corresponding part of the experimental data.

Only the low-energy negative parity states can be discussed, since the excitation of neutrons from the $\nu \pi 2p_{1/2}$ orbital are not allowed in the chosen model space. In good agreement with the discussion above, the lowest $3^- - 6^-$ states have a dominant contribution from the $\pi 2p_{3/2} \nu 1g_{9/2}$ configuration (from 90% to 99%), while the second multiplet
2− − 7− arises mainly from the coupling of π 1f5/2 and ν 1g9/2 orbitals (≈ 80% for 4−, 5− states). The 62− state lies at 1.1 MeV and is not seen at the scale of the figure. The inversion of the 3− and 6− states is not essential, since it is within the precision of the schematic shell model. The only possible 1+ state in this model space, corresponding to the π 1g9/2 ν 1g9/2 configuration, is positioned at 2.354 MeV, in rather good agreement with the experimental value of 1.980 MeV.

To validate further the predictions made and to get an insight into the structure of other possible states, we have also performed large-scale shell-model calculations using a realistic effective interaction as given by a G-matrix calculation [34] with the modified monopole part [64, 87]. The model space consists of the 1f5/2, 2p3/2, 2p1/2, 1g9/2 orbitals outside the 56Ni-core without any restrictions on their occupation.

The results of the diagonalization, performed with the shell-model code ANTOINE [96, 97], are also shown in figure 4.6 and are in rather good agreement with the experimental data. The calculations show more mixing between the different configurations; however, the main components of the lowest states can be clearly selected (see table 4.1). As follows from this table, the contribution of the proposed π 2p3/2 ν 1g9/2 configuration to the first 6−, 3−, 4− and 5− states is more than 52%, supporting the calculations using a more schematic force presented before. The second largest configuration is always π 2p3/2 ν (1f5/2 1g9/2) of about 18–20%. The contributions of other configurations do not exceed 6%.

The structure of the lowest 1+ and 2+ states is dominated by the proton particle-neutron hole π 2p3/2 ν (2p1/2 1g9/2) configuration, with the second largest component being given by the π 2p3/2 ν (1f5/2 2p1/2 1g9/2) configuration, as can be seen in table 4.1.

The calculated magnetic moments of the isomers are given in the last column of table 4.1 and are in very good agreement with the measured values [98].

The states belonging in the extreme single-particle shell model to the second negative parity multiplet, 2−− 7− from the π 1f5/2 ν 1g9/2 configuration, are predicted by the present realistic calculations to have more strongly mixed wave functions. The first 2−, 7− states and the second 3− − 6− states placed by the calculation at energies between 1275 keV (for the 2− state) and 1797 keV (for the 7− state) do not contain a single component contributing more than 18%.

The same is valid for the next excited 1+ states: all of them represent a complex mixture of many different pure configurations. Surprisingly, we do not find in the present calculation (at least within the 10 lowest 1+ states) the 1+ state with the dominant π 1g9/2 ν 1g9/2 configuration, experimentally seen at 1980.1 keV. The precise origin of this deficiency is not well understood as yet.

4.3 Proton Monopole Shift in Neutron-Rich Cu

In this section, we study the proton monopole shift in neutron-rich Cu-nuclei. The interest in neutron-rich nuclei around 68Ni and in particular the questioned magicity of 78Ni has recently motivated the global study of low-energy nuclear structure for both odd-A Cu nuclei [85] at the LISOL facility in Louvain-la-Neuve and odd-odd Cu-nuclei at ISOLDE, Cern [89, 90] up to very neutron-rich species. Figure 4.7 contains the selected states of odd-A Cu with spin and parity quantum numbers of the valence proton oscillator shell
Table 4.1: Structure of the lowest states in $^{70}$Cu as follows from the shell-model calculations with the realistic effective interaction [34]. The magnetic moments of the isomers calculated with the effective spin $g$-factors ($\langle g^{x y}_{\nu} \rangle_{\text{eff}} = 0.7 \langle g^{x y}_{\nu} \rangle_{\text{free}}$) are given in the last column.

<table>
<thead>
<tr>
<th>$I^\pi$</th>
<th>$E_{\text{exp}}$ (keV)</th>
<th>$E_{\text{th}}$ (keV)</th>
<th>configuration</th>
<th>(%)</th>
<th>$\mu_{\text{exp}}$ ($\mu_N$) [98]</th>
<th>$\mu_{\text{th}}$ ($\mu_N$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$6^-$</td>
<td>0</td>
<td>0</td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(59%)</td>
<td>(+)1.50(7)(8)</td>
<td>1.56</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(18%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$3^-$</td>
<td>101.1</td>
<td>87</td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(56%)</td>
<td>(-)3.50(7)(11)</td>
<td>-3.28</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(18%)</td>
<td></td>
<td></td>
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<tr>
<td>$4^-$</td>
<td>228.5</td>
<td>336</td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(52%)</td>
<td></td>
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<tr>
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<td></td>
<td></td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(18%)</td>
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<tr>
<td>$5^-$</td>
<td>506.6</td>
<td>582</td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(52%)</td>
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<tr>
<td></td>
<td></td>
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<td>(20%)</td>
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<td>1275</td>
<td>$\pi^1f_{5/2}2^1g_{9/2}$</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>$\pi^1f_{5/2}2^1g_{9/2}$</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
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<td></td>
<td></td>
<td>$\pi^1f_{5/2}2^1g_{9/2}$</td>
<td>(10%)</td>
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<tr>
<td>$1^+$</td>
<td>242.4</td>
<td>383</td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
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<td>(+)1.86(4)(6)</td>
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<tr>
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<td></td>
<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
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<tr>
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<td>317</td>
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<td>$\pi^2p_{3/2}2^1g_{9/2}$</td>
<td>(13%)</td>
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above \( Z = 28 \): \( 2p_{3/2}, 1f_{5/2}, 2p_{1/2}, 1g_{9/2} \). The ground state of odd-\( A \) Cu-nuclei up to \( ^{73}\text{Cu} \) is \( 3/2^- \) conform with the occupation of the \( 2p_{3/2} \) orbital. As seen from figure 4.7, the \( 5/2^- \) state starts to drop drastically in energy for nuclei with \( A > 69 \) and might be expected to become the ground state in heavy odd-\( A \) Cu.

### 4.3.1 Monopole Shift

For the description of the Cu-nuclei we have chosen the shell-model space consisting out of four valence orbitals: \( 2p_{3/2}, 1f_{5/2}, 2p_{1/2}, \) and \( 1g_{9/2} \), for both neutrons and protons, outside the \( ^{56}\text{Ni} \)-core (see figure 4.8). This model space contains all necessary degrees of freedom to describe low-energy nuclear structure.

Since we are interested in the variation of the proton single-particle energies, and the neutrons occupy several single-particle orbitals, we investigate the proton monopole shift, as defined in (2.39):

\[
\tilde{\epsilon}_j = \epsilon_j + \sum_{j'} \tilde{E}(\pi j) (2j + 1) v_{j'}^2.
\]

\( \tilde{E}(\pi j) \) is the average matrix element as defined in (2.8):

\[
\tilde{E}(\pi j) = \frac{\sum_J (2J+1) \langle j, j; J | V_{\pi \nu} | j, j; J \rangle}{\sum_J (2J+1)}.
\]

The neutron occupation probabilities \( v_{j'}^2 \) have been obtained by solving the BCS equations using a pairing Hamiltonian [29]:

\[
H = -G \sum_{j, j', m > 0, m' > 0} (-1)^{j+m} (-1)^{j'+m'} a_{j, m}^\dagger a_{j', -m'} a_{j', -m} a_{j, m}.
\]

The strength of the pairing interaction was chosen to reproduce the pairing gaps in neighboring even-even Ni-isotopes [80] resulting in a dependence \( G = 23/A \) MeV.
Figure 4.8: Experimental single-particle energy levels outside the $^{56}\text{Ni}^{28}$ core. On the left, the single-particle proton energies, obtained from the lowest states of $^{57}\text{Cu}^{28}$; on the right, the single-particle neutron energies, obtained from the lowest states of $^{57}\text{Ni}^{29}$. Data from \cite{99}.

In the present work we have restricted ourselves to two types of the effective interaction. First, we consider the $\delta$-interaction with the spin-exchange term \cite{29}:

$$V = -V_0(1 - \alpha + \alpha \vec{\sigma}_\pi \cdot \vec{\sigma}_\nu)\delta(\vec{r}_\pi - \vec{r}_\nu).$$ \hfill (4.6)

The two parameters, the overall strength $V_0$ and the strength $\alpha$ of the exchange term are to be adjusted to the experimental data in odd-odd nuclei from the mass region one is studying.

The geometrical properties of the zero-range interaction, even including spin-exchange contributions, allow to obtain a very simple analytical expression for the monopole shift:

$$\tilde{\epsilon}_{j_\pi} = \epsilon_{j_\pi} - V_0(1 - \alpha) \sum_{j_\nu} F^0_{n_\pi l_\pi n_\nu l_\nu} (2j_\nu + 1)\nu_{j_\nu}^2,$$ \hfill (4.7)

where $F^0_{n_\pi l_\pi n_\nu l_\nu}$ are Slater integrals. In order to derive this result, we had to make use of a peculiar property of the Wigner $3j$-symbols, as described in appendix B.

We stress the fact that since the average proton-neutron matrix element from the $\delta$-interaction entering (4.7) does not depend on $j_\pi$, the relative shift for spin-orbit partners (see e.g. the result for the $2p_{1/2}$ and $2p_{3/2}$ orbitals in figure 4.10(b)) stays constant and remains equal to the difference of the original single-particle energies ($\epsilon_{j_\pi} - \epsilon_{j'_\pi}$).

For the Cu-isotopes, we have determined the parameters of (4.6) to be $V_0 = 400$ MeV-fm$^3$ and $\alpha = 0.1$. These values suit the systematics known from the description of heavier isotopes \cite{100} and they result in two-body matrix elements of the same order as
those of the realistic interaction which will be described below. The chosen interaction also gives a reasonable, although slightly stretched, spectrum of $^{58}$Cu [101] (and see figure 4.9).

The second type of interaction used here is a realistic one, obtained from the $G$-matrix through a Brueckner-Hartree-Fock procedure [34] and modified further for a monopole correction [64, 87] following the recipe of [63] to account for the saturation properties. The interaction works very well in the description of Ni- and Cu-isotopes, reproducing many known spectroscopic properties [64].

In figures 4.10 and 4.11 we compare the experimental energy centroids (figure 4.10(a)) with the results of the calculations according to equation (4.3) with two types of the interaction (figures 4.10(b) and 4.10(c)).

Figure 4.10(b) contains the results obtained using the $\delta$-force. For $^{57}$Cu, the lowest states are given by the empirical values $\epsilon_{f_n}$. These values are modified by the two-body interaction. Effective single-proton energies for the $1f_{5/2}$ and $1g_{9/2}$ states first move up, when neutrons are filling the $pf$ orbitals, and then (from $^{69}$Cu) go down relative to the $2p_{3/2}$ state as the neutron $1g_{9/2}$ orbital starts to be filled. This is governed by the relative magnitude of the centroids of the interaction. In particular, the drastic lowering of the $1f_{5/2}$ and $1g_{9/2}$ orbitals stems from more attractive $E(1f_{5/2}1g_{9/2})$ and $E(1g_{9/2}2g_{9/2})$ values relative to $E(2p_{3/2}1g_{9/2})$. The energy of the $2p_{1/2}$ orbital stays unchanged with respect to the $2p_{3/2}$ ground state as has been mentioned before. At $A = 79$ we observe a crossing between the effective $2p_{1/2}$ and $1f_{5/2}$ states; however, the $\delta$-interaction does not reproduce the expected crossing of the effective $2p_{3/2}$ and $1f_{5/2}$ orbitals.

In figure 4.10(c), we present the results obtained with the realistic effective interaction described above. Only diagonal proton-neutron matrix elements contribute to the expression (4.3). Though the overall trend obtained from both types of the interaction remains the same, as follows from the similar character of the matrix elements, there are certain distinctions. First, the energy of the $2p_{1/2}$ orbital varies relative to the $2p_{3/2}$ ground state orbital (see figure 4.10(c)). Secondly, the proton $1f_{5/2}$ orbital decreases steeper as neutrons are added to the $1g_{9/2}$ orbital, and for $^{79}$Cu the inversion of the $1f_{5/2}$ and $2p_{3/2}$ orbitals is predicted, compared to the use of the $\delta$-interaction.

We point out that the lack of agreement between the variation of the effective $1g_{9/2}$ single-proton state and the experimental $9/2^+$ level is due to the fact that the single-particle strength of the $1g_{9/2}$ state lies higher up and the lowest state which is plotted in figure 4.10(a), due to the lack of experimental data, contains only a small fraction of that (see tables 4.2, 4.3, 4.4 and 4.5).

### 4.3.2 Large-Scale Shell-Model Calculations

In order to get an insight into additional correlations that cause a variation of the single-particle centroids of the proton $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ states beyond the monopole shift, we have carried out large-scale shell-model calculations using the same realistic effective interaction as described above. The model space consists of the $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, $1g_{9/2}$ orbitals outside the $^{56}$Ni-core, truncated in case of $^{67}$Cu, $^{63,65,68}$Cu and $^{71}$Cu (up to 3, 4 and 8 particles, respectively, were allowed to occupy the $1g_{9/2}$ orbital). The calculations were done using the shell-model code OXBASH [102]. The single-particle centroids for the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ states have been obtained by taking into
Figure 4.9: The spectrum of $^{58}\text{Cu}$ obtained from experiment and with various interactions. Only the levels below 2 MeV are shown. The left most panel represents the experimental spectrum [101]. The second panel shows the spectrum obtained with the realistic effective interaction [34]. The third panel represents the effect of the delta-interaction, with parameters $V_0 = 400 \text{ MeV-fm}^3$ and $\alpha = 0.1$. The last panel shows the quadrupole force with strength $\chi = -0.02 \text{ MeV}$. 
Figure 4.10: (a) Experimental centroids when data are available (see tables 4.2, 4.3, 4.4 and 4.5) or lowest states of a given spin and parity in odd-A Cu-isotopes. (b), (c) Theoretical evolution of the single-particle energies in odd-A Cu-isotopes due to the monopole part of (b) the proton-neutron δ-interaction and (c) realistic interaction \cite{34}, respectively. (d) Shell-model centroids derived from the exact diagonalization using the realistic interaction.

account up to about 400-800 excited states weighted with their spectroscopic factors (in order to exhaust the sum rule for $T_f = T_i - \frac{1}{2}$ transfer up to 98% or to get a reasonable saturation of the total value for truncated spaces), and they are shown in figure 4.10(d). The wave functions of the corresponding Ni-isotopes have been calculated without any restrictions of the model space.

The total spectroscopic strength in proton stripping reactions to the states with $T_f = T_i - \frac{1}{2}$ is given by the following sum rule \cite{25}:

$$C^2 \sum_f \frac{2J_f + 1}{2J_i + 1} S_f(nlj)$$

$$= \frac{T_i + T_{iz}}{2T_{iz}(2T_i + 1)} \left[ (T_i + T_{iz} + 1) \langle \tilde{n}_+ (j) \rangle_{j_i,j_i} - (T_i - T_{iz} + 1) \langle \tilde{n}_- (j) \rangle_{j_i,j_i} \right]. \quad (4.8)$$

$J_i, J_f$ are the spin and $T_i, T_f$ the isospin quantum numbers of the initial and final states.
Figure 4.11: (a), (b) The same as in (c) of figure 4.10, but implying normal filling of the neutron orbitals, without the BCS approach: (a) is normal filling, (b) inverse filling of the neutron $1f_{5/2}$ and $2p_{1/2}$ orbitals. The arrows in figure 4.10(b) below the plot indicate schematically the normal filling of the neutron single-particle orbitals in Cu-isotopes.

(as indicated in tables 4.2, 4.3, 4.4 and 4.5 where the average number of neutron holes in the ground state of the Ni-isotopes is taken from the shell-model diagonalization.

A remarkable result is that the centroids shown in figure 4.10(d) are rather close to those obtained by the analytical approach (4.3) as shown in figure 4.10(c). The wiggles in the behaviour of the shell-model $1g_{9/2}$ centroid in figure 4.10(d) for $^{65-69}$Cu are most probably related to the truncations of the model space which is otherwise too large to be treated numerically. The monopole energy shift incorporates the effects of a certain class of residual interactions (self-energy correction of the proton single-particle energy because of proton-neutron interactions and neutron pairing) on the bare proton single-particle energy within the model space, as expressed by equation (4.3).

A comparison of these results thus illuminates the question of what type of correlations is important in the calculation of the energy shifts beyond the monopole shift. A rather good agreement between the centroids of figures 4.10(c) and 4.10(d) confirms that the basic ingredients of the single-particle centroid variations are already taken into account by equation (4.3). This is a most interesting and valuable result.

To illustrate the importance of the pairing effects, we plot in figure 4.11(a) the effective single-proton energies obtained from the monopole Hamiltonian with normal filling of the single-particle orbitals by neutrons (the approach chosen in [26, 30, 63, 103, 104]). It is seen that through the occupation probabilities, the pairing force (figure 4.10(c)) smoothens significantly the single-particle behaviour. Figure 4.11(b) shows the same evo-
4.3 Proton Monopole Shift in Neutron-Rich Cu

Figure 4.12: The lowest $3/2^-, 5/2^-, 1/2^-$ and $9/2^+$ states in odd-$A$ Cu-isotopes. (a) experimental values; (b) as obtained from the shell-model diagonalization with the realistic interaction.

According to the results of figure 4.11(a), but with a different order of filling of neutrons orbitals (neutron $2p_{1/2}$ is filled before neutron $1f_{5/2}$). The behaviour of the proton single-particle orbitals does not have a zigzag structure in this case, but the maximum of the centroids is shifted to $^{68}\text{Cu}$, compared to the calculations with pairing effects (figures 4.10(b) and 4.10(c)). Let us note that physically the order of filling chosen in figure 4.11(a) is more realistic than that implied in figure 4.11(b), as follows from the experimental spectra of $^{67,69}\text{Ni}$ (neutron single-particle orbital $2p_{3/2}$ is higher than $1f_{5/2}$ in these nuclei).

Since the lowest-lying $J^\pi = 1/2^-, 3/2^-, 5/2^-$ and $9/2^+$ states represent only a fraction of the total proton single-particle strength, we compare the energies of the lowest $1/2^-, 3/2^-, 5/2^-$ and $9/2^+$ experimental states (figure 4.12(a)) and theoretical states obtained from the large-scale diagonalization (figure 4.12(b)). In general, we remark a very good agreement with the experimental data due to the quality of the effective interaction.

By comparing the results of figures 4.10(c), 4.10(d) and 4.12(b), it is clear that the correlations beyond the monopole approximation are necessary to understand the detailed fine structure of the energy variations for the lowest $1/2^-, 5/2^-$ and $9/2^+$ levels. This is particularly the case for the $1/2^-$ and $5/2^-$ levels where specific kinks, related to a possible shell closure at $N = 40$, are clearly seen in the diagonalization. The general trend of the $9/2^+$ level, as obtained from diagonalization, is quite different compared to the monopole shift. These effects are obviously a result of interactions of the pure single-particle configurations with many of the excited configurations with the same $J^\pi$ value.

4.3.3 Comparison with Experimental Centroids

Since we are interested in the variation of the proton single-particle energies, it is consistent to compare our theoretical results with the experimental centroids of the $2p_{3/2}, 1f_{5/2}$.
Figure 4.13: Proton-stripping spectroscopic factors into the lowest $3/2^-, 5/2^-, 1/2^-$, and $9/2^+$ states, respectively, in odd-$A$ Cu-isotopes, obtained from the shell-model diagonalization with the realistic interaction. The values are normalized to the shell-model sum rule.

$2p_{1/2}$ and $1g_{9/2}$ single-proton states, defined as:

$$E(nlj) = \frac{\sum_k S^k_{nlj} E^k_{J=j}}{\sum_k S^k_{nlj}},$$  \hspace{1cm} (4.10)

where $S^k_{nlj}$ are spectroscopic factors for a proton transfer (to the $(nlj)$ single-particle state), and $E^k_{J=j}$ is the experimental excitation energy of the $k$th state with $J = j$ (both $S^k_{nlj}$ and $E^k_{J=j}$ are taken from [99, 105, 106, 107, 108, 109] and [85]).

Unfortunately, the data on spectroscopic factors is rather scarce and differs significantly from one experiment to another. In tables 4.2, 4.3, 4.4 and 4.5, we summarize the available spectroscopic strength for the states of interest in $^{59}$Cu, $^{61}$Cu, $^{63}$Cu and $^{65}$Cu, respectively. The experimental centroids are plotted in figure 4.10(a). For those states (isotopes) for which no experimental data exists, only the lowest state of a given spin is indicated. As seen from the tables, the sum rule (for the transfer to both $T_f = T_i \pm \frac{1}{2}$ states) is far from being accomplished, especially for the $9/2^+$ states. Thus, one should be cautious with the trends of the experimental ‘centroids’ for this particular state.

Finally, in figure 4.13, we summarize the spectroscopic factors of the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ proton stripping from the $^{\text{A-1}}$Ni-core into the lowest-lying $1/2^-$, $3/2^-$, $5/2^-$ and $9/2^+$ states of $^{\text{A}}$Cu, respectively, as provided by the shell-model diagonalization.

The spectroscopic factors have been normalized to the sum rule presented in equation 4.9. The absolute spectroscopic factors for the lowest states of a given spin are shown in table 4.2, 4.3, 4.4 and 4.5 in comparison with the available experimental data on $^{59-65}$Cu. The calculated spectroscopic factors are in rather good agreement for the lowest $3/2^-$ and $1/2^-$ states (within 20%); however, the disagreement increases for the $5/2^-$ and $9/2^+$ states in these isotopes. It is not clear, at present, what the origin of these
Table 4.2: Available experimental data on spectroscopic factors of the lowest $3/2^-$, $5/2^-$, $1/2^-$ and $9/2^+$ states in $^{59}$Cu (taken from Ni(d,n) or Ni($^3$He,d) proton-stripping reaction studies [99, 105, 106, 107, 108, 109]). The sum rule refers to the proton transfer to both, $T_f = T_i \pm \frac{1}{2}$ states, while the shell-model sum rule is given for the states with $T_f = T_i - \frac{1}{2}$ only. The calculated spectroscopic factors for the lowest states of a given spin are indicated as well. The energies $E_{\text{exp}}$, absolute experimental centroids and relative experimental centroids are in MeV.

<table>
<thead>
<tr>
<th>$^I^E_{\text{exp}}$</th>
<th>$C^2S(2J + 1)$ (exp)</th>
<th>$C^2S(2J + 1)$ total (exp)</th>
<th>sum rule (shell model)</th>
<th>sum rule (shell model) absolute (exp)</th>
<th>centroid absolute (exp)</th>
<th>centroid relative (exp)</th>
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<td>$\frac{9}{2}^+$</td>
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<td>4.31</td>
<td>6.724</td>
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Table 4.3: Available experimental data on spectroscopic factors of the lowest $3/2^-, 5/2^-, 1/2^-$ and $9/2^+$ states in $^{61}\text{Cu}$ (taken from Ni(d,n) or Ni($^3\text{He,d}$) proton-stripping reaction studies [99, 105, 106, 107, 108, 109]). The sum rule refers to the proton transfer to both, $T_f = T_i + \frac{1}{2}$ states, while the shell-model sum rule is given for the states with $T_f = T_i - \frac{1}{2}$ only. The calculated spectroscopic factors for the lowest states of a given spin are indicated as well. The energies $E_{\text{exp}}$, absolute experimental centroids and relative experimental centroids are in MeV.

<table>
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<th>$I^\pi$</th>
<th>$E_{\text{exp}}$</th>
<th>$C^2S(2J + 1)$</th>
<th>$C^2S(2J + 1)$</th>
<th>sum rule</th>
<th>$C^2S(2J + 1)$</th>
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<td>(shell model)</td>
<td>(exp)</td>
<td>absolute</td>
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<td>0.06</td>
<td>0.008</td>
<td>1.668</td>
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<td>0.96</td>
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<td>2.721</td>
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<td>4.04</td>
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<td>2.94</td>
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Table 4.4: Available experimental data on spectroscopic factors of the lowest $3/2^-$, $5/2^-$, $1/2^-$ and $9/2^+$ states in $^{63}$Cu (taken from Ni(d,n) or Ni($^3$He,d) proton-stripping reaction studies [99, 105, 106, 107, 108, 109]). The sum rule refers to the proton transfer to both, $T_f = T_i \pm \frac{1}{2}$ states, while the shell-model sum rule is given for the states with $T_f = T_i - \frac{1}{2}$ only. The calculated spectroscopic factors for the lowest states of a given spin are indicated as well. The energies $E_{\text{exp}}$, absolute experimental centroids and relative experimental centroids are in MeV.

<table>
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<tr>
<th>$I^\pi$</th>
<th>$E_{\text{exp}}$</th>
<th>$C^2 S(2J + 1)$ (exp)</th>
<th>$C^2 S(2J + 1)$ total (exp)</th>
<th>sum rule (shell model)</th>
<th>sum rule (shell model)</th>
<th>centroid absolute (exp)</th>
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<td>$\frac{5}{2}^-$</td>
<td>0.962</td>
<td>1.92</td>
<td></td>
<td></td>
<td>0.40</td>
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<td></td>
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<tr>
<td></td>
<td>1.412</td>
<td>2.70</td>
<td></td>
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<td>1.56</td>
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<tr>
<td></td>
<td>2.337</td>
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<td></td>
<td></td>
<td>0.78</td>
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<tr>
<td></td>
<td>3.225</td>
<td>0.30</td>
<td>5.4</td>
<td>6</td>
<td>5.489</td>
<td>1.226</td>
<td>1.435</td>
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<tr>
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<td>0.90</td>
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<tr>
<td></td>
<td>2.062</td>
<td>0.29</td>
<td>1.67</td>
<td>2</td>
<td>1.800</td>
<td>0.912</td>
<td>0.703</td>
</tr>
<tr>
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<td></td>
<td></td>
<td>3.24</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.970</td>
<td>0.51</td>
<td>5.81</td>
<td>10</td>
<td>8.648</td>
<td>2.635</td>
<td>2.425</td>
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</table>
Table 4.5: Available experimental data on spectroscopic factors of the lowest $3/2^-, 5/2^-, 1/2^-$ and $9/2^+$ states in $^{65}\text{Cu}$ (taken from Ni(d,n) or Ni($^3\text{He,d}$) proton-stripping reaction studies [99, 105, 106, 107, 108, 109]). The sum rule refers to the proton transfer to both, $T_f = T_i \pm \frac{1}{2}$ states, while the shell-model sum rule is given for the states with $T_f = T_i - \frac{1}{2}$ only. The calculated spectroscopic factors for the lowest states of a given spin are indicated as well. The energies $E_{\text{exp}}$, absolute experimental centroids and relative experimental centroids are in MeV.

<table>
<thead>
<tr>
<th>$I^\pi$</th>
<th>$E_{\text{exp}}$</th>
<th>$C^2S(2J + 1)$ (exp)</th>
<th>$C^2S(2J + 1)$ total (exp)</th>
<th>sum rule (shell model)</th>
<th>sum rule (shell model)</th>
<th>centroid absolute (exp)</th>
<th>centroid relative (exp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{65}\text{Cu}$</td>
<td>$\frac{3}{2}^-$</td>
<td>0</td>
<td>3.08</td>
<td>2.92</td>
<td>0.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.725</td>
<td>0.06</td>
<td>3.38</td>
<td>4</td>
<td>3.898</td>
<td>0.196</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>2.329</td>
<td>0.24</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\frac{5}{2}^-$</td>
<td>1.113</td>
<td>1.14</td>
<td>2.40</td>
<td>2.13</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.623</td>
<td>0.36</td>
<td>3.9</td>
<td>6</td>
<td>5.694</td>
<td>1.519</td>
<td>1.323</td>
</tr>
<tr>
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<td>0.770</td>
<td>1.30</td>
<td>1.64</td>
<td>2</td>
<td>1.01</td>
<td>1.883</td>
<td>1.069</td>
</tr>
<tr>
<td>$\frac{9}{2}^+$</td>
<td>2.526</td>
<td>3.80</td>
<td>3.80</td>
<td>10</td>
<td>0.76</td>
<td>8.970</td>
<td>2.526</td>
</tr>
</tbody>
</table>
differences is. It may be due to a lack of experimental data, but it may also point out certain deficiencies in the realistic interaction presently used. As for the whole series of Cu-isotopes, the calculations show in figure 4.13 that only the $3/2^-$ ground state remains more or less a pure single-particle state. The lowest $1/2^-$ state is predicted to carry about half of the $2p_{1/2}$ single-particle strength. The lowest $5/2^-$ state shows much more mixing for $^{61-69}$Cu. This is in line with experimental observations of a few $5/2^-$ states in these isotopes even at low energies. Finally, the $9/2^+$ state is predicted to be a rather pure single-particle $1g_{9/2}$ state only for light isotopes. Starting from $^{67}$Cu, the single-proton strength almost vanishes. In order to test these predictions, more precise data on spectroscopic factors and level spin and parity assignments would be very helpful.

### 4.3.4 Conclusion

In conclusion, it becomes clear that using both simple effective and realistic forces in order to derive the corresponding monopole energy shifts, the experimental proton single-particle centroids are, at present, only moderately described. This comparison is hampered by the lack of reliable and extensive experimental results on one-nucleon transfer reactions.

An interesting point is a reproduction of a lowering in the $1f_{5/2}$ energy centroid, once the $N = 40$ neutron number is passed, in particular using realistic forces. We also remark that correlations that define the monopole energy shift, as defined in equation (4.3), are consistent with the theoretical single-particle energy centroid resulting from a diagonalization of the full energy matrix, encompassing all possible residual interactions within the large model space. This result is an interesting one and has to be studied in other mass regions too. Although the energies obtained from the diagonalization in the large model space and corresponding to the lowest state of each spin and parity, follow the corresponding experimental energies rather well and exhibit interesting fine structure, the theoretical centroid, using a significant number of the eigenstates, becomes rather smooth again. At the same time, more experimental data on the structure of nuclei from the mass region would serve as a good testing ground for the present results and the interactions used.

### 4.4 Spectroscopy of $^{70-78}$Cu

#### 4.4.1 Residual Interactions and Shell-Model Study of Energy Levels in Odd-Odd Cu-Isotopes

In principle, the odd-odd nuclei $^{70-78}$Cu can be described within the context of large-scale shell-model calculations. The starting point for such a calculation would be the $^{56}$Ni$_{28}$ core, with the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ orbitals as the valence space for both protons and neutrons. However, since we concentrate on this particular set of five Cu-nuclei, in which the filling of the neutron $1g_{9/2}$ orbital is playing an essential role, we consider these nuclei as consisting out of a doubly-magic $^{68}$Ni$_{40}$-core coupled with the respective valence nucleons. This implies that there is only one valence proton, and one to nine valence neutrons. The model space for the proton consists out of the orbitals $2p_{3/2}$,
Table 4.6: Energies of the proton single-particle states in $^{69}$Cu, regarded as a $^{68}$Ni-core coupled with one valence proton.

<table>
<thead>
<tr>
<th>$\pi$ single-particle state</th>
<th>$\epsilon_{js}$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1g_{9/2}$</td>
<td>2.553</td>
</tr>
<tr>
<td>$1f_{5/2}$</td>
<td>1.214</td>
</tr>
<tr>
<td>$2p_{1/2}$</td>
<td>1.110</td>
</tr>
<tr>
<td>$2p_{3/2}$</td>
<td>0.000</td>
</tr>
</tbody>
</table>

The energy levels in the schematic approach are obtained in the following way. The proton single-particle energies have to be corrected for the monopole shift [110]: when the neutrons start filling the $1g_{9/2}$ single-particle level, the relative proton single-particle energies change because of the larger radial overlap between the proton $1f_{5/2}$ – neutron $1g_{9/2}$ orbitals compared to the proton $2p_{3/2}$ and $2p_{1/2}$ – neutron $1g_{9/2}$ overlap. These corrected single-proton energies $\tilde{\epsilon}_{js}$ are expressed as:

$$\tilde{\epsilon}_{js} = \epsilon_{js} + 10n_{1g_{9/2}} \tilde{E}(j_\pi 1g_{9/2}),$$

(4.11) with $\tilde{E}(j_\pi 1g_{9/2})$ defined as:

$$\tilde{E}(j_\pi 1g_{9/2}) = \frac{\sum_j \langle j_\pi 1g_{9/2}, J | V | j_\pi 1g_{9/2}, J \rangle (2J + 1)}{\sum_j (2J + 1)},$$

(4.12) describing the average matrix element of the proton-neutron interaction, and $n_{1g_{9/2}}$:

$$n_{1g_{9/2}} = \frac{N - 40}{10},$$

(4.13) is the occupation probability of the $\nu 1g_{9/2}$ single-particle level. This change in single-proton energy is illustrated in figure 4.14. The $1f_{5/2}$ orbital comes down in energy relative to the $2p_{1/2}$ and $2p_{3/2}$ orbitals. If one uses a residual quadrupole-quadrupole force, the monopole shifts become trivially zero. In order to improve the ‘realistic’ character of the schematic study using the residual quadrupole-quadrupole interaction, the monopole energy shifts obtained with the delta-interaction are used.

The filling of the neutron $1g_{9/2}$ orbital can, to a good approximation, be described by means of a one-quasi-particle excitation with energy $E_{1g_{9/2}}$ [28].

Besides the neutron one-quasi-particle energy and proton single-particle energies, we also need the two-body matrix elements coupling the proton orbital $j_\pi$ with the filling neutron $1g_{9/2}$ orbital to compute the energy levels. The filling of the neutron $1g_{9/2}$ orbital is approximated by a neutron one quasi-particle configuration (indicated by the tilde, hence: $1g_{9/2}$). These matrix elements can be expressed as:

$$\langle j_\pi 1g_{9/2}, J | V | j_\pi 1g_{9/2}, J \rangle = (1 - n_{1g_{9/2}}) \langle j_\pi 1g_{9/2}, J | V | j_\pi 1g_{9/2}, J \rangle + n_{1g_{9/2}} \langle j_\pi 1g_{9/2}^{-1}, J | V | j_\pi 1g_{9/2}^{-1}, J \rangle.$$

(4.14)
This is a linear combination of particle-particle and particle-hole matrix elements, and as such, particularly sensitive to the filling of the neutron orbital. So the interaction changes from a pure particle-particle interaction in $^{70}\text{Cu}$ to a pure particle-hole interaction in $^{78}\text{Cu}$.

The energy of a particular configuration with a proton moving in the orbital $j_\pi$ and the neutrons filling the $1g_9/2$ orbital is then expressed as:

$$E_{1g_9/2} + \tilde{\varepsilon}_{j_\pi} + \langle j_\pi|\tilde{1}g_9/2, J|V_{\delta/QQ}|j_\pi, \tilde{1}g_9/2, J \rangle.$$ (4.15)

In the present study, we focus on the proton $2p_3/2$ and $1f_5/2$ coupled to the neutron orbital $1g_9/2$. This gives rise to a multiplet with spin and parity of $3^-, 4^-, 5^-, 6^-$ and $2^-, 3^-, 4^-, 5^-, 6^-, 7^-$, respectively. Including also the non-diagonal matrix elements and diagonalizing the small matrices, one obtains the final energy spectrum. We investigate the evolution of the energy levels as a function of neutron number and discuss the results in the next subsection. In this highly truncated model space we study the effect of the two different schematic interactions between the valence proton and the valence neutrons.

First, we consider the effect of a quadrupole-quadrupole proton-neutron interaction, defined as:

$$V_{QQ} = \chi \left( \sqrt{\frac{m \omega}{\hbar}} r_\pi \right)^2 \left( \sqrt{\frac{m \omega}{\hbar}} r_\nu \right)^2 \tilde{Y}_2(\Omega_\pi) \cdot \tilde{Y}_2(\Omega_\nu),$$ (4.16)

where the strength $\chi$ is given by $\chi = -0.02$ MeV. The strength has been obtained by fitting the theoretical $2p_3/2 \nu 1g_9/2$ multiplet splitting to the experimental splitting in the lowest-lying levels in $^{70}\text{Cu}$. This strength then fixes the structure of other proton-neutron multiplets and also their relative variation as a function of neutron number.

Secondly, we study the effect of a zero-range interaction with spin exchange, where the interaction has the following form:

$$V_\delta = -V_0 (1 - \alpha + \alpha \vec{\sigma}_\pi \cdot \vec{\sigma}_\nu) \delta(\vec{r}_\pi - \vec{r}_\nu),$$ (4.17)
with \( V_0 \) the strength of the interaction, equal to \( V_0 = 400 \text{ MeV} \cdot \text{fm}^3 \). The amount of spin exchange is determined by the parameter \( \alpha \), which can vary from 0 to 1, and equals \( \alpha = 0.1 \) in the present calculations.

Finally, a large-scale shell-model calculation was performed using the realistic force determined by Hjorth-Jensen and co-workers \[34\], with the ANTOINE code \[96, 97\]. Naturally, we no longer use a highly-restricted model space but a larger one: the \( 2p_{3/2}, 2p_{1/2}, 1f_{5/2}, 1g_{9/2} \) orbitals, for both protons and neutrons. The input values for the neutron and proton single-particle energies differ from the ones we used in the schematic study: now we use the single-particle energies of one neutron or one proton coupled to a \( ^{56}_{28}\text{Ni}_{28} \)-core.

### 4.4.2 Discussion and Comparison With the Energy Spectra of Odd-Odd Cu-Isotopes

In the upper part of figure \[4.15\], we consider the multiplets \( \pi 2p_{3/2} \nu 1g_{9/2} \) (a) and \( \pi 1f_{5/2} \nu 1g_{9/2} \) (b) in an independent way (no mixing) for the QQ-interaction. A clear dependence on the neutron number \( N \), hence the occupation probability \( n_{1g_{9/2}} \), results, which is of course very much like the behaviour encountered when applying Paar’s parabolic rule \[93\]. One notices the switching of the multiplet ordering in each multiplet with respect to the \( N = 45 \) mid-shell situation from a particle-particle into a particle-hole energy spectrum. For the lowest levels, originating from the \( \pi 2p_{3/2} \nu 1g_{9/2} \) multiplet, this implies a change of the \( 3^– \) and \( 6^– \) levels into the \( 5^– \) and \( 4^– \) levels as lowest-lying levels, which seems consistent with the experimental changes in possible ground-state spins. In constructing the energy splitting in the second multiplet \( \pi 1f_{5/2} \nu 1g_{9/2} \), the relative energy spacing between the \( \pi 1f_{5/2} \) and \( \pi 2p_{3/2} \) orbitals as well as the monopole variation in this \( \pi 1f_{5/2} \) level, compared to the reference value of 1.214 MeV (the dashed line in figure \[4.15\]) in \(^{70}\text{Cu}\), has been included for the various neutron numbers.

In the same figure \[4.15\], we compare the above results using the QQ-interaction with the results of the \( \delta \)-interaction ((c) and (d)). The results are rather similar, but the symmetry with respect to the \( N = 45 \) mid-shell point does no longer hold (because the particle-particle and particle-hole matrix elements are no longer related by a simple change in sign). Moreover, the ordering in the lowest multiplet \( \pi 2p_{3/2} \nu 1g_{9/2} \) now gives the correct result when compared with the experimental energy spectrum observed in \(^{70}\text{Cu}\). This is probably due to the more ‘realistic’ properties of the zero-range character of the \( \delta \)-interaction when comparing, e.g. the two-body matrix elements with those of the realistic interaction of \[34\].

In a next step, we go beyond lowest order and we explicitly consider the coupling between the multiplets \( \pi 2p_{3/2} \nu 1g_{9/2}, \pi 1f_{5/2} \nu 1g_{9/2} \) and \( \pi 2p_{1/2} \nu 1g_{9/2} \). The results, derived by diagonalizing the small energy matrices, are presented in figure \[4.16\], for both (a) the quadrupole-quadrupole and (b) \( \delta \)-interaction. The results become slightly more realistic but no major changes show up in the spectrum, compared to the results derived from the independent multiplets only. The general outcome remains the turning over of the multiplet ordering going from a specific particle-particle character (at \( N = 41 \)) towards the reversed ordering corresponding with the particle-hole character (at \( N = 49 \)).

A comparison is also made with the results obtained using the realistic interaction determined by \[34\] (using the shell-model code ANTOINE \[96, 97\]). The resulting energy
4.4 Spectroscopy of $^{70-78}$Cu

Figure 4.15: Independent $\pi 2p_{3/2} - \nu 1g_{9/2}$ and $\pi 1f_{5/2} - \nu 1g_{9/2}$ multiplets, using a quadrupole interaction ((a) and (b), respectively) and a $\delta$-interaction ((c) and (d), respectively). The dashed line indicates the 1.214 MeV $\pi 1f_{5/2}$ level of $^{70}\text{Cu}$.

One notices that the relative ordering of the $3^{-}$ and $6^{-}$ levels is reversed compared to the experimental situation in $^{70}\text{Cu}$ for both schematic interactions. For the $\delta$-interaction, the energy difference becomes tiny, whereas the realistic force correctly describes the experimental ordering. For the position of the experimental $2^{-}$ state (again in $^{70}\text{Cu}$), the specific $J$-dependence in the two-body matrix elements using a $\delta$-interaction seems to account much better for this result, compared to the QQ-interaction. Here, the realistic force predicts the $2^{-}$ level too high in excitation energy. This clear deviation seems to be related to much stronger configuration mixing present in the wave function for the lowest $2^{-}$ and $7^{-}$ states (the $\pi 1f_{5/2} - \nu 1g_{9/2}$ component is not the dominant one) and to the specific character of the interaction derived in [34].

From the three calculations, it is clear that the first $5^{-}$ state comes down in excitation energy as the neutron number increases and even becomes the ground state in $^{78}\text{Cu}$ (in close agreement with the indications from the present experiments). The second $4^{-}$ state has come down very much, as well as as the second $5^{-}$ state. It is rather remarkable that the lowest energy states in $^{78}\text{Cu}$ are the ones with relatively high spin, but this comes from the change of particle-particle to particle-hole behaviour.

When we compare the level structure in figure 4.16 with the levels suggested by the experiment, we remark that in general the theoretical results predict low-lying levels with
4 Copper Isotopes

Figure 4.16: Mixing of the $\pi 2p_{3/2} l^2 \bar{g}_{9/2}$, $\pi 1f_{5/2} l^2 \bar{g}_{9/2}$ and $\pi 2p_{1/2} l^2 \bar{g}_{9/2}$ multiplets, using (a) the quadrupole-quadrupole interaction and (b) the $\delta$-interaction, compared to the results (c) obtained from the large-scale diagonalizations using the realistic interaction \cite{34}.
higher spins than the experiment would suggest.

There is at present very little information about the ground-state spin and parity values for the isotopes lying in between, $^{72}$Cu, $^{74}$Cu and $^{76}$Cu: the theoretical calculations suggest ground states that (in the light of the accuracies in the above theoretical descriptions) might be consistent with an overall value of $3^{-}$. This would not be inconsistent with the present assignments of (1-3) in $^{72}$Cu, (2,3) in $^{74}$Cu and (3,4) in $^{76}$Cu, but more detailed experimental studies of these odd-odd Cu nuclei are needed in order to learn about the characteristics of the proton-neutron interaction, as well as of the monopole shifts in this particular region of the nuclear chart.
5 Bismuth Isotopes

5.1 Introduction

It has been known that the shell structure of nuclei with a very large proton or neutron excess differs considerably from the one of nuclei near stability [8]. One of the major contributions to the single-particle energies comes from the proton-neutron interaction, in particular for medium-heavy (Cu, Sb) and heavy nuclei as has been recognized [22, 23, 24].

Within a shell-model approach, the description of the nuclear mean field is obtained from the monopole part of the nuclear Hamiltonian [26, 30, 63, 70] (see chapter 2). The eigenvalues of the monopole part of the Hamiltonian were shown to provide the effective single-particle energies [26] and should reproduce the experimentally observed single-particle (hole) energies for both protons and neutrons in nuclei adjacent to a closed-shell configuration.

In this respect, the Pb-region forms a particularly interesting region to study the monopole energy shifts, since the starting proton and neutron single-particle energies are very well known from the nuclei surrounding $^{208}$Pb, i.e. $^{207}$Tl, $^{207}$Pb, $^{209}$Bi and $^{209}$Pb (see [111] and references therein) (see figure 5.1).

Moving away from the $Z = 82, N = 126$ configuration, much less experimental information on the particular variation of these single-particle energies is known.

In this chapter, we aim to study the single-particle variation (monopole shift) for the odd-mass Bi-nuclei with changing neutron number, using the method discussed in chapter 2 and applied in chapter 4 to study the odd-mass Cu-nuclei. The experimental information concerning the odd-mass Bi-nuclei, and in particular the variation of the lowest-lying configuration with spin-parity $J^\pi$ corresponding to the proton single-particle configurations $1h_9/2$, $2f_{7/2}$ and $1i_{13/2}$ is rather limited, and is given in figure 5.2.

We shall make use of the effective interaction of Kuo-Herling [112, 113]. The starting point of Kuo and Herling was the bare nucleon-nucleon Hamada-Johnston potential, applied to the $^{208}$Pb mass region. This effective interaction was later modified by Warburton and Brown [114], and was shown to give particularly good agreement with experimental data known at that time. It describes the structure of the odd-odd $^{210}$Bi-nucleus very well [114]. More recently, Caurier et al. [115] used this particular effective interaction to study the $N = 126$ configuration for the Po-Pu region, still adjusting slightly the monopole two-body matrix elements for the $\pi 1h_9/2 \pi 1i_{13/2}$ configuration. This configuration is important when dealing with the high-spin structure in these nuclei.

Besides the use of the realistic effective Kuo-Herling interaction, we also study the energy shifts originating from schematic interactions, in order to appreciate the effect
Figure 5.1: Experimental single-particle energies near the $Z = 82, N = 126$ shell closures. The data are obtained from $^{209}$Pb, $^{207}$Pb, $^{209}$Bi and $^{207}$Tl. Energies are in keV, relative to the closed shells. Figure taken from [111].
5.2 Spectroscopy of $^{210}$Bi

5.2.1 The Shell-Model Space

Since the odd-mass Bi-nuclei are described as the doubly-magic $^{208}$Pb-core with one extra proton and a varying number of neutron valence particles ($N > 126$) or holes ($N < 126$), our starting point will be the single-particle energies taken from the data given in figure 5.1. The method to determine the monopole energy shift, caused by the effective proton-neutron interaction, as a function of changing neutron number $N$, has been described in the previous chapters. Hereby, the filling of the neutron orbitals is not treated in a naive way, but pairing correlations to the lowest order have been included.

The shell-model space that is used, follows from the data on nuclei around the doubly-magic $^{208}$Pb-core. The energies of the proton and neutron single-particle orbitals are given in figure 5.1. In view of the experimental information (see figure 5.1), we study in particular the proton in the $\pi 1h_{9/2}$, $\pi 2f_{7/2}$ and $\pi 1i_{13/2}$ orbitals. For the neutrons filling the orbitals above $N = 126$, we consider the full $\nu 2g_{9/2}$, $\nu 1i_{11/2}$, $\nu 1j_{15/2}$, $\nu 3d_{5/2}$, $\nu 4s_{1/2}$, $\nu 2g_{7/2}$, $\nu 3d_{3/2}$ space. The neutron holes can occupy the orbitals $\nu 3p_{1/2}$, $\nu 2f_{5/2}$, $\nu 3p_{3/2}$, $\nu 1i_{13/2}$, $\nu 2f_{7/2}$ and $\nu 1h_{9/2}$, respectively.

In principle, this large model space should allow us to determine the monopole shift up to the extreme neutron-rich and neutron-deficient Bi-isotopes. Since in the very neutron-deficient Bi-nuclei, approaching the neutron mid-shell region at $N = 104$, deformation effects start playing an important role [116], we do not progress beyond $N = 116$. Combined with the lack of experimental data on the heavier Bi-isotopes, we limit our approach to the $^{199-219}$Bi-isotopes ($N = 116 - 136$).

Figure 5.2: Experimental lowest states with spin-parity $J^\pi$ corresponding to the proton single-particle configurations $1h_{9/2}$, $2f_{7/2}$ and $1i_{13/2}$. The data on $^{213}$Bi and $^{215}$Bi are taken from [111] and references therein, the other data are extracted from [99].

of particular force components that are implicitly present within the realistic effective interaction. We also present calculations on the variations in the energy spectra for the odd-odd Bi-nuclei including the calculated monopole shifts.
In order to evaluate the proton monopole shift as expressed in equation (2.39), we need the occupation probabilities $v_j^2$ for the neutron orbitals in the appropriate model spaces ($N > 126$, $N < 126$). Since we do not aim at studying a full Hartree-Fock plus BCS approach, we can obtain a rather good approximation to the $v_j^2$ values by using the constant pairing force defined in expression (2.20) of chapter 2. The pairing strength $G$ has been obtained by fitting the theoretical pairing gap to the experimental pairing gap, and is equal to $G = 30/A$ MeV [117]. The occupation probabilities are obtained by solving the BCS equations for this pairing force.

5.2.2 Effective Proton-Neutron Interactions

A crucial part in calculating the monopole shift is to obtain a proton-neutron interaction that reproduces as well as possible the odd-odd spectrum in $^{210}$Bi, with $^{210}$Bi containing just a single proton and a single neutron moving outside the doubly-closed shell nucleus $^{208}$Pb. This imposes important constraints on any proton-neutron interaction.

Here, we make use of the effective two-body interaction of Kuo and Herling [112, 113], modified by Warburton and Brown [114]. This force has been shown to provide an excellent description for the $A = 210 - 212$ nuclei [114]. We have included a mass dependence in the two-body matrix elements of the realistic effective interaction through the factor $(A_0/A)^{1/3}$, with $A$ being the mass of the nucleus under study, and $A_0 = 208$ the mass of the core nucleus $^{208}$Pb.

We also study the monopole energy shift using some schematic forces such as a zero-range (delta) and finite-range (central) interaction (with spin-exchange). The quadrupole-quadrupole proton-neutron force, known to not produce any monopole energy shift [100], is used to study the energy spectrum of the odd-odd Bi-isotopes.

Since we are dealing with schematic two-body forces, their parameters have been fitted to the $^{210}$Bi-nucleus: it can be considered as a two-body system, consisting out of a proton and a neutron outside the closed $^{208}$Pb core. Figure 5.3 gives the experimental results for the lowest $J^e = 0^- - 9^-$ multiplet of $^{210}$Bi [99], along with the results obtained for the $\delta$-interaction. This multiplet corresponds to the proton in the $\pi h_{9/2}$ orbital and the neutron in the $\nu 2g_{9/2}$ orbital, outside the $^{208}$Pb-core. The parameters of the various schematic interactions have been obtained in such a way as to obtain the best possible agreement with the experimental level splitting of the $0^- - 9^-$ multiplet of $^{210}$Bi, in particular with the $8^-$ level at 0.583 MeV. The realistic interaction reproduces the spectrum very well.

The schematic interactions used in this chapter have been discussed extensively in chapter 3, and we will only list their parameters here:

- a $\delta$-interaction including spin-exchange (see expression (3.35) in chapter 3), with strength $V_0$ and spin-exchange parameter $\alpha$ fitted to the lowest experimental $0^- - 9^-$ multiplet of $^{210}$Bi. We found that a strength $V_0 = 444$ MeV-fm$^3$ and $\alpha = 0.1$ give the best agreement.

- a quadrupole-quadrupole interaction (see expression (3.36)) with strength $\chi$ has been fitted in the same way as for the delta-interaction, and a value of $\chi = -0.003$ MeV gives the best agreement with the experimental lowest $0^- - 9^-$ multiplet of $^{210}$Bi. We decided not to go beyond the third decimal in $\chi$ in our fit, since the
Figure 5.3: Lowest $0^- - 9^-$ multiplet for $^{210}$Bi. The left-most column represents the experimental data from [111] and references therein; the second column gives the result for the modified interaction of Kuo and Herling [114]; the third column gives the multiplet splitting obtained from the $\delta$-interaction with spin-exchange, and the last column the splitting obtained with the QQ-interaction.
energy difference between the experimental $8^-$ level and the $8^-$ level obtained by
the QQ-force is very small. The QQ-force does not produce a monopole shift [100],
but it will be used to study the evolution of the lowest states in odd-odd Bi-isotopes
in section 5.4.

- a central interaction with finite range (see expression (3.10)) has been chosen to
study the evolution of the proton single-particle energy levels. We do not use the
full expression (3.10) of the central force, but we limit ourselves to the following
two terms:

\[ V_C(1, 2) = V_0(r) + V_{\sigma r}(r) \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2. \]  

(5.1)

The strengths $V_0$ and $V_{\sigma r}$ are arbitrarily set to $V_0 = V_{\sigma r} = 10$ MeV each. Also, the
two-body matrix elements are mass-dependent through the factor $(A_0/A)^{1/3}$, as we
did for the realistic effective interaction.

Ideally, all four terms of the central force (3.10) would be incorporated in a fit to
the experimental spectrum of $^{210}$Bi, as well as the two-body tensor force (3.27)
and the two-body spin-orbit force (3.29). Here, we are interested in the effect that
one particular part of the central force has on the evolution of the single-particle
energy levels. It is of course entirely possible to obtain a good value for the strength
parameters by fitting them to the experimental spectrum of $^{210}$Bi, but no single force
component would ever be used to study the spectroscopic properties of a nucleus.
As such, the values for the strength parameters of the central force listed here are not
intended to result in the best possible reproduction of the experimental spectrum of
$^{210}$Bi, but rather to give a quantitative idea of the evolution of the neutron monopole
shift.

### 5.3 Proton Monopole Shift in Odd Bi-Isotopes

Since the Bi-isotopes have only one proton outside the doubly-magic $^{208}$Pb-core, the lowest
states having spin and parity $J^\pi = 9/2^-, 7/2^-$ and $13/2^+$ contain to a large extent the
single-proton configurations $1h_9/2$, $2f_7/2$ and $1i_{13/2}$, respectively. In order to com-
pare the calculated monopole shifts ($\epsilon_j$) for these three proton orbitals with the energy
centroids for these configurations, we need information about spectroscopic factors. Un-
fortunately there is not enough (consistent) data available on the $^{199–209}$Bi isotopes [99].
Hence, we compare the monopole shift with the experimental lowest-lying energy lev-
els. In figure 5.4(a) we show the lowest-lying experimental energy levels with spin-parity
corresponding to the proton single-particle orbitals $1h_9/2$, $2f_7/2$ and $1i_{13/2}$.

The monopole energy shifts for the proton $1h_9/2$, $2f_7/2$ and $1i_{13/2}$ single-particle orbitals,
as a function of changing neutron number $N$, are compared for various interactions
in figure 5.4. In figure 5.4(b) and 5.4(c), the results for the Kuo-Herling and $\delta$-interaction
(including spin-exchange), respectively, are given. The correspondence between these
two forces is remarkable, even though the specific proton-neutron two-body matrix el-
ments show some clear differences (as illustrated in the energy spectrum of $^{210}$Bi in
figure 5.3), in particular for the low spin values. Because of the small weight $(2J + 1)$ of
the low-spin states when averaging the two-body matrix elements (see expression (2.8)),
there is no substantial difference between the monopole energy shifts calculated using the
Figure 5.4: Proton monopole shift: comparison with (a) the experimental lowest states (data on $^{213}$Bi and $^{215}$Bi from [111] and references therein, other data from [99]), and the contributions from various interactions: (b) realistic interaction, (c) $\delta$-interaction with spin-exchange, (d) Wigner-force, (e) $\vec{\sigma} \cdot \vec{\partial} \vec{\tau} \cdot \vec{\sigma}$-term with radial dependence of Yukawa type ($\mu = 0.70$ fm$^{-1}$), (f) central interaction $1 + \vec{\sigma} \cdot \vec{\partial} \vec{\tau} \cdot \vec{\sigma}$ with radial dependence of Yukawa type ($\mu = 0.70$ fm$^{-1}$).
Kuo-Herling interaction and $\delta$-force. We can thus conclude that the schematic structure of this simple $\delta$-force corresponds very well with the structure of the effective Kuo-Herling force, as far as the monopole energy shifts are concerned.

However, both the delta-interaction and the Kuo-Herling interaction predict the $2f_{7/2}$ level slightly too high compared to the experimental lowest state $7/2^-$. Unfortunately, there exist almost no data on the corresponding spectroscopic factors $S(2f_{7/2})$ [99]; hence, a comparison of the effective single-particle energies with the experimental centroids is not feasible. Nevertheless, we expect the monopole shift to be the driving mechanism behind the evolution of the single-particle energies.

The results using a central force with a finite-range potential of Yukawa type (with $\mu = 0.70 \text{ fm}^{-1}$), are shown in figure 5.4(d) for the Wigner-force ($V_{\sigma\tau} = 0 \text{ MeV}$), in figure 5.4(e) the admixture (1 + $\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu$, $\tilde{\tau}_\pi \cdot \tilde{\tau}_\nu$) for the Wigner-force, and in figure 5.4(f) the admixture (1 + $\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu$, $\tilde{\tau}_\pi \cdot \tilde{\tau}_\nu$). We do not consider the $(\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu)$ component, since this term does not result in a relative change in the $N$-dependence of the $\tilde{\epsilon}_{j\nu}$ values.

The spin-isospin exchange component $(\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu, \tilde{\tau}_\pi \cdot \tilde{\tau}_\nu)$ is producing a pronounced increase of the proton $2f_{7/2}$ single-particle energy relative to the reference $1h_{9/2}$ single-particle energy for $N < 126$, compared to the pure Wigner-term. The $\pi 1i_{13/2}$ single-particle energy is slightly increasing for $N > 126$ for the $\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu$, $\tilde{\tau}_\pi \cdot \tilde{\tau}_\nu$-term, contrary to the effect induced by the Wigner-force. In figure 5.4(f) the admixture 1 + $\tilde{\sigma}_\pi \cdot \tilde{\sigma}_\nu$, $\tilde{\tau}_\pi \cdot \tilde{\tau}_\nu$ is displayed. The experimentally observed decrease of the $\pi 2f_{7/2}$ orbital for $N > 126$ is reproduced, albeit it less steep.

### 5.4 Lowest-Multiplet Structure in Odd-Odd Bi-Isotopes

Once the parameters of the delta-interaction and the quadrupole-quadrupole force have been determined, as described in the previous section, one can study the evolution of the lowest-lying proton-neutron multiplet $\pi 1h_{9/2}/2g_{9/2}$ as a function of the filling of the neutron $2g_{9/2}$ orbital, starting from $^{210}$Bi and going towards $^{218}$Bi. The $\pi 1h_{9/2}/2g_{9/2}$ coupling results in the $0^- - 9^- \text{ multi-plet}$.

The necessary ingredients to study the evolution of this multiplet are the proton effective single-particle energies $\tilde{\epsilon}_{j\nu}$, the neutron one-quasi-particle energies, and the proton-neutron two-body particle–quasi-particle matrix elements. The proton does not change its particle character, but the neutron does: when the neutrons start filling the $\nu 2g_{9/2}$ orbital, they can be described as particles; when the $\nu 2g_{9/2}$ orbital is almost full, it is more convenient to describe the neutrons as holes. A better way to describe this change from particle to hole character is to describe the neutrons as quasi-particles. As a result, the proton-neutron two-body matrix elements are expressed as a linear combination of a particle-particle and a particle-hole matrix element:

$$
\langle j_\pi j_\nu, J | V | j_\pi j_\nu, J \rangle = (1 - v^2_{j,\nu}) \langle j_\pi j_\nu, J | V | j_\pi j_\nu, J \rangle + v^2_{j,\nu} \langle j_\pi j_\nu^{-1}, J | V | j_\pi j_\nu^{-1}, J \rangle,
$$

(5.2)

with $v^2_{j,\nu}$ the occupation probability of a neutron in orbital $j_\nu$. Since the neutrons are filling a single orbital $j_\nu = 2g_{9/2}$, $v^2_{j,\nu}$ can be approximated using the simple relation:

$$
v^2_{j,\nu} = \frac{n_{j,\nu}}{(2j_\nu + 1)},
$$

(5.3)
5.4 Lowest-Multiplet Structure in Odd-Odd Bi-Isotopes

with \( n_{j\nu} \) being the numbers of neutrons present in orbital \( j\nu \).

The expression of the proton-particle–neutron-quasi-particle matrix element results in a switching from a typical proton-neutron particle-particle spectrum at the beginning of the neutron \( \nu^2 g_{9/2} \) orbital into a typical proton-neutron particle-hole spectrum when the neutron \( \nu^2 g_{9/2} \) orbital has been filled with 10 neutrons. This is illustrated in figure 5.5, for both the \( \delta \)-interaction including spin-exchange in panel (b), for a pure quadrupole-quadrupole force in panel (c), and using the realistic Kuo-Herling interaction in panel (d). There is an overall similarity in these energy spectra: the change from the low spin \( J^\pi = 0^-, 1^- \) states as the lowest excited states in \( ^{210}\text{Bi} \), into a highly-compressed multiplet structure near mid-shell i.e. \( ^{214}\text{Bi} \), and into the situation where the \( J^\pi = 5^-, 6^-, 7^- \) levels are the lowest states. The details are clearly different, depending on the residual proton-neutron interaction.

This ‘turning-over’ in the proton-neutron spectrum with increasing neutron number, when neutrons are filling the \( \nu^2 g_{9/2} \) orbital, is most clearly seen using a quadrupole-quadrupole force. In this case, the particle-hole matrix element has the opposite sign of the particle-particle matrix element (but the same absolute value), and so expression (5.2) reduces to the form:

\[
\langle j_{\pi j\nu}, J | V_{QQ} | j_{\pi j\nu}, J \rangle = (1 - 2v_{j\nu}^2) \langle j_{\pi j\nu}, J | V_{QQ} | j_{\pi j\nu}, J \rangle. \tag{5.4}
\]

Moreover, the particle-particle spectrum (multiplet energy splitting) follows a parabolic form as a function of \( J(J+1) \). In the particle-particle case, this parabola has the \( J^\pi = 0^- \) as the lowest-lying state; at mid-shell, there is an exact degeneracy \( (u_{j\nu}^2 = v_{j\nu}^2) \); and for the particle-hole case, the lowest-lying state is the \( J^\pi = 6^- \) state (see also Paar [93]). This parabolic structure results in high-spin isomers in the lighter Bi-nuclei, and into a high-spin \( (6^-, 7^-) \) ground state in \( ^{216,218}\text{Bi} \) [111, 118], and this is also seen when using the other forces.
Table 5.1: Experimental data on the lowest $0^- - 9^-$ states in $^{210-218}$Bi; the data has been extracted from [99]. All energies are in MeV.

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>E</th>
<th>$J^\pi$</th>
<th>E</th>
<th>$J^\pi$</th>
<th>E</th>
<th>$J^\pi$</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{210}$Bi</td>
<td>0^-</td>
<td>0.047</td>
<td>$^{212}$Bi</td>
<td>0^-</td>
<td>0.239</td>
<td>$^{214}$Bi</td>
<td>0^- , 1^-</td>
</tr>
<tr>
<td>1^-</td>
<td>0.000</td>
<td>1^-</td>
<td>0.000</td>
<td>1^-</td>
<td>0.000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2^-</td>
<td>0.320</td>
<td>2^-</td>
<td>0.115</td>
<td>(2^-)</td>
<td>0.053</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3^-</td>
<td>0.348</td>
<td>(3^-)</td>
<td>0.213</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4^-</td>
<td>0.503</td>
<td>(4^-)</td>
<td>0.251</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>5^-</td>
<td>0.439</td>
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<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>6^-</td>
<td>0.550</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7^-</td>
<td>0.433</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8^-</td>
<td>0.583</td>
<td>(8^- , 9^-)</td>
<td>0.250</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9^-</td>
<td>0.271</td>
<td></td>
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</tr>
</tbody>
</table>
5.4 Lowest-Multiplet Structure in Odd-Odd Bi-Isotopes

Figure 5.5: Panel (a) gives the experimental [99] lowest-lying states with spin-parity corresponding to the $0^- - 9^-$ multiplet in $^{210}_{83}$Bi$_{127}$ (see also table 5.1). In panel (b), the $\pi_1 h_9/2 \nu_2 g_{9/2}$ multiplet splitting due to the $\delta$-force is shown; in panel (c), the splitting due to the QQ-force, and in panel (d), the splitting caused by the modified Kuo-Herling interaction [114]. All energies are in MeV.
6 \( N = 51 \) Isotones

6.1 Introduction

After discussing the typical situation of a single proton outside a closed proton shell (Cu \((Z = 29), \) Bi \((Z = 83)\)), we study the \( N = 51 \) isotones which form an interesting example of nuclei where the variation of the neutron single-particle energies can be investigated. Nuclei in this mass region are particularly important to understand astrophysics processes.

Almost half of the elements with mass number \( A > 60 \) which can be found in nature, have been produced by the rapid neutron-capture process, or \( r \)-process, most probably in supernova explosions (e.g. [119] and references therein). Depending on the location of the \( r \)-process path in the astrophysical models, different nuclear abundances occur [120, 121]. Calculations of Surman and Engel [122] have pointed out that particular nuclei relatively close to stability can have a significant effect on the neutron-capture rates, hence, the abundance patterns: nuclei near closed shells have small neutron separation energies, and the level densities near the neutron thresholds are expected to be low. Consequently, one expects direct neutron-capture to make a significant contribution to the overall neutron-capture rate.

Due to the lack of experimental data on (direct) neutron-capture rates, various models exist. These models need detailed information on the nuclear structure properties such as reaction cross sections, energy levels, spins, parities, electromagnetic transition probabilities, single-particle spectroscopic factors, and nuclear density distributions. Different nuclear structure models result in different direct neutron-capture rates, and a different \( r \)-process path [123].

Recent \((d, p)\) experiments on \(^{83}\)Ge and \(^{85}\)Se [124, 125, 126, 127] have provided new data on neutron single-particle states in these \( N = 51 \) isotones, and have sparked new interest in the \( 28 < Z < 50, N = 50 \) region.

Another point of interest is the evolution of the shell structure going from \(^{78}\)Ni to \(^{100}\)Sn at the proton drip line, as pointed out by Grawe et al. [128, 129]. The doubly-magic \(^{100}\)Sn-core has been studied in [130, 131, 132].

In the present chapter, we study the evolution of the neutron single-particle energy levels for \( N = 51 \) as a function of changing proton number \( Z \), spanning the entire \( 28 \leq Z \leq 50 \) major shell.
6.2 Spectroscopy of $^{90}$Y

6.2.1 The Shell-Model Space

We use $^{88}$Sr as a closed core in our shell-model calculations. This approximation turns out to be quite good for nuclei in the close vicinity, e.g. $^{89}$Sr and $^{92}$Zr. More recent validation for this assumption is reported in [133]. There, both a $^{88}$Sr and $^{90}$Zr-core have been used in extensive shell-model calculations for a wider range of Zr-isotopes. It turns out [133] that $^{88}$Sr is a good core to describe nuclei up to $^{96}$Zr; from there on, heavier nuclei such as $^{90}$Zr and $^{94}$Sr might be better cores. This points out some flaws in the realistic effective interaction used, and in the (limited) model space. The overall agreement between theoretical calculations by [133, 134, 135, 136] and the experimental data provides strong support for $^{88}$Sr as a closed core for nuclei around $Z = 40$ and $N = 50$.

The model space consists of the proton orbitals between the $Z = 28$ and $Z = 50$ major shells, and the neutron orbitals between the $N = 50$ and $N = 82$ major shells. Since we consider $^{88}$Sr as a closed core, excitations into the proton orbitals $1g_{9/2}$ and $2p_{1/2}$ correspond with particle excitations, whereas excitations into the $2p_{3/2}$ and $1f_{5/2}$ orbitals correspond with hole excitations. The neutron orbitals $2d_{5/2}$, $3s_{1/2}$, $2d_{3/2}$, $1g_{7/2}$ and $1h_{11/2}$ correspond with particle excitations for the $N = 51$ nuclei.

The proton and neutron single-particle energies used in this work are the ones listed in Table II of [133], and they are given schematically in figure 6.1. The energies of the proton hole states are taken from the experimental data on $^{87}$Rb [99].

The $N = 51$ isotones have a single neutron in the model space, which makes them well-suited to study the neutron monopole shift. We make use of the analogue of expression (2.39) to compute the neutron monopole shift:

$$
\bar{e}_{j\nu} = \epsilon_{j\nu} + \sum_{j\pi} E_{j\pi j\nu} (2j\pi + 1) v_{j\pi}^2, \quad (6.1)
$$

and the occupation probabilities $v_{j\pi}^2$ are obtained using the pairing Hamiltonian (see (2.20)) with constant pairing strength $G = 23/A$ MeV. This strength has been obtained by fitting the theoretical pairing gap to the experimental pairing gap [117].

6.2.2 Effective Proton-Neutron Interactions

The effective realistic nucleon-nucleon interaction used to study the $N = 51$ isotones is the interaction developed by M. Hjorth-Jensen [137], based on the charge-symmetry breaking potential of Machleidt et al. [138], and is similar to the one developed by Holt et al. [133]. It is an effective interaction based on meson exchange models for the free nucleon-nucleon interaction. The effective interaction is obtained in a $G$-matrix approach.

In a shell-model calculation, it provides a good qualitative reproduction of the energies and $E2$ transition rates of the $^{90}$--$^{98}$Zr isotopes. A drawback of this interaction is the fact that it is only defined for the proton orbitals $1g_{9/2}$ and $2p_{1/2}$, so we cannot use it to study the $N = 51$ isotones with proton number $Z < 38$. We have included a mass dependence in the two-body matrix elements of the realistic effective interaction through the factor $(A_0/A)^{1/3}$, with $A$ being the mass of the nucleus under study, and $A_0 = 88$ the mass of the core nucleus $^{88}$Sr.
6.2 Spectroscopy of $^{90}$Y

<table>
<thead>
<tr>
<th>Energy [MeV]</th>
<th>Single-particle State</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.500</td>
<td>1h$_{11/2}$</td>
</tr>
<tr>
<td>2.630</td>
<td>1g$_{7/2}$</td>
</tr>
<tr>
<td>2.230</td>
<td>2d$_{3/2}$</td>
</tr>
<tr>
<td>1.260</td>
<td>3s$_{1/2}$</td>
</tr>
<tr>
<td>0.900</td>
<td>1g$_{9/2}$</td>
</tr>
<tr>
<td>0.000</td>
<td>2p$_{1/2}$</td>
</tr>
<tr>
<td>0.000</td>
<td>2d$_{5/2}$</td>
</tr>
<tr>
<td>0.402587</td>
<td>1f$_{5/2}$</td>
</tr>
</tbody>
</table>

Figure 6.1: Single-particle energies near the $Z = 38$, $N = 50$ shell. The proton and neutron single-particle energies are the ones used in [133]; the proton single-hole energies are obtained from the experimental data on $^{87}$Rb [99]. The energies are in MeV, relative to the closed shell. The proton shell gap of 3.5415 MeV is obtained from the experimental proton separation energies of $^{89}$Y and $^{88}$Sr [99].

Besides a realistic effective interaction, we also make use of schematic two-body forces in order to study the spectrum sensitivity to such schematic choices. The parameters characterizing the various forces have been obtained by fitting to the experimental spectrum of $^{90}$Y, since $^{90}$Y can be mainly considered as a two-particle system (one proton and one neutron) outside the closed $^{88}$Sr-core. The experimental spectrum of $^{90}$Y is shown in figure 6.2, along with the spectra obtained by the realistic effective interaction in the middle column and the delta-interaction in the right-most column.

It is seen that the lowest $2^-$, $3^-$ states originate from the $2p_{1/2}(\pi)2d_{5/2}(\nu)$ proton-neutron configuration mainly. The next group of positive parity states ($2^+ - 7^+$) results from the $1g_{9/2}(\pi)2d_{5/2}(\nu)$ proton-neutron coupling primarily. One also notices the nearby $0^-$, $1^-$ states with a mainly $2p_{1/2}(\pi)2s_{1/2}(\nu)$ proton-neutron character. The realistic interaction clearly shows the best agreement when comparing with the experimental data.

The schematic forces used here (delta-interaction with spin-exchange, central force) have been presented before in chapter 3, and we will only briefly list the values of their respective strength parameters:

- a $\delta$-interaction including spin-exchange (see expression (3.35)). A strength $V_0 = 500$ MeV-fm$^3$ and a spin-exchange parameter $\alpha = 0.2$ give the best agreement with
Figure 6.2: Spectrum of $^{90}$Y. The left most column represents the experimental spectrum [99]. The middle column gives the spectrum obtained using the realistic effective interaction [137] in our model space, and the right-most column gives the spectrum obtained using the delta-force with spin-exchange.
the spectrum of \(^{90}\text{Y}\), as can be seen in the right-most column of figure 6.2.

- a central interaction, keeping only the first (proportional to \(V_0\)) and last term (proportional to \(V_{\sigma\tau}\)) of expression (3.10). As a result, we have the same form (5.1) of the central interaction as for the Bi-isotopes in chapter 5. The strengths are arbitrarily set to \(V_0 = V_{\sigma\tau} = 20\) MeV. Also, the two-body matrix elements are mass-dependent through the factor \((A_0/A)^{1/3}\), as we did for the realistic effective interaction.

The choice for this particular form of the central force has been discussed earlier in chapter 5 for the Bi-isotopes.

### 6.3 Neutron Monopole Shift in Odd \(N = 51\) Isotones

In this section, the experimental data on the evolution of the neutron single-particle energy levels of the \(N = 51\) isotones will be compared with the results obtained with the various interactions (both realistic and schematic). These studies try to shed light on the changing neutron single-particle energy levels, or the so-called neutron monopole shift.

#### 6.3.1 Experimental Centroids

The available experimental data on the neutron single-particle energy levels are given in figure 6.3. The upper frame 6.3(a) represents the experimental centroids, for those single-particle levels where spectroscopic factors are available. We have limited our approach to spectroscopic factors obtained through \((d, p)\)-reactions. The available experimental data on the lowest \(5/2^+, 1/2^+, 7/2^+, 3/2^+\) and \(11/2^-\) states and the corresponding spectroscopic factors for \(^{83}\text{Ge}, ^{85}\text{Se}, ^{87}\text{Kr}, ^{89}\text{Sr}, ^{91}\text{Zr}\) and \(^{93}\text{Mo}\) are shown in tables 6.1 and 6.2. The data on \(^{89}\text{Sr}\) from the work of Cleary [139] has been decreased with a factor 1/1.25 in order to renormalize the total \(5/2^+\) spectroscopic strength from 1.25 to the sum rule limit of 1.0.

The experimental lowest-lying states with spin and parity \(J^z\) equal to the corresponding neutron single-particle levels are given in figure 6.3(b). Both centroids and lowest-lying levels exhibit the same overall behaviour (up to \(Z = 42\)).

#### 6.3.2 Neutron Monopole Shift

In this section, we study the effect of the filling proton orbitals on the neutron single-particle energy levels, with the realistic and schematic interactions listed in the previous section.

The comparison between the experimental centroids and the neutron monopole shifts with various interactions is given in figure 6.4.

Figure 6.4(b) gives the neutron monopole shift obtained using the realistic effective interaction of M. Hjorth-Jensen [137]. Since this interaction is only defined for the proton orbitals \(1g_{9/2}\) and \(2p_{1/2}\), we cannot use it to study the monopole shift for the \(N = 51\) isotones with proton number \(Z < 38\). The filling of the proton \(1g_{9/2}\) orbital lowers the neutron \(1g_{7/2}\) orbital, due to the strongly attractive nature of the interaction between
Figure 6.3: Comparison between (a) the experimental centroids, listed in table 6.1 and table 6.2, and (b) the experimental lowest states, and each $J^\pi$ value matches the quantum numbers of the corresponding neutron single-particle levels.
Figure 6.4: Neutron monopole shift: comparison with (a) the experimental centroids, and the contributions from various interactions: (b) realistic interaction [137], (c) $\delta$-interaction with spin-exchange, (d) Wigner-term of the Yukawa force, (e) $\vec{\sigma} \cdot \vec{\sigma} \cdot \vec{r}$-term with radial dependence of Yukawa type ($\mu = 0.70$ fm$^{-1}$), (f) central interaction $(1 + \vec{\sigma} \cdot \vec{\sigma} \cdot \vec{r})$ with radial dependence of Yukawa type ($\mu = 0.70$ fm$^{-1}$).
Table 6.1: Available experimental data on spectroscopic factors of the lowest $5/2^+$, $1/2^+$, $7/2^+$, $3/2^+$ and $11/2^-$ states in $^{85}$Ge, $^{85}$Se, $^{87}$Kr and $^{89}$Sr taken from $(d,p)$ neutron-stripping reactions. The data on $^{85}$Ge are from [124] and on $^{85}$Se from [125]. The data on $^{87}$Kr is extracted from the online nuclear data sheets [99]. The data on $^{89}$Sr come from [139]. In the case of $^{83}$Ge, $^{85}$Se and $^{87}$Kr, there is very little spectroscopic data available. Hence, the centroids listed here should be regarded as lower limits for the ‘real’ centroids, since the latter will lie higher in energy.

<table>
<thead>
<tr>
<th>$^A$Element</th>
<th>$^J$Spin</th>
<th>$E_{exp,i}$ (MeV)</th>
<th>$S_i$</th>
<th>$\sum_i S_i$ (MeV)</th>
<th>centroid$_{abs}$ (MeV)</th>
<th>centroid$_{rel}$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{85}$Ge</td>
<td>$5/2^+$</td>
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<td>0.30</td>
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spin-orbit partners $j_>(\pi l g_9/2)$ and $j_<(\nu l g_7/2)$. The $\pi l g_9/2$ ($j_>$) has a similar effect on the $\nu l h_{11/2}$ ($j_>$) orbital, albeit less pronounced because of the difference in the orbital quantum number $l$, and hence the reduced overlap of the radial wave functions. The lowering of the $\nu 3s_{1/2}$ with decreasing proton number (between $Z = 42$ and $Z = 38$) is reproduced, but the steep decrease is not. However, since the experiments in [124] and [125] have only measured half of the spectroscopic strength of a pure single-particle configuration, it is expected that the experimental centroid of the $1/2^+$ level lies at a higher energy.

The effect of the $\delta$-force with spin-exchange is illustrated in figure 6.4(c). As has been pointed out earlier for the Cu-isotopes in chapter 4 and appendix B, the spin-orbit partners $\nu 2d_{5/2}$ and $\nu 2d_{3/2}$ show no relative change. The filling of the $\pi l g_9/2$ orbital pulls down the $\nu l g_{7/2}$ and $\nu l h_{11/2}$ orbitals, and again, the decrease of the $\nu l h_{11/2}$ orbital is less steep because of the different orbital angular momentum $l$. Below $Z = 34$, the $\nu l g_{7/2}$ goes up
### Table 6.2: Available experimental data on spectroscopic factors of the lowest $5/2^+$, $1/2^+$, $7/2^+$, $3/2^+$ and $11/2^-$ states in $^{91}$Zr and $^{93}$Mo, taken from $(d, p)$ neutron-stripping reactions. The data are extracted from the online nuclear data sheets [99].

<table>
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<th>$E_{exp,i}$ (MeV)</th>
<th>$S_i$</th>
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because of the emptying of the $\pi 1f_{5/2}$ orbital.

The effect of a Wigner-force ($V_0 = 20$ MeV and $V_{\sigma\tau} = V_\sigma = V_\tau = 0$ MeV in expression (3.10)) is illustrated in figure 6.4(d). Without the spin-isospin exchange term ($\bar{\sigma}_\pi \cdot \bar{\sigma}_\nu \bar{r}_\pi \cdot \bar{r}_\nu$), the spin-orbit partners $\nu 2d_{5/2}$ and $\nu 2d_{3/2}$ do not show any relative change either.

The effect of the fourth term ($V_{\sigma\tau} = 20$ MeV and $V_0 = V_\sigma = V_\tau = 0$ MeV in expression (3.10)) of the central force is shown in figure 6.4(e). The effect of the $(\bar{\sigma}_\pi \cdot \bar{\sigma}_\nu \bar{r}_\pi \cdot \bar{r}_\nu)$ term on the neutron single-particle energy levels with changing proton number is clearly visible. As protons fill the $1g_{9/2}$ orbital, the $\nu 1g_{7/2}$ and $\nu 1h_{11/2}$ orbitals come down in energy. The $(\bar{\sigma}_\pi \cdot \bar{\sigma}_\nu)(\bar{r}_\pi \cdot \bar{r}_\nu)$-term causes a steep lowering of the $\nu 3s_{1/2}$ orbital with decreasing proton number $Z$ ($Z < 40$), i.e. with the emptying of the $\pi 2p_{1/2}$ and $\pi 2p_{3/2}$ orbitals, which is also seen experimentally.

Finally, the neutron monopole shift (2.39) caused by the central force ($V_0 = V_{\sigma\tau} = 20$ MeV and $V_\sigma = V_\tau = 0$ MeV in expression (3.10)) is shown in figure 6.4(f). The steep decrease of the $\nu 3s_{1/2}$ orbital for $Z < 40$ is reproduced, as well as the lowering of the $\nu 1g_{7/2}$ and $\nu 1h_{11/2}$ levels for $Z > 40$ (filling of the $\pi 1g_{9/2}$ orbital).
7 Monopole Shift: The Role of Different Nucleon-Nucleon Force Components

7.1 Introduction

In the previous chapters we have studied the monopole shift of proton and neutron single-particle energies in various mass regions, in particular for the $Z = 29$ Cu-isotopes (chapter 4), the $Z = 83$ Bi-isotopes (chapter 5) and the $N = 51$ isotones (chapter 6), and we have made extensive comparisons with the available experimental data. At present, there is still a clear lack of spectroscopic information, such as one-nucleon transfer data and the corresponding spectroscopic factors, that hampers the construction of single-particle energy centroids.

The performed calculations of the monopole shifts in these mass regions made use of (i) realistic effective interactions, based on the $G$-matrix and adjusted further to reproduce a large number of experimental data in an optimal way, and (ii) schematic forces. The latter calculations, in particular using a zero-range interaction, even including spin-exchange, exhibit specific shortcomings when comparing to the available experimental data, in particular for the Cu-isotopes ($Z = 29$) and for the $N = 51$ nuclei. Some of these shortcomings are rather general in scope and are due to the specific structure of the zero-range force including spin-exchange (see equations (3.34) and (3.35)). Inspecting the experimental monopole shifts, one notices particular variations between the $(n f_{5/2}, n g_{9/2})$ partners $1f_{5/2}$ and $1g_{9/2}$ when filling the neutron $1g_{9/2}$ orbital in the Cu-nuclei, as well as between the $1g_{7/2}$ and $1h_{11/2}$ neutron single-particle orbitals when filling the proton $1g_{9/2}$ orbital in the $N = 51$ nuclei, respectively.

In order to explore the underlying mechanisms that may give rise to these experimental observations, we carry out a study of the general structures observed in the monopole shifts, concentrating on the different components also present in realistic nucleon-nucleon forces. Thereby we focus on the various spin, isospin and spin-isospin exchange components in the nucleon-nucleon (NN) forces.
7 Monopole Shift: The Role of Different Nucleon-Nucleon Force Components

### 7.2 Generic Features of Monopole Shifts for Different NN-Force Components

Besides the realistic effective interactions in the detailed studies of the preceding chapters, we have made use of two types of schematic forces in order to compare with the experimental data.

- The first is the use of a zero-range force with spin exchange:

\[
V_\delta(1, 2) = -V_0(1 - \alpha + \alpha \vec{\sigma}_1 \cdot \vec{\sigma}_2) \delta \vec{r}_1 \cdot \vec{r}_2. \tag{7.1}
\]

The spin-exchange term is particularly important in order to reproduce details in the nuclear energy spectra, especially for odd-odd nuclei that are very sensitive to this term. The spin-exchange term, however, does not give rise to any variation in the proton single-particle energy of spin-orbit partners when filling neutron orbitals in a given series of isotopes. This feature is due to the specific analytic structure of the two-body matrix elements of the \(\delta\)-force, including spin-exchange, and has been explicitly discussed in chapter 4 when discussing the Cu-isotopes (see also appendix B). This relation holds approximately when the monopole variation for the single-particle energy level is studied for orbitals that have radial wave functions that are very similar in structure (such as the \(1f_{5/2}\) and the \(1g_{9/2}\) proton single-particle orbitals in the Cu-nuclei): in the example both have the same radial quantum number \(n = 1\) and thus the radial wave functions have no node, but are very similar.

- Next, we make use of a general finite-range central potential, including the various spin, isospin and spin-isospin exchange terms:

\[
V_C(1, 2) = V_0(r) + V_\pi(r) \vec{\tau}_1 \cdot \vec{\tau}_2 + V_\sigma(r) \vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_{\pi\tau}(r) \vec{\tau}_1 \cdot \vec{\tau}_2, \tag{7.2}
\]

with the Yukawa type radial dependence for all radial dependences \(V_0(r), V_\pi(r), V_\sigma(r)\) and \(V_{\pi\tau}(r)\):

\[
V_i(r) = -V_i e^{-\mu r}. \tag{7.3}
\]

\(V_i\) is the strength of the radial dependence, and \(\mu = 0.70\) fm\(^{-1}\). We have checked that other finite-range potentials such as an exponential form, a Gaussian form and others, yield very similar results. The two-body matrix elements of these force components have been discussed extensively in chapter 3 and appendix A. Our aim here is to study the relative monopole shifts using the separate terms that show up in equation (7.2) in order to evaluate specific effects in those energy variations. These effects will be illustrated in the next section for the Cu \((Z = 29)\) and the \(N = 51\) nuclei in more detail.

- Since both the zero-range interaction including spin-exchange of (7.1) and the central force of (7.2) result in vanishing (or very small) relative energy shifts for spin-orbit partners, and the isospin-dependent terms in the central potential affect the monopole shifts in a subtle way, we are motivated to study the effect of non-central nucleon-nucleon two-body forces such as a tensor force:

\[
V_T(1, 2) = V_T(r) \left( \vec{Y}_2(\vec{r}) \cdot [\vec{\sigma}_1 \vec{\sigma}_2]^{(2)} \right) \left( v_0 + v_\pi(\vec{\tau}_1 \cdot \vec{\tau}_2) \right), \tag{7.4}
\]
and the non-local two-body spin-orbit interaction:

\[ V_{lS}(1, 2) = V_{lS}(r) \vec{l} \cdot \vec{S}, \]  

(7.5)

with \( \vec{l} \) the relative orbital angular momentum operator, and \( \vec{S} \) the total spin of the two-nucleon system \( \vec{S} = \vec{s}_1 + \vec{s}_2 \).

We notice that for the tensor force, only the isospin-exchange term gives rise to non-vanishing average matrix elements and therefore produces non-zero energy shifts. We also like to point out that in most cases, two-body matrix elements for the two-body tensor-interaction are evaluated by transforming to the relative and center-of-mass coordinates of the two-nucleon system. It is, however, very illuminating to evaluate the two-body matrix elements also in a standard \( jj \)-coupling scheme by using the multipole decomposition. In this way, one has to rewrite the tensor force in a form that separates into operators acting on nucleon 1 and nucleon 2 separately. This is still rather easy to do for a zero-range force, but for the tensor interaction this is an involved calculation (see [140]).

7.3 Application in Various Mass Regions

Here, we study the contributions of the different NN-force components, as outlined in section 7.2, to the monopole energy shifts and this in both the Cu-isotopes \((Z = 29)\) and the \(N = 51\) isotopes as typical examples for both proton and neutron monopole-shifted single-particle energy levels. A number of rather general conclusions, which are also corroborated by further explorations in other mass regions, i.e. the F-isotopes \((Z = 9)\) [141], the K-isotopes \((Z = 19)\) [141], the Bi-isotopes \((Z = 83)\) and the \(N = 29\) isotones [141], can be drawn from those results.

A peculiar feature shows up when comparing these different sets of monopole variations amongst themselves but keeping an eye on the experimental data. Neither the zero-range interaction (with or without spin-exchange term) nor the central force (also including \( \sigma \cdot \sigma, \tau \cdot \tau \) and \( \sigma \cdot \sigma \tau \cdot \tau \)) with radial dependence of Yukawa type reproduces a significant variation in the \( \pi 1g_9/2 \) versus the \( \pi 1f_5/2 \) energy shift when filling the \( \nu 1g_9/2 \) orbital of the Cu-isotopes (see figures 7.1 and 7.2). We present the analogous results on the \( \nu 1g_7/2 \) versus the \( \nu 1h_{11/2} \) energy shift when filling the \( \pi 1g_9/2 \) orbital of the \( N = 51 \) isotones in figures 7.4 and 7.5, showing the experimental centroids and the monopole shifts induced by the realistic interaction, zero-range interaction, and central force components with radial dependence of Yukawa type (pure central term, \( \vec{\sigma} \cdot \vec{\sigma}, \vec{\tau} \cdot \vec{\tau} \) and \( \vec{\sigma} \cdot \vec{\sigma} \vec{\tau} \cdot \vec{\tau} \)).

On the other hand, the tensor force including the isospin-exchange term, exhibits a very systematic relative variation which is observed experimentally (within the restrictions of the presently available data on the single-particle structure of the observed low-lying levels). To a good extent, this variation is also seen in the calculations of the monopole shifts using realistic effective interactions. The effect of the tensor force on the monopole shifts is illustrated in figure 7.3 for the Cu-isotopes, and in figure 7.6 for the \( N = 51 \) isotones. In order to clearly demonstrate the pure effect of the tensor force, we have adopted normal filling of the neutron orbitals in the Cu-isotopes and of the proton orbitals in the \( N = 51 \) orbitals. We also show the effect of the two-body spin-orbit force
Figure 7.1: Proton monopole shift in the odd-\(A\) Cu-isotopes for various interactions. Panel (a) represents the experimental centroids when data are available (see tables 4.2, 4.3, 4.4 and 4.5) or lowest states of a given spin and parity; (b) realistic effective interaction [34]; (c) \(\delta\)-force (see expression (3.35)) with \(V_0 = 400 \text{ MeV-fm}^3\) and \(\alpha = 0.1\).
Figure 7.2: Proton monopole shift in the odd-\( A \) Cu-isotopes for various parameter combinations of the central force as defined in expression (3.10): (a) Wigner term: \( V_0 = -20 \) MeV, \( V_\alpha = V_\tau = V_{\sigma\tau} = 0 \) MeV; (b) \( V_\tau = 15 \) MeV, \( V_0 = V_\sigma = V_{\sigma\tau} = 0 \) MeV; (c) \( V_{\sigma\tau} = -10 \) MeV, \( V_0 = V_\sigma = V_\tau = 0 \) MeV. The radial dependence is of Yukawa type, with \( \mu = 0.70 \) fm\(^{-1}\). The strengths of the Wigner and \( \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 \) term of the central interaction have been fitted to the experimental spectrum of \( ^{58}\text{Cu} \); the strength of the \( \vec{\tau}_1 \cdot \vec{\tau}_2 \) term has been chosen such as to obtain good agreement between the average matrix elements computed with the \( \vec{\tau}_1 \cdot \vec{\tau}_2 \) term and the ones obtained with the realistic effective interaction \([34, 64, 87]\).
on the monopole shifts. The strength of the tensor force and the spin-orbit interaction, respectively, have been set arbitrarily.

The monopole energy shifts discussed in the Cu ($Z = 29$) and $N = 51$ mass regions are corroborated by the study of single-particle monopole shifts in a large set of nuclei including the F ($Z = 9$), Sb ($Z = 51$) isotopes as well as the $N = 29$ isotones [141]. They all point out the generic result that proton-neutron matrix elements of the type $\langle j^\nu_\ell^\nu_\sigma, J | V | j^\sigma_\ell^\sigma_\nu, J \rangle$ with $j^\nu_\ell = \ell^\nu + 1/2$ and $j^\nu_\sigma = \ell^\nu - 1/2$ are regularly more attractive than those of the type $\langle j^\sigma_\ell^\sigma_\nu, J | V | j^\nu_\ell^\nu_\sigma, J \rangle$ and $\langle j^\nu_\ell^\nu_\sigma, J | V | j^\nu_\ell^\nu_\sigma, J \rangle$. This property of the force has been recognized earlier in studies of those mechanisms responsible for the onset of deformation [23, 24, 142]. A similar trend has been revealed from experimental and theoretical studies of light neutron-rich nuclei and the particular reason for that observation, namely the dominant effect of the $\sigma \cdot \sigma T \cdot T$ term in the central part of the effective proton-neutron interaction has been proposed [26]. In that particular case, the orbitals appearing in the two-body matrix elements given above were restricted to be spin-orbit as well as proton-neutron partners originating from the same major shell (indicating that the orbitals $j^\nu_\ell, j^\nu_{\ell-1}$ reduce to the $j^\nu_\ell, j^{\nu-1}_\ell$ single-particle states). These results are nicely illustrated in figure 7.7 for the tensor force as applied to the odd-mass F-isotopes ($Z = 9$) where we observe the relative proton single-particle monopole shifts as a function of neutron number $N$ when filling the neutron $sd$-shell and the next $1f_{7/2}$ orbital.

We illustrate the above outcome for the two-body tensor force for the monopole energy shifts in a schematic way in figure 7.8. These opposite effects are most clearly expressed by the sum rule for monopole shifts of the two neutron spin-orbit partner orbitals $j^{\nu}_\ell (= \ell^\nu + 1/2)$ and $j^{\nu}_{\ell-1} (= \ell^\nu - 1/2)$ caused by a filling of the proton $j^{\nu}_\ell (\ell^\nu \neq \ell^\nu')$.
expression (7.6) is equally valid when the protons are filling the \( j_{<} \) orbital. This sum rule does not hold any longer if we loosen the restriction of having to work with spin-orbit partners but consider orbitals \( j_{>}' = l' + 1/2 \) and \( j_{<}' = l'' - 1/2 \) \((l' \neq l'')\) and which are characterized by radial wave functions of very similar character (the same radial quantum number \( n \)). A typical illustration of this situation shows up in the study of the \( N = 51 \) isotones when we follow the monopole energy shift of the \( 1g_{7/2} \) and \( 1h_{11/2} \) neutron orbitals when filling the proton \( 1g_{9/2} \) orbital, depicted schematically in the left panel of figure 7.9. Likewise, when emptying the proton orbital \( 1f_{5/2} \) in these \( N = 51 \) isotones when we study the lighter nuclei of this series, the same relative shifts appear in the right panel of figure 7.9. There is some experimental indication that this is indeed the case for these nuclei although the data set is too small to be conclusive.

So, there is quite a robust outcome when exploring the characteristics of the monopole
Figure 7.5: Neutron monopole shift in the odd-$A \, N = 51$ isotones for various parameter combinations of the central force as defined in expression (3.10): (a) Wigner term: $V_0 = 20$ MeV, $V_\sigma = V_\tau = V_{\sigma \tau} = 0$ MeV; (b) $V_\tau = -20$ MeV, $V_0 = V_\sigma = V_{\sigma \tau} = 0$ MeV; (c) $V_\sigma = 20$ MeV, $V_0 = V_\sigma = V_\tau = 0$ MeV. The radial dependence is of Yukawa type, with $\mu = 0.70$ fm$^{-1}$. The strengths of the various terms of the central interaction have been set arbitrarily.

energy shift using the two-body tensor force.

(i) Due to the specific character of the two-body tensor force (which resembles the interaction between two magnetic dipoles in electromagnetism), this force only acts between states of which the total intrinsic spin of the two-body system is $S = 1$.

(ii) There is no interaction between two particle states in which the relative angular momentum $l = 0$, due to the presence of the spherical harmonic $Y^2_2$.

(iii) The monopole energy shifts following from the tensor force when one of the orbitals is a $ns1/2$ orbital, vanish, as follows from the multipole composition $[140]$ and angular momentum algebra.

(iv) For light nuclei ($p$-shell, $sd$-shell nuclei), the monopole energy shifts for a set of spin-orbit partners of a given charge (proton or neutron) are opposite in sign when
7.3 Application in Various Mass Regions

Figure 7.6: Neutron monopole shift in the odd-$A$ $N = 51$ isotones for the tensor force of (3.27) ($v_{t0} = v_{tt} = 50$ MeV) and the spin-orbit interaction of (3.29) ($V_{IS} = 20$ MeV). In this particular case, we show the absolute variation of the single-particle energy levels, contrary to the relative variation shown in earlier figures. Here, we have applied normal filling of the proton orbitals, instead of the earlier adopted BCS approach, in order to demonstrate the pure effect of the tensor force and the spin-orbit interaction. The radial dependence is of Yukawa type with $\mu = 0.70$ fm$^{-1}$.

Figure 7.7: Absolute variation of the proton single-particle energies in the F-isotopes ($Z = 9$), obtained with a tensor force (see expression (3.27)) with strengths $v_{t0} = v_{tt} = 50$ MeV.
Figure 7.8: Schematic illustration of the effect of a proton in the $j_{\pi}^\nu$ orbital on the neutron $j_{\nu}^\pi$ and $j_{\pi}^\nu$ single-particle energies, induced by the two-body tensor force. The $j_{\pi}^\nu - j_{\nu}^\pi$ interaction is repulsive, pushing the $j_{\nu}^\pi$ level up in energy, while the $j_{\pi}^\nu - j_{\pi}^\nu$ interaction is attractive, bringing down the $j_{\nu}^\nu$ energy level.

Figure 7.9: Schematic illustration of the effect of the tensor force on the neutron $1g_{7/2}$ and $1h_{11/2}$ orbitals in the $N = 51$ isotones when filling the proton $1g_{9/2}$ orbital (on the left) or when emptying the proton $1f_{5/2}$ orbital (on the right).
Figure 7.10: The two-body matrix elements for the tensor force are the largest for the isospin-exchange term, coupling the proton $j_\ell = l - 1/2$ orbital with the neutron $j_{\nu} = l + 1/2$ orbital (or the proton $j_{\nu}$ with the neutron $j_\ell$ orbital). On the right, we give a schematic representation of the interaction mechanism of the spin-exchange term of the tensor force, expressed by $\vec{\sigma} \cdot \vec{\delta} \vec{\tau} \cdot \vec{\tau}$.

filling one or the other of the spin-orbit partners of the other charge state (neutron or proton, respectively). This is consistent with the fact that the interaction matrix elements are maximal for spin-orbit proton-neutron partners (see schematic figure 7.10).

(v) For medium-heavy and even heavy nuclei, the above feature concerning the monopole energy shift remains valid even when we relax on the condition that we are considering spin-orbit partners. It holds as long as we consider proton (neutron) orbitals of the type $n_\ell j_{\nu} = l + 1/2$ and $n_\nu j_\ell = l' - 1/2 (l' \neq l)$ interacting with neutrons (protons) filling an orbital of the type $n'_{\nu}, j''_{\nu} = l'' \pm 1/2$ (with high $j''_{\nu}$ orbitals in particular). This effect, seen in both the $Z = 51$ and $N = 51$ nuclei, is opposite to the argument that the monopole energy shifts are mainly governed by the radial overlap of the proton and neutron orbitals. It might be a unique probe to test the presence of two-body tensor effects when describing single-particle variations over a large interval of nuclei (isotopes or isotones).

We comment in particular on the items (iv) and (v). It is indeed so that the interaction amongst proton and neutron orbitals that are at the same time spin-orbit partners is particularly strong. This follows as well from the use of a proton-neutron interaction of central type with the form $\int f(r) \sigma_\pi \cdot \sigma_\nu \tau_\pi \cdot \tau_\nu$ as has been discussed at some length by Otsuka et al. [143]. We like to stress that the proton-neutron tensor force induces the same effect as the $\sigma_\pi \cdot \sigma_\nu \tau_\pi \cdot \tau_\nu$ force, but the tensor force also contains the results highlighted under item (v). So, the particular variations in the monopole energy shifts discussed under (v) imply the need of including two-body tensor forces in the proton-neutron channel.
7.4 Conclusion

After the analysis carried out in the study of each individual NN-force component, there are unambiguous indications that a two-body tensor force component is needed in order to describe experimental monopole energy shifts, for both the lighter nuclei and heavy nuclei with an important neutron excess. These results are consistent with calculations that were carried out by Otsuka et al. [143].

There are a number of interesting remarks to be made at this point about the importance of this particular NN-force.

a. Theoretical analysis of the NN-potential, using a $1/N_c$-expansion (with $N_c = 3$ the number of colours) [144], has indicated that the most important terms contributing to the nucleon-nucleon potential are the Wigner term of the central potential, the $\sigma \cdot \sigma \tau \cdot \tau$ term and the tensor force including the isospin-exchange term. They appear in the same order of the expansion and are the leading terms.

b. This is in line with the underlying $\pi$ and $\rho$ meson exchange picture giving rise to the potentials that are characterized in coordinate space by both a Yukawa radial shape multiplied by a tensor and spin force with isospin-exchange included (see expression (3.1) in chapter 3). Of course, this holds on the level of the realistic NN-interactions between free nucleons. In order to derive an effective in-medium two-body interaction starting from the more basic free nucleon-nucleon force, one has to construct the corresponding $G$-matrix including specific core-polarization effects (incorporating the use of limited model spaces). One expects that these effective interactions, based on the $G$-matrix, retain the fundamental features of the tensor and spin-exchange (including isospin-exchange), as present in the bare NN-force: e.g. the Kuo-Brown and modified Kuo-Brown interactions for the $sd$ and $fp$ shell-model spaces [62, 63, 68, 69, 70], effective interactions in the $f_{pg9/2}$ shell-model space of M. Hjorth-Jensen and collaborators [34], Kuo and Herling for the Pb-region [112, 113], ... In fact, it seems that those realistic effective interactions exhibit these properties as is illustrated by the fact that the monopole energy shifts, evaluated for the various mass regions, always provide the best description of the experimentally observed behaviour. Moreover, the individual two-body matrix elements using those $G$-matrix interactions exhibit the properties as described under the items (iv) and (v) in the previous section.

c. There remains a problem when using schematic forces: it is difficult, at present, to have a good idea of the relative importance of the pure central term viz-a-viz the $\sigma_x \cdot \sigma_{\mu} \tau_{\nu} \cdot \tau_{\nu}$ and $\sigma_x \cdot \sigma_{\mu} \tau_{\mu} \cdot \tau_{\nu}$ and the tensor force (with isospin-exchange) on the basis of fitting to energy levels and monopole shifts. Some recent work in that respect has been carried out by Otsuka et al. [26, 143] and Dobaczewski [145]. A possible suggestion is that one maps out the $G$-matrix interactions that are presently in use for various regions of the nuclear mass table in a basis of independent invariant operators that characterize the fundamental nucleon-nucleon force (see section 3.2 in chapter 3). By using the geometrical properties of these different two-body operators, one can derive a set of equations and perform a least-squares fit to the
two-body matrix elements of the $G$-matrix in the various mass regions. However, this is work that is situated beyond the scope of the present study.
8 Conclusions

In this work, we have tried to answer the question of what happens with the nuclear shell structure when we move out of the valley of $\beta$-stability and what the driving mechanism behind the observed changes is. Experimental and theoretical research suggests that the shell structure of nuclei with an extreme $N/Z$ ratio (the so-called exotic nuclei) can differ from the one of stable nuclei.

Nuclear shell structure is guided by specific numbers of protons and neutrons that provide additional stability to the nucleus. These magic numbers are related to an important ansatz in the description of the atomic nucleus: the nucleons are treated as independent particles whose characteristics are governed by a mean field. The link between the independent particle motion in the nuclear mean field, and the two-body interaction between the nucleons in the many-body system of the atomic nucleus, is made via Hartree-Fock theory: starting from a two-body interaction, a mean field can be developed via an iterative and self-consistent process. However, this technique is well-suited for nuclei for which there exists a good initial guess for the two-body interaction; when moving out of the valley of $\beta$-stability and going towards the exotic nuclei, there is less data to base an interaction on. How to proceed?

It turns out that the nuclear shell model can provide us with a simple yet elegant method to study the evolution of the magic numbers towards neutron-rich and neutron-deficient nuclei outside the valley of $\beta$-stability. The nuclear Hamiltonian can be decomposed in multipoles, of which the monopole part takes into account the lowest-order corrections of the single-particle energy with varying nucleon number, i.e. the self-energy correction of the proton (neutron) energy when neutrons (protons) are filling the neutron (proton) valence space. This evolution of the self-energy corrected single-particle energy is called the monopole shift. Next, we study lowest-order pairing corrections among the identical nucleons, introduced via the BCS approach. It turns out that they play an important role in the monopole energy shift. We have compared the monopole energy shifts, including lowest-order pairing corrections, with the energy centroids, incorporating all residual correlations as obtained from large-scale shell-model calculations. An interesting result is that the monopole shift is in remarkable agreement with the calculated full single-particle energy centroid and also corresponds quite well with the experimental centroids (when available).

The dominant role in this study is played by the two-body proton-neutron interaction. We have studied the effect of two types of interactions: realistic effective interactions and schematic interactions. Some of the realistic effective interactions in our approach are based on the $G$-matrix: a many-body technique that starts from the bare nucleon-nucleon force, and that brings in the nuclear medium effects. Various interactions exist, each providing a very good description of a particular mass region. The schematic interactions
are based on general symmetry principles, and we study general central forces, two-body
tensor and spin-orbit forces and zero-range interactions.

We have applied our technique to the study of the evolution of proton (neutron) single-
particle energy levels (monopole shifts) with varying neutron (proton) number in various
mass regions. Thereby, we have focused on nuclei differing from a doubly-closed shell
nucleus by one extra or one missing nucleon, since the lowest-lying states in such nuclei
are most likely to carry most of the single-particle strength. The odd-$A$ Cu-isotopes ($Z =
29$), the odd-$A$ Bi-isotopes ($Z = 83$) and the odd-$A$ $N = 51$ isotones meet that condition.
We have compared our theoretical predictions with the available experimental data.

The monopole energy shifts obtained with the realistic effective interaction generally
agree quite well with the experimental centroids (when available). The lack of agree-
ment seen in the Cu-isotopes is due to missing experimental data on the single-particle
spectroscopic factors, and perhaps also to deficiencies in the effective interaction.

The zero-range interaction with spin-exchange has some interesting analytical prop-
erties (no relative monopole shift for spin-orbit partners), and despite its simple structure,
it produces monopole shifts that agree rather well with the experimental centroids, but it
exhibits specific shortcomings for particular single-particle orbitals.

We have also studied central interactions including spin ($\mathbf{s}_1 \cdot \mathbf{s}_2$), isospin ($\mathbf{t}_1 \cdot \mathbf{t}_2$) and
spin-isospin ($\mathbf{s}_1 \cdot \mathbf{t}_2 \mathbf{t}_1 \cdot \mathbf{t}_2$) exchange components. The spin-exchange term does not cause
any variation in the proton (neutron) single-particle energies when filling neutron (proton)
orbitals in a given series of isotopes (isotones). Only the terms which include isospin-
exchange (with or without spin-exchange) contribute to the monopole shift. However, the
central force, including spin-, isospin- and spin-isospin exchange, cannot account on itself
for the observed single-particle energy variations, and it shows similar shortcomings as in
the case of the zero-range interaction.

The tensor force, including the isospin-exchange term, can account for some of the
systematic single-particle energy changes observed, due to its peculiar properties for specific
combinations of single-particle orbitals. It turns out that proton-neutron matrix ele-
mments of the type $\langle j_\pi^Z j_\nu^L, J | V | j_\pi^Z j_\nu^L, J \rangle$ or $\langle j_\pi^Z j_\nu^L, J | V | j_\pi^Z j_\nu^L, J \rangle$ (with $j_\pi^Z = l^\pi + 1/2$ and
$j_\nu^Z = l^\nu - 1/2$) are regularly more attractive than those of the type $\langle j_\pi^Z j_\nu^L, J | V | j_\pi^Z j_\nu^L, J \rangle$ and
$\langle j_\pi^Z j_\nu^L, J | V | j_\pi^Z j_\nu^L, J \rangle$. These opposite effects are most clearly expressed by a sum
rule for monopole shifts of the two neutron spin-orbit partner orbitals $j_\nu^L (= l^\nu + 1/2)$ and
$j_\pi^Z (= l^\pi - 1/2)$ caused by a filling of the proton $j_\pi^Z (l^\pi \neq l^\nu)$ orbital:

$$
(2j_\pi^Z + 1) \tilde{E}(j_\pi^Z j_\nu^L) + (2j_\nu^L + 1) \tilde{E}(j_\pi^Z j_\nu^L) = 0. \quad (8.1)
$$

This expression is equally valid when protons are filling the $j_\pi^Z$ orbital. The tensor force
shows the same properties as the spin-isospin exchange term of the central interaction,
but the latter does not fulfill the sum rule of (8.1). Since the experimental results seem
to follow the trend suggested by the tensor force, this implies that the two-body tensor
force has to be included in the description of the changing single-particle energies over a
certain mass region.

To conclude, we can say that we have performed a detailed analysis of the mechanisms
behind the possible change of the single-particle energies when moving towards exotic
nuclei. We have shown that the monopole shift provides an interesting description of the
observed effects. The need to include the tensor force in the description of nuclear
data is demonstrated. However, more work still needs to be done: more data about the
single-particle spectroscopic factors for exotic nuclei is desirable, and data about other mass regions is very welcome. Also, the relative contributions of the various two-body forces are not clear yet, and more work in this direction will be carried out.
A Proton-Neutron Two-Body Matrix Elements

A.1 Notation - Conventions - Some Frequently Used Expressions

We outline the notation and conventions used in this work. Some of the properties or relations often used in the calculation of two-body matrix elements are listed here. Proof of the relations and more elaborate discussions, as well as properties of $3j$-, $6j$- and $9j$-symbols, can be found in [25, 28, 146].

- $a$ stands for the state of a nucleon characterized by the quantum numbers $n_a, l_a, j_a$:
  \[ a \equiv n_a, l_a, j_a. \]  
  \[(A.1)\]

- $\alpha$ stands for all the quantum numbers of a nucleon in state $a$:
  \[ \alpha \equiv n_a, l_a, j_a, m_a, t_{za}. \]  
  \[(A.2)\]
  with $m_a$ the projection of the total angular momentum $j_a$, and $t_{za}$ the $z$-projection of the isospin of the nucleon in state $a$.

- $a^\dagger_\alpha$ is an operator which creates a particle in state $\alpha$:
  \[ a^\dagger_\alpha \equiv a^\dagger_{n_a l_a j_a m_a(t_{za})}. \]  
  \[(A.3)\]
  It is a spherical tensor operator of rank $j_a$. We also often use $a^\dagger_{j_a m_a}$ as a notation for the creation operator, with $j_a$ shorthand for $j_a = n_a l_a j_a$, in order to express the dependence on the magnetic quantum number explicitly.

- $a_\alpha$ is an operator which annihilates a particle in state $\alpha$; based on this operator, the spherical tensor operator $\tilde{a}_\alpha$ can be defined:
  \[ \tilde{a}_\alpha = \tilde{a}_{j_a, m_a} \equiv (-1)^{j_a + m_a} a_{j_a, -m_a}. \]  
  \[(A.4)\]

- The operators $a_\alpha$ and $a^\dagger_\beta$ obey the following anticommutation relations:
  \[ \{a_\alpha, a^\dagger_\beta\} = \delta_{\alpha\beta}. \]  
  \[(A.5)\]
Based on the creation operators, a coupled operator $A^+(j_a j_b, JM)$ can be defined, a spherical tensor operator of rank $J$ that creates a normalized two-particle state:

$$A^+(j_a j_b, JM) = \frac{1}{\sqrt{1 + \delta_{ab}}} \left[ a^+_j a^+_j \right]^J_M.$$  \hspace{1cm} (A.6)

- $\tilde{A}(j_a j_b, JM)$ is a coupled two-particle annihilation operator:

$$\tilde{A}(j_a j_b, JM) = \frac{-1}{\sqrt{1 + \delta_{ab}}} \left[ \tilde{a}_j \tilde{a}_j \right]^J_M$$

$$= (-1)^{J+M} A(j_a j_b, J-M).$$  \hspace{1cm} (A.8)

- $U(j_a j_b, JM)$ is a coupled particle-hole operator:

$$U(j_a j_b, JM) = \left[ a^+_j \tilde{a}_j \right]^J_M.$$  \hspace{1cm} (A.9)

It has the following properties:

$$U^+(j_a j_b, JM) = (-1)^{j_a-j_b+M} U(j_b j_a, J-M),$$

$$U(j_a j_a, 00) = \frac{1}{j_a} n_{j_a},$$  \hspace{1cm} (A.10)

with $n_{j_a}$ the number operator in the $j_a$ shell:

$$n_{j_a} = \sum_{m_a} a^+_j a^+_j a^+_{j_a, m_a}.$$  \hspace{1cm} (A.12)

- $\hat{x}$, with $x$ an integer or a half-integer, stands for $\sqrt{2x+1}$, and this short-hand notation will be used throughout this work (no confusion should be possible with operators).

- Wigner-Eckart theorem for a spherical tensor operator of rank $k$ and order $\kappa$:

$$\langle \alpha j m | T^{(k)}(\kappa) | \alpha' j' m' \rangle = (-1)^{j-k} \left( \begin{array}{ccc} j & k & j \\ -m & \kappa & m \end{array} \right) \langle \alpha j || T^{(k)} || \alpha' j' \rangle.$$  \hspace{1cm} (A.13)

Here, and in following expressions, $\alpha$, $\alpha'$, $\alpha_1$, $\alpha_2$, $\alpha'_1$ and $\alpha'_2$ stand for all the quantum numbers needed to uniquely specify the state involved.

- Reduction rule for the reduced matrix element of a tensor operator $T^{(k)}(1, 2)$ that is a tensor product of spherical tensor operators acting on two independent subsystems:

$$T^{(k)}(1, 2) = \left[ T^{(k_1)}(1) \otimes T^{(k_2)}(2) \right]^{(k)}.$$  \hspace{1cm} (A.14)

The reduction rule is given by:

$$\langle \alpha_1 j_1, \alpha_2 j_2; J || T^{(k)}(1, 2) || \alpha'_1 j'_1, \alpha'_2 j'_2; J' \rangle$$

$$= \hat{J} \hat{J}' k \left\{ \begin{array}{ccc} j_1 & j_2 & J \\ j'_1 & j'_2 & J' \\ k_1 & k_2 & k \end{array} \right\} \langle \alpha_1 j_1 || T^{(k_1)} || \alpha'_1 j'_1 \rangle \langle \alpha_2 j_2 || T^{(k_2)} || \alpha'_2 j'_2 \rangle.$$  \hspace{1cm} (A.15)
A.2 Delta-Interaction With Spin-Exchange

The delta-interaction with spin-exchange provides a simple analytical form for the nuclear two-body interaction, and can be used to characterize some of the salient features observed in the energy spectra of nuclei containing a proton-neutron system outside of a closed-shell core. It is expressed as:

\[ V = V_0 (1 + \alpha \sigma_\pi \cdot \sigma_\nu) \delta(\tilde{r}_\pi - \tilde{r}_\nu). \]  

(A.20)

\( V_0 \) describes the interaction strength, and is expressed in units MeV\cdotfm\(^3\). The minus sign indicates the attractive nature of the force. The parameter \( \alpha \) indicates the degree of spin-exchange, and lies in the interval \([0, 1]\). \( V_0 \) and \( \alpha \) are fitted to the experimental energy spectrum of the odd-odd nucleus adjacent to a closed shell, in order to fix the specific proton-neutron characteristics in the given mass region.

Assume a proton in orbital \( j_\pi \) with quantum numbers \((n_\pi, l_\pi, j_\pi)\) and a neutron in orbital \( j_\nu \) with quantum numbers \((n_\nu, l_\nu, j_\nu)\); using \( jj \)-coupling, the two-body matrix

\[ \langle \alpha_1 j_1, \alpha_2 j_2; J \rangle \Big| \mathbf{T}^{(k)}(1, 2) \Big| \mathbf{U}^{(k)}(2) \Big| \alpha_1' j_1', \alpha_2' j_2'; J' \rangle \nonumber \]

\[ = (-1)^{j_2 + j_1' + J} \begin{pmatrix} j_1 & j_2 & J \\ j_2' & j_1' & k \end{pmatrix} \langle \alpha_1 j_1 \rangle \langle \alpha_1' j_1' \rangle \times \langle \alpha_2 j_2 \rangle \langle \alpha_2' j_2' \rangle \delta_{J J'}. \]  

(A.16)

If one of the operators is a unit operator, the reduction rule is given by:

\[ \langle \alpha_1 j_1, \alpha_2 j_2; J \rangle \Big| \mathbf{T}^{(k)}(1) \Big| \mathbf{U}^{(k)}(2) \Big| \alpha_1' j_1', \alpha_2' j_2'; J' \rangle \nonumber \]

\[ = \begin{pmatrix} j_1 & j_2 & J \\ j_2' & j_1' & k \end{pmatrix} \times \langle \alpha_1 j_1 \rangle \langle \alpha_1' j_1' \rangle \delta_{j_2 j_2' \alpha_2} \]  

(A.17)

\[ \langle \alpha_1 j_1, \alpha_2 j_2; J \rangle \Big| \mathbf{T}^{(k)}(2) \Big| \mathbf{U}^{(k)}(2) \Big| \alpha_1' j_1', \alpha_2' j_2'; J' \rangle \nonumber \]

\[ = \begin{pmatrix} j_1 & j_2 & J \\ j_2' & j_1' & k \end{pmatrix} \times \langle \alpha_2 j_2 \rangle \langle \alpha_2' j_2' \rangle \delta_{j_1 j_1'} \]  

(A.18)

The harmonic oscillator radial wave functions \( R_{nl}(r) \) are defined to be positive at the origin.

The total angular momentum \( \tilde{j} \) is obtained by coupling the spin angular momentum \( \tilde{s} \) and the orbital angular momentum \( \tilde{l} \) in the following order:

\[ \tilde{j} = \tilde{l} + \tilde{s}. \]  

(A.19)
A Proton-Neutron Two-Body Matrix Elements

Element can be written as:

\[
\langle j_\pi j_\nu; JM | V_\delta | j'_\pi j'_\nu; JM \rangle = -V_0 \langle j_\pi j_\nu; JM | \delta(\hat{r}_\pi - \hat{r}_\nu) | j'_\pi j'_\nu; JM \rangle
\]

\[
\quad - \alpha V_0 \langle j_\pi j_\nu; JM | (\hat{\sigma}_\pi \cdot \hat{\sigma}_\nu - 1) \delta(\hat{r}_\pi - \hat{r}_\nu) | j'_\pi j'_\nu; JM \rangle
\]

\[
= \text{term 1} + \text{term 2}. \quad (A.21)
\]

The first step is to expand the delta-interaction in the complete set of functions \( P_k(\cos \theta_{12}) \). A general central interaction \( V(|\vec{r}_1 - \vec{r}_2|) \) can be written as [146]:

\[
V(|\vec{r}_1 - \vec{r}_2|) = \sum_{k=0}^{\infty} v_k(r_1, r_2) P_k(\cos \theta_{12}). \quad (A.22)
\]

\( P_k(\cos \theta_{12}) \) are the Legendre polynomials, which can be decomposed using the spherical harmonics:

\[
P_k(\cos \theta_{12}) = \frac{4\pi}{2k + 1} \sum_{n=-k}^{k} (-1)^n Y_n^k(\Omega_1) Y_n^k(\Omega_2), \quad (A.23)
\]

and \( \theta_{12} \) denotes the angle between the two position vectors \( \vec{r}_1 \) and \( \vec{r}_2 \). The function \( v_k(r_1, r_2) \) is defined as:

\[
v_k(r_1, r_2) = \frac{2k + 1}{2} \int_{-1}^{1} V(|\vec{r}_1 - \vec{r}_2|) P_k(\cos \theta_{12}) d \cos \theta_{12}. \quad (A.24)
\]

An expansion similar to (A.22) can be applied to the delta-force \( \delta(\vec{r}_1 - \vec{r}_2) \):

\[
\delta(\vec{r}_1 - \vec{r}_2) = \sum_{k=0}^{\infty} \frac{\delta(r_1 - r_2) 2k + 1}{r_1 r_2} \frac{1}{4\pi} P_k(\cos \theta_{12}), \quad (A.25)
\]

and the function \( v_k(r_1, r_2) \) has the form:

\[
v_k(r_1, r_2) = \frac{\delta(r_1 - r_2) 2k + 1}{r_1 r_2} \frac{1}{4\pi}. \quad (A.26)
\]

Now, the term without spin-dependence is calculated first:

\[
\text{term 1} = -V_0 \langle j_\pi j_\nu; JM | \delta(\hat{r}_\pi - \hat{r}_\nu) | j'_\pi j'_\nu; JM \rangle
\]

\[
= -V_0 \sum_{k=0}^{\infty} f_k^{(1)} F_k. \quad (A.27)
\]

Using the radial wave functions:

\[
R_{nl}(r) = \frac{u_{nl}(r)}{r}, \quad (A.28)
\]

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the Slater integrals $F^k$ and the factors $f_k^{(1)}$ become:

$$F^k = \int_0^\infty u_{n_l, r}(r) u_{n_l', r'}(r') v_k(r, r') u_{n_l, r}(r) u_{n_l', r}(r) dr d\rho$$

$$= \int_0^\infty u_{n_l, r}(r) u_{n_l', r}(r') \frac{\delta(r - r')}{r^2} 2k + 1 \frac{4\pi}{4\pi}$$

$$\times u_{n_l, r}(r) u_{n_l', r}(r) dr d\rho$$

$$= \frac{2k + 1}{4\pi} \int_0^\infty u_{n_l, r}(r) u_{n_l', r}(r) \frac{1}{r^2} u_{n_l, r}(r) u_{n_l', r}(r) dr$$

$$= (2k + 1) F^0, \quad (A.29)$$

and:

$$f_k^{(1)} = \frac{4\pi}{2k + 1} \langle j_\pi j'_\nu; JM| \vec{Y}_k(\Omega_\pi) \cdot \vec{Y}_k(\Omega_\nu)| j'_\pi j'_\nu; JM \rangle$$

$$= \frac{4\pi}{2k + 1} (-1)^{j_\nu + j'_\nu + J} \left\{ \begin{array}{ccc}
 j_\pi & j'_\nu & J \\
 j'_\nu & j_\pi & k \\
 \end{array} \right\}$$

$$\times \langle j_\pi || \vec{Y}_k(\Omega_\pi) || j'_\nu \rangle \langle j'_\nu || \vec{Y}_k(\Omega_\nu) || j'_\nu \rangle. \quad (A.30)$$

$\langle j_\pi || \vec{Y}_k(\Omega_\pi) || j'_\nu \rangle$ can be written as:

$$\langle j_\pi || \vec{Y}_k(\Omega_\pi) || j'_\nu \rangle = (-1)^{j_\pi - 1/2} \sqrt{\frac{(2j_\pi + 1)(2j'_\nu + 1)(2k + 1)}{4\pi}}$$

$$\times \left( \begin{array}{ccc}
 j_\pi & k & j'_\nu \\
 -1/2 & 0 & 1/2 \\
 \end{array} \right) \frac{1}{2} \left( 1 + (-1)^{l_\pi + l'_\nu + k} \right) (-1)^{l_\pi + l'_\nu + 1 - j_\pi - j'_\nu}, \quad (A.31)$$

where convention (A.19) $\vec{j} = \vec{i} + \vec{s}$ for the coupling order of the momenta is used. After carefully rewriting the expression for term 1 and using the orthogonality properties of the $3j$-symbols, one gets for term 1 the result:

$$\text{term 1} = -V_0 \frac{F^0}{4} \sqrt{(2j_\pi + 1)(2j'_\nu + 1)(2j_\nu + 1)(2j'_\nu + 1)}$$

$$\times \left( \begin{array}{ccc}
 j_\pi & j'_\nu & J \\
 1/2 & -1/2 & 0 \\
 \end{array} \right) \left( \begin{array}{ccc}
 j_\pi & j'_\nu & J \\
 1/2 & -1/2 & 0 \\
 \end{array} \right)$$

$$\times \left[ (-1)^{j_\nu - j'_\nu} \left( (-1)^{l_\nu + l'_\nu} + (-1)^{l_\nu + l'_\nu} \right) + \frac{1}{4J(J + 1)} \right] S(j_\nu, j_\pi, J) S(j'_\nu, j'_\pi, J). \quad (A.32)$$

The factors $S(j_\nu, j_\pi, J)$ and $S(j'_\nu, j'_\pi, J)$ stand for:

$$S(j_\nu, j_\pi, J) = (2j_\nu + 1) + (2j_\pi + 1)(-1)^{j_\pi + j_\nu + J},$$

$$S(j'_\nu, j'_\pi, J) = (2j'_\nu + 1) + (2j'_\pi + 1)(-1)^{j'_\pi + j'_\nu + J}. \quad (A.33)$$
Term 2 is calculated in the following way:

\[
\text{term 2} = -\alpha V_0 (j_\pi j_\nu ; JM)(\vec{\sigma}_\pi \cdot \vec{\sigma}_\nu - 1)\delta(\vec{r}_\pi - \vec{r}_\nu) |j'_\pi j'_\nu ; JM\rangle
\]

\[
= -\alpha V_0 \sum_{k=0}^{\infty} f_k^{(2)} F^k. \tag{A.34}
\]

The factor \( f_k^{(2)} \) becomes:

\[
f_k^{(2)} = \frac{4\pi}{2k+1} (j_\pi j_\nu ; JM)(\vec{\sigma}_\pi \cdot \vec{\sigma}_\nu - 1)(\vec{Y}_k(\Omega_\pi) \cdot \vec{Y}_k(\Omega_\nu)) |j'_\pi j'_\nu ; JM\rangle
\]

\[
= \frac{4\pi}{2k+1} \sum_{L,S,L',S'} \hat{L}\hat{S}\hat{L'}\hat{S'}\hat{j}_\pi j_\nu j'_\pi j'_\nu
\]

\[
\times \left\{ \begin{array}{ccc} l_\pi & l_\nu & L \\ 1/2 & 1/2 & S \end{array} \right\} \left\{ \begin{array}{ccc} l'_\pi & l'_\nu & L' \\ 1/2 & 1/2 & S' \end{array} \right\}
\]

\[
\times \langle (l_\pi l_\nu) L(\frac{11}{2}) S ; JM | (\vec{\sigma}_\pi \cdot \vec{\sigma}_\nu - 1) (\vec{Y}_k(\Omega_\pi) \cdot \vec{Y}_k(\Omega_\nu)) |(l'_\pi l'_\nu) L'(\frac{11}{2}) S' ; JM\rangle. \tag{A.35}
\]

The matrix element can be rewritten as:

\[
\langle (l_\pi l_\nu) L(\frac{11}{2}) S ; JM | (\vec{\sigma}_\pi \cdot \vec{\sigma}_\nu - 1) (\vec{Y}_k(\Omega_\pi) \cdot \vec{Y}_k(\Omega_\nu)) |(l'_\pi l'_\nu) L'(\frac{11}{2}) S' ; JM\rangle
\]

\[
= \sum_{M_L,M_S,M'_L,M'_S} \langle LM_L,SM_S;JM | LM'_L,S'M'_S;JM\rangle
\]

\[
\times \langle (l_\pi l_\nu) LML | \vec{Y}_k(\Omega_\pi) \cdot \vec{Y}_k(\Omega_\nu) |(l'_\pi l'_\nu) L'M'_L\rangle
\]

\[
\times \langle (\frac{11}{2}) S M_S | \vec{\sigma}_\pi \cdot \vec{\sigma}_\nu - 1 |(\frac{11}{2}) S' M'_S\rangle. \tag{A.36}
\]

After the necessary angular momentum algebra, term 2 has the form:

\[
\text{term 2} = -2\alpha V_0 F^{0}\hat{j}_\pi j_\nu j_\pi j_\nu \hat{l}_\pi \hat{l}_\nu (-1)^{j_\nu + j'_\nu + l_\pi + l'_\pi + J}
\]

\[
\times \left\{ \begin{array}{ccc} j_\pi & j_\nu & J \\ l_\pi & 1/2 & \end{array} \right\} \left\{ \begin{array}{ccc} j'_\pi & j'_\nu & J \\ l'_\pi & 1/2 & \end{array} \right\}
\]

\[
\times \left( \begin{array}{ccc} l_\pi & l_\nu & J \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} l'_\pi & l'_\nu & J \\ 0 & 0 & 0 \end{array} \right)
\]

\[
= -\alpha V_0 F^{0}\hat{j}_\pi j_\nu j_\pi j_\nu (-1)^{j_\nu + j'_\nu + l_\pi + l'_\pi + J} (1 + (-1)^{l_\pi + l'_\pi + J})
\]

\[
\times \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & -1/2 & 0 \end{array} \right) \left( \begin{array}{ccc} j'_\pi & j'_\nu & J \\ 1/2 & -1/2 & 0 \end{array} \right). \tag{A.37}
\]

Summing term 1 and term 2, and rewriting the 3j-symbols as Clebsch-Gordan coefficients, one obtains the final expression for the two-body \( \delta \)-interaction matrix element:
A.3 Quadrupole-Quadrupole Interaction

The quadrupole-quadrupole interaction is defined as:

\[
V_{QQ} = \chi \left( \sqrt{\frac{m\omega}{\hbar}} r_\pi \right)^2 \left( \sqrt{\frac{m\omega}{\hbar}} r_\nu \right)^2 \tilde{Y}_2(\Omega_\pi) \cdot \tilde{Y}_2(\Omega_\nu) = \chi \tilde{Q}_\pi \cdot \tilde{Q}_\nu. \tag{A.39}
\]

\(\chi\) is the interaction strength, expressed in units MeV, and can be obtained through fitting to the experimental data on odd-odd nuclei adjacent to closed shells. The proton-neutron two-body matrix element in \(jj\)-coupling is expressed as:

\[
\langle j_\pi j_\nu; JM | \tilde{Q}_\pi \cdot \tilde{Q}_\nu | j'_\pi j'_\nu; JM \rangle
= \chi (-1)^{J-M} \begin{pmatrix} J & 0 & 0 & J \\ -M & 0 & 0 & M \end{pmatrix} \langle j_\pi j_\nu; J||\tilde{Q}_\pi \cdot \tilde{Q}_\nu||j'_\pi j'_\nu; J \rangle
= \chi (-1)^{j_\nu + j_\pi + J} \begin{pmatrix} j_\pi & j_\nu & 0 & J \\ j'_\pi & j'_\nu & 0 & 2 \end{pmatrix} \left( \frac{m\omega}{\hbar} \right)^2
\times \langle n_\pi l_\pi | r_\pi^2 | n'_\pi l'_\pi \rangle \langle j_\pi || \tilde{Y}_2(\Omega_\pi) || j'_\pi \rangle \langle j_\nu || \tilde{Y}_2(\Omega_\nu) || j'_\nu \rangle. \tag{A.40}
\]

The radial matrix elements are the radial overlap integrals:

\[
\langle n_\pi l_\pi | r_\pi^2 | n'_\pi l'_\pi \rangle = \int_0^\infty R_{n_\pi l_\pi}(r_\pi)r_\pi^2 R_{n'_\pi l'_\pi}(r_\pi) r_\pi^2 dr_\pi, \\
\langle n_\nu l_\nu | r_\nu^2 | n'_\nu l'_\nu \rangle = \int_0^\infty R_{n_\nu l_\nu}(r_\nu)r_\nu^2 R_{n'_\nu l'_\nu}(r_\nu) r_\nu^2 dr_\nu. \tag{A.41}
\]

Using (A.31) and the analogous expression for the neutrons, one gets the final result:

\[
\langle j_\pi j_\nu; JM | V_{QQ} | j'_\pi j'_\nu; JM \rangle
= \frac{\chi}{16\pi} (-1)^{J_j J_\nu} \begin{pmatrix} j_\pi & j_\nu & 0 & J \\ j'_\pi & j'_\nu & 0 & 2 \end{pmatrix} \left( \frac{m\omega}{\hbar} \right)^2 \times
\times \langle n_\pi l_\pi | r_\pi^2 | n'_\pi l'_\pi \rangle \langle n_\nu l_\nu | r_\nu^2 | n'_\nu l'_\nu \rangle
\times \langle j'_\pi - 1/2, j_\pi 1/2|20 \rangle \langle j'_\nu 1/2, j_\nu - 1/2|20 \rangle. \tag{A.42}
\]
A.4 Other Forces

The matrix elements for a general central potential, two-body tensor force and two-body spin-orbit force can be calculated using a common method. Since one uses central radial potentials, only the relative two-particle coordinates appear (besides spin and isospin operators) and it is beneficial to transform the $jj$-coupled two-particle wave functions into the $LS$-coupled basis. The starting point is the expression for a normalized antisymmetric two-particle state in $LS$-coupling:

$$
|((l_a l_b)_{LS}, JMTM_T)_{\text{n.a.s.}} = \frac{1}{\sqrt{2(1 + \delta_{n_a n_b} \delta_{l_a l_b})}} (1 - \hat{P}_{12}^{\nu} \hat{P}_{12}^{\sigma} \hat{P}_{12}^{T}) |((l_a(1) l_b(2))_{LS}, JMTM_T) = \frac{1}{\sqrt{2(1 + \delta_{n_a n_b} \delta_{l_a l_b})}} \sum_{N\Lambda l} (1 - (-1)^{l+\Lambda+S+T}) \times \langle n_a l_a, n_b l_b : L|n l, N\Lambda : L \rangle |((\Lambda)_{LS}, JMTM_T) = \frac{1}{\sqrt{2(1 + \delta_{n_a n_b} \delta_{l_a l_b})}} \sum_{N\Lambda l} (1 - (-1)^{l+\Lambda+S+T}) \times \langle n_a l_a, n_b l_b : L|n l, N\Lambda : L \rangle (-1)^{l+\Lambda-L} |(\Lambda)_{LS}, JMTM_T \rangle. \tag{A.43}
$$

The operators $\hat{P}_{12}^{\nu}$, $\hat{P}_{12}^{\sigma}$ and $\hat{P}_{12}^{T}$ have been defined in equations (3.11), (3.12) and (3.14), respectively. The coefficient $\langle n_a l_a, n_b l_b : L|n l, N\Lambda : L \rangle$ is called a Moshinsky bracket and defines the transformation from a product of harmonic oscillator wave functions $R_{n_a l_a}(r_1)R_{n_b l_b}(r_2)$ to a product of harmonic oscillator wave functions $R_{n l}(r)R_{N\Lambda}(R)$, with $r = |\vec{r}_1 - \vec{r}_2|$ and $R = |\frac{1}{2}(\vec{r}_1 + \vec{r}_2)|$ the relative and center-of-mass coordinates, respectively [147]. The transformation guarantees the correct total orbital angular momentum $\vec{L}$:

$$\vec{l}_a + \vec{l}_b = \vec{L} = \vec{l} + \vec{\Lambda}. \tag{A.44}$$

Now, the transition from $jj$-coupling to $LS$-coupling is done via angular momentum recoupling, resulting in the following expression for the normalized antisymmetrized two-particle state:

$$
|((j_a j_b)_{JMTM_T})_{\text{n.a.s.}} = \frac{1}{\sqrt{2(1 + \delta_{ab})}} (1 - \hat{P}_{12}^{\nu} \hat{P}_{12}^{\sigma} \hat{P}_{12}^{T}) |((j_a j_b)_{JMTM_T}) = \sum_{L S J} \left( \begin{array}{ccc} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & S & J \end{array} \right) \sqrt{1 + \delta_{n_a n_b} \delta_{l_a l_b}} \frac{1 + \delta_{ab}}{1 + \delta_{ab}} |(l_a l_b)_{LS}, JMTM_T\rangle_{\text{n.a.s.}} = \frac{1}{\sqrt{2(1 + \delta_{ab})}} \sum_{L S J} \left( \begin{array}{ccc} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & S & J \end{array} \right) \sum_{N\Lambda l} (1 - (-1)^{l+\Lambda+S+T}) \times \langle n_a l_a, n_b l_b : L|n l, N\Lambda : L \rangle (-1)^{l+\Lambda-L} |(\Lambda)_{LS}, JMTM_T \rangle. \tag{A.45}
$$
Here, $j_a$ is shorthand writing for $j_a = n_a l_a j_a$. The factor \( \binom{l_a}{l_b}{1/2}j_a{1/2}j_b \) is the modified 9j-symbol:

\[
\binom{l_a}{l_b}{1/2}j_a{1/2}j_b = \frac{\hat{g}_{a} \hat{g}_{b} \hat{S}}{\hat{g}_{a} \hat{g}_{b} \hat{S}} \left\{ \begin{array}{c}
l_a \\
l_b \\
L \\
\end{array} \left| \begin{array}{c}
1/2 \\
1/2 \\
S \\
J \\
\end{array} \right. \right\} \frac{\hat{g}_{a} \hat{g}_{b} \hat{S}}{\hat{g}_{a} \hat{g}_{b} \hat{S}} \left\{ \begin{array}{c}
l_a \\
l_b \\
L \\
\end{array} \left| \begin{array}{c}
1/2 \\
1/2 \\
S \\
J \\
\end{array} \right. \right\} . \quad (A.46)
\]

The interaction matrix element for a normalized antisymmetrized two-particle state then becomes:

\[
\langle (j_a j_b) JMTM_T | V(1, 2) | (j_c j_d) JMTM_T \rangle_{a.a.s.} = \frac{1}{2\sqrt{(1 + \delta_{ab})(1 + \delta_{cd})}} \sum_{L' S' J'} \left( \binom{l_a}{l_b}{1/2}j_a{1/2}j_b \right) \left( \binom{l_c}{l_d}{1/2}j_c{1/2}j_d \right) \\
\times \sum_{n l N A} \sum_{n' l' N' A'} \left( 1 - (-1)^{l + S + T} \right) \left( 1 - (-1)^{l' + S' + T} \right) \\
\times \langle n_a l_a, n_b l_b : L | n_l N A : L \rangle \langle n_c l_c, n_d l_d : L' | n_l' N' A' : L' \rangle \\
\times (-1)^{l + A - L + l' + N' - L'} \\
\times \langle (A) L S, JMTM_T | V(1, 2) | (A') L' S', JMTM_T \rangle . \quad (A.47)
\]

Using the recoupling:

\[
\left\{ \begin{array}{c}
\tilde{A} + \tilde{I} = \tilde{L} \\
\tilde{L} + \tilde{S} = \tilde{J}
\end{array} \Rightarrow \left\{ \begin{array}{c}
\tilde{I} + \tilde{S} = \tilde{J} \\
\tilde{A} + \tilde{J} = \tilde{J}
\end{array} \right\} \right. \quad (A.48)
\]

the matrix element \( \langle (A) L S, JMTM_T | V(1, 2) | (A' L') S', JMTM_T \rangle \) can be rewritten as:

\[
\langle (A) L S, JMTM_T | V(1, 2) | (A' L') S', JMTM_T \rangle = \sum_{J J'} (-1)^{\Lambda + l + S + J} \hat{L} \hat{J} \left\{ \begin{array}{c}
\Lambda \\
J
\end{array} \right| \hat{L} \hat{J} \left\{ \begin{array}{c}
l \\
J
\end{array} \right. \\
\times (-1)^{\Lambda' + l' + S' + J'} \hat{L'} \hat{J'} \left\{ \begin{array}{c}
\Lambda' \\
J'
\end{array} \right| \hat{L'} \hat{J'} \left\{ \begin{array}{c}
l' \\
J'
\end{array} \right. \\
\times \langle (A) L S, JMTM_T | V(1, 2) | (A' L') S', JMTM_T \rangle \\
\times \langle (A) L S, JMTM_T | V(1, 2) | (A' L') S', JMTM_T \rangle \\
\times \langle (I S) JMTM_T | V(1, 2) | (I' S') JMTM_T \rangle . \quad (A.49)
\]

The factor \( U(A I J S; L J) \) has been defined as:

\[
U(A I J S; L J) \equiv (-1)^{\Lambda + l + S + J} \hat{L} \hat{J} \left\{ \begin{array}{c}
\Lambda \\
S
\end{array} \right| \hat{L} \hat{J} \left\{ \begin{array}{c}
l \\
J
\end{array} \right. \right\} . \quad (A.50)
\]
Inserting expression (A.49) into equation (A.47), the matrix element becomes:

\[
\langle (a,b)JM | V(1,2) | (c,d)JM \rangle_{n.a.s.} = \\
\frac{1}{2\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} \sum_{LL'S'} \begin{pmatrix} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & S & J \end{pmatrix} \begin{pmatrix} l_c & 1/2 & j_c \\ l_d & 1/2 & j_d \\ L' & S' & J \end{pmatrix} \\
\times \sum_{n',n''} \sum_{\Lambda} \left( 1 - (-1)^{l+S+T} \right) \left( 1 - (-1)^{l'+S'+T} \right) \left( -1 \right)^{l+l'-L-L'} \\
\times \langle n_a l_a, n_b l_b : L | n_l, N\Lambda : L \rangle \langle n_c l_c, n_d l_d : L' | n''_l', N\Lambda : L' \rangle \\
\times \sum_{J} \langle \Lambda IJS; L,J \rangle \langle \Lambda'IJS' ; L',J \rangle \\
\times \langle \langle lS,JMTM_T | V(1,2) | (l'S')JMTM_T \rangle \rangle \tag{A.51}
\]

This expression provides us with an excellent starting point for the computation of the matrix elements of any purely central potential, as well as for the two-body tensor force and the two-body spin-orbit force, as will be shown in the next subsections.

Expression (A.51) has been obtained in the isospin formalism; the relation between the interaction matrix element in isospin formalism and proton-neutron formalism is given by the following expression [148]:

\[
\langle (a,b)JM | V(1,2) | (c,d)JM \rangle_{n.a.s.} = \\
\frac{\sqrt{1+\delta_{ab}} \sqrt{1+\delta_{cd}}}{2} \left( \langle (a,b)JM = 0M_T | V(1,2) | (c,d)JM = 0M_T \rangle_{n.a.s.} \right) \\
+ \langle (a,b)JM = 1M_T | V(1,2) | (c,d)JM = 1M_T \rangle_{n.a.s.} \right). \tag{A.52}
\]

A.4.1 General Central Potential

We make use of the central potential as defined in equation (3.26):

\[
V_C(1,2) = V_C(r) \sum_{i,j=\{1,3\}} a_{ij} \hat{\Pi}. \tag{A.53}
\]

Using the expressions:

\[
\langle \langle lS,JMTM_T | V_C(1,2) | (l'S')JMTM_T \rangle \rangle \\
= \langle \langle lS,JMTM_T | V_C(r) \sum_{i,j=\{1,3\}} a_{ij} \hat{\Pi} | (l'S')JMTM_T \rangle \rangle \\
= \delta_{l''} \langle n_l | V_C | n''_l' \rangle \langle SMSTM_T | \sum_{i,j=\{1,3\}} a_{ij} \hat{\Pi} | SM'TSTM_T \rangle, \tag{A.54}
\]

and:

\[
\langle SMSTM_T | \sum_{i,j=\{1,3\}} a_{ij} \hat{\Pi} | SMSTM_T \rangle = a_{(2T+1)(2S+1)}, \tag{A.55}
\]
the expression for the matrix element of the central force becomes:

\[
\langle (j_a j_b)J M T M_T | V_C(1, 2) | (j_c j_d)J M T M_T \rangle_{\text{n.a.s.}} = \frac{1}{2\sqrt{(1 + \delta_{ab})(1 + \delta_{cd})}} \sum_{LL'S} \begin{pmatrix} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & S & J \end{pmatrix} \begin{pmatrix} l_c & 1/2 & j_c \\ l_d & 1/2 & j_d \\ L' & S & J \end{pmatrix} \times \sum_{nN\Lambda n'} \left( 1 - (-1)^{l+L+S+T} \right) \left( 1 - (-1)^{l'+L'+S+T} \right) \left( -1 \right)^{L+L'} \\
\times \langle n_{l_a} l_{b}, n_{l_b} : L | n_{l_c} l_{d} : L' | n'_{l}, \Lambda : L \rangle \langle n_{l_{c}} l_{d} : L' | n'_{l}, \Lambda : L' \rangle \\
\times (2J + 1)U(\Lambda lJS; L J)U(\Lambda lJS; L' J) \langle n'_{l} | V_{C} | n_{l} \rangle a_{(2T+1)(2S+1)}. \tag{A.56}
\]

\[\text{A.4.2 Two-Body Tensor Force}\]

The two-body tensor force is defined as in equation (3.27):

\[
V_T(1, 2) = V_T(r) \left( v_{t_0} + v_{tt} \vec{r}_1 \cdot \vec{r}_2 \right) \left( \frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \\
= \sqrt{\frac{24\pi}{5}} V_T(r) \left( v_{t_0} + v_{tt} \vec{r}_1 \cdot \vec{r}_2 \right) \left( \vec{Y}_2(\Omega_r) \cdot [\vec{\sigma}_1 \vec{\sigma}_2]^2 \right). \tag{A.57}
\]

Inserting this expression (A.49) results in:

\[
\langle (lS)J M T M_T | \sqrt{\frac{24\pi}{5}} V_T(r) \left( v_{t_0} + v_{tt} \vec{r}_1 \cdot \vec{r}_2 \right) \left( \vec{Y}_2(\Omega_r) \cdot [\vec{\sigma}_1 \vec{\sigma}_2]^2 \right) | (l'S')J M T M_T \rangle \\
= \sqrt{\frac{24\pi}{5}} \left( -1 \right)^{s+s'+j} \left\{ \begin{array}{cccc} l & S & S' & J \\ l' & S' & S & J' \end{array} \right\} \langle nl | V_T | n'l' \rangle \langle l||\vec{Y}_2(\Omega_r)||l' \rangle \\
\times \langle S | [\vec{\sigma}_1 \vec{\sigma}_2]^2 | S' \rangle \langle TM_T | (v_{t_0} + v_{tt} \vec{r}_1 \cdot \vec{r}_2) | TM_T \rangle \\
= \sqrt{\frac{24\pi}{5}} \left( -1 \right)^{s+s'+j} \left\{ \begin{array}{cccc} l & S & S' & J \\ l' & S' & S & J' \end{array} \right\} \langle nl | V_T | n'l' \rangle \frac{\hat{P}}{\sqrt{4\pi}} (-1)^{l'} \langle l'0l0|20 \rangle \\
\times 2\sqrt{5} \delta_{S1}\delta_{S'1} \left( v_{t_0} + v_{tt} \left( 2T(T+1) - 3 \right) \right) \\
= \sqrt{24} \left( -1 \right)^{j+1} \left\{ \begin{array}{cccc} l & 1 & 1 & J \\ l' & 1 & 1 & J' \end{array} \right\} \langle nl | V_T | n'l' \rangle \frac{\hat{P}}{\sqrt{4\pi}} (-1)^{l'} \langle l'0l0|20 \rangle \delta_{S1}\delta_{S'1} \\
\times \left( v_{t_0} + v_{tt} \left( 2T(T+1) - 3 \right) \right). \tag{A.58}
\]

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Finally, the two-body tensor force interaction matrix element has the form:

\[
\langle (j_a j_b) J MT M_T | V_T (1, 2) | (j_c j_d) J MT M_T \rangle_{\text{n.a.s.}} = \frac{\sqrt{6}}{\sqrt{1 + \delta_{ab}(1 + \delta_{cd})}} \sum_{LL'} \left( \begin{array}{cc} l_a & 1/2 \\ b_a & 1/2 \\ L & 1 & J \end{array} \right) \left( \begin{array}{cc} l_c & 1/2 \\ d_c & 1/2 \\ L' & 1 & J' \end{array} \right) \\
\times \sum_{n\Lambda n'L} \sum_{n'l'} \left( 1 - (-1)^{l+1+T} \right) \left( 1 - (-1)^{l'+1+T} \right) (-1)^{l+l'-L-L'} \\
\times \langle n_a l_a, n_b l_b : L | nl, \Lambda : L \rangle \langle n_c l_c, n_d l_d : L' | n'l', \Lambda : L' \rangle \\
\times U(\Lambda l J 1; L J) U(\Lambda' l' J 1; L' J) (-1)^{J+1} \left\{ \begin{array}{ccc} l & 1 & J \\ 1 & l' & 2 \end{array} \right\} \\
\times \langle n l | V_T | n'l' \rangle \hat{\mathbf{T}} (l' \ell l 0 | 20) \left[ v_{10} + v_{l} (2T(T+1) - 3) \right].
\] (A.59)

**A.4.3 Two-Body Spin-Orbit Force**

The two-body spin-orbit force is defined as in equation (3.29):

\[ V_{ls}(1, 2) = V_{ls}(r) \mathbf{i} \cdot \mathbf{S}. \] (A.60)

Implementing this expression in (A.49) gives:

\[
\langle (lS) J MT M_T | V_{ls}(r) \mathbf{i} \cdot \mathbf{S} | (l'S') J MT M_T \rangle = \langle (lS) J MT M_T | V_{ls} \frac{1}{2} (\mathbf{J} \cdot \mathbf{J} - \mathbf{i} \cdot \mathbf{S} \cdot \mathbf{S}) | (l'S') J MT M_T \rangle. \] (A.61)

Substitution of this equation into equation (A.51) gives as a final result:

\[
\langle (j_a j_b) J MT M_T | V_{ls}(1, 2) | (j_c j_d) J MT M_T \rangle_{\text{n.a.s.}} = \frac{1}{4 \sqrt{1 + \delta_{ab}(1 + \delta_{cd})}} \sum_{LL'S} \left( \begin{array}{cc} l_a & 1/2 \\ b_a & 1/2 \\ L & S & J \end{array} \right) \left( \begin{array}{cc} l_c & 1/2 \\ d_c & 1/2 \\ L' & S & J \end{array} \right) \\
\times \sum_{n\Lambda n'L} \sum_{n'l'} \left( 1 - (-1)^{l+S+T} \right)^2 (-1)^{L+L'} \\
\times \langle n_a l_a, n_b l_b : L | nl, \Lambda : L \rangle \langle n_c l_c, n_d l_d : L' | n'l', \Lambda : L' \rangle \\
\times \langle n l | V_{ls} | n'l' \rangle \\
\times \sum_{J} U(\Lambda l J S; L J) U(\Lambda l J S; L' J) \\
\times \left( J (J + 1) - S (S + 1) - l (l + 1) \right). \] (A.62)
B Some Special Interaction Properties

B.1 Delta-Interaction

The average matrix element, defined in (2.8), for the delta-interaction (3.35) shows some interesting properties. The starting point is the diagonal matrix element for the delta-interaction, based on expression (A.32):

\[
\langle j_\pi j_\nu; JM|V_\delta|j_\pi j_\nu; JM \rangle = -V_0(2j_\pi + 1)(2j_\nu + 1) \times \left[ (1 - 2\alpha - 2\alpha(-1)^J) \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & -1/2 & 0 \end{array} \right)^2 + \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & 1/2 & -1 \end{array} \right)^2 \right].
\]  

(B.1)

In order to calculate the average matrix element, some summation properties can be used:

\[
\sum_J (2J + 1) \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & -1/2 & 0 \end{array} \right)^2 = 1, \quad (B.2)
\]

\[
\sum_J (2J + 1) \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & 1/2 & -1 \end{array} \right)^2 = 1. \quad (B.3)
\]

In the calculations, the expression:

\[
\sum_J (-1)^J(2J + 1) \left( \begin{array}{ccc} j_\pi & j_\nu & J \\ 1/2 & -1/2 & 0 \end{array} \right)^2,
\]

also appears, for which no standard result exists in the literature on angular momentum algebra (e.g. [149]). It turns out that in the most general case, the expression vanishes, i.e.:

\[
\sum_J (-1)^J(2J + 1) \left( \begin{array}{ccc} j & j' & J \\ m & -m & 0 \end{array} \right)^2 = 0, \quad (B.5)
\]

due to the peculiar summation properties of the $3j$-symbols for any $m$-value:

\[
\sum_{J=\text{even}} (-1)^J(2J + 1) \left( \begin{array}{ccc} j & j' & J \\ m & -m & 0 \end{array} \right)^2 = \frac{1}{2}, \quad (B.6)
\]

\[
\sum_{J=\text{odd}} (-1)^J(2J + 1) \left( \begin{array}{ccc} j & j' & J \\ m & -m & 0 \end{array} \right)^2 = -\frac{1}{2}. \quad (B.7)
\]
Such summations over the odd or even values of the angular momentum appear quite often when evaluating matrix elements using angular momentum algebra. The resulting value for the average matrix element thus becomes:

\[ \overline{E}(J_{\pi},J_{\nu}) = -V_0 F^0 (1 - \alpha). \] (B.8)

Here, \( F^0 \) is the Slater integral, as encountered in expression (A.23). An important remark is that expression (B.8) for the average matrix element of the delta-interaction does not depend on the \( j \) quantum numbers of the orbitals, it only depends on the \( n \) and \( l \) quantum numbers through the Slater integral. Another important feature is that the spin-exchange term does not contribute to the average matrix element – the average matrix element for interactions of the form \( \vec{\sigma}_1 \cdot \vec{\sigma}_2 \) vanishes.

Based on relation (2.17), the average matrix element for a proton particle (hole) and a neutron hole (particle) has the form:

\[ \overline{E}(J_{\pi},J_{\nu}) = V_0 F^0 (1 - \alpha). \] (B.9)

The same remarks are valid.

### B.2 Multipole-Multipole Interaction

The average matrix element for any multipole-multipole interaction, and in particular the quadrupole-quadrupole interaction (3.36), identically becomes zero, since only the monopole part of the residual proton-neutron interaction contributes to the shift in the single-particle energies [100, 150]. This can be proven easily, given a general separable multipole residual interaction:

\[ V_{\pi \nu} = \sum_\lambda \chi_\lambda r_\pi^\lambda r_\nu^\lambda \vec{Y}_\lambda(\Omega_\pi) \cdot \vec{Y}_\lambda(\Omega_\nu). \] (B.10)

The proton-neutron two-body matrix elements for this interaction are given by:

\[ \langle j_{\pi} j_{\nu} ; J M | V_{\pi \nu} | j_{\pi} j_{\nu} ; J M \rangle = \sum_\lambda (-1)^{j_{\pi} + j_{\nu} + J} \chi_\lambda \left\{ \begin{array}{ccc} j_{\pi} & j_{\nu} & J \\ j_{\nu} & j_{\pi} & \lambda \end{array} \right\} \times \langle \pi || r_\pi^{J} \vec{Y}_\lambda^J(\Omega_\pi) || j_{\nu} \rangle \langle j_{\nu} || r_\nu^{J} \vec{Y}_\lambda^J(\Omega_\nu) || j_{\nu} \rangle. \] (B.11)

If one inserts the result (B.11) into the numerator of (2.8), one obtains:

\[ \sum_J (2J + 1) \langle j_{\pi} j_{\nu} ; J | V_{\pi \nu} | j_{\pi} j_{\nu} , J \rangle = \sum_J (2J + 1) \sum_\lambda (-1)^{j_{\pi} + j_{\nu} + J} \chi_\lambda \left\{ \begin{array}{ccc} j_{\pi} & j_{\nu} & J \\ j_{\nu} & j_{\pi} & \lambda \end{array} \right\} \times \langle \pi || r_\pi^{J} \vec{Y}_\lambda^J(\Omega_\pi) || j_{\nu} \rangle \langle j_{\nu} || r_\nu^{J} \vec{Y}_\lambda^J(\Omega_\nu) || j_{\nu} \rangle = \sum_J \sum_\lambda (2J + 1)(-1)^{j_{\pi} + j_{\nu} + J} \left\{ \begin{array}{ccc} j_{\pi} & j_{\nu} & J \\ j_{\nu} & j_{\pi} & \lambda \end{array} \right\} F(j_{\pi}, j_{\nu}, \lambda), \] (B.12)
with $F(j_\pi, j_\nu, \lambda)$ totally independent of $J$ and given by:

$$
F(j_\pi, j_\nu, \lambda) = \chi_\lambda \langle j_\pi || r_\pi^\lambda Y_\lambda(\Omega_\pi) || j_\nu \rangle \langle j_\nu || r_\nu^\lambda Y_\lambda(\Omega_\nu) || j_\nu \rangle. 
$$ (B.13)

Using the relation:

$$
\sum_J (2J + 1)(-1)^{j_\pi + j_\nu + J} \left\{ \begin{array}{ccc} j_\pi & j_\nu & J \\ j_\pi & j_\nu & \lambda \end{array} \right\} = \sqrt{(2j_\pi + 1)(2j_\nu + 1)} \delta_{\lambda 0}, 
$$ (B.14)

(B.12) reduces to:

$$
\sum_J (2J + 1) \langle j_\pi j_\nu, J | V_{\pi \nu} | j_\pi j_\nu, J \rangle = \sqrt{(2j_\pi + 1)(2j_\nu + 1)} F(j_\pi, j_\nu, \lambda = 0), 
$$ (B.15)

clearly demonstrating that only the monopole ($\lambda = 0$) component of a multipole-multipole force contributes to the average matrix element.
C Publications

The results presented in this work have been published and presented in the following papers:


D Nederlandstalige samenvatting

In dit werk hebben we ons gebogen over de vraag “Wat gebeurt er met de schillenstructuur van de atoomkern wanneer we de vallei van β-stabiliteit verlaten, en wat is het mechanisme achter de waargenomen veranderingen?”. Experimenteel en theoretisch onderzoek suggereert dat de ordening van de schillenmodel-ééndeeltjestoestanden (ook schillenstructuur genoemd) in atoomkernen met een groot proton- of neutronoverschot (de zogenaamde exotische atoomkernen) merkbaar kan afwijken van de gekende schillenstructuur in stabiele atoomkernen.

De referentiepunten bij het bestuderen van de schillenstructuur in de atoomkern zijn de magische getallen: dit zijn welbepaalde aantallen protonen en neutronen die resulteren in extra stabiliteit (verhoogde bindingsenergie of kleinere kernmassa) vergeleken met naburige atoomkernen. Deze magische getallen houden verband met een belangrijke aanname in de beschrijving van de atoomkern: we beschouwen de nucleonen (protonen en neutronen) als onafhankelijk bewegende fermionen in een centrale potentiaal. De link tussen deze onafhankelijk bewegende nucleonen in het gemiddeld veld van de atoomkern en de tweedeeltjesinteractie tussen de nucleonen die het veeldeeltjessysteem van de atoomkern bepalen, wordt gevormd door Hartree-Fock-theorie (HF-theorie). In HF-theorie start men van een tweedeeltjesinteractie, waarbij men met behulp van iteratieve en zelf-consistente methodes een gemiddeld veld afleidt. Deze techniek is erg geschikt voor atoomkernen waarvoor men een goede initiële benadering voor de tweedeeltjesinteractie heeft. Verlaat men echter de vallei van β-stabiele atoomkernen, dan zijn er veel minder experimentele gegevens beschikbaar om een goede interactie op te baseren. Hoe kunnen we dit probleem aanpakken?

Het schillenmodel van de atoomkern biedt ons een eenvoudige en elegante manier om de evolutie van de magische getallen te bestuderen, wanneer we onze aandacht verschuiven van de vallei van β-stabiele kernen naar de neutron- en protonrijke atoomkernen. We verwachten dat de schillenstructuur van de neutron- en protonrijke atoomkernen anders is dan die van de β-stabiele atoomkernen. Een belangrijke rol in de studie van de veranderingen wordt gespeeld door de proton-neutron residuelle tweedeeltjesinteractie, die een essentieel onderdeel uitmaakt van de Hamiltoniaan die de atoomkern beschrijft.

In hoofdstuk 2 tonen we aan dat de tweedeeltjesinteractie in de Hamiltoniaan kan geschreven worden als een som van multipooltermen. De monopoolterm in deze decompositie beschrijft de laagste-orde energiecorrectie van de ééndeeltjesenergie met veranderend proton- of neutronaantal. Deze laagste-orde correctie is niets anders dan de self-energiecorrectie van het proton (neutron) wanneer neutronen (protonen) de neutron-valentieruimte (proton-valentieruimte) opvullen (zie figuur D.1).

De evolutie van de ééndeeltjesenergie gecorrigeerd met de self-energie, ook wel monopoolver-
Figuur D.1: Figuur bovenaan: zelfenergie-correctie voor het protonorbitaal $j_\pi$ als functie van het veranderend neutronaantal $n_{j\nu}$, waarbij de neutronen verdeeld worden over de orbitalen $j_{\nu_1}, \ldots, j_{\nu_n}$. Figuur onderaan: de laagste-orde BCS-correctie voor de proton-één-deeltjesenergie $\epsilon_{j_\pi}$ houdt in dat de neutronen als gevolg van de paarkracht een distributie over de verschillende neutronorbitalen met een bezettingswaarschijnlijkheid $v_{j\nu}^2$ vertonen. Dit resultert in een ééndeeltjesenergie met een zelfenergie-correctie, of effectieve proton-ééndeeltjesenergie $\tilde{\epsilon}_{j_\pi}$.
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Dutch

The monopole shift, also known as the proton-neutron two-body interaction, is described by the following formula (in the case of the monopole shift of the proton-one-nucleon energy as a function of changing neutron number):

$$\varepsilon_{j_n} = \varepsilon_{j_n} + \sum_{j_v} \tilde{E}(j_{\pi},j_{\nu})n_{j_\nu}. \quad (D.1)$$

Hereby describes the effective proton-one-nucleon energy, $\varepsilon_{j_n}$ is the proton-one-nucleon energy of a proton-orbital net outside the double-magic core, $n_{j_\nu}$ is the number of neutrons in the neutron-orbital $j_\nu$, and $\tilde{E}(j_{\pi},j_{\nu})$ is the core matrix element:

$$\tilde{E}(j_{\pi},j_{\nu}) = \frac{\sum_{2J+1}(2J+1) \langle j_{\pi}j_{\nu}, J | V_{\pi\nu} | j_{\pi}j_{\nu}, J \rangle}{\sum_{2J+1}}. \quad (D.2)$$

We also bring in the effect of the lowest-order corrections caused by the isobaric force between the identical nucleons into account. We treat the isobaric force via the BCS method. Through this, a distribution of neutrons over the available orbitals $j_\nu$, described by specific occupation probabilities $v^2_{j_\nu}$.

Even using (D.1) for the proton-monopole shift, we obtain with a result:

$$\varepsilon_{j_n} = \varepsilon_{j_n} + \sum_{j_v} \tilde{E}_{j_{\pi},j_{\nu}}(2j_{\nu} + 1)v^2_{j_\nu}. \quad (D.3)$$

We compare the monopole shift, including the lowest-order pair corrections, with the energy centroids $E_{j_{\pi},j_{\nu}}$ calculated as a weighted average of energy eigenvalues $E^{(i)}(J)$ with the same spin and parity as the one-nucleon state, with the corresponding spectroscopic factor $S(J^{(i)}; j)$:

$$\bar{\varepsilon}_j \equiv \frac{\sum_{i} E^{(i)}(J) S(J^{(i)}; j)}{\sum_{i} S(J^{(i)}; j)}. \quad (D.4)$$

The theoretical energy-centroids are obtained by means of large-scale shell model calculations. As already mentioned, the residual proton-neutron two-body interaction plays a crucial role. In chapter 3 we give a brief description of the used nucleon-nucleon interactions in the study of the monopole shift in different mass regions. In particular, we focus on (i) microscopic effective interactions (based on the construction of the $G$-matrix associated with a given free nucleon-nucleon force), (ii) phenomenological effective interactions, and (iii) schematic two-body interactions. In this dissertation we use both $G$-matrix interactions (Kuo-Brown, Kuo-Herling, Hjorth-Jensen) and other schematic interactions (nul-dracht $\delta(\vec{r}_1 - \vec{r}_2)$-force, quadrupole force, and more general central two-body interactions, and also a two-body tensor- and spin-basis force).

In the above described model, we have applied to the study of the evolution of the one-nucleon energies (monopole shift) of the proton-orbitals (neutron-orbitals) as a function of changing neutron number (proton number), and this in different mass regions. Hereby we have our main attention on atom cores that do not belong to a
extra of ontbrekend nucleon verschillen van een dubbelmagische atoomkern; de laagst gelegen energietoestanden in zulke kernen bezitten het grootste deel van de ééndehoekjessterkte. De Cu-isotopen \((Z = 29)\), Bi-isotopen \((Z = 83)\) en de \(N = 51\) isotonen voldoen aan deze voorwaarde, en we vergelijken onze theoretische voorspellingen voor deze kernen met de beschikbare experimentele gegevens in respectievelijk hoofdstuk 4, 5 en 6. kracht en de deltakracht, dan zien we dat de multipletten in het begin van het \(\nu 1g9/2\) orbitaal een deeltjes-karakter vertonen, en de grondtoestand wordt gegeven door toestanden met een lage spin, zoals bijvoorbeeld \(3^-\) in \(^{70}\text{Cu}\). Wanneer het \(\nu 1g9/2\) orbitaal bijna volledig gevuld is met neutronen, zoals in \(^{78}\text{Cu}\), dan vertoont het multiplet eerder een gaten-karakter, en voorspellen de berekeningen voor de grondtoestand configuraties met een hogere spin, zoals \(6^-\) voor \(^{78}\text{Cu}\). De resultaten van grootschalige schillenmodelberekeningen komen over het algemeen vrij goed overeen met de theoretische resultaten bekomen door middel van de schematische interacties. Vergelijken we met de beschikbare experimentele gegevens, dan geven de theoretische berekeningen grondtoestanden met een iets hogere spin.

In hoofdstuk 5 bestuderen we de Bi-isotopen. We onderzoeken het effect van een microscopische effectieve interactie (gebaseerd op de \(G\)-matrix) en een deltakracht op de proton-monopoolverschuiving in de Bi-isotopen. De sterke en de spin-uitwisselingsparameter van de deltakracht worden gefit aan het experimentele spectrum van \(^{210}\text{Bi}\). We beschouwen de \(^{199–219}\text{Bi}\) -isotopen als een \(^{208}\text{Pb}\)-romp waaraan 1 proton in het \(\pi 1h9/2, \pi 2f7/2\) of \(\pi 1i13/2\) orbitalen gekoppeld is; de neutronen kunnen zowel deeltjes zijn \((N > 126)\) verdeeld over de \(\nu 2g9/2, \nu 1i11/2, \nu 1j15/2, \nu 3d5/2, \nu 4s1/2, \nu 2g7/2\) en \(\nu 3d3/2\) orbitalen, als gaten \((N < 126)\) verdeeld over de \(\nu 3p1/2, \nu 2f5/2, \nu 3p3/2, \nu 1i13/2, \nu 2f7/2\) en \(\nu 1h9/2\) orbitalen.

De deltakracht en de microscopische effectieve interactie vertonen een vrij grote gelijkenis qua verloop van de proton-monopoolverschuivingen voor \(N > 126\), maar geen van beide reproduceert de sterke daling van de \(7/2^-\) toestand (hoofdzakelijk \(\pi 2f7/2\)) die experimenteel wordt waargenomen. Vervolgens onderzoeken we het effect op de monopoolverschuivingen van een centrale kracht, bestaande uit een Wigner-term en een spin-isospin-uitwisselingsterm. De sterkte van de twee termen wordt arbitrair bepaald. Geen van beide termen afzonderlijk, noch de combinatie van de twee termen slaagt erin de geobserveerde systematische trends te reproduceren.

Op dezelfde manier als voor de Cu-isotopen onderzoeken we ook voor de oneven-\(^{210–218}\text{Bi}\)-kerne de structuur van de laagste multipletten. We beschouwen de evolutie van het proton \(1h9/2 – \text{neutron} 2g9/2\) multiplet (resulterend in toestanden met spin en pariteit \(J^\pi = 0^- – 9^-\)) als functie van het aantal neutronen in het \(\nu 2g9/2\) orbitaal. De neutronen worden ook hier beschreven als quasi-deeltjes. De effecten van een deltakracht, een kwadrupoolkracht en een microscopische effectieve interactie worden vergeleken met het experimenteel waargenomen verloop (waar mogelijk – zie tabel 5.1). Ook hier wordt de overgang van deeltje-deeltjestructuur naar deeltje-gatstructuur waargenomen. De multipletsplitsing geïnduceerd door de kwadrupoolkracht volgt, net zoals in de Cu-isotopen, een parabolisch verloop als functie van \(J(J + 1)\). Dit parabolisch verloop resulteert in isomere toestanden met vrij hoge \(J\)-waarde in de lichtere Bi-isotopen, wat overeenkomt met de experimentele waarnemingen. In de zwaardere \(^{216,218}\text{Bi}\) -isotopen zorgt dit voor een grondtoestand met een een hoge \(J^\pi (6^-, 7^-)\).
In hoofdstuk 6 bestuderen we de $N = 51$ isotonenreeks. Hierbij vertrekken we van de $^{88}$Sr-romp, en onderzoeken we de neutron-monopoolverschuiving als functie van veranderend protonaantal $28 \leq Z \leq 50$. Het neutron kan zich in het $2d_{5/2}$, $3s_{1/2}$, $2d_{3/2}$, $1g_{7/2}$ of $1h_{11/2}$ orbitala bevinden. De protonen zijn zowel deeltjes verdeeld over de orbitalen $1g_{9/2}$ en $2p_{1/2}$, als gaten verdeeld over de orbitalen $2p_{3/2}$ en $1f_{5/2}$. Het effect van een microscopische effectieve interactie, een deltakracht en een centrale interactie (Wigner-term en spin-isospin-uitwisselingsterm) op de neutron-monopoolverschuivingen wordt vergeleken met de experimentele resultaten (centroïden waar mogelijk – zie tabellen 6.1 en 6.2). De sterke en de spin-uitwisselingsparameter van de deltakracht worden bekomen via een fit aan het experimentele spectrum van $^{90}$Y. De sterktes van de termen in de centrale kracht worden arbitrair bepaald.

Op het eerste gezicht reproduceert de realistische effectieve interactie de experimenteel waargenomen trend in de monopoolverschuivingen vrij goed. Door een gebrek aan data voor $Z > 44$, en het feit dat de realistische effectieve interactie niet gedefinieerd is voor $N < 38$, is het echter moeilijk een uitspraak te doen over het verloop over een groter massagebied. De deltakracht reproduceert ook vrij goed de waargenomen evolutie in de monopoolverschuiving, behalve de opvallende afname in excitatie-energie van het $\nu 3s_{1/2}$ orbitala voor $Z < 40$. De Wigner-term in de centrale interactie reproduceert de sterke daling van het $\nu 1g_{7/2}$ orbitala wanneer protonen het $\pi 1g_{9/2}$ orbitala opvullen ($Z > 40$), maar geeft geen goede overeenkomst voor het verloop van de andere orbitalen. De spin-isospin-uitwisselingsterm $\tilde{\sigma}_1 \cdot \tilde{\sigma}_2 \tilde{\tau}_2 \cdot \tilde{\tau}_2$ reproduceert de sterke afname in excitatie-energie van het $\nu 3s_{1/2}$ orbitala voor $Z < 40$, maar geeft geen bevredigende resultaten voor de andere orbitalen. Een geschikte combinatie van deze twee termen in de centrale interactie reproduceert de experimenteel waargenomen trend vrij goed.

Tenslotte trachten we in hoofdstuk 7 de bekomen resultaten voor de monopoolverschuiving (variatie in proton- of neutron-ééndeeltjesenergie) voor $Z = 29$, $Z = 83$ en $N = 51$ meer algemeen te analyseren, gebruik makend van zowel microscopische effectieve interacties als meer schematische effectieve interacties. We merken op dat in het algemeen de $G$-matrix-kracht de experimentele energievorschuivingen vrij goed beschrijft. De studie van meer eenvoudige schematische interacties vertoont duidelijke tekortkomingen. Teneinde te analyseren welke specifieke componenten, aanwezig in de microscopische effectieve interacties, verantwoordelijk zijn voor deze verschillen, bestuderen we systematisch het gedrag van de set van 8 interacties: $\{1, \tilde{\sigma}_1 \cdot \tilde{\sigma}_2, S_{12}, \tilde{\Gamma} \cdot \tilde{S}\} \otimes \{1, \tilde{\tau}_1 \cdot \tilde{\tau}_2\}$. Op die manier zonderen we het generieke gedrag voor elk van deze termen af.

Uiteindelijk blijkt dat enkel de tensorkracht, inclusief de isospin-uitwisselingsterm, een aantal van de geobserveerde systematische veranderingen in de ééndeeltjesenergieën reproduceert. De tensorkracht vertoont bijzondere kenmerken voor welbepaalde combinaties van ééndeeltjesorbitalen. Het resultaat is dat proton-neutron-matrixelementen van het type $\langle j_\sigma^p j_{\zeta}^\nu \gamma_j^\nu, J|V|j_\sigma^p j_{\zeta}^\nu, J\rangle$ of $\langle j_\sigma^p j_{\zeta}^\nu, J|V|j_\sigma^p j_{\zeta}^\nu, J\rangle$ (met $j_\sigma^p = l^\pi + 1/2$ en $j_{\zeta}^\nu = l^\nu - 1/2$) in het algemeen meer aantrekkelijk zijn dan matrixelementen van het type $\langle j_\sigma^p j_{\zeta}^\nu, J|V|j_\sigma^p j_{\zeta}^\nu, J\rangle$ en $\langle j_\sigma^p j_{\zeta}^\nu, J|V|j_\sigma^p j_{\zeta}^\nu, J\rangle$ (zie ook figuur D.2). Dit effect wordt kwalitatief beschreven door een somregel voor monopoolverschuivingen van de twee neutron-spin-baan-partnerorbitalen $j_{\zeta}^\nu(=l^\nu + 1/2)$ en $j_{\zeta}^\nu(=l^\nu - 1/2)$, waarbij die monopoolver-
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Figuur D.2: Schematische illustratie van het effect van een proton in het orbitaal $j^\pi_z$ op de neutron $j'^\nu_z$- en $j'^\nu_x$-ééndeeltjesenergieën, veroorzaakt door de tweedeeltjestensorinteractie. De $j^\pi_x - j'^\nu_x$-interactie is afstotend; de $j^\pi_x - j'^\nu_z$-interactie is aantrekkend.

De schuiving veroorzaakt wordt door het vullen van het proton $j^\pi_x$-orbitaal ($l^\pi \neq l'^\nu$):

$$(2j'^\nu_x + 1)E(j^\pi_x j'^\nu_x) + (2j'^\nu_z + 1)E(j^\pi_z j'^\nu_z) = 0.$$  \hspace{1cm} (D.5)

Deze somregel is ook geldig wanneer protonen het $j^\pi_x$-orbitaal opvullen. De tensorkracht vertoont dezelfde eigenschappen als de spin-isospin-uitwisselingsterm van de centrale kracht, maar deze laatste voldoet niet aan de somregel (D.5). Vermits de experimentele resultaten lijken te voldoen aan de trend gesuggereerd door de tensorkracht, geeft dit een sterke aanwijzing voor de noodzaak tot het implementeren van de tweedeeltjes-tensorkracht in de beschrijving van de veranderende ééndeeltjesenergieën in een bepaald massagegebied. Dit wijst erop dat in het bijzonder de tweedeeltjes-tensorkracht effectief aanwezig is in de $G$-matrix, geconstrueerd als microscopische effectieve interactie in de verschillende massagebieden zoals bestudeerd in dit proefschrift.

Om te besluiten kunnen we zeggen dat we een gedetailleerde analyse hebben gemaakt van het mechanisme dat geobserveerd wordt in de veranderingen van de ééndeeltjesenergieën wanneer we exotische atoomkernen onderzoeken. We hebben aangetoond dat de monopoolverschuiving een interessante beschrijving van de geobserveerde effecten biedt, en we hebben ook aangetoond dat het noodzakelijk is om de tweedeeltjes-tensorkracht bij de beschrijving van gegevens over de atoomkernen te betrekken. Meer gegevens over spectroscopische factoren van ééndeeltjestoestanden in exotische atoomkernen zijn wenselijk, en gegevens over andere massagebieden zijn eveneens welkom. Ook zijn de relatieve bijdragen van de verschillende tweedeeltjesinteracties nog niet bepaald. Meer werk in deze
richting staat op het programma.
Bibliography


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