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Calculation of two-quasiparticle excitations of heavy nuclei

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Abstract

Two-quasiparticle excited states in heavy and superheavy nuclei are studied. The single-particle level structure is obtained in the frame of modified TCSM. The pairing correlations is treated at the BCS level. Special attention is given to the description of blocking effect. Where it is possible the results are compared with experimental data. For superheavy nuclei ^{258,260}Fm, ^{260,262,264}No two-quasiparticles states with high angular momentum are predicted.

1 Introduction

Investigation of properties of superheavy nuclei and newly discovered isotopes of known nuclei is one of actively developing areas of nuclear physics. The modern experimental techniques allow to gain an information not only on the characteristics of the ground state but also on the structure of the excitation spectra of exotic nuclei. Special interest is related to the study of low-lying two-quasiparticle excitations with high value of angular momentum as these excitations might lead to the long-lived isomeric states. Moreover the spectroscopic study of one- and two-quasiparticle states and isomers in the heaviest nuclei is up to date because of the problem of unambiguous identification of new superheavy nuclei.

With the growth experimental interest to this problem, the requirement for theoretical predictions appears. There are many different models which are suited to describe excited spectra of heavy nuclei. One can note, for example, various realizations of mean field and shell models [1, 2]. Among them it is worth to emphasize the microscopic-macroscopic approach based on the two-center shell model (TCSM) [3] as one of the most efficient and developed models dealing with structure of superheavy nuclei. The parameteres of this approach were set so to describe the spins and parities of the ground state of known heavy nuclei (the rare earth nuclei, actinides, and superheavy nuclei). This modification was made to improve its predictive power of the model in the region of interest.

In this work we study two-quasiparticle excitations in various isotopes of Yb, Hf, W, Os, Pt, Hg, Fm, No elements. The modified TCSM was used to obtain the single-particle level structure and ground state shape parametrization of chosen nuclei. The pairing was described at the BCS level and the excitations are built from the independent quasiparticles. The blocking effect was taken into account explicitly. Two-quasiparticle excitations with the high angular momentum values were calculated and compared with experiment.

2 Theoretical background

This work is based on the microscopic-macroscopic method. First the shape parameters of the ground state was defined using the TCSM. For these parameters the single-particle spectrum of the corresponding nucleus was calculated. Using these single-particle spectra the equations of independent quasiparticle models of Soloviev [4, 5] was solved for the ground state and for the lowest two-quasiparticle excitations. In the description of two-quasiparticle excitations the blocking effect was taken into account. The details of each step of the calculations are presented below.

2.1 Two center shell model

For calculation of single particle energy spectrum used in this work two center shell model (TCSM) is used.

Two-center shell model allows us to calculate the potential energy surface and describe the nuclear shape from the ground state to formation of two fission fragments using the following set of collective coordinates: $\lambda = l/(2R_0), \eta, \epsilon, \beta_1, \beta_2$. The elongation $\lambda = l/(2R_0)$ measures the length l of the system in units of the diameter $2R_0$ of the spherical nucleus. The transition of the nucleons through the neck is described by the mass asymmetry η. The neck parameter $\epsilon = E_0/E'$ is defined by the ratio of the actual barrier height E_0 to the barrier height E' of the two-center oscillator. The deformations $\beta_i = a_i/b_i$ of axial symmetric fragments are defined by the ratio of their semiaxes (Figure1). For compact nuclear shapes near the ground state, one can set $\epsilon = 0$ and $\eta = 0$. Hence, there are only three parameters: λ, β_1, and β_2 to describe the deformations of various multipolarities. The case of $\beta_1 = \beta_2 = \beta$, which is treated to obtain single particle energy spectrum used here, means the absence of the static deformations of odd multipolarities [6].

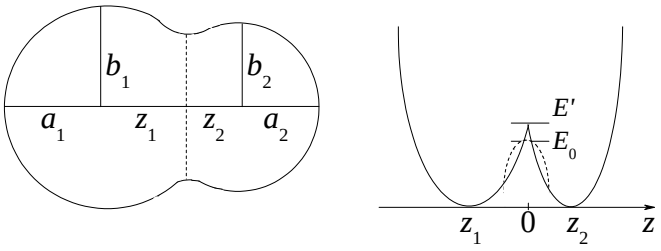


Figure 1: The potential along the z-axis and the associated nuclear shape. The designations of the geometrical quantities have been indicated and the definition of the parameter $\epsilon = E'/E_0$ is explained.

The single-particle Hamiltonian in this model is written in cylinder coordinates and has the spin-orbital term and l^2-term as usual for the Nilsson-type model.

$$H = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\rho, z) + V_{LS} + V_{l^2}, \tag{1}$$

where single particle potential $V(\rho, z)$ is parametrized for symmetric nucleus near the ground state [7].

2.2 Pairing correlations

Treating of the pairing correlations is very important. As it is well known the pairing interaction strongly affects the structure of an atomic nucleus. This interaction manifests itself in many different aspects. One of the clearest signatures of that are the lowering of energies of even-even nuclei with

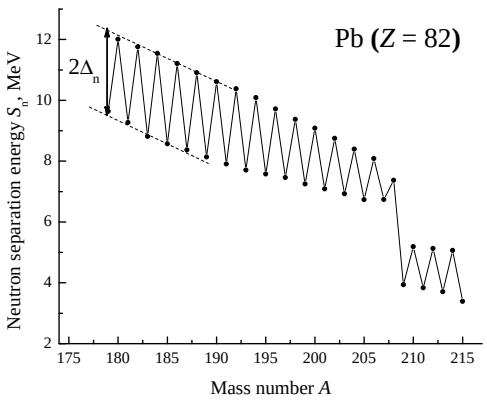


Figure 2: Neutron separation energy dependence on the mass number in Pb isotopes.

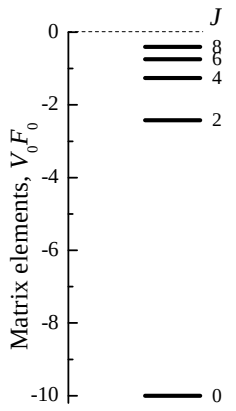


Figure 3: The two-body interaction matrix elements.

respect to their odd-mass neighbors and that the values of spin and parity for all even–even nuclei in the ground state are $J^P = 0^+$.

The pairing is the short-range part of the nuclear residual interaction. Let us consider the Hamiltonian with the pair interaction between nucleons [4, 5]:

$$H_0 = H_{av} + H_{pair}. \tag{2}$$

Neutron and proton systems are considered independently, so (2) can be written as

$$H_0 = H_0(p) + H_0(n). \tag{3}$$

Because of that we are considering here only neutron systems. Expressions for proton systems can be obtained in complete analogy.

Nucleon pairing is the additional attraction between two nucleons of the same type. The attraction lowers their total energy by an amount $2\Delta_n$, where Δ_n is called the pairing gap or the odd-even staggering (OES). The excitation corresponding one broken pair has the pairing energy $2\Delta_n$ above the ground state and the same value is between even-even and odd-even mass surfaces or difference in nucleon separation energies of adjacent nuclei (Figure2).

The residual interaction responsible for coupling to angular momentum zero must thus be attractive and of short range to provide the desired correlation. Using, for example, an attractive δ-function interaction in fact produces a spectrum in which the energy depends on the total angular momentum J and the state with $J = 0$ is the lowest [8]. As an example, consider the two-particle interaction of identical nucleons ($S = 0$, $T = 1$) in the $j = 9/2$ shell by using the δ-potential (see AppendixA,[9]). The two-nucleon interaction matrix element is given by

$$\langle \Psi | \hat{V}_{int} | \Psi \rangle = -V_0 F_0 (2j+1)^2 \begin{pmatrix} j & j & J \\ 1/2 & -1/2 & 0 \end{pmatrix}^2, \tag{4}$$

Table 1: The two-body interaction matrix elements for different values of the total angular momentum J

J	0	2	4	6	8
Matrix Elements	-10	-2.42	-1.26	-0.76	-0.40

where $V_0 = const$ – amplitude of interaction, F_0 is the radial integral and it is not depend on j and J. J can be only even because of the Pauli exclusion principle: $J = 0,\ 2,\ ...\ 2j-1$. So one can calculate the part of matrix element which depends on angular momenta.

As can be seen from Table1 and Figure3, the interaction for the $J = 0$ pair is much stronger than for the $J \neq 0$ pairs. This suggests that we may simplify the interaction in a single j shell by making the approximation that only the $J = 0$ channel contributes.

The Hamiltonian of the pair interaction in general form is written as

$$H = \sum_{f,f'} T'(f,f') a^\dagger_f a_{f'} - \frac{1}{4} \sum_{f_1 f_2 f'_1 f'_2} G(f_1, f_2; f'_2, f'_1) a^\dagger_{f_1} a^\dagger_{f_2} a_{f'_2} a_{f'_1}, \tag{5}$$

where f is the complex of all quantum numbers which are describing nucleon state. From the quantum numbers it is necessary to extract $\sigma = \pm 1$. States with different signs of σ are conjugate under the reflection time operation. It could be sign of moment projection on the symmetry axis of the nucleus for instance.

With the abbreviation $G(f_1, f_2; f'_2, f'_1) \equiv G_N$ we have the pure pairing interaction ($J = 0$ state on Figure3), or just the pairing interaction, H_{pair} for a single j shell as [10]

$$H_{pair} = -G_N \sum_{s,s'} a^\dagger_{s+} a^\dagger_{s-} a_{s'-} a_{s'+} \tag{6}$$

2.3 Equations

We consider as a starting point of the single particle energies Fermi energy level. Then (5) become

$$H_0(n) = \sum_{s\sigma} (E_0(s) - \epsilon_F) a^\dagger_{s\sigma} a_{s\sigma} - G_N \sum_{s,s'} a^\dagger_{s+} a^\dagger_{s-} a_{s'-} a_{s'+}, \tag{7}$$

The nucleon number conservation condition must be also imposed:

$$N = \sum_{s\sigma} \langle \Psi | a^\dagger_{s\sigma} a_{s\sigma} | \Psi \rangle, \tag{8}$$

where $\langle \Psi | ... | \Psi \rangle$ means averaging for considered state. Creation and annihilation operators obey the relations:

$$a^\dagger_{s\sigma} a_{s'\sigma'} + a_{s'\sigma'} a^\dagger_{s\sigma} = \delta_{ss'} \delta_{\sigma\sigma'}, \tag{9}$$

$$a_{s\sigma} a_{s'\sigma'} + a_{s'\sigma'} a_{s\sigma} = 0, \tag{10}$$

$$a^\dagger_{s'\sigma'} a^\dagger_{s\sigma} + a^\dagger_{s\sigma} a^\dagger_{s'\sigma'} = 0. \tag{11}$$

Let us commit a linear canonical transformation corresponding to transition from particle operators to quasiparticle operators:

$$a_{s\sigma} = u_s\alpha_{s,-\sigma} + \sigma v_s\alpha^{\dagger}_{s\sigma}, \tag{12}$$

$$a^{\dagger}_{s\sigma} = u_s\alpha^{\dagger}_{s,-\sigma} + \sigma v_s\alpha_{s\sigma}, \tag{13}$$

where u_s, v_s – real functions. Operators $\alpha^{\dagger}_{s,\sigma}$, $\alpha_{s',\sigma'}$ must obey the same relations (9)–(11):

$$\begin{aligned}\delta_{ss}\delta_{\sigma\sigma} = (u_s\alpha^{\dagger}_{s,-\sigma} + \sigma v_s\alpha_{s\sigma})(u_s\alpha_{s,-\sigma} + \sigma v_s\alpha^{\dagger}_{s\sigma}) + (u_s\alpha_{s,-\sigma} + \sigma v_s\alpha^{\dagger}_{s\sigma})(u_s\alpha^{\dagger}_{s,-\sigma} + \\ +\sigma v_s\alpha_{s\sigma}) = u_s^2(\alpha^{\dagger}_{s-\sigma}\alpha_{s-\sigma} + \alpha_{s-\sigma}\alpha^{\dagger}_{s-\sigma}) + v_s^2\sigma^2(\alpha_{s\sigma}\alpha^{\dagger}_{s\sigma} + \alpha^{\dagger}_{s\sigma}\alpha_{s\sigma}) = \\ = u_s^2\delta_{-\sigma-\sigma} + v_s^2\delta_{\sigma\sigma} = 1.\end{aligned} \tag{14}$$

It follows that u_s, v_s must satisfy the condition

$$\eta_s = u_s^2 + v_s^2 - 1 = 0. \tag{15}$$

Suppose that the ground state of the even neutron number system is quasiparticle vacuum. Then the wave function of this state:

$$\alpha_{s\sigma}|\Psi_0\rangle = 0, \langle\Psi_0|\alpha^{\dagger}_{s\sigma} = 0, \tag{16}$$

for any $s\sigma$.

To find the average value of $H_0(n)$ under the Ψ_0-state one need to calculate $\langle\Psi_0|a^{\dagger}_{s\sigma}a_{s\sigma}|\Psi_0\rangle$ and $\langle\Psi_0|a^{\dagger}_{s+}a^{\dagger}_{s-}a_{s'-}a_{s'+}|\Psi_0\rangle$:

$$\begin{aligned}\langle\Psi_0|a^{\dagger}_{s\sigma}a_{s\sigma}|\Psi_0\rangle = \langle\Psi_0|(u_s\alpha^{\dagger}_{s,-\sigma} + \sigma v_s\alpha_{s\sigma})(u_s\alpha_{s,-\sigma} + \sigma v_s\alpha^{\dagger}_{s\sigma})|\Psi_0\rangle = \\ = /\text{using (16)}/ = v_s^2\langle\Psi_0|\alpha_{s\sigma}\alpha^{\dagger}_{s\sigma}|\Psi_0\rangle = v_s^2,\end{aligned} \tag{17}$$

$$\begin{aligned}\langle\Psi_0|a^{\dagger}_{s+}a^{\dagger}_{s-}a_{s'-}a_{s'+}|\Psi_0\rangle = u_sv_su_{s'}v_{s'}\underbrace{\langle\Psi_0|\alpha_{s+}\alpha^{\dagger}_{s+}\alpha_{s'+}\alpha^{\dagger}_{s'+}|\Psi_0\rangle}_{=1} + \\ +v_s^2v_{s'}^2\langle\Psi_0|\alpha_{s+}\alpha_{s-}\alpha^{\dagger}_{s'-}\alpha^{\dagger}_{s'+}|\Psi_0\rangle - u_sv_sv_{s'}^2\langle\Psi_0|\alpha_{s+}\alpha^{\dagger}_{s+}\alpha^{\dagger}_{s'-}\alpha^{\dagger}_{s'+}|\Psi_0\rangle - \\ -u_{s'}v_{s'}v_s^2\langle\Psi_0|\alpha_{s+}\alpha_{s-}\alpha_{s'+}\alpha^{\dagger}_{s'+}|\Psi_0\rangle = u_sv_su_{s'}v_{s'} + \delta_{ss'}v_s^4.\end{aligned} \tag{18}$$

Then the average value of (7) can be written as

$$\langle\Psi_0|H_0(n)|\Psi_0\rangle = 2\sum_s(E_0(s) - \epsilon_F)v_s^2 - G_N\Big(\sum_s u_sv_s\Big)^2 - G_N\sum_s v_s^4. \tag{19}$$

One need to make the renormalization of the single-particle energy values $E(s) = E_0(s) - \frac{G_N}{2}v_s^2$. Therefore (19) become

$$\langle\Psi_0|H_0(n)|\Psi_0\rangle = 2\sum_s(E(s) - \epsilon_F)v_s^2 - G_N\Big(\sum_s u_sv_s\Big)^2. \tag{20}$$

Determine functions u_s, v_s from the minimum condition of (20) by using the variational principle. There is connection (15) between them hence it is necessary to introduce additional

Lagrange multiplier μ_s. Then variations δu_s and δv_s can be considered independently. Extremum condition is written as

$$\delta\Big\{\langle\Psi_0|H_0(n)|\Psi_0\rangle + \sum_s \mu_s\eta_s\Big\} = 0. \tag{21}$$

After the variation one obtain two equations

$$4(E(s)-\epsilon_F)v_s - 2G_N u_s \sum_{s'} u_{s'}v_{s'} - 2\mu_s v_s = 0, \tag{22}$$

$$-2G_N v_s \sum_{s'} u_{s'}v_{s'} - 2\mu_s u_s = 0. \tag{23}$$

Now we need to exclude μ_s: $u_s(22) - v_s(23)$. We obtain equation

$$2(E(s)-\epsilon_F)u_s v_s - G_N(u_s^2 - v_s^2)\sum_{s'} u_{s'}v_{s'} = 0, \tag{24}$$

which must be supplemented by equation

$$N = 2\sum_s v_s^2. \tag{25}$$

The value $2v_s^2$ is the particle density of the s state and the value $2u_s^2 = 2(1-v_s^2)$ is the hole density. The equation (24) has two solutions: $u_s v_s = 0$ and $u_s v_s \neq 0$. We will consider only the second one. Introduce correlation function (pairing gap):

$$\Delta_n = G_N \sum_s u_s v_s, \tag{26}$$

and define u_s and v_s functions as

$$u_s^2 = \frac{1}{2}\Big(1 + \frac{E(s)-\epsilon_F}{\varepsilon(s)}\Big), \tag{27}$$

$$v_s^2 = \frac{1}{2}\Big(1 - \frac{E(s)-\epsilon_F}{\varepsilon(s)}\Big). \tag{28}$$

Substitute (26), (27), (28) in (24) and obtain

$$u_s v_s = \frac{1}{2}\frac{\Delta_n}{\varepsilon(s)}. \tag{29}$$

On the other hand, from (27), (28) one can see that

$$u_s^2 v_s^2 = \frac{1}{4}\frac{\varepsilon(s)^2 - (E(s)-\epsilon_F)^2}{\varepsilon(s)^2}. \tag{30}$$

From (29) and (30) it can be obtained that

$$\varepsilon(s) = \sqrt{\Delta_n^2 + (E(s)-\epsilon_F)^2}. \tag{31}$$

From substitution (29) in (26) and taking into account (25) there is the system of equations for defining Δ_n and ϵ_F:

$$1 = \frac{G_N}{2} \sum_s \frac{1}{\sqrt{\Delta_n^2 + (E(s) - \epsilon_F)^2}}, \tag{32}$$

$$N = \sum_s \Big(1 - \frac{E(s) - \epsilon_F}{\sqrt{\Delta_n^2 + (E(s) - \epsilon_F)^2}}\Big). \tag{33}$$

Using (20) and (26) obtain the expression for ground state energy of the system:

$$\mathscr{E}_0^n = \sum_s 2E(s)v_s^2 - \frac{\Delta_n^2}{G_N}. \tag{34}$$

These equations were carried out in [4, 5].

2.4 Blocking effect

Basic equations derived in the previous section (32), (33) however need to be clarified for the quasiparticle excited states by strict taking into account the Pauli exclusion principle and the requirement of particle number conservation in average. It means that the presence of the unpaired particles affects on the superfluid properties of the system. This influence has been called blocking effect. Double-degenerate level at which there is one nucleon is excluded from consideration since filling levels is taking place by nucleon pairs, or the level is blocked. With the effect taking into account it is necessary to solve the variational problem for each of the excited states of the system. It boils down to that the calculation of the properties of certain states, the levels at which there are quasiparticles are not taken into account. For a system consisting of an odd neutron number equations take the form

$$1 = \frac{G_N}{2} \sum_{s \neq s_2} \frac{1}{\sqrt{\Delta_n^2(s_2) + (E(s) - \epsilon_F(s_2))^2}}, \tag{35}$$

$$N = 1 + \sum_{s \neq s_2} \Big(1 - \frac{E(s) - \epsilon_F(s_2)}{\sqrt{\Delta_n^2(s_2) + (E(s) - \epsilon_F(s_2))^2}}\Big), \tag{36}$$

where s_2 is the excluded state – for ground state it is F-state and for the first excited state it is $(F+1)$-state (see Figure4). Hence the expression for energy changes too:

$$\mathscr{E}_0(s_2) = E(s_2) + \sum_{s \neq s_2} 2E(s)v_s^2(s_2) - \frac{\Delta_n^2(s_2)}{G_N}. \tag{37}$$

To find the energy of quasiparticle excitation on the Figure4 one need to subtract energies for F- and $(F+1)$-states:

$$E^*(F \to F+1) = \mathscr{E}_0(F+1) - \mathscr{E}_0(F). \tag{38}$$

Consider even-even nuclei. In this case equations for ground state stay the same (32), (33). But for excited state which corresponds to breaking of nucleon pair there will be two excluded states s_1, s_2, $s_1 \neq s_2$ (see Figure5). Equations for excited state take the form

$$1 = \frac{G_N}{2} \sum_{s \neq s_1, s_2} \frac{1}{\sqrt{\Delta_n^2(s_1, s_2) + (E(s) - \epsilon_F(s_1, s_2))^2}}, \tag{39}$$

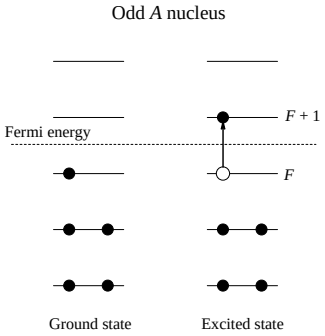


Figure 4: Formation of excited state in odd A nucleus.

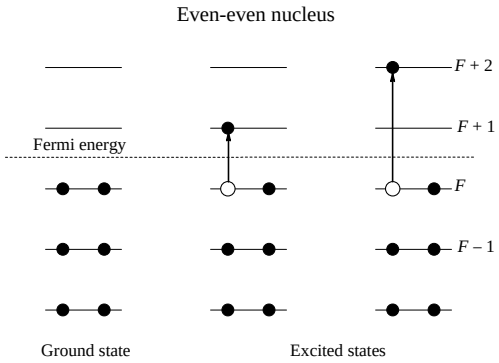


Figure 5: Formation of excited state in even-even nucleus.

$$N = 2 + \sum_{s \neq s_1, s_2} \Big(1 - \frac{E(s) - \epsilon_F(s_1, s_2)}{\sqrt{\Delta_n^2(s_1, s_2) + (E(s) - \epsilon_F(s_1, s_2))^2}}\Big), \tag{40}$$

And the energy of the certain state $s_1 \to s_2$

$$\mathscr{E}_0(s_1, s_2) = E(s_1) + E(s_2) + \sum_{s \neq s_1, s_2} 2E(s) v_s^2(s_1, s_2) - \frac{\Delta_n^2(s_1, s_2)}{G_N}. \tag{41}$$

s_1, s_2 can take different values $F \pm i$, $i = 0, 1, 2,...$ The more i is, the more excited energy is. Energies of quasiparticle excitations are determined by the difference

$$E^*(s_1 \to s_2) = \mathscr{E}_0(s_1, s_2) - \mathscr{E}_0^n, \tag{42}$$

where $\mathscr{E}_0^n$ is defined by (34).

3 Realization

Even-even nuclei and two quasiparticle neutron excitations were considered. Solving equations (39) and (40) was carried out by using *Wolfram Mathematica*.

First nuclear parameters (mass number `A`, proton number `Z` and neutron number `n=A-Z`), parameter `Gn = const/A` and single particle spectrum ϵ`n` (which is calculated from the modified TCSM, see Appendix2.1) are introduced. Next one can find the last filled level. For nucleus with even neutron number that is:
`F` = `n/2`;

Levels which will be subsequently excluded from consideration `s1`, `s2` are defined regarding to `F` level:
`s1` = `F`;
`s2` = `F` + `1`;

Equations for ground state are

$\texttt{f10} = \sum_{\texttt{k=1}}^{\texttt{Nn}} \frac{1}{\texttt{EqpN[[k]]}} - \frac{2}{\texttt{Gn}} == 0;$

$\texttt{f20} = (\texttt{A} - \texttt{Z}) - \sum_{\texttt{k=1}}^{\texttt{Nn}} (1 - \frac{\epsilon\texttt{n[[k]]} - \texttt{Ln}}{\texttt{EqpN[[k]]}}) == 0;$

where the table of energies (31) $\texttt{EqpN} = \texttt{Table}[\sqrt{(\epsilon\texttt{n[[j]]} - \texttt{Ln})^2 + \texttt{Dn}^2/\texttt{Gn}};, \{\texttt{j}, 1, \texttt{Nn}\}]$ is introduced for ease, $\texttt{Nn} = \texttt{Length}[\epsilon\texttt{n}]$ and Ln is the Fermi energy level. For excited state we must to exclude two levels:

$\texttt{f11} = \sum_{\texttt{k=1}}^{\texttt{Nn}} \frac{1}{\texttt{EqpN[[k]]}} - \frac{1}{\texttt{EqpN[[s1]]}} - \frac{1}{\texttt{EqpN[[s2]]}} - \frac{2}{\texttt{Gn}} == 0;$

$\texttt{f21} = (\texttt{A} - \texttt{Z} - 2) - \sum_{\texttt{k=1}}^{\texttt{Nn}} (1 - \frac{\epsilon\texttt{n[[k]]} - \texttt{Ln}}{\texttt{EqpN[[k]]}}) + (1 - \frac{\epsilon\texttt{n[[s1]]} - \texttt{Ln}}{\texttt{EqpN[[s1]]}}) + (1 - \frac{\epsilon\texttt{n[[s2]]} - \texttt{Ln}}{\texttt{EqpN[[s2]]}}) == 0;$

Solutions are found by using `FindRoot`. `Dn` is the unknown pairing gap Δ_n. `Ln00`, `Dn00` are the solutions for ground state. The value of `Dn00` must be equal to the corresponding result of calculation in the modified TCSM (see Appendix2.1). To do this one need to print the value `Dn00`. Satisfaction of this condition is accomplished by changing constant `Gn`. For ground state:

```
wn00 = FindRoot[f10,f20, Ln, 40, 60, Dn, -0.60, 0.60,MaxIterations -> 500,
AccuracyGoal -> 8];
Ln00 = wn00[[1, 2]];
Print["Dn gr st"]
Dn00 = Abs[wn00[[2, 2]]]
```

As a result of this part of the program we have the constant G_n, the ground state pairing gap Δ_n, the Fermi energy level ϵ_F, the ground state energy $\mathscr{E}_0^n$ and the excitation without taking into account blocking effect $E^*(s_1 \to s_2)$:

```
Dn gr st
0.932768
```

$\texttt{EqpN00} = \texttt{Table}[\sqrt{(\epsilon\texttt{n[[j]]} - \texttt{Ln00})^2 + \texttt{Dn00}^2/\texttt{Gn}};, \{\texttt{j}, 1, \texttt{Nn}\}];$

$\texttt{En00} = \sum_{\texttt{s=1}}^{\texttt{Nn}} \epsilon\texttt{n[[s]]}(1 - \frac{\epsilon\texttt{n[[s]]} - \texttt{Ln00}}{\texttt{EqpN00[[s]]}}) - \texttt{Dn00}^2/\texttt{Gn};$`(*ground state energy*)`

`Eexc=EqpN00[[s1]]+EqpN00[[s2]];(*excitation without blocking*)`

The same procedure takes place for excited state. Here the solutions of equations are denoted `Ln01, Dn01`. And for excited state energy we have

$\texttt{En01} = \sum_{\texttt{s=1}}^{\texttt{Nn}} \epsilon\texttt{n[[s]]}(1 - \frac{\epsilon\texttt{n[[s]]} - \texttt{Ln01}}{\texttt{EqpN01[[s]]}}) - \epsilon\texttt{n[[s1]]}(1 - \frac{\epsilon\texttt{n[[s1]]} - \texttt{Ln01}}{\texttt{EqpN01[[s1]]}}) - \epsilon\texttt{n[[s2]]}(1 - \frac{\epsilon\texttt{n[[s2]]} - \texttt{Ln01}}{\texttt{EqpN01[[s2]]}}) +$

$+\epsilon\texttt{n[[s1]]} + \epsilon\texttt{n[[s1]]} - \texttt{Dn01}^2/\texttt{Gn};$

or simpler

$\texttt{En01} = \sum_{\texttt{s=1}}^{\texttt{Nn}} \epsilon\texttt{n[[s]]}(1 - \frac{\epsilon\texttt{n[[s]]} - \texttt{Ln01}}{\texttt{EqpN01[[s]]}}) + \epsilon\texttt{n[[s1]]}(\frac{\epsilon\texttt{n[[s1]]} - \texttt{Ln01}}{\texttt{EqpN01[[s1]]}}) + \epsilon\texttt{n[[s2]]}(\frac{\epsilon\texttt{n[[s2]]} - \texttt{Ln01}}{\texttt{EqpN01[[s2]]}}) - \texttt{Dn01}^2/\texttt{Gn};$

Hence the excited state energy with taking into account blocking effect is

```
Eexc_bl = En01 - En00;
```

Table 2: For nuclei $N = 94$.

Nucleus $^A\mathrm{X}(N = 94, Z)$	$F \to F+1$	$F \to F+2$	$F-1 \to F+1$	$F-1 \to F+2$
$^{158}\mathrm{Gd}(94, 64)$	0.58	0.64	0.64	0.68
$^{160}\mathrm{Dy}(94, 66)$	0.56	0.61	0.69	0.70
$^{162}\mathrm{Er}(94, 68)$	0.54	0.62	0.68	0.69
[4]	0.65	0.67	0.65	0.67

To check how the program works one can look at how calculated particle and hole number

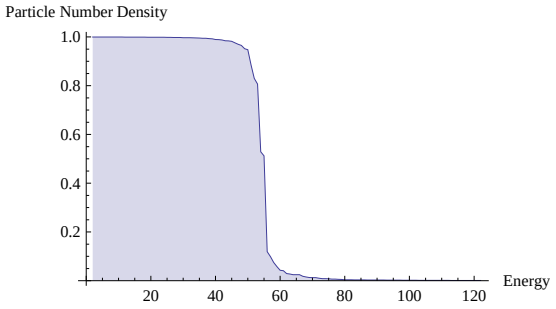


Figure 6: Particle number density dependence v_s^2 on the energy.

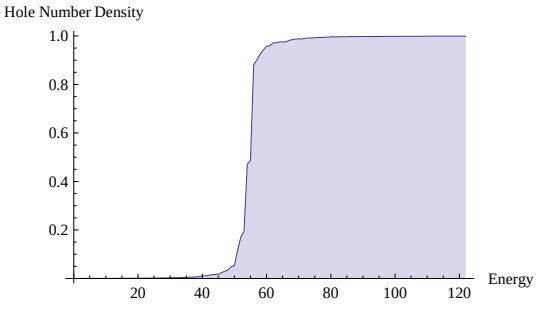


Figure 7: Hole number density dependence u_s^2 on the energy.

Table 3: For nuclei $N = 96$.

Nucleus ^{A}X$(N = 96, Z)$	$F \to F+1$	$F \to F+2$	$F-1 \to F+1$	$F-1 \to F+2$
^{160}Gd$(96, 64)$	0.45	0.63	0.54	0.66
^{162}Dy$(96, 66)$	0.60	0.62	0.61	0.62
^{164}Er$(96, 68)$	0.61	0.65	0.63	0.66
[4]	0.56	0.70	0.58	0.70

densities depend on the energy. It is clearly seen from Figure6 and Figure7 that according to (27) and (28) $u_s^2 + v_s^2 = 1$.

To test excitation energy calculations taking into account blocking effect comparison with the results [4] was carried out. The relations of the correlation functions of two-quasiparticle states to the ground states Δ_n^*/Δ_n are presented on Table2 and Table3, where $F_1 \to F_2$ denotes the considered transition. In [4] corresponding relations are given for deformed nuclei with $\beta_0 = 0.3$. Deviation can be related to difference of considered single particle energy spectrum or constant G_n.

4 Results

Our model was applied to the various isotopes of Yb, Hf, W, Os, Pt, Hg, Fm, No elements. The results of calculations are presented on Figures 8-12 and in Table 4. As one can see energies of two-quasiparticle excitations obtained in our calculations are close to the experimental data.

It is important to emphasize that the inclusion of blocking effect significantly improves the results. As it was shown in [6] if the blocking effect is neglected the calculation overestimates the energies of these states. On Figure 8 the energies of two-quasiparticle states for ^{182,184}Hf, ^{190,192}Hg are shown both with and without blocking. Experimental energies are denoted by crosses (here and further experimental data are from [11, 12]), "2qp" means calculated two quasiparticle excitations without blocking effect and "2qp+bl" means corresponding energies with blocking effect. There are values of used constant G_nA, pairing gap for ground state Δ_n and pairing gap for excited state $(F \to F+1)$ Δ_n^* under the spectra.

One can see that taking into account blocking effect improves results and deviation from

experimental data become smaller. Blocking reduces energies of two-quasiparticle excitations approximately on 30%. This reduction is in agreement with phenomenological value used in [3]. The reason for this is the decrease of the correlation function Δ_n in case of blocking the levels close to the Fermi surface.

In general results of calculations are in a quite agreement with experiment. The same can be observed on Figure9, Figure10 and Figure11. Figure12 a) shows the spectrum of ^{256}Fm – experimental data and calculated energies. For isotopes ^{258,260}Fm and ^{260,262,264}No there is no experimental data, so one can make some predictions by using model discussed above. Results are presented on Figure12 b).

It is interesting that the change of Δ_n^* is strongly different from nucleus to nucleus. In some cases there are vanishing correlation function Δ_n^* of excited states ($F \to F+1$) (Table4). One of possible explanations could be the irregularities of the single particle spectrum in the vicinity of the Fermi surface.

For example as one can see from Figure 13 these irregularities lead to the sparse single-particle spectra for W isotopes. In these isotopes the correlation functions of excited states are close to zero.

The effect of irregularities of single-particle spectra is especially pronounced on the Figure 14 for isotopes of Hf. For ^{176,178,180}Hf the spectra around the Fermi surface are less dense than in average. As a result blocking leads to the significant reduction of Δ_n. Oppositely in ^{182}Hf, spectrum is more dense than in average and the effect of blocking is weaker. Isotope ^{184}Hf represents the intermediate case.

The strong changes of the correlation functions due to the blocking effect doesn't lead however to drastic changes in the energies of two-quasiparticle excitations. These energies vary much smoother comparing with the Δ_n and the deviation between theory and experiment does not increase (see Figure15).

The influence of spectra irregularities on the correlation function is obvious in the seniority model. This model deals with the situation when N particles located on the shell consists of 2Ω degenerate states. According to this model [9] the correlation function can be written as

$$\Delta_n \sim \sqrt{\frac{N}{2\Omega}}\sqrt{1-\frac{N}{2\Omega}}. \tag{43}$$

It is seen from (43), Δ_n is largest when the shell is half filled ($N = \Omega$) and is the weakest when the shell is completely filled or empty ($N = 2\Omega, 0$, respectively). In the single particle energy spectrum completely filled shell is equivalent to presence of energy gap. Therefore from Figure14 can be seen that blocking effect contributes to the presence of the gap $\sim$1.5 MeV.

5 Conclusions

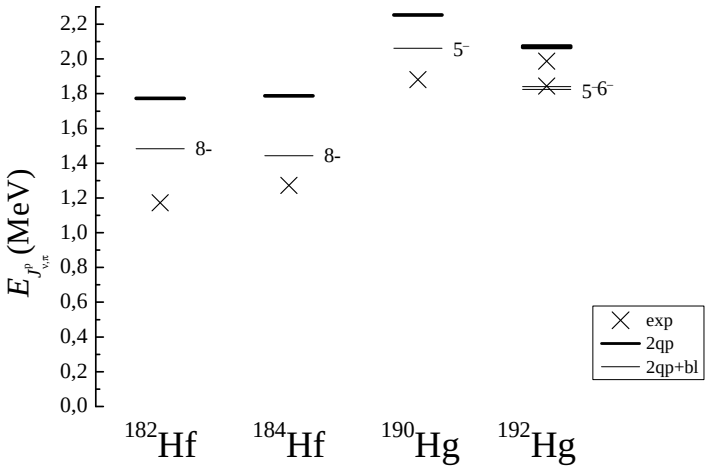
Two quasiparticle low-lying excitations with high values of angular momenta were calculated by using general equations of superfluid nuclear model with inclusion of blocking effect. It was checked on even-even nuclei with mass number A around 180 and then it was applied to predict the excited states of ^{258,260}Fm and ^{260,262,264}No. In general deviations from experimental data are about 300 keV and less.

Using the same methods one can obtain one quasiparticle and three quasiparticle excitations in odd-A nuclei. It turns out that low-lying excited levels can be interpreted in the framework of quasiparticle approach.

Table 4: Nuclei with $\Delta_n^* \sim 0$.

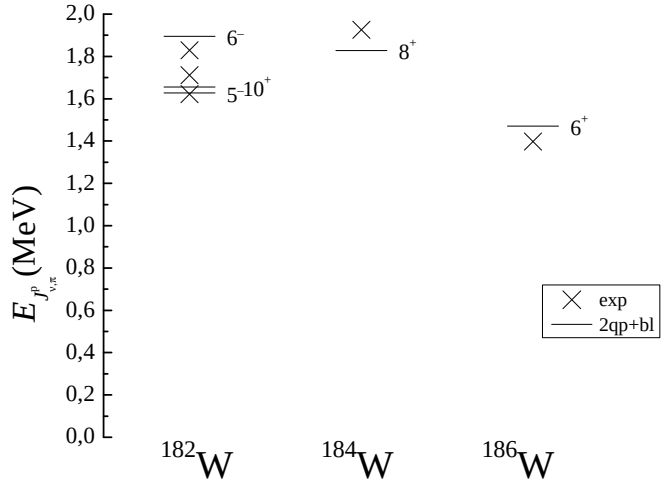
Nucleus ^{A}X(N,Z)	Δ_n of ground state	Δ_n^* of $F \to F+1$
^{174}Yb$(104,70)$	0.664	0
^{176}Yb$(106,70)$	0.713	0
^{176}Hf$(104,72)$	0.665	0
^{178}Hf$(106,72)$	0.708	0
^{180}Hf$(108,72)$	0.727	0
^{178}W$(104,74)$	0.756	0
^{180}W$(106,74)$	0.705	0
^{182}Pt$(104,78)$	0.754	0

During this work I have studied shell model approaches to the nuclear structure. Especially I have learned two-center shell model which was used in this work to obtain single-particle spectra. I have learned how to derive the equations of superfluid nuclear model. In order to solve these equations I have studied *Wolfram Mathematica*. Working on the problem of description of nuclear excitations I have thoroughly studied the influence of blocking effect on the pairing correlation functions.



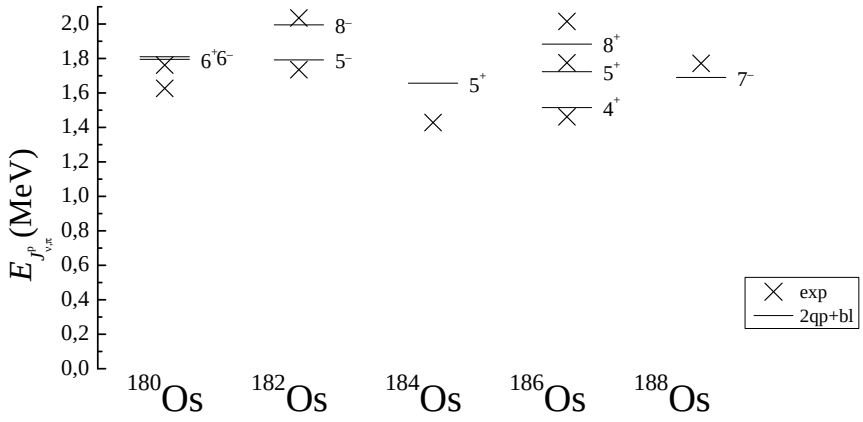
G_n=const/A, const = 14,26	14,41	15,14	15,14
Δ_n = 0,86	0,83	1,08	1,03
Δ_n^* = 0,54	0,35	0,84	0,78

Figure 8: Spectra of Hf and Hg isotopes.



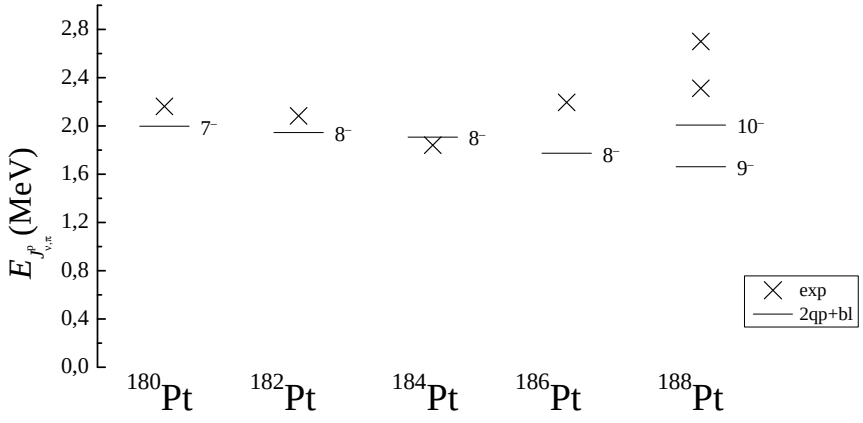
G_n=const/A, const = 14,26	14,41	14,46
Δ_n = 0,71	0,81	0,83
Δ_n^* = 0,29	0,28	0,48

Figure 9: Spectra of W isotopes.



G_n=const/A, const = 14,66	14,66	14,54	14,51	14,41
Δ_n = 0,95	0,91	0,85	0,81	0,82
Δ_n^* = 0,65	0,63	0,43	0,46	0,54

Figure 10: Spectra of Os isotopes.



G_n=const/A, const = 14,54	14,57	14,80	14,68	14,81
Δ_n = 0,79	0,75	1,05	1,00	0,95
Δ_n^* = 0,54	0,48	0,81	0,75	0,66

Figure 11: Spectra of Pt isotopes.

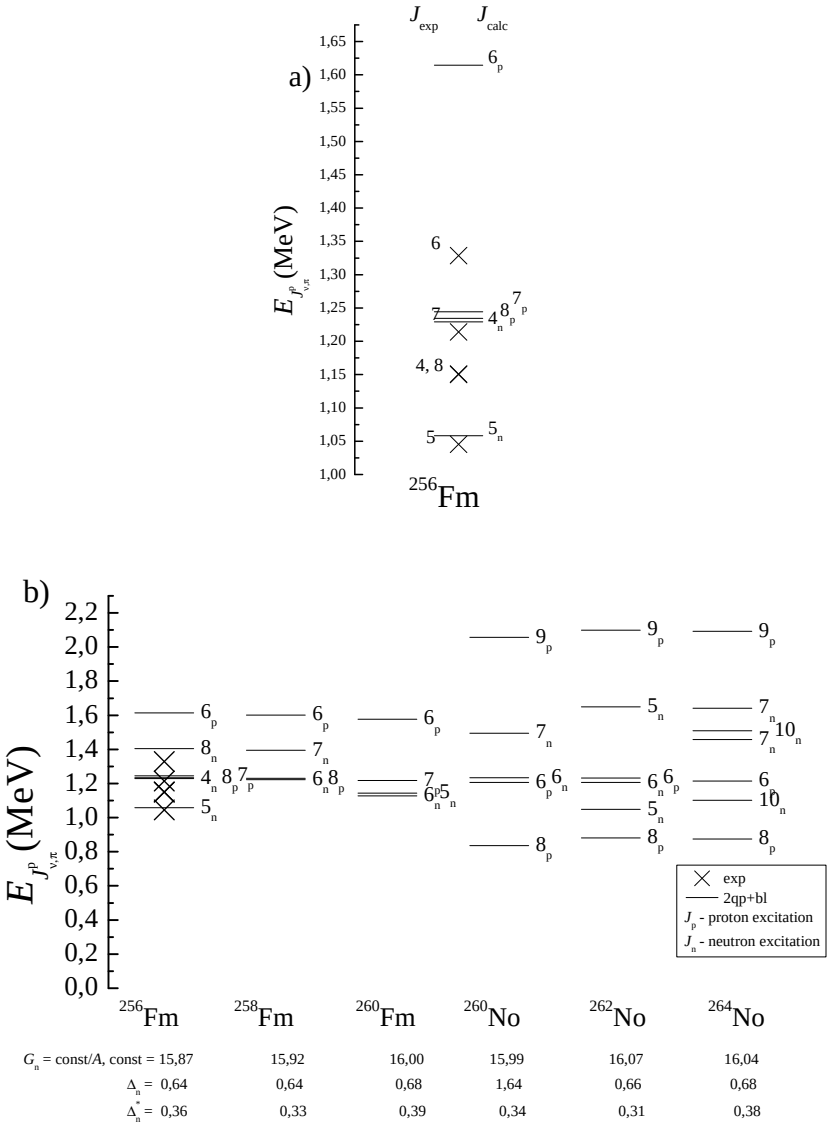


Figure 12: a) Spectrum of ^{256}Fm isotope; b) Calculated energies for Fm and No isotopes.

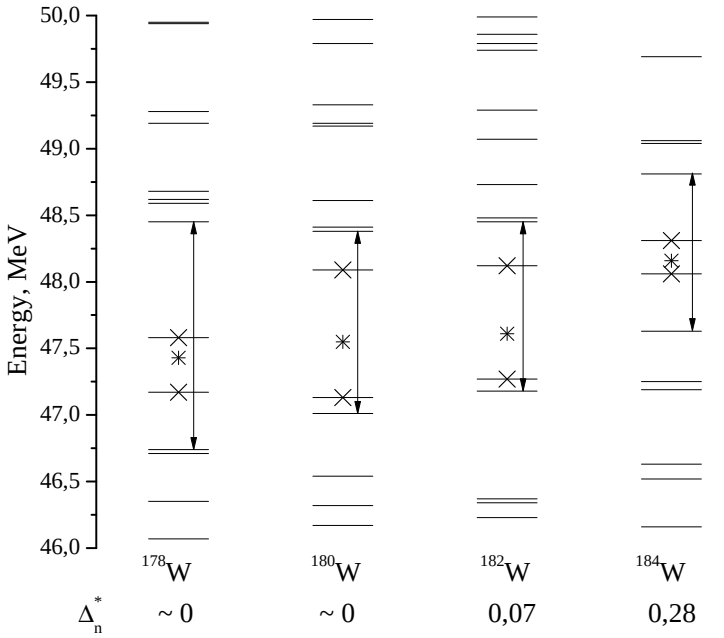


Figure 13: Single particle energy spectra of W isotopes.

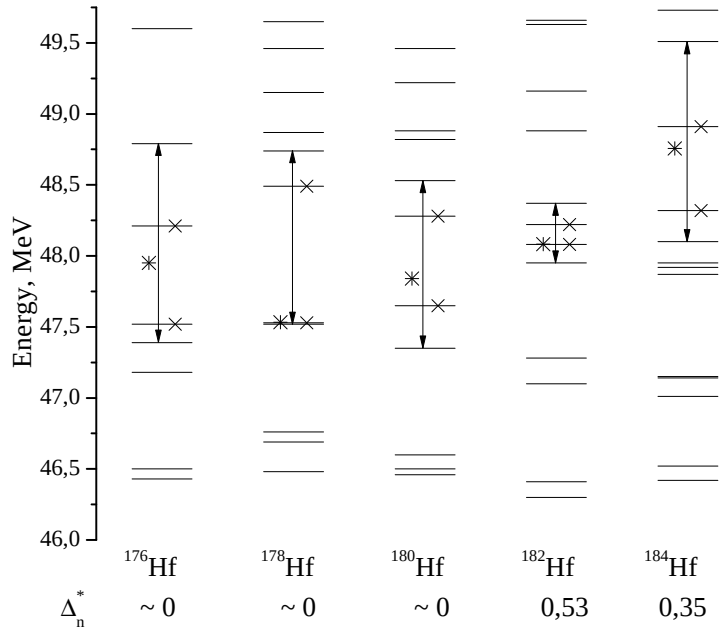


Figure 14: Single particle energy spectra of Hf isotopes. Fermi energy is indicated by stars, blocked levels are indicated by crosses. Under the spectra there are correlation functions of excited state. Correlation functions of ground state are in Table4.

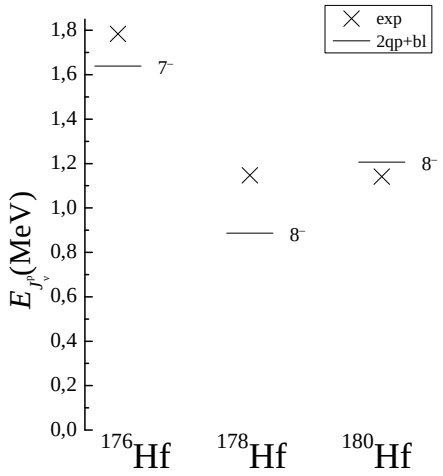


Figure 15: Spectra of Hf isotopes, results of two quasiparticle excitation calculations and their comparison with experiment.

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A Matrix elements in δ-potential

Most expressions which are used below are taken from [13]. Potential:

$$\hat{V}_{int} = V_0 \delta(\vec{r_1} - \vec{r_2}) \tag{44}$$

Equation:

$$\hat{V}_{int}|\Psi\rangle = \Delta E|\Psi\rangle \tag{45}$$

It means to find eigen values one need to find matrix elements:

$$\Delta E = \langle\Psi|\hat{V}_{int}|\Psi\rangle \tag{46}$$

δ-function can be written as

$$\delta(\vec{r_1} - \vec{r_2}) = \frac{1}{r_1 r_2}\delta(r_1 - r_2)\sum_{\lambda\mu} Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2) \tag{47}$$

Two nucleon wave function

$$\Psi_{m_1 m_2}(\vec{r_1}, \vec{r_2}) = \Phi_1(\vec{r_1})\Phi_2(\vec{r_2}) - \Phi_2(\vec{r_1})\Phi_1(\vec{r_2}) \tag{48}$$

In LM basis

$$\Psi_{LM}(\vec{r_1}, \vec{r_2}) = \sum_{m_1 m_2} C^{LM}_{lm_1 lm_2}(\Phi_1(\vec{r_1})\Phi_2(\vec{r_2}) - \Phi_2(\vec{r_1})\Phi_1(\vec{r_2})) \tag{49}$$

where Φ_1, Φ_2 - basis functions. $1, 2$ imply dependence on all quantum numbers of particle 1 and particle 2 respectively.

$$\Phi_1 = \frac{R_{nl}(r_1)}{r_1}Y_{lm_1}(\Omega_1) \tag{50}$$

Taking into account the above

$$\langle\Psi|\hat{V}_{int}|\Psi\rangle = V_0 \int \delta(r_1 - r_2)\frac{R^2_{nl}(r_1)R^2_{nl}(r_2)}{r_1^3 r_2^3}\sum_{m'_1 m'_2 m_1 m_2} C^{L'M'}_{lm'_1 lm'_2}C^{LM}_{lm_1 lm_2}[Y^*_{lm'_1}(\Omega_1)Y^*_{lm'_2}(\Omega_2) - \tag{51}$$

$$-Y^*_{lm'_2}(\Omega_1)Y^*_{lm'_1}(\Omega_2)][\sum_{\lambda\mu} Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2)][Y_{lm_1}(\Omega_1)Y_{lm_2}(\Omega_2) - Y_{lm_2}(\Omega_1)Y_{lm_1}(\Omega_2)]dV.$$

Volume element in spherical coordinates

$$dV = dV_1 dV_2 = r_1^2 r_2^2 \sin\theta_1 \sin\theta_2 dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2. \tag{52}$$

The dependence on r can be extracted and written as the radial integral

$$F_0 = \int \frac{R^4_{nl}(r)}{r^2}dr. \tag{53}$$

$$\langle\Psi|\hat{V}_{int}|\Psi\rangle = V_0 F_0 \sum_{\lambda\mu}\int [Y^*_{lm_1}(\Omega_1)Y^*_{lm_2}(\Omega_2) - Y^*_{lm_2}(\Omega_1)Y^*_{lm_1}(\Omega_2)]Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2) \tag{54}$$

$$[Y_{lm_1}(\Omega_1)Y_{lm_2}(\Omega_2) - Y_{lm_2}(\Omega_1)Y_{lm_1}(\Omega_2)]d\Omega_1 d\Omega_2.$$

Integral of the spherical harmonics multiplication:

$$\int\limits_0^{2\pi} d\phi \int\limits_0^{\pi} d\theta \sin\theta Y_{l_1 m_1}(\theta,\phi)Y_{l_2 m_2}(\theta,\phi)Y^*_{l_3 m_3}(\theta,\phi) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}} C^{l_3 0}_{l_1 0 l_2 0} C^{l_3 m_3}_{l_1 m_1 l_2 m_2}. \tag{55}$$

Symmetry property:

$$Y^*_{lm}(\Omega) = (-1)^m Y_{l-m}(\Omega). \tag{56}$$

The integral (54) represents the sum of the four integrals and to each of them the expression (55) can be applied:

$$\int Y^*_{lm'_1}(\Omega_1)Y^*_{lm'_2}(\Omega_2)Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2)Y_{lm_1}(\Omega_1)Y_{lm_2}(\Omega_2)d\Omega_1 d\Omega_2 = \tag{57}$$

$$= \int Y^*_{lm'_1}(\Omega_1)Y_{\lambda\mu}(\Omega_1)Y_{lm_1}(\Omega_1)d\Omega_1 \int Y^*_{lm'_2}(\Omega_2)Y^*_{\lambda\mu}(\Omega_2)Y_{lm_2}(\Omega_2)d\Omega_2 =$$

$$= (-1)^\mu (C^{l0}_{\lambda 0 l 0})^2 \frac{2\lambda+1}{4\pi} C^{lm'_1}_{\lambda\mu l m_1} C^{lm'_2}_{\lambda -\mu l m_2}.$$

$$-\int Y^*_{lm'_1}(\Omega_1)Y^*_{lm'_2}(\Omega_2)Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2)Y_{lm_2}(\Omega_1)Y_{lm_1}(\Omega_2)d\Omega_1 d\Omega_2 = \tag{58}$$

$$= -(-1)^\mu (C^{l0}_{\lambda 0 l 0})^2 \frac{2\lambda+1}{4\pi} C^{lm'_1}_{\lambda\mu l m_2} C^{lm'_2}_{\lambda -\mu l m_1}.$$

$$-\int Y^*_{lm_2}(\Omega_1)Y^*_{lm_1}(\Omega_2)Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2)Y_{lm_1}(\Omega_1)Y_{lm_2}(\Omega_2)d\Omega_1 d\Omega_2 = \tag{59}$$

$$= -(-1)^\mu (C^{l0}_{\lambda 0 l 0})^2 \frac{2\lambda+1}{4\pi} C^{lm'_2}_{\lambda\mu l m_1} C^{lm'_1}_{\lambda -\mu l m_2}.$$

$$\int Y^*_{lm_2}(\Omega_1)Y^*_{lm_1}(\Omega_2)Y_{\lambda\mu}(\Omega_1)Y^*_{\lambda\mu}(\Omega_2)Y_{lm_2}(\Omega_1)Y_{lm_1}(\Omega_2)d\Omega_1 d\Omega_2 = \tag{60}$$

$$= (-1)^\mu (C^{l0}_{\lambda 0 l 0})^2 \frac{2\lambda+1}{4\pi} C^{lm'_2}_{\lambda\mu l m_2} C^{lm'_1}_{\lambda -\mu l m_1}.$$

Then to each term we apply the expression for the multiplication of four Clebsch–Gordan coefficients:

$$\sum_{\beta\gamma\epsilon\phi} C^{a\alpha}_{b\beta c\gamma} C^{d\delta}_{e\epsilon f\phi} C^{b\beta}_{e\epsilon g-\eta} C^{c\gamma}_{f\phi j-\mu} = \sum_{kx} (-1)^{j+g-k} \sqrt{(2b+1)(2c+1)(2d+1)(2k+1)} \tag{61}$$

$$C^{kx}_{g\eta j\mu} C^{a\alpha}_{d\delta k-x} \begin{Bmatrix} a & b & c \\ d & e & f \\ k & g & j \end{Bmatrix}.$$

At the same time using the index permutation, where it is appropriate:

$$C^{c\gamma}_{a\alpha b\beta} = (-1)^{a+b-c} C^{c\gamma}_{b\beta a\alpha} = (-1)^{a-\alpha} \sqrt{\frac{2c+1}{2b+1}} C^{b-\beta}_{a\alpha c-\gamma} \tag{62}$$

The sum along x disappears, since because of the coefficients symmetry properties – $x = 0$. Taking into account

$$\sum_{\mu}(-1)^{\lambda+\mu}C^{k0}_{\lambda-\mu\lambda\mu} = \sqrt{2\lambda+1}\delta_{k0} \tag{63}$$

we find out that the $k = 0$ as well. Then, applying the following three expressions

$$C^{L'M'}_{LM00} = \delta_{LL'}\delta_{MM'} \tag{64}$$

$$\begin{Bmatrix} L & l & l \\ L & l & l \\ 0 & \lambda & \lambda \end{Bmatrix} = \frac{(-1)^{2l+L+\lambda}}{\sqrt{(2L+1)(2\lambda+1)}}\begin{Bmatrix} l & l & L \\ l & l & \lambda \end{Bmatrix} \tag{65}$$

$$\sum_{f\phi}(-1)^{2c}\sqrt{(2e+1)(2f+1)}C^{f\phi}_{b\beta d\delta}C^{c\gamma}_{a\alpha f\phi}\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} = C^{e\epsilon}_{b\beta a\alpha}C^{c\gamma}_{d\delta e\epsilon} \tag{66}$$

We come to a simple form of the matrix element

$$\Delta E_L = \langle\Psi|\hat{V}_{int}|\Psi\rangle = -\frac{V_0F_0}{\pi}(2l+1)^2\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{67}$$

It means, if we take $l = 1$ then the total orbital angular momentum takes values of $L = 0, 1, 2$. So we have diagonalized matrix 3x3, without taking into account the multiplier $-V_0F_0/\pi$ (you can see here that L can be only even)

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{6}{5} \end{pmatrix} \tag{68}$$

Then by using transition from LS coupling to jj coupling [14]

$$\Delta E_J = (2j+1)^2\sum_{LS}(2L+1)(2S+1)\begin{Bmatrix} l & l & L \\ 1/2 & 1/2 & S \\ j & j & J \end{Bmatrix}^2\Delta E_L, \tag{69}$$

and taking into account that for identical particles $S = 0$ one has

$$\begin{Bmatrix} l & l & L \\ 1/2 & 1/2 & 0 \\ j & j & J \end{Bmatrix} = \begin{Bmatrix} j & j & J \\ l & l & L \\ 1/2 & 1/2 & 0 \end{Bmatrix} = \delta_{JL}\delta_{\frac{1}{2}\frac{1}{2}}\frac{(-1)^{J+1/2+j+l}}{\sqrt{2(2J+1)}}\begin{Bmatrix} j & j & J \\ l & l & 1/2 \end{Bmatrix} \tag{70}$$

After applying the transformation

$$\begin{pmatrix} a & a' & c \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} a & a' & c \\ b & b' & 1/2 \end{Bmatrix} = -\frac{1}{\sqrt{(2a+1)(2a'+1)}}\begin{pmatrix} b & b' & c \\ 1/2 & -1/2 & 0 \end{pmatrix} \tag{71}$$

one can obtain the expression for matrix element (4).