CALCULATION OF THE SPECTRUM OF THE NUCLEUS $_{86}Rn^{218}$

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The spectrum of the nucleus $_{86}Rn^{218}$, which has ten extra nucleons, is computed. It is shown that the self-consistent potential $V_C + V_S$ and the pairing potential V_p determined from nuclei with one and two nucleons outside the closed shells allow the calculation of the lower excited states in many-nucleon problems. The good agreement between the computed and the experimental binding energies of the ten nucleons indicates that the effect on the energy of forces of a different type, if they exist at all, must be small. It is found that the second excited state in the spectrum of Rn^{216} must actually be a 0^+ state, in contrast to the assignment 2^+ which has been chosen in analogy with the vibrational spectra. It is shown that besides the experimentally observed levels there is a large number of as yet unobserved levels. The fractional parentage coefficients for the removal of one and two particles have been computed for all states with $^3/_2 \leq j \leq {}^{13}/_2$.

In the present paper are considered even-even nuclei with more than four nucleons outside doubly closed shells. The investigation of nuclei of such complexity will allow us to establish how well a self-consistent potential augmented by two-body forces describes their structure and the character of their excited states. In this sense the present paper is a logical continuation of previously published work [1-5] where consecutively were considered nuclei with one, two and four extra nucleons. In the present paper are reported the results of calculations of the spectrum of the nucleus Rn^{218} which has six neutrons and four protons outside of the closed shells.

THE BASIC ASSUMPTIONS

We briefly enumerate the fundamental assumptions on which our calculations are based.

1. The self-consistent potential which acts on the individual nucleons is determined by the spectrum of nuclei with one nucleon outside doubly closed shells. It consists of a central potential $V_C(r)$ and of a quadrupole part $V_S(r)$. The central potential is

$$V_C(r_i) = \frac{V_0}{1+e^{\alpha(r_i-r_0)}} - \lambda\left(\frac{\hbar}{2Mc}\right)^2 \frac{\mathbf{l}_i\mathbf{s}_i}{r_i}\frac{\partial V}{\partial r_i}. \quad (1)$$

The parameters α, λ, V_0 were determined by comparison of the calculated spectra of a number of such nuclei with the experimental data. The radial functions R_{nlj} were also obtained. For further work we used the functions of Bi^{209} and Pb^{209} which were obtained with the optimum values of the parameters, viz., $\alpha = 1.15$ $\lambda = 25$, $V_0 = 57$ MeV for protons, and $V_0 = 43$ MeV for neutrons.

The quadrupole potential was taken to be

$$V_S(\mathbf{r}_i) = -\varkappa(r_i)\sqrt{\frac{\hbar\omega}{2C}}\sum_\mu [b_\mu + (-1)^\mu b^+_{-\mu}]\, Y_{2\mu}(\vartheta_i, \varphi_i). \quad (2)$$

Here b^+ and b are the phonon creation and annihilation operators. The parameters $\hbar\omega$ and C were determined from the quadrupole moments Q and from the E2 transition probabilities: $\hbar\omega = 3$ MeV, $C = 1000 - 2000$ MeV. For the radial matrix elements we have the estimate $\langle n|\kappa(r_i)|n'\rangle \approx (-1)^{n+n'}$ 40 MeV (n, n' are the radial quantum numbers).

2. In nuclei with more than one particle outside the closed shells the short range residual forces play an important part. They were taken to have the form

$$V_p(ik) = -(v_s\pi_s + v_t\pi_t)\exp(-|\mathbf{r}_i - \mathbf{r}_k|^2/\rho^2), \quad (3)$$

where $\pi_s = {}^1/_4(1 - \sigma_1\cdot\sigma_2)$ and $\pi_t = {}^1/_4(3 + \sigma_1\cdot\sigma_2)$ are the singlet and triplet projection operators, and ρ is the range of the forces. We emphasize that this form of the forces is sufficiently general. It follows from [2-4] that the parameters v_s and v_t for the pairs nn, pp, and np are approximately the same and are $v_s \approx 35$ MeV, and $v_t \approx 15$ MeV. The effective range is $\rho \approx 2f$. In the following it is assumed that no new forces appear as the number of nucleons outside of the core increases, and that the parameters of the potential and the pairing forces remain unchanged.

FUNDAMENTALS OF THE COMPUTATION METHOD

The total Hamiltonian of the system is

$$\hat{H} = \sum_i \hat{H}_0(i) + \hat{H}_S + \sum_i V_S(i) + \sum_{i<k} V_p(ik). \qquad (4)$$

Here

$$\hat{H}_0 = -\left(\frac{\hbar^2}{2M}\right)\Delta + V_C, \quad \hat{H}_S = \hbar\omega\left(\frac{5}{2} + \sum_\mu b_\mu^+ b_\mu\right);$$

$\hat{H}_S$ is the Hamiltonian of the nuclear surface which executes quadrupole vibrations with energy $\hbar\omega$. Such a Hamiltonian has to be introduced to account for the coupling of the valence nucleons with the core nucleons.

The single-particle and the phonon wave functions are the eigenfunctions of the operators

$$\hat{H}_0 | ljm\rangle = E_l | ljm\rangle,$$

$$\hat{H}_S \left| NRM_R\right\rangle = \left(N + \tfrac{5}{2}\right)\hbar\omega \left| NRM_R\right\rangle,$$

where N is the number of phonons with energy $N\hbar\omega$.

The complete orthogonal system of functions belonging to the operator $\sum_i \hat{H}_0(i) + \hat{H}_S$ will be all the possible functions of the form $|J_nJ_p : J; NR : IM\rangle$, which are constructed according to the angular momentum coupling rules with Clebsch-Gordan coefficients from the neutron function (whose angular momentum we denote by J_n), the proton wave function (angular momentum J_p), and the phonon wave function $|NRM_R\rangle$. The neutron wave function itself (and also the proton wave function) is constructed by vector coupling different functions of the form $|j^n \alpha J\rangle$ which is fully antisymmetric in all neutrons. (Here j is the angular momentum of the individual nucleons, J is the angular momentum of the configuration j^n, and α designates all the other quantum numbers necessary to specify the state j^n.)

The function which corresponds to filling the levels j_1 and j_2 with neutrons and the levels j_3 and j_4 with protons is written in the form

$$|(j_1^{n_1}\alpha_1 J_1, j_2^{n_2}\alpha_2 J_2 : J_n)_a\ (j_3^{n_3}\alpha_3 J_3, j_4^{n_4}\alpha_4 J_4 : J_p)_a : J : NR : IM\rangle. \qquad (6)$$

A function containing a larger number of levels is written in an analogous fashion.

The solution of the Schrödinger equation with Hamiltonian (4) can be represented as

$$|IM\rangle = \sum_\beta c_\beta^I\ |J_nJ_p : J : NR : IM\rangle,$$

where, in general, the sum goes over the complete set of eigenfunctions of the operator $\sum_i \hat{H}_0(i) + \hat{H}_S$. Inserting such a function into the equation $\hat{H}\psi = E\psi$ one obtains after the usual manipulations the energy matrix. Its diagonalization yields then the eigenvalues of the operator H and the values of the coefficients C_β^I.

The matrix elements of the interactions nn, pp, and np can be represented as sums of two-body matrix elements using fractional parentage coefficients. Similarly the matrix elements of the interaction V_S are given by sums involving fractional parentage coefficients. The appropriate formulae were derived but we shall not give them here due to their cumbersome form.

The characteristics of fractional parentage coefficients are discussed in many papers. However, actual numerical computations exist only for angular momenta up to $j = 7/2$.[1)] We have therefore computed the fractional parentage coefficients for all angular momenta $3/2 \le j \le 13/2$. Basic for the computations was a recurrence relation [7] which gives the fractional parentage coefficients for the configurations $|j^n J\rangle$ in terms of those for the configurations $|j^{n-1}\alpha' J'\rangle$. However one has to keep in mind that:

1) the wave function $|j^n J\rangle$ may not correspond to some well defined seniority s but may be a linear combination of several functions with seniorities $s'' - 1$ and $s'' + 1$ and with the given angular momentum J (s'' is the seniority of the parent state);

2) the obtained set of linearly independent functions with angular momentum J will not be orthogonal.

Therefore in the computation of the fractional parentage coefficients one has to adhere to a definite sequence and to find such mutually orthogonal linear combinations of the functions which correspond to the desired value of s.

CALCULATION OF THE SPECTRUM OF $_{86}Rn^{218}$

After computation of the fractional parentage coefficients, we programmed the BÉSM-2 electronic computer to calculate arbitrary diagonal and off-diagonal matrix elements. The energy matrix was investigated in detail for I = 0, 2, 4. All single-particle states with an excitation energy of up to 3 MeV were considered, i.e., six neutron levels and five proton levels (see Fig. 1). Even with this limitation the number of states contributing to each angular momentum state is very large. However, not all states have an equal in-

[1)] A number of papers, e.g. [6], contain errors for the case of more than half-filled shells.

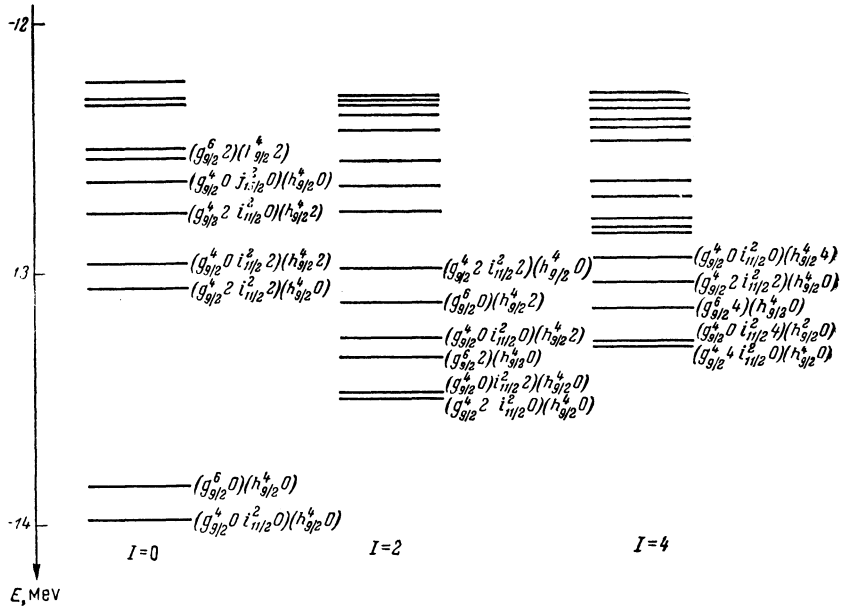

FIG. 2. The lowest excited states of the ten nucleons of Rn^{218}, taking into account the single particle energies and the diagonal elements of the residual interaction. The configurations are indicated to the right. The energy is counted from the single particle ground state energy.

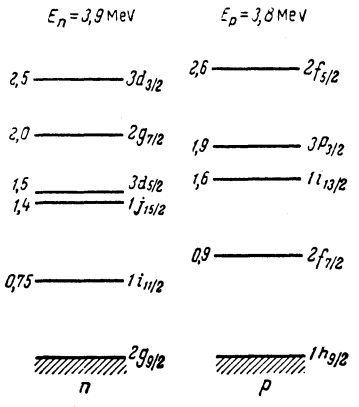

FIG. 1. Single-particle excited state levels of the nuclei Pb^{209} and Bi^{209}.

fluence on the positions of the lowest levels. One thus must select judiciously that finite number of states which determine the position of the low levels.

To begin with, the diagonal elements were computed and the low levels were examined in the diagonal approximation. Figure 2 shows that the level density is very high, and that it increases with increasing I. The close lying lowest levels for each I are associated with the states $|(g^6_{9/2}\,J_n)a\,(h^4_{9/2}\,J_p)_a\,JM\rangle$ and $|(g^4_{9/2}\,J_1\,i^2_{11/2}\,J_2 : J_n)a\,(h^4_{9/2}\,J_p)\,a\,JM\rangle$.[2)]

The selection of states was performed so as to obtain as high an accuracy as possible for the few lowest levels for each I. For each of the three to seven lowest levels, all off-diagonal matrix elements were computed, i.e. the first few rows and columns of the energy matrix were constructed.

[2)]In this respect the spectrum of Rn^{218} differs from that of Po^{212}.

Then the quantity $a^2_{ik}/|a_{ii} - a_{kk}|$ was evaluated, where a_{ik} is an off-diagonal matrix element, and a_{ii} and a_{kk} are the corresponding diagonal matrix elements. For I = 0 and I = 2 those rows and columns of the energy matrix were stricken out for which $a^2_{ik}/|a_{ik} - a_{kk}| < 0.005$.

This way a matrix of rank 31 was obtained for I = 0 and of rank 55 for I = 2 and I = 4. However, we had to limit ourselves to a somewhat lower accuracy for the case I = 4 since there the density of low lying levels is considerably higher. One thus would have to diagonalize a matrix of higher rank than 55, which is difficult with the BÉSM-2.

We can estimate the influence of the states not included by second order perturbation theory. Remaining within the open shell, we get an additional shift of approximately 0.05 MeV for the low levels with I = 0 and I = 2 and approximately 0.15 MeV for those with I = 4. In order to check on the manner in which the positions of the low levels change with increasing order of the matrix, a number of matrices of different rank were diagonalized for I = 0 and I = 2. In varying the rank of the matrix and investigating the dependence of its eigenvalues on the rank, we essentially use a certain analog of the Ritz method.

In Fig. 3 we have plotted the first eigenvalues for I = 0 and I = 2 against the rank of the matrix. The last points which correspond to a matrix of rank one hundred have been obtained by perturbation theory. It should be noted that it is of equal importance to consider the pp, nn, and np off-diagonal elements. To illustrate this point we give two matrices of the sixth order taken from the energy matrices for I = 0 and I = 2 (see Table I).

Table I. Sixth rank energy matrices for I = 0 and I = 2

			$I=0$			
$(g^6_{9/2}0)\,(h^4_{9/2}0)$	−13.85	−0.3	−0.62*	0.07		
$(g^4_{9/2}0i^2_{11/2}0)\,(h^4_{9/2}0)$	−0.3	−13.99		−0.56	−0.62*	0.84
$(g^6_{9/2}2)\,(h^4_{9/2}2)$	−0.62*		−12.54		−0.2	
$(g^4_{9/2}2i^2_{11/2}2)\,(h^4_{9/2}0)$	0.07	−0.56		−13.06		
$(g^4_{9/2}2i^2_{11/2}0)\,(h^4_{9/2}2)$		−0.62*	−0.2		−12.76	
$(g^4_{9/2}0i^2_{11/2}0)\,(h^2_{9/2}0i^2_{13/2}0)$		0.84				−11.34
			$I=2$			
$(g^6_{9/2}0)\,(h^4_{9/2}2)$	−13.12	−0.3			−0.28*	
$(g^4_{9/2}0i^2_{11/2})\,(h^4_{9/2}2)$	−0.3	−13.27	−0.3*	−0.28*		
$(g^4_{9/2}0i^2_{11/2}2)\,(h^4_{9/2}0)$		−0.3*	−13.49	−0.25	−0.03	0.84
$(g^4_{9/2}2i^2_{11/2}0)\,(h^4_{9/2}0)$		−0.28*	−0.25	−13.49	0.2	
$(g^6_{9/2}2)\,(h^4_{9/2}0)$	−0.28*		−0.03	0.2	−13.34	
$(g^4_{9/2}0i^2_{11/2}2)\,(h^2_{9/2}0i^2_{13/2}0)$			0.84			−10.8

*Off-diagonal elements of the np interaction.

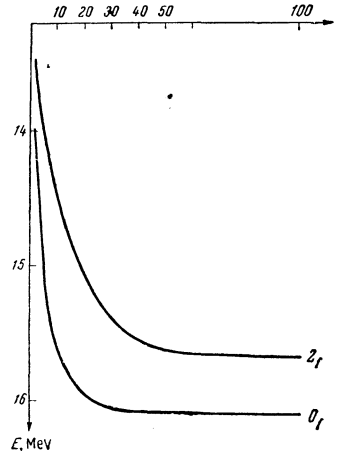

FIG. 3. Dependence of the first excited states with I = 0 and I = 2 on the size of the matrix.

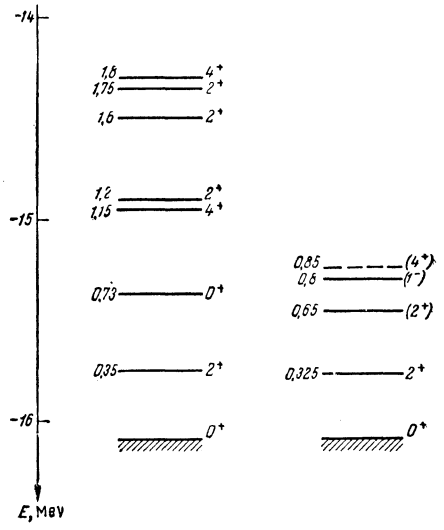

FIG. 4. Level scheme of Rn^{218} for spins 0, 2, and 4. To the right is shown the experimental level scheme. The energy on the ordinate is counted from the single particle ground state.

The np off-diagonal elements are indicated by an asterisk.

Inclusion of the Coulomb interaction will decrease the separation of the levels with I = 0 and I = 2 further by approximately 0.05 MeV and those with I = 0 and I = 4 by about 0.1 MeV. The final level scheme is depicted in Fig. 4. The experimental level scheme is shown to the right.

In the experimental papers [8] the third excited state which lies at 0.65 MeV has been given the tentative spin and parity assignment 2^+. This is based on the analogy with the level sequence in vibrational nuclei. The calculation shows that it must have the quantum numbers 0^+. The second 2^+ level lies at a higher energy (see Fig. 4). The experimentally observed 1^- level can be explained as follows. The 1^- levels are obtained from configurations of the form

$$|(g^6_{9/2}J_n)_a\,(h^3_{9/2}J_3 i_{13/2}:J_p)_a J=1^-\rangle,$$
$$|(g^4_{9/2}J_1 i^2_{11/2}J_2:J_n)_a\,(h^3_{9/2}J_3 i_{13/2}:J_p)_a\,J=1^-\rangle,$$
$$|(g^5_{9/2}J_1 j_{15/2}:J_n)_a\,(h^4_{9/2}J_p)\,J=1^-\rangle.$$

Many such configurations exist. However, they lie high above the ground state since they are associated with the breaking of a pair of protons (or neutrons) and the raising of one of the protons (neutrons) to the level $i_{13/2}(j_{15/2})$. Therefore the first 1^- level appears at approximately 2.5 MeV despite of the large number of 1^- states and their strong interaction.

So far we have discussed single particle excited states and have neglected "particle-hole" excitations of the core. Actually the core excita-

Table II. Expansion coefficients c^{I}_{β} for the wave functions of some states of Rn^{218}

$(j_1^{n_1} J_1 j_2^{n_2} J_2 : J_n)_a$	$(j_3^{n_3} J_3 j_4^{n_4} J_4 J_p)$	J	N	R	0_1	0_2
	$I=0$					
$(g_{9/2}^6 0)$	$(h_{9/2}^4 0)$	0	0	0	0.38	0.72
$(g_{9/2}^4 0 i_{11/2}^2 0 : 0)$	$(h_{9/2}^4 0)$	0	0	0	0.70	−0.33
$(g_{9/2}^6 2)$	$(h_{9/2}^4 2)$	0	0	0	0.12	0.25
$(g_{9/2}^6 0)$	$(h_{9/2}^2 0 f_{7/2}^2 0 : 0)$	0	0	0	0.05	0.10
$(g_{9/2}^6 0)$	$(h_{9/2}^2 0 i_{13/2}^2 0 : 0)$	0	0	0	−0.08	−0.16
$(g_{9/2}^4 0 g_{7/2}^2 0 : 0)$	$(h_{9/2}^4 0)$	0	0	0	0.10	0.10
$(g_{9/2}^4 2 i_{11/2}^2 2 : 0)$	$(h_{9/2}^4 0)$	0	0	0	0.20	−0.17
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 2)$	0	0	0	0.23	−0.16
$(g_{9/2}^4 2 i_{11/2}^2 0 : 2)$	$(h_{9/2}^4 2)$	0	0	0	0.18	−0.10
$(g_{9/2}^4 0 i_{11/2}^2 0 : 0)$	$(h_{9/2}^2 0 i_{13/2}^2 : 0)$	0	0	0	−0.14	0.06
$(g_{9/2}^4 0 j_{15/2}^2 0 : 0)$	$(h_{9/2}^4 0)$	0	0	0	−0.17	−0.05
$(g_{9/2}^6 2)$	$(h_{9/2}^4 0)$	2	1	2	−0.12	−0.28
$(g_{9/2}^6 0)$	$(h_{9/2}^4 2)$	2	1	2	−0.10	−0.23
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 0)$	2	1	2	−0.22	0.15
$(g_{9/2}^4 2 i_{11/2}^2 0 : 2)$	$(h_{9/2}^4 0)$	2	1	2	−0.16	0.10
$(g_{9/2}^4 0 i_{11/2}^2 0 : 0)$	$(h_{9/2}^4 2)$	2	1	2	−0.16	0.10
	$I=2$					
$(j_1^{n_1} J_1 j_2^{n_2} J_2 : J_n)_a$	$(j_3^{n_3} J_3 j_4^{n_4} J_4 : J_p)$	J	N	R	2_1	2_2	2_3
$(g_{9/2}^6 0)$	$(h_{9/2}^4 2)$	2	0	0	0.06	0.40	−0.35
$(g_{9/2}^4 0 i_{11/2}^2 0 : 0)$	$(h_{9/2}^4 2)$	2	0	0	0.32	0.21	0.17
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 0)$	2	0	0	0.67	−0.29	−0.23
$(g_{9/2}^4 2 i_{11/2}^2 0 : 2)$	$(h_{9/2}^4 0)$	2	0	0	0.33	0.40	0.57
$(g_{9/2}^6 2)$	$(h_{9/2}^4 0)$	2	0	0	0.07	0.56	−0.43
$(g_{9/2}^4 2 i_{11/2}^2 2 : 0)$	$(h_{9/2}^4 2)$	2	0	0	0.13	0.05	0.10
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^2 0 i_{13/2}^2 0 : 0)$	2	0	0	−0.13	0.06	0.06
$(g_{9/2}^6 2)$	$(h_{9/2}^2 0 i_{13/2}^2 0 : 0)$	2	0	0	−0.02	−0.13	0.10
$(g_{9/2}^4 2 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 0)$	2	0	0	−0.12	0.06	0.05
$(g_{9/2}^4 2 i_{11/2}^2 4 : 2)$	$(h_{9/2}^4 0)$	2	0	0	0.19	−0.14	−0.12
$(g_{9/2}^4 0 i_{11/2}^2 4 : 4)$	$(h_{9/2}^4 2)$	2	0	0	0.22	−0.14	−0.12
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 2)$	2	0	0	−0.12	0.06	0.05
$(g_{9/2}^4 2 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 2)$	2	0	0	0.13	0.02	0.07
$(g_{9/2}^4 2 i_{11/2}^2 2 : 3)$	$(h_{9/2}^4 2)$	2	0	0	0.04	−0.15	−0.21
	$I=2$					
$(j_1^{n_1} J_1 j_2^{n_2} J_2 : J_n)_a$	$(j_3^{n_3} J_3 j_4^{n_4} J_4 : J_p)$	J	N	R	2_1	2_2	2_3
$(g_{9/2}^4 2 i_{11/2}^2 2 : 4)$	$(h_{9/2}^4 2)$	2	0	0	0.19	0.02	0.09
$(g_{9/2}^6 2)$	$(h_{9/2}^4 2)$	4	1	2	−0.02	−0.14	0.12
$(g_{9/2}^6 0)$	$(h_{9/2}^4 0)$	0	1	2	−0.02	−0.24	0.23
$(g_{9/2}^4 0 i_{11/2}^2 0 : 0)$	$(h_{9/2}^4 0)$	0	1	2	−0.21	−0.09	−0.16
$(g_{9/2}^4 0 i_{11/2}^2 4 : 4)$	$(h_{9/2}^4 0)$	4	1	2	−0.17	0.12	0.10
$(g_{9/2}^4 2 i_{11/2}^2 2 : 4)$	$(h_{9/2}^4 0)$	4	1	2	−0.15	−0.01	−0.05
$(g_{9/2}^4 0 i_{11/2}^2 2 : 2)$	$(h_{9/2}^4 2)$	4	1	2	−0.15	0.03	0.02

tions have a negligible influence on the even-parity low excited states. However, when investigating levels of the opposite parity one has to take into account the "particle-hole" excitations. Thus one has to consider in addition to the interaction of filled single particle orbitals also that of hole states associated with core excitations if one wants to obtain correct position of the 1^- levels. This will lead to considerable lowering of the first 1^- state and it must depress it to the experimentally observed position.

In Table II are given the expansion coefficients C^I_β of the wave functions of Rn^{218} in terms of the eigenfunctions of $\sum_i^{10}\hat{H}_0(i) + \hat{H}_S$.

It is of interest to compare the experimental and the calculated binding energies of the ground state. The single particle energy of six neutrons and four protons is $(-3.9 \times 6 - 3.8 \times 4) = -38.6$ MeV. The computed pairing energy and the interaction energy with the surface is for a ground state -16.1 MeV. The Coulomb energy for the repulsion of the four protons equals 2.5 MeV. Thus the computed separation energy is 52.2 MeV. The observed separation energy for ten nucleons in Rn^{218} is 50.8 MeV. It should be remembered that the basic assumption was that the excited nucleons interact only through residual pairing forces. The obtained result indicates that any additional forces of a different type, if they exist at all, make a small contribution.

In order to determine how sensitive the obtained results are to changes of the parameters, we varied them within certain not too large ranges. In Fig. 5 we show the motion of some levels due to changes of the single particle energy of the state $i_{11/2}$. This change can be generated by a change of the surface diffuseness parameter of the potential V_C. In Fig. 6 the position of the first few levels with I = 0 and I = 2 is shown if the parameters v_S, v_t and C are varied, with $\hbar\omega$ = 3 MeV. From this it is evident that the level sequence 0 – 2 – 0 is maintained for all these changes, and that the best agreement with experiment obtains at v_S = 35 MeV, v_t = 15 MeV, and C = 1000 to 2000 MeV, i.e., the same parameters which have earlier [2-5] been found to be optimal. From the same figure we see that the V_S-interaction does not change significantly the position and the character of the levels.

The probabilities of γ transitions between the different states of Rn^{218} were also computed. Here only the most important components of the wave functions were used. Therefore the accuracy

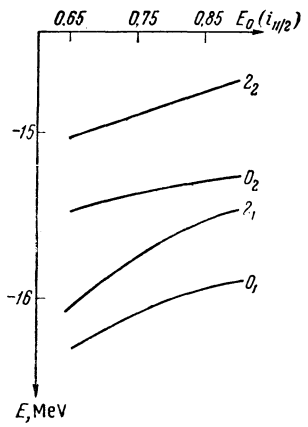

FIG. 5. Position of the first levels with I = 0 and I = 2 as a function of the single particle energy of the state $i_{11/2}$.

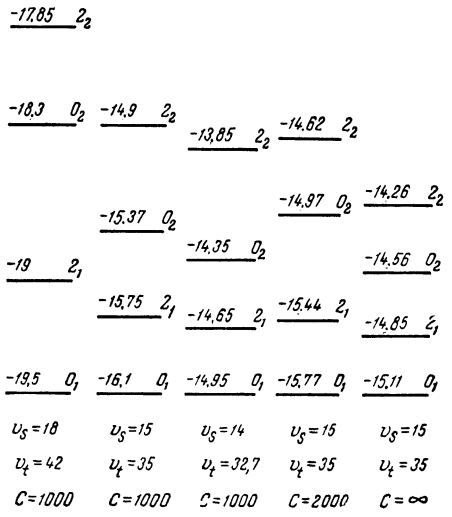

FIG. 6. Positions of the first states with I = 0 and I = 2 for several values of the parameters v_S, v_t and C. The energies are given to the left (all values in MeV).

of these computations is relatively small. However, the obtained results indicate that the probabilities of the E2 transitions $2_1 \rightarrow 0_1$ and $0_2 \rightarrow 2_1$ are roughly the same. The transition $2_2 \rightarrow 2_1$ is an E2 + M1 mixture where the E2 contribution is smaller than in the transitions $2_1 \rightarrow 0_1$ and $0_2 \rightarrow 2_1$. Furthermore, the level 2_2 must have a strong transition to the ground state 0_1. All these results must be experimentally checked.

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250