EFFECTIVE PROTON-PROTON INTERACTION FOR $2p_{1/2}$ AND $1g_{9/2}$ ORBITS

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The effective interaction energies were deduced from the latest experimental data for ^{91}Nb. The other set of parameters was determined directly from the data for ^{90}Zr. Obtained parameters were compared with those published previously. Using two-body parameters, the energy levels for ^{90}Zr, ^{91}Nb and ^{92}Mo were computed.

1. Introduction

In nuclear shell-model calculations, one can parametrize the residual interaction between the extra-core nucleons in many different ways. In the calculation the interaction is diagonalized within a limited number of configurations. Through these calculations one attempts to define a mathematically simple interaction which simulates the effects of the realistic nucleon-nucleon interaction, which is mathematically singular. The realistic interaction is expected to produce considerable configuration mixing. Hence, the interactions studied with a limited number of configurations are called the effective residual interactions.

In the calculation only the matrix elements of the interaction in the two-nucleon configurations appear. The number of matrix elements used as parameters can be reduced only by considering the lowest dominant configurations.

Nuclei of the mass-90 region are rather well described by $2p_{1/2}$ and $1g_{9/2}$ protons outside an inert core, that is ^{88}Sr. A common feature of the theoretical calculations [1–3] is the application of two-body matrix elements as parameters to fit the experimental data taken for nuclei of the region in question. Usually one applies well established experimental levels as much as possible. The effective parameters which can be obtained in such a way, reproduce (not very exactly) the positions of the levels belonging to the simple multiplets. On the other hand, in such an analysis one cannot say much about the tendency of the parameters to change with the variation of the extra-core particle number.

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Results presented in this work are an attempt to obtain sets of parameters from single neighbouring nuclei. The effective parameters were obtained from the latest experimental data for ^{91}Nb [4] (Section 3). The other set of parameters was determined directly from the data for ^{90}Zr (Section 4). Both sets of parameters were used to calculate the energy level positions in ^{90}Zr, ^{91}Nb and ^{92}Mo.

2. *Notation and sign convention*

In the present work the following convention will be used. Values of the many-particle matrix-elements, as well as total nuclear binding energies (TNBE) are positive, and this is why the single-particle energies are negative. The two-body effective parameters V_J (with $J = 0, 2, 4, 6$ and 8 in the case of $g_{9/2}$ orbits) can be obtained within the accuracy of a constant, the value of which depends on the zero energy position. Expression $\langle M^{\mathrm{Nb}}\rangle_J$ denotes the diagonal 3-particle matrix-element for spin J, if the energy scale is adjusted at the ground state of ^{91}Nb (J must be different from 9/2). Its value is equals directly to the energy of the state with spin J. $\langle M\rangle_J$ denote this same matrix-element but taken relative to the ground state of the ^{88}Sr core.

The following expression is valid:

$$\langle M^{\mathrm{Nb}}\rangle_J = \langle M\rangle_J + 3C_1 \tag{1}$$

with $3C_1 = DBE\,(\mathrm{Nb, Sr}) + 3C_g$, where C_g denotes the single particle energy for a proton in the $1g_{9/2}$ orbit, *DBE* is the difference between *TNBE*'s. In order to calculate the *TNBE*, the proper atomic mass value must be substituted into equation

$$TNBE(Z, N) = ZM_{\mathrm{H}} + NM_{\mathrm{n}} - {}_{Z}M_{N}^{\mathrm{A}} - E_{\mathrm{b}}(Z, N)/c^2, \tag{2}$$

where M_{H} is the hydrogen mass, M_{n} is the neutron mass, ${}_{Z}M_{N}^{\mathrm{A}}$ is the atomic mass of the atom with Z protons and N neutrons. The term $E_{\mathrm{b}}(Z, N)$ is an estimate of the total electronic binding energy with the value ranging from 76.4 keV for strontium to 91.2 keV for niobium within an accuracy of 10% [5].

Thus

$$DBE(\mathrm{Nb, Sr}) = TNBE(^{91}\mathrm{Nb}) - TNBE(^{88}\mathrm{Sr}) \tag{3}$$

or

$$DBE(\mathrm{Nb, Sr})\ [\mathrm{keV}] = 931476\,\{3(M_{\mathrm{H}}) + M(^{88}\mathrm{Sr}) - M(^{91}\mathrm{Nb})\} - \Delta E_{\mathrm{b}}\ [\mathrm{keV}],$$

where $\Delta E_{\mathrm{b}} = E_{\mathrm{b}}(\mathrm{Nb}) - E_{\mathrm{b}}(\mathrm{Sr}) \approx 15$ keV and M being expressed in atomic mass units

Relation between the matrix-elements in the vertical energy scale is presented in Fig. 1 The following relations can be obtained in a similar way as in Eq. 1

$$E(^{89}Y,\ J = 9/2) = DBE(\mathrm{Y, Sr}) + C_g = 914\ \mathrm{keV}, \tag{4}$$

$$E(^{89}\mathrm{Y},\ J = 1/2) = DBE(\mathrm{Y, Sr}) + C_p = 0\ \mathrm{keV}$$

Taking $DBE(Y, Sr) = 7068$ keV [6] we get values of single particle energies for protons in the orbit $1g_{9/2}$ and $2p_{1/2}$,

$$C_g = -6154 \text{ keV} \quad \text{and} \quad C_p = -7068 \text{ keV}.$$

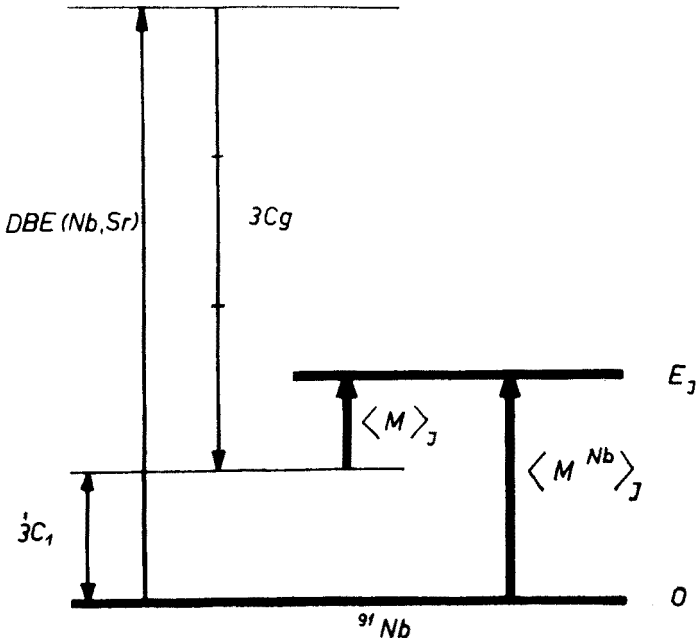

Fig. 1. Graphical representation of many-particle matrix-elements

As was already pointed out the relation

$$V_J^{Nb} = V_J + C_1 \tag{5}$$

is also valid in our notation. Effective parameters determined relative to the ^{91}Nb ground state can be quite easily replaced by those obtained relative to the Sr ground state (^{88}Sr is a core).

3. *Calculation of the two-body effective parameters from* ^{91}Nb

Nuclear shell model calculations with a limited number of configurations are frequently realized. If the configuration space is restricted to the $1g_{9/2}$ and $2p_{1/2}$ single particle states, one needs the following two-body effective parameters:

$$\langle (g_{9/2})^2 | V | (g_{9/2})^2 \rangle_J = V_J \quad \text{with} \quad J = 0, 2, 4, 6, 8,$$

$$\langle (p_{1/2})^2 | V | (p_{1/2})^2 \rangle_{J=0} = V_{pp},$$

$$\langle (p_{1/2})^2 | V | (g_{9/2})^2 \rangle_{J=0} = V_{pg},$$

$$\langle (p_{1/2}g_{9/2})\,|V|\,(p_{1/2}g_{9/2})\rangle_{J=4} = V_{4M},$$
$$\langle (p_{1/2}g_{9/2})\,|V|\,(p_{1/2}g_{9/2})\rangle_{J=5} = V_{5M}. \tag{6}$$

It is convenient to replace the V_{pp} parameter by $Z = V_{pp} - 2\delta$, where $\delta = C_g - C_p$ (δ = 914 keV from the experimental difference of the energy levels in ^{89}Y).

3.1. Determination of $V_k - V_0$ from negative parity states

The differences between the two-body matrix-elements $V_k - V_0$ (with $k = 2, 4, 6$ and 8) can be obtained from the negative parity states. This was already done in our previous experimental work [4], where the following expression was used

$$V_J - V_0 = (E_{J+1/2} - E_{1/2^-}) + (E_{J-1/2} - E_{J+1/2})\frac{J}{2J+1}, \tag{7}$$

J denotes the total angular momentum of two protons at the $g_{9/2}$ orbits. Let β denote a splitting parameter. It can be obtained as mean value of the $(E_{J+1/2} - E_{J-1/2})/(2J+1)$ terms. In the present analysis the $5/2^-$ level was not included because the appropriate energy difference was much smaller than in other cases (25 keV, comparing with 35.5 keV for other levels). One can verify the determined quantities using them as parameter values for calculating energy differences between the positive parity states belonging to the $(g_{9/2})^3$ configuration. Their values agree very well with the experiment.

3.2. Determination of V_J from positive parity states

The diagonal matrix-elements in the three-particle configuration for spin different from 9/2 can be presented as a linear combinations of V_2, V_4, V_6 and V_8. Taking experimental values of energy levels belonging to the $(g_{9/2})^3$ configuration one gets a set of linear equations with only 4 unknown parameters which are V_2^{Nb}, V_4^{Nb}, V_6^{Nb} and V_8^{Nb}. The solution of these equations gives the serched four values. Comparing these results with those obtained earlier (in Sect. 3.1), one calculates the value of V_0^{Nb}. As was mentioned in Section 2, it is quite easy to replace values of V_J^{Nb} by V_J using equation (5).

3.3. Determination of V_{pg}, Z, V_{4M} and V_{5M}

The nondiagonal part of the matrix of interaction has the form

$$\begin{array}{l} (p_{1/2})^2 g_{9/2} \\ (g_{9/2})^3 v = 1 \\ (g_{9/2})^3 v = 3 \end{array} \begin{pmatrix} X & Y & 0 \\ Y & \langle M_1\rangle & \langle M_2\rangle \\ 0 & \langle M_2\rangle & \langle M_3\rangle \end{pmatrix} \tag{8}$$

where elements $\langle M_1\rangle$, $\langle M_2\rangle$ and $\langle M_3\rangle$ are linear combinations of V_0, V_2, V_4, V_6 and V_8 (already known).

$$X = Z + 2\alpha = V_{pp} - 2\delta + (9V_{4M} + 11V_{5M})/10,$$
$$Y = \sqrt{8/10}\, V_{pg}. \tag{9}$$

The problem is to find such values of X and Y for which after diagonalization, the eigenvalues would be equal to the experimental energy values decreased by $3C_1$.

The proper values of X and Y gave the best least squares fit. Parameters V_{pg} was directly determined from Y value.

Values of α and also the V_{4M} and V_{5M} can be derived from X after substituting a proper values for Z. The latter one was determined in analysis with additional experimental data taken from ^{90}Zr. In a similar way as in ^{91}Nb, the nondiagonal part of the matrix of interaction for ^{90}Zr has the form

$$\begin{matrix}(p_{1/2})^2 \\ (g_{9/2})^2\end{matrix}\begin{pmatrix}Z & V_{pg} \\ V_{pg} & V_0\end{pmatrix}. \tag{10}$$

After diagonalization the eigenvalue should equal to the experimental energies of the 0^+ states descreased by some constant, the value of which is the mean of differences between real energy levels with spin 2^+, 4^+, 6^+ and 8^+ and proper values of the V_J. The least squares fit gives the best value of Z from which $\alpha = (9V_{4M}+11V_{5M})/20$ is determined. Combining two equations with α and spliting parameters $\beta = (V_{5M}-V_{4M})/10$ one can obtain V_{4M} and V_{5M}.

The analysis described above was performed with the NIOBAN computer program, which was especially written to solve this problem. Starting from the experimental ^{91}Nb energy levels the program calculates all needed two-body effective parameters as well as the theoretical positions of ^{90}Zr, ^{91}Nb and ^{92}Mo levels, which belong to the adequate

TABLE I

Comparison of the parameters obtained from ^{90}Zr, ^{91}Nb experimental data and the others published before

Parameters in keV	Zr	Nb	[a]AT	[b]BGL	[c]GS
V_0	−1978	−1789	−1770	−1719	−1707
V_2	−940	−680	−570	−603	−613
V_4	−49	38	220	164	144
V_6	322	243	550	508	450
V_8	463	509	690	570	565
V_{pp}	−685	−685	−557	−484	−542
V_{pg}	839	847	863	901	853
V_{4M}	527	640	—	690	714
V_{5M}	107	285	—	175	195
C_p	−7068	−7068	−7104	−7094	−7125
C_g	−6154	−6154	−6310	−6255	−6247

[a]AT — Auerbach, Talmi [1], [b]BGL — Ball, Grory, Larsen [2], [c]GS — Gloeckner, Serduke [3].

proton configuration within $p_{1/2}-g_{9/2}$ configuration space. Calculations can be done both with a seniority concerving interaction and the one which exactly includes the off-diagonal matrix-elements. To determine the level positions, the lowest energy state was set

to zero, and in the case of negative parity states the energy scale was fitted to the certain well established level.

A few sets of parameters were obtained which depend on the number of levels included in the analysis. The parameters corresponding with the well established levels $5/2^+$, $7/2^+$, $13/2^+$ $17/2^+$ and $21/2^+$ spins are nearly the same as those obtained from the all known positive parity states in ^{91}Nb, belonging to the $(g_{9/2})^3$ configuration. Table I contains parameters computed by NIOBAN as well as other calculated directly from experimental data for ^{90}Zr and described in [1-3].

4. *Calculation of the two-body effective parameters from* ^{90}Zr

Having accepted our convention, one is able to calculate effective two-body interactions from the experimental data for ^{90}Zr. The following expression is valid

$$V_J = V_J^{\mathrm{Zr}} - C_2 \tag{11}$$

with $J = 2, 4, 6, 8$, $V_J^{\mathrm{Zr}} = E_J$ and $C_2 = DBE(\mathrm{Zr}, \mathrm{Sr}) + 2C_g = 3126$ keV. V_J were easily obtained after substituting the proper energy levels [7].

The nondiagonal part of the matrix of interaction has a form already specified in Section 3.3 (expression 10). The eigenvalues of this matrix are equal to the experimental energies of 0^+ states decreased by C_2. The solution of the eigenequations with $Z = -2513$ keV determined $V_0 = -1978$ keV and $V_{pg} = 839$ keV. The V_{4M} and V_{5M} can be calculated from the relations

$$V_{4M} = E_{4-} - C_3, \qquad V_{5M} = E_{5-} - C_3, \tag{12}$$

where $C_3 = DBE(\mathrm{Zr}, \mathrm{Sr}) + C_p + C_g$. Numerical values of the parameters are listed in Table I.

5. *Discussion*

The parameters mentioned in Table I were used to calculate the energy levels for ^{90}Zr, ^{91}Nb and ^{92}Mo. The matrix elements which are nondiagonal in the seniority scheme were included in the analysis. Calculations were done also with the interaction in which the seniority is conserved.

Table II contains a list of the energy levels for ^{91}Nb. The level positions were calculated by NIOBAN using the parameters presented in Table I. The root mean square (rms) deviation per level was also calculated for every case to compare the parameters. As can be seen, the rms deviation per level has practically this same value for nonconservation of seniority as for seniority conservation. As an example of the obtained results the following wave functions are given:

$\psi_1^2 = 0.308\,(p_{1/2}^2 g_{9/2}) + 0.686\,(g_{9/2}^3 v = 1) + 0.006\,(g_{9/2}^3 v = 3)$

or $\psi_2^2 = 0.305\,(p_{1/2}^2 g_{9/2}) + 0.695\,(g_{9/2}^3)$ for the 1637 keV in ^{91}Nb.

$\psi_1^2 = 0.6797\,(p_{1/2}^2\, g_{9/2}^2) + 0.3199\,(g_{9/2}^4 v = 2) + 0.0004\,(g_{9/2}^4 v = 4)$

or $\psi_2^2 = 0.685\,(p_{1/2}^2 g_{9/2}^2) + 0.315\,(g_{9/2}^4)$ for the 2761 keV 8^+ state in ^{92}Mo.

TABLE II

Energy levels for ^{91}Nb calculated using the parameters presented in Table I

Spin	E_{exp}	Parameters from ^{91}Nb seniority conservation	nonconservation	Parameters Gs seniority conservation	nonconservation	Parameters from ^{90}Zr seniority conservation	nonconservation
$1/2^-$	104.5	104.5		104.5		104.5	
$3/2^-$	1311.0	1319.7		1354.2		1268.5	
$5/2^-$	1186.3	1142.1		1094.7		1058.5	
$7/2^-$	2120.0	2109.1		2215.0		2243.5	
$9/2^-$	1790.0	1789.3		1747.9		1865.5	
$11/2^-$	2413.0	2384.4		2624.8		2698.5	
$13/2^-$	1983.4	1922.6		1950.1		2152.5	
$15/2^-$	2660.0	2722.2		2843.6		2923.5	
$17/2^-$	2033.4	2118.3		1961.3		2209.5	
$9/2^+$	.0	.0	.0	.0	.0	.0	.0
$3/2^+$	—	2412.1	2411.9	2595.7	2595.8	2560.0	2560.0
$5/2^+$	1965.0	1968.2	1968.0	2196.7	2196.8	2098.6	2098.7
$7/2^+$	1581.0	1584.6	1584.4	1574.4	1574.8	1366.0	1366.1
$9/2^+$ $v=1$	1637.0	1637.0	1636.7	1704.5	1704.2	1649.4	1648.8
$9/2^+$ $v=3$	2631.0	2547.2	2553.8	2783.9	2784.4	2791.1	2792.0
$11/2^+$	2330.0	2394.8	2394.6	2462.0	2462.0	2413.2	2413.3
$13/2^+$	2291.0	2281.7	2281.5	2369.1	2369.1	2311.4	2311.5
$15/2^+$	2902.0	2961.1	2960.8	3221.0	3221.1	3319.2	3319.3
$17/2^+$	3110.0	3108.1	3107.9	3180.8	3180.8	3271.9	3272.0
$21/2^+$	3467.0	3471.3	3471.1	3527,9	3527.9	3693.8	3693.9
rms deviation per level		42.55	41.80	133.66	133.71	182.35	182.42

For a comparison of the energy levels for ^{91}Nb, Fig. 2 is included.

Table III gives a list of the energy levels for ^{90}Zr.

Configuration space involved in the present analysis gives 23 positive and 20 negative parity levels for ^{92}Mo whereas only 9 levels are experimentally known. ^{92}Mo level positions were calculated using the parameters obtained from ^{90}Zr and ^{91}Nb as well as other parameters published elsewhere. In all cases the accuracies of the rms deviation are similar but not as good as in the case of levels of ^{90}Zr and ^{91}Nb.

The following comments can be made:

1. On the average, the admixture of the seniority nonconserving part of the wave-function is of the order of 10^{-3}.

2. Parameters obtained from the same nuclei give a small rms deviation per level but do not reproduce the energy spectrum so well for other nuclei.

3. It is hoped, that determination of the parameters from the neighbouring nuclei will give a possibility of finding some regularity in changes of their values if the number of extra core particles is varied.

For the solution of this problem more exact experimental data, specially for ^{92}Mo, ^{93}Tc and ^{94}Ru are needed.

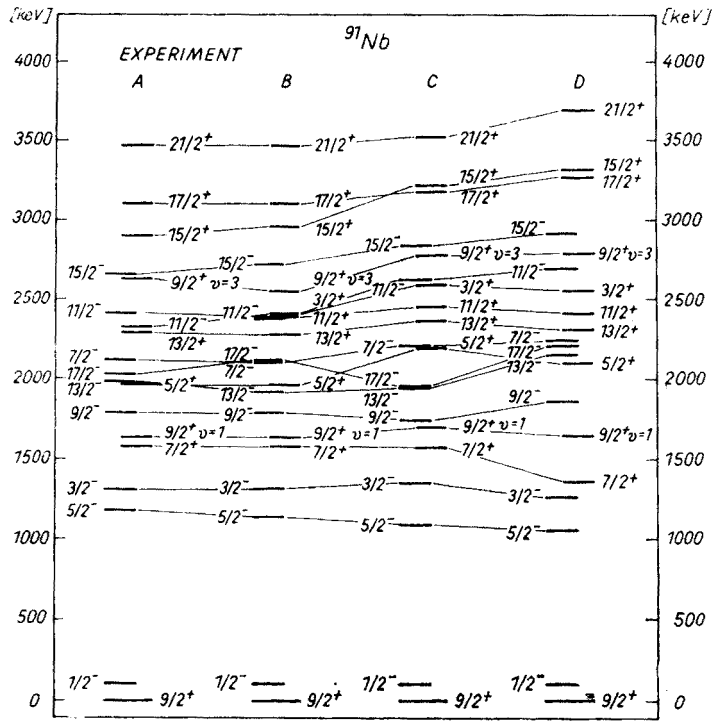

Fig. 2. Experimental and theoretical level scheme for ^{91}Nb: A — level scheme taken from [4], B, C, D — calculated energy levels using the parameters obtained from ^{91}Nb, published in [3] and from ^{90}Zr, respec tively

TABLE III

Energy levels for ^{90}Zr calculated using the parameters presented in Table I

Spin	E_{exp} in keV ^{90}Zr	Parameters obtained from		
		^{91}Nb	GS	^{90}Zr
0^+	.0	.0	.0	.0
0^+	1760.7	1843.2	1805.5	1761.0
2^+	2186.2	2392.4	2292.2	2186.0
4^+	3076.8	3110.7	3049.2	3077.0
6^+	3447.8	3315.0	3355.2	3448.0
8^+	3589.0	3581.8	3470.2	3589.0
5^-	2318.7	2318.7	2318.7	2318.7
4^-	2738.9	2673.9	2837.7	2738.7
rms deviation per level		95.12	76.20	0.18

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