1 and 2. Our new value is significantly different from and significantly more precise than the best value previously available, i.e., from the 1960 Mass Table. Agreement with the 1964 Mass Table gives some confidence in its accuracy.

Note added in proof. Since our measurements were completed, new experimental values for the chlorine isotopes have been reported from Minnesota [J. L. Benson and W. H. Johnson, Jr., Phys. Rev. Letters **13**, 724 (1964)]. Expressed in terms of mass excesses, so that they can be compared easily with the earlier values in Figs. 1 to 3, these new Minnesota values are: $Cl^{37}=-34\,096.7\pm0.6\,\mu u$, $Cl^{35}=-31\,146.4\pm0.6\,\mu u$, $Cl^{37}-Cl^{35}=-2\,950.3\pm0.6\,\mu u$.

ACKNOWLEDGMENT

We are grateful to Professor Mattauch for sending us a preprint of the 1964 Atomic Mass Table.

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Energy Levels of Pb^{210} from Shell Theory*

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The present calculations for Pb^{210} have been based upon the double-closed-shell-core model with harmonic-oscillator wave functions. All two-neutron configurations of the $2g_{9/2}$, $1i_{11/2}$, $1j_{15/2}$, $3d_{5/2}$, $4s_{1/2}$, $2g_{7/2}$, $3d_{3/2}$ main shell are included. A singlet-even Gaussian effective interaction with parameters determined by low-energy proton-proton scattering and zero triplet-odd effective interaction give, within 50 keV, the binding energy of the two outer nucleons determined from experimental data and the energies of four excited states which have been experimentally identified. An empirical relation between matrix elements for slightly different parameters is described. It indicates that the interaction and the harmonic-oscillator parameter ν used here also give the general agreement with experiment which had been obtained for Pb^{206} with similar parameters. Calculations with a Yukawa singlet-even interaction and with additional attractive and repulsive central and central+tensor triplet-odd effective interactions were made for Pb^{210}; they all lead to somewhat worse agreement. None of these interactions is, however, definitely excluded by the present data. Level schemes, tables of level energies and of some wave functions, and detailed formulas for the calculation of γ-ray transition probabilities are given. A model for the 2.15-MeV $\frac{1}{2}^-$ state of Pb^{209} is also discussed.

I. BACKGROUND OF THE CALCULATION

IN recent years calculations have indicated that energies of low states of nuclei near a double-closed-shell-core nucleus relative to the energy of such a nucleus can often be obtained from a shell-theoretical description with one or two single-particle states and matrix elements of the type

$$\mathfrak{M}(j_1j_2,j_1'j_2',J)=\langle j_1j_2J\,|\,V(1,2)\,|\,j_1'j_2'J\rangle. \quad (1)$$

Each single-particle state is described by the quantum numbers n_i, l_i, j_i; the first two numbers have been omitted in (1). In these investigations[1] by the "method of effective interactions," only a few matrix elements (1) appear; they are determined by the best fit to a large number of data. Often the fit of this theoretical model is excellent. It suggests that the detailed physical framework of the shell theory may have considerable validity at least in some regions of the periodic system.

Already long before enough data had become available for these investigations, *calculations* of the matrix elements (1) were made with simple assumptions for the two-nucleon interaction $V(1,2)$. These matrix elements are then used in larger calculations, which often take into account a considerable number of single-particle states. Nevertheless, there is usually less accurate agreement between such calculations and experiment than with the method of effective interactions.

A very striking exception, however, are the calculations by Kearsley[2] and True and Ford[3] for the nucleus Pb^{206}. There is now at least some indication from experimental data concerning the spins and parities of 19 excited states of this nucleus.[4] Three of these are tentatively identified as due to core excitation. Their excitation energies are approximately equal to those of probably corresponding excited states in the nucleus Pb^{208}. The measured energies of the 16 remaining excited states differ by an average of 2.7% from energies calculated with a singlet-even interaction between the outer nucleons.[5] Calculations have also been made for

* Part of this work was done under the auspices of the U. S. Atomic Energy Commission. Calculations were made at the Computer Center, University of California, Berkeley.

[1] I. Talmi, Rev. Mod. Phys. 34, 704 (1962).

[2] M. J. Kearsley, Nucl. Phys. 4, 157 (1957).

[3] W. W. True and K. W. Ford, Phys. Rev. **109**, 1675 (1958).

[4] *Nuclear Data Sheets*, compiled by K. Way *et al.* (Printing and Publishing Office, National Academy of Sciences—National Research Council, Washington 25, D. C.), NRC 61-4-110 to 126.

[5] W. W. True and K. W. Ford, Ref. 3, Table VIII.

two more complicated models which include an interaction between the outer nucleons and the surface of the core. One such calculation[6] leads to about equally good agreement with the energies now available; another[7] to considerably poorer agreement.

The calculations with the simple model which had been used for Pb^{206} can also be made for Pb^{210}, which has two neutrons outside the Pb^{208} core. Such calculations are described in the present paper. A harmonic-oscillator single-particle potential is used. Single-particle energies are taken from the experimental spectrum of Pb^{209}. A model for the $1/2^-$ state in this spectrum will be discussed (Sec. II). Results for both Gaussian and Yukawa singlet-even interactions (Sec. III) are given. The effects of additional central and central+tensor triplet-odd interactions are also investigated (Sec. V). For all interactions, the diagonal and off-diagonal matrix elements (1) for all configurations arising from all single-particle levels of the $N=127$ to 184 neutron shell have been calculated, by the recent method of Horie and Sasaki[8] (Sec. IV). Multiple-precision fixed-point arithmetic[9] was used in the calculation of these matrix elements on a digital computer.[10]

After the computational part of the present paper (Sec. IV. 2) was completed, new experimental data on Pb^{210} were published.[11] They provide a welcome opportunity for a more extensive comparison between theory and experiment.

II. LEVELS OF Pb^{209}

In the reaction $Pb^{208}(d,p)Pb^{209}$ eight levels of Pb^{209} with excitation below 3 MeV have been identified.[12] One of these is especially weak; its probable spin and parity assignment is $1/2^-$. The other seven are stronger and their probable assignments are those of the seven single-particle levels of the $N=127$ to 184 shell. The levels are shown in Fig. 1. It is noteworthy that the next highest state strongly excited in this (d,p) reaction is at 3.97 MeV, that is, 1.45 MeV above the $3d_{3/2}$ level.[12]

A detailed calculation for the $1/2^-$ state at 2.15 MeV would require diagonalization of a matrix for two-particle+one-hole configurations. A calculation with a zero-range interaction, without configuration interaction, has led to an estimate of the energy of this state.[13] A simplified model will be discussed here. It is based on the assumption that the two particles are in the same state as in the lowest state for Pb^{210}, with $J'=0$. This state is taken to be a superposition of the states $j^2\,J'=0$

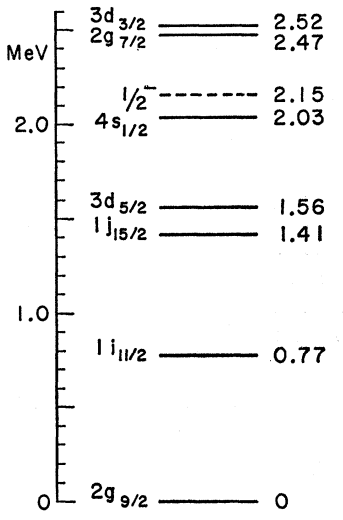

FIG. 1. The energies $\Delta(j)$ of the states below 3 MeV which have been identified in the reaction $Pb^{208}(d,p)Pb^{209}$ (Ref. 12). Each level except the $1/2^-$ level, represented by a dashed line, has a single-particle assignment.

of several configurations (Sec. V). Then the hole state must be $3p_{1/2}$, to give $J=1/2$. This situation can also be pictured as two particles in the $N=127$ to 184 shell with a Pb^{207} $1/2^-$ core. The energy differences between the following two pairs of nuclei should be equal:

$$Pb^{208}\ 0^+,\quad Pb^{207}\ 1/2^-\quad \text{and}\quad Pb^{210}\ 0^+,\quad Pb^{209}\ 1/2^-.$$

For Pb^{210} the interaction between the $3p_{1/2}$ neutron and the two outer neutrons has been neglected. With the masses of the ground states of these nuclei (Sec. V, Ref. 27), one obtains an excitation energy $\mathcal{E}=2.197$ MeV for the Pb^{209} $1/2^-$ state.

Another estimate for $\mathcal{E}$ based upon the same model can be made in a quite different way. This estimate requires the energy ϵ needed to excite one particle from a $3p_{1/2}$ state of the core into a $2g_{9/2}$ state outside the core. This energy will now be estimated in two ways: (a) The first estimate is $\epsilon=3.34$ MeV, the average of 3.198 and 3.475 MeV, the energies of the 5^- and 4^- excited states[14] of Pb^{208}. The $Pb^{207}(d,p)Pb^{208}$ experiments[12] suggest that these states are mainly $(2g_{9/2})(3p_{1/2})^{-1}$. The fact that these states differ in energy by 0.277 MeV indicates that ϵ actually depends somewhat upon the relative orientation of the spins $\frac{1}{2}$ and $\frac{9}{2}$ of the Pb^{207} core and the outer particle. (b) Another estimate of ϵ can be based upon the assumption that the energy differences between the following pairs of nuclei should be equal:

$$Pb^{209}\ \tfrac{9}{2}^+,\quad Pb^{208}\ (2g_{9/2})(3p_{1/2})^{-1}\quad \text{and}\quad Pb^{208}\ 0^+,\quad Pb^{207}\ \tfrac{1}{2}^-.$$

With the experimental masses (Ref. 27), one obtains $\epsilon=3.432$ MeV.

A state of $(2g_{9/2})^2(1p_{1/2})^{-1}$ would have energy $\sim\epsilon$ relative to $(2g_{9/2})^1$ if there were no interaction between the outer nucleons. Actually, there will be appreciable interaction, and their wave function will again be assumed to be that for the ground state of Pb^{210} with

[6] Reference 3, Table XVI.
[7] V. N. Guman, Yu. I. Kharitonov, L. A. Sliv, and G. A. Sogomonova, Nucl. Phys. **28**, 192 (1961).
[8] H. Horie and K. Sasaki, Progr. Theoret. Phys. (Kyoto) **25**, 475 (1961).
[9] R. M. Baer and M. G. Redlich, Commun. Assoc. Computing Machinery **7**, 657 (1964).
[10] M. G. Redlich and R. M. Baer (unpublished).
[11] P. Weinzierl, E. Ujlaki, G. Preinreich, and G. Eder, Phys. Rev. **134**, B257 (1964).
[12] P. Mukherjee and B. L. Cohen, Phys. Rev. **127**, 1284 (1962).
[13] H. Pollak, Bull. Classe Sci. Acad. Roy. Belg. **47**, 1035 (1961).
[14] These are the second and third excited states of Pb^{208}. The first excited state at 2.165 MeV, with 3^-, does not involve the configuration $(2g_{9/2})(3p_{1/2})^{-1}$.

admixtures to $(2g_{9/2})^2$ and with binding energy approximately 1.25 MeV, from experiment as well as from calculations (Sec. V). Therefore, the actual excitation energy of the $1/2^-$ state in Pb^{209} should be approximately $\mathcal{E}=3.34-1.25=2.09$ MeV with the first ϵ, and 2.18 MeV with the second ϵ. The close agreement of these estimates with the measured energy may, however, be accidental, and this model may not be accurate.

In the present paper the single-particle energies will be assumed to be those of the remaining seven levels in Fig. 1. The possibility that the $1j_{15/2}$ and $1i_{11/2}$ levels should be interchanged[12] will be examined.

III. EFFECTIVE INTERACTIONS BETWEEN THE OUTER NUCLEONS

The interaction of (1) will be written as

$$V(1,2)=\sum_X V_X(1,2)\,P_X, \tag{2}$$

where P_X is one or a linear combination of exchange operators. The subscript X can be W, M, B, or H; the corresponding operators are $P_W=1$, $P_M=$space-coordinate exchange operator, $P_B=$spin-coordinate exchange operator and $P_H=P_MP_B$. The operator P_X can also be any linear combination of the preceding four operators. In particular, operators P_X with $X=$SE (singlet even), TE (triplet even), and TO (triplet odd) will be used here.

Only the singlet-even and triplet-odd interactions are needed for Pb^{210}. In the present calculation, the singlet-even interaction between two free protons at <3.6 MeV with the parameters of Jackson and Blatt[15] will be used. The detailed shape is not determined by these data; here, Gaussian and Yukawa potentials will be used. They are written as

$$V_{\rm SE}(1,2)=V_0\exp(-r^2/r_n^2), \tag{3}$$

with $V_0=-31.61$ MeV and $r_n=1.7765$ F, and

$$V_{\rm SE}(1,2)=V_0\,e^{-r/r_n}/(r/r_n), \tag{4}$$

with $V_0=-47.31$ MeV and $r_n=1.1653$ F. The potentials (3) and (4) are based upon the effective ranges and scattering lengths of Table IX, Ref. 15. These differ only slightly from more recent data.[16] It will be seen in Sec. IV.1 that the nuclear matrix elements are not sensitive to changes of the order $\sim 5\%$ in the effective range, or the related parameter r_n.

Calculations have been made with two different assumptions for the triplet-odd interaction. The first is simply

$$V_{\rm TO}(1,2)=\alpha V_{\rm SE}(1,2), \quad \text{Yukawa or Gaussian} \tag{5}$$

where α is a constant. The second is based upon the triplet-even (TE) interaction

$$V_{\rm TE}(1,2)=V_0\left[\frac{e^{-r/r_{cn}}}{r/r_{cn}}+\gamma S_{12}\frac{e^{-r/r_{tn}}}{r/r_{tn}}\right], \tag{6}$$

with the tensor operator S_{12}. Feshbach and Schwinger[17] calculated tables of the sets of parameters for which the interaction (6) will describe the TE neutron-proton scattering at low energies and the properties of the ground state of the deuteron. Here the following parameters will be used:

$$r_{cn}=1.1653\text{ F},\quad V_0=-41.73\text{ MeV},$$
$$r_{tn}=1.5350\text{ F},\quad \gamma=0.7820.$$

The range parameter r_{cn} has been chosen equal to the r_n for the SE interaction (4). The remaining parameters are determined by the fit to experimental data.[18] The second assumption for the TO interaction is now

$$V_{\rm TO}(1,2)=-0.5\,V_{\rm TE}(1,2), \tag{7}$$

with $V_{\rm TE}(1,2)$ given by (6).

There is no *a priori* reason to assume that these interactions should also be accurate for the outer nucleons in a nucleus, which are expected to have much larger energies. Some recent calculations for Bi^{210} and Po^{210} were based on an interaction with a Gaussian SE part which had considerably different parameters.[19] In the present paper, however, the consequences for Pb^{210} of interactions based upon the low-energy data will be examined.

IV. DETAILS OF THE MODEL AND THE CALCULATIONS

1. The Harmonic-Oscillator Parameter ν

The harmonic-oscillator single-particle potential contains just one parameter[20] ν. For all states of the $N=127$ to 184 shell except $1j_{15/2}$, the equation

$$\langle nlj|r^2|nlj\rangle=15/(2\nu) \tag{8}$$

holds. The wave functions have a factor $\exp(-\frac{1}{2}\nu r^2)$.

The range/radius parameter λ, defined by Horie and Sasaki,[8] is useful for calculations with either Gaussian or Yukawa interactions. With r_n defined by (3) or (4), this parameter is given by

$$\lambda=r_n(\tfrac{1}{2}\nu)^{1/2}. \tag{9}$$

An empirical rule. If $\mathfrak{M}_1$ and $\mathfrak{M}_2$ are two central-interaction matrix elements of type (1) for Pb^{210}, for either Gaussian or Yukawa shape, with $V_{0,1}$, λ_1, and $V_{0,2}$, λ_2, respectively, then

$$\mathfrak{M}_2/\mathfrak{M}_1\approx V_{0,2}\,\lambda_2^2/V_{0,1}\,\lambda_1^2, \tag{10}$$

[15] J. D. Jackson and J. M. Blatt, Rev. Mod. Phys. **22**, 77 (1950).
[16] M. A. Preston, *Physics of the Nucleus* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1962).
[17] H. Feshbach and J. Schwinger, Phys. Rev. **84**, 194 (1951).
[18] These parameters differ slightly from one of the sets given by Feshbach and Schwinger, Ref. 17, Table V. An interpolation has been made, by means of their Rule 4, p. 199.
[19] Y. E. Kim and J. O. Rasmussen, Nucl. Phys. **47**, 184 (1963).
[20] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

if λ_2 and λ_1 differ by $\sim 5\%$ or less. In the region of parameter λ values used in the present paper, the rule (10) is usually accurate to about $\pm\frac{1}{2}x\%$ if λ_2 and λ_1 differ by $x\%$. Occasionally, a very large deviation appears; the largest found was $2.5x\%$.

This rule originated with the observation that matrix elements $\mathfrak{M}$ of type (1) change only slightly with changes in the effective range r_0 of the two-nucleon interaction, for a given v. Such changes affect the well depth parameter s only slightly, but affect r_n very strongly, as is seen from Jackson and Blatt, Ref. 15, Eqs. (11.3 G) and (11.3 Y). The depth V_0 is given by

$$V_0 = cs r_n^{-2} = \tfrac{1}{2} cs v \lambda^{-2},$$

with c equal to a constant which depends upon the shape of the interaction. Here, cs is almost constant when r_0 and r_n are changed, and (10) leads to approximately the same matrix elements for two interactions differing by a few percent in r_n or r_0.

Equivalent v for Pb^{206}. The calculations[2,3] for Pb^{206} had been made with potentials which differed somewhat from (3) and (4). With the above rule, the results of True and Ford[5] are approximately those obtained with (3) and $v = 0.20539$ F^{-2}. The λ values differ by $x = 1.4\%$. The results of Kearsley[2] are equivalent to (4) plus (5) with $\alpha = -0.559$, and $v = 0.16832$. Here, the λ values differ by $x = 5.8\%$.

2. The Horie-Sasaki Method

The two-nucleon potential $V_X(1,2)$ of (2) will be written as

$$V_X(1,2) = V_{X0}(r) + V_{X2}(r)\, S_{12}. \tag{11}$$

The subscript κ of $V_{X\kappa}(r)$ equals 0 for the central and 2 for the tensor interactions. Matrix elements of each term of (11) can be calculated for harmonic-oscillator wave functions by use of the Horie-Sasaki method.[8] In this method, each such matrix element is expressed as a linear combination of radial integrals $K_m^{(\kappa)}$, which depend only upon $V_{X\kappa}(r)$ and v. The coefficients of the $K_m^{(\kappa)}$ are independent of $V_{X\kappa}(r)$ and v. The subscript m takes integer values ≤ 14 for states up to and including $1j_{15/2}$. Thus,

$$\langle j_1 j_2 J | V_{X\kappa}(r)\, P_X Q_\kappa | j_1' j_2' J \rangle = \sum_m C_m(j_1 j_2, j_1' j_2', J; X, \kappa)\, K_m^{(\kappa)} \tag{12}$$

with $Q_0 = 1$, and $Q_2 = S_{12}$. The coefficients C_m can be expressed as $d^{1/2}\, e/f$, with d, e, and f integers, when harmonic-oscillator single-particle wave functions are used. The $K_m^{(\kappa)}$ are related[21] to the $J_m^{(\kappa)}$ defined in Ref. 8 by

$$K_m^{(\kappa)} = J_m^{(\kappa)} \times 2^m/(2m+1)!!. \tag{13}$$

These K integrals can be written as simple linear combinations of the Talmi integrals I_l of Ref. 20.

[21] H. Horie (unpublished work).

For the zero-range central interaction

$$V_{X0}(r) P_X = r^{-2}\, \delta(r)\, P_X, \tag{14}$$

and the singular zero-range tensor interaction

$$V_{X2}(r) P_X S_{12} = r^{-4}\, \delta(r)\, P_X S_{12}, \tag{15}$$

the K integrals $K_m^{(\kappa)}$ have the nonzero values $K_m^{(0)} = (2v^3/\pi)^{1/2}$ for $m \geq 0$ and $K_m^{(2)} = (2m+3) I_1/5$ for $m \geq 1$. Here, I_1 is a Talmi integral.[20] These values permit a check of the coefficients C_m, because the matrix elements of (14) and (15) can be calculated in an entirely independent way for both central[22] and tensor[23] interactions.

The calculations of this paper have been carried out on an IBM 7090/94 computer. Multiple-precision fixed-point arithmetic[9] was used throughout (a) the calculation of the coefficients C_m and (b) the separate calculation of the zero-range matrix elements needed to check the values of each set of these coefficients.[10] Decimal approximations were not used for any part of the calculations (a) or (b).

Double-precision floating-point arithmetic was used, however, in FORTRAN II programs for the calculation of the K integrals for Gaussian and Yukawa interactions with range >0. These integrals depend upon the range/radius parameter λ of Eq. (9). The integrals calculated by the programs for both Gaussian and Yukawa interactions for the values $\lambda = 0.2$ (0.1) 1.0 have been compared with tables[21] and some additional calculations, all made with a desk calculator.

After the C_m and the $K_m^{(\kappa)}$ have been calculated, the simple final steps of Eq. (12) are carried out, also with double-precision floating-point arithmetic. However, only a few sample checks have been made of this part of the calculation. No separate, entirely independent check of each final matrix element for range >0 has been made. Therefore, the accuracy of these matrix elements is less certain than that of the coefficients C_m. A check of the programs for the final matrix elements has, however, been made for the $N = 83$ to 126 shell. Energies obtained from diagonalization of matrices for this shell with the model and parameters of True and Ford[5] have been compared with all energies of their Table VIII. The average magnitude of the difference between an energy of their table and that calculated with the present method is below 2 keV. The largest discrepancy is 7 keV.

3. The Shell Model for Pb^{210}

There are 28 configurations of the type

$$n_1 l_1 j_1, \quad n_2 l_2 j_2$$

[22] N. Newby, Jr. and E. J. Konopinski, Phys. Rev. **115**, 434 (1959); A. de-Shalit, Phys. Rev. **91**, 1479 (1953).

[23] The diagonal matrix elements of the interactions (15) have been calculated for configurations $(nl)^2$ in L–S coupling by M. Moshinsky, Nucl. Phys. **8**, 19 (1958). A general formula has since been derived by the author (unpublished work).

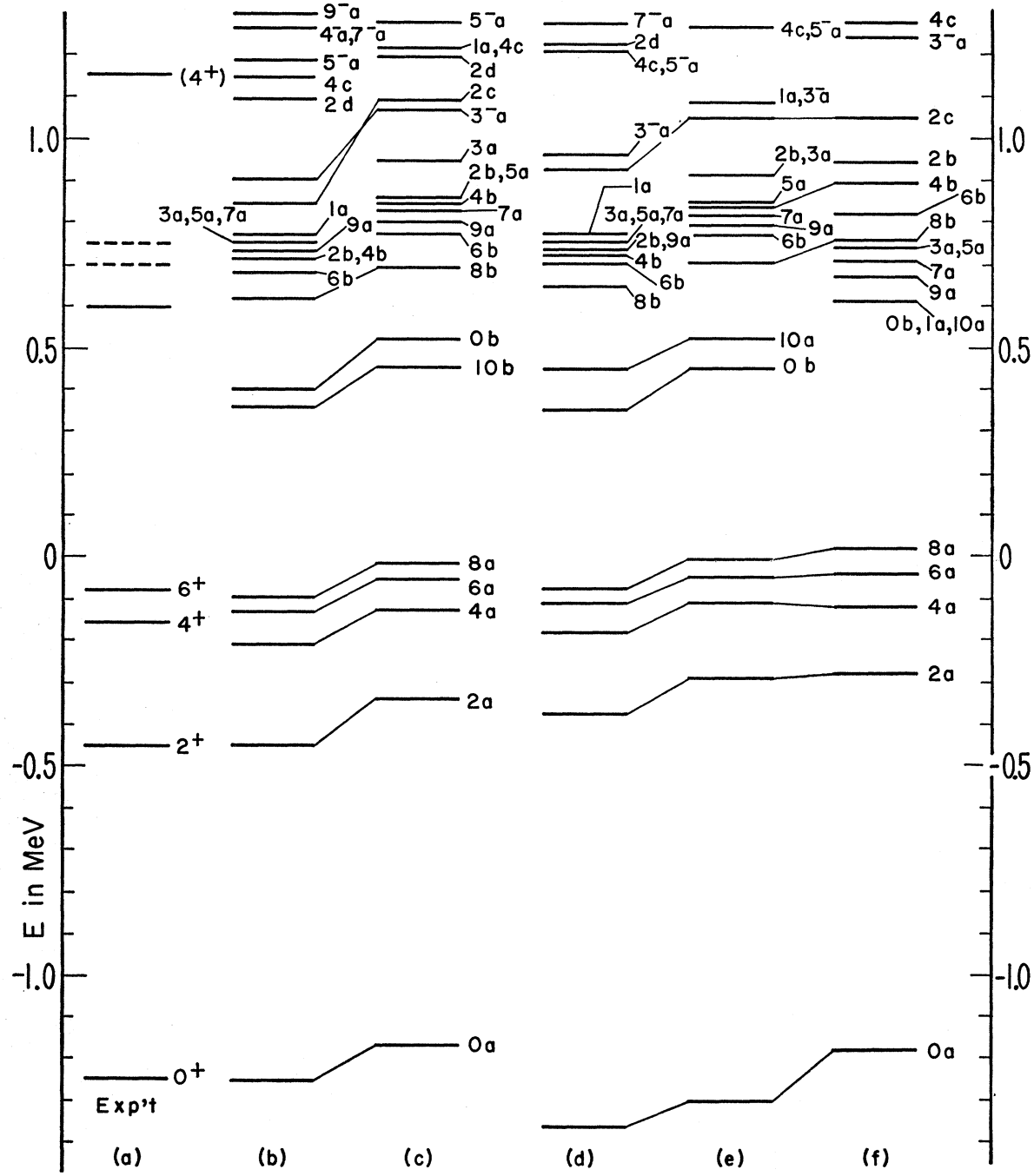

FIG. 2. (a) Observed levels of Pb^{210}. The ordinate is the energy of interaction between the two outer nucleons. The energy of the nucleons in the ground state is taken from data as -1.250 MeV. The remaining schemes show calculated levels: (b) Gaussian SE interaction. (c) Gaussian SE+repulsive TO interaction, from Eqs. (3) and (5) with $\alpha=-0.5$. (d) Yukawa SE interaction. (e) Yukawa SE+repulsive TO interaction from Eqs. (4) and (5) with $\alpha=-0.559$. (f) Yukawa SE+Feshbach-Schwinger central+tensor TO interaction, from Eq. (7). The radius parameter ν equals 0.20539 F^{-2} for both (b) and (c), and 0.18457 F^{-2} for (d), (e), and (f). Theoretical levels with parity + are labeled Jx; those with parity − are labeled $J^{-}x$. Here, x indicates the order, with $x=a$ for the lowest state.

for the seven single-particle states of Fig. 1. Taking into account the permitted values of J for each configuration, there are altogether 141 states with two neutrons in the $N=127$ to 184 shell. All diagonal and off-diagonal (interconfiguration) matrix elements for all these states have been calculated, for each interaction and each set of parameters described in Sec. V. An earlier calculation based upon a model which includes an interaction between the outer nucleons and the surface of the core took into account five single-particle states.[7]

The diagonal single-particle energies will be denoted $\Delta(j_i)$. They are taken relative to the energy of the $2g_{9/2}$ state (see Fig. 1). Matrices of the type

$$A=\|\mathfrak{M}(j_ij_k,j_{i'}j_{k'},J)+[\Delta(j_i)+\Delta(j_k)]\delta_{ii'}\delta_{kk'}\|\,, \quad (16)$$

with $\mathfrak{M}$ from (1), were formed for all possible values of J and parity. They were diagonalized on the computer. Each diagonalization was checked by substitution of each eigenvalue ϵ_i and its corresponding eigenvector B_i into the matrix equation $AB_i=\epsilon_iB_i$.

In these calculations, all conventions of Racah[24,25] have been followed. In particular, spin and orbital angular momentum couple in the order

$$\mathbf{s}+\mathbf{l}=\mathbf{j}. \quad (17)$$

The signs of the radial wave functions and the parameter ν are those of Talmi[20] and Horie and Sasaki.[8]

V. RESULTS OF THE CALCULATIONS

1. Experimental Data

It will be assumed here that the binding energy of an outer neutron in the $2g_{9/2}$ or in a higher state due to its interaction with the core does not change with the addition of a second outer neutron. If such a neutron is added to Pb^{209}, it will, however, interact not only with the core, but also with the other outer neutron. The state of lowest energy will be a superposition of states of $(2g_{9/2})^2$ and higher configurations. Here, B will denote the binding energy of the two outer neutrons in their lowest state minus the binding energy which they would have in the lowest state [configuration $(2g_{9/2})^2$] if each outer nucleon interacted only with the core, that is, if the interaction between the outer nucleons were exactly zero. B is given by

$$B=S_n(Pb^{210})-S_n(Pb^{209}), \quad (18)$$

where S_n is a neutron separation energy. The energy B can be obtained from three sources: (i) recent data[26] on $S_n(Pb^{209})$, on the reaction $Bi^{209}(n,\gamma)Bi^{210}$, and the β^--decay energies of Pb^{209} and Pb^{210}; (ii) a new table of masses of heavy elements[27]; (iii) the 1961 Table of Nuclidic Masses.[28] These values of B are compared with the calculation using the singlet-even Gaussian interaction (3) and $\nu=0.20539$ F^{-2}, described in Part 2 of this section, and plotted in Fig. 2(b):

Experimental data	(i)	1.243 ± 0.029 MeV,
	(ii)	1.235 MeV,
	(iii)	1.273 ± 0.070 MeV.
Theory, SE Gaussian		1.254 MeV.

In Fig. 2 (a), experimental energies are plotted. The energy of the ground state is taken as $-B=-1.250$ MeV. The energies of the excited states are then given by the data of Weinzierl, Ujlaki, Preinreich, and Eder.[11]

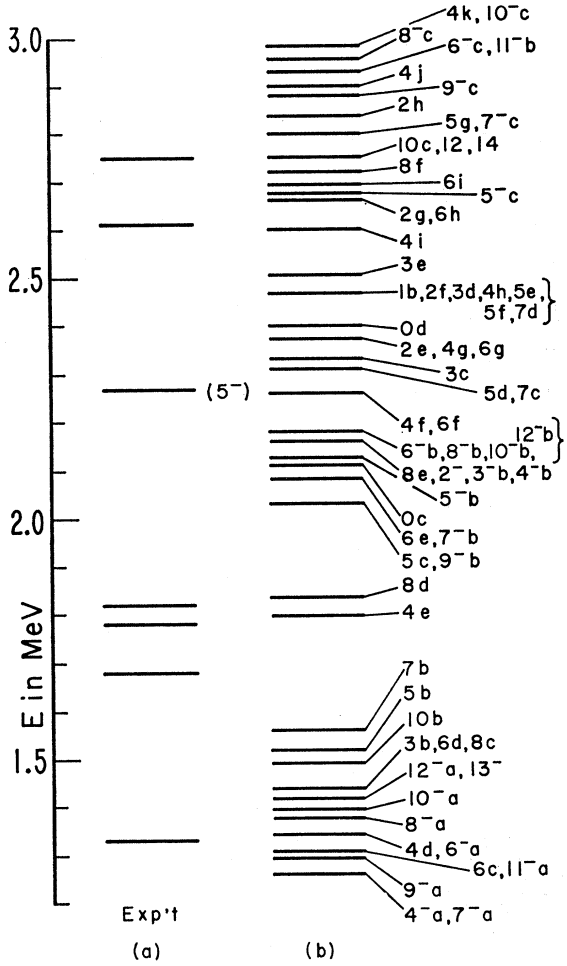

FIG. 3. Continuation of the level schemes of Fig. 2 (a) and (b) up to energy $E=3.0$ MeV (energy of excitation 4.25 MeV). Part (a) shows the observed levels, Part (b), those calculated for the Gaussian SE interaction. Experimental results indicate that the (5^-) state with $E=2.27$ MeV (excitation 3.52 MeV) is core-excited. (The level 11^-b should be at 1.94 MeV instead of 2.94 MeV.)

[24] G. Racah, Phys. Rev. **62**, 438 (1942); Physica **16**, 651 (1950).
[25] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic Press Inc., New York, 1963).
[26] Reference 4, NRC 5-3-88 to 121 (May 1963).
[27] V. E. Viola, Jr., and G. T. Seaborg (to be published).
[28] L. A. König, J. H. E. Mattauch, and A. H. Wapstra, Nucl. Phys. **31**, 18 (1962).

2. Results for Several Interactions

Each of the theoretical level schemes of Fig. 2 (b)–(f) will be described separately, and some calculations for which no schemes are given will be discussed. The levels with parity + are labeled Jx, and those with parity − are labeled J^-x. Here $x=a, b, c, \cdots$, denotes the order of the states; the lowest state with J is Ja. For some J, there is only one state; then the label x is omitted. The energy of the state Jx due to the two-nucleon interaction is denoted $E(Jx)$; it is the ordinate of Fig. 2. In many instances there are two or more states with calculated energies which differ only by a few keV. For all these states only one line is drawn and it is marked with the labels of all the states, separated by commas.

Figure 2 (b) shows the results for the Gaussian interaction (3) between nucleons in SE states only. The interaction is zero for TO states. The radius parameter ν equals 0.20539 F^{-2}. This value leads to approximately the best agreement with all energies now available. From Eq. (7), the square root of the expectation value of r^2 for all single-particle states except $1j_{15/2}$ is given by

$$\langle r^2\rangle^{1/2}=6.043\text{ F}=1.017\times 210^{1/3}\text{ F}.$$

The above value of ν happens to be also the value which leads to the results of True and Ford[5] for Pb^{206}, from the empirical rule of Sec. IV. 1. Another calculation (not shown) has been made for the exact interaction and ν of True and Ford. The average difference between the energies of this calculation and those of Fig. 2 (b) is far below 1%. The maximum absolute energy difference for all levels is 15 keV.[29]

Figure 2 (c) gives the levels for the same SE interaction and ν as for Fig. 2 (b), with the additional repulsive central TO interaction (5) with $\alpha=-0.5$. The results are rather similar to those for the SE interaction alone. There is, however, a sharp difference in $E(1a)$ for the two interactions: The value for Fig. 2 (b) is 0.770 MeV; for Fig. 2 (c), it is 1.213 MeV. A separate calculation has been made for an attractive TO interaction (5) with $\alpha=+0.5$. The resulting levels are displaced relative to those of Fig. 2 (b) by approximately the same magnitudes as those of Fig. 2 (c), but in the opposite direction.

Figure 2 (d) shows the results for the central Yukawa interaction (4), between SE states only. Here, $\nu=0.18457$. This parameter is considerably larger than the $\nu=0.16832$ determined by the fit to the work of Kearsley.[2] From the rule of Eq. (10), the magnitudes of the matrix elements increase approximately linearly with ν, if the other parameters are kept fixed. The magnitude of the energy of the lowest state with each J, obtained after diagonalization of the matrix, also usually increases with ν, although not necessarily linearly. The large ν of Fig. 2 (d) has been chosen in an attempt to fit the energy of the 2^+ state. We see that the calculated $|E(2a)|$ is still too small, although $|E(0a)|$ is too large.

Figure 2 (e) gives results for the same SE interaction and ν, with the repulsive central TO interaction used by Kearsley, that is, (5) with $\alpha=-0.559$. It is still not possible to fit both the binding energy of the ground state and the excitation energy of the first 2^+ state. In Pb^{206} there is a similar, but smaller discrepancy.[2] The state $1a$ lies appreciably higher than for the SE interaction, as in the Gaussian level schemes.

Two further calculations with Yukawa shape and a central TO interaction equal to −0.559 times the SE interaction have been made. For the first, the same potential as in Fig. 2(e) was used, but a smaller harmonic-oscillator parameter, namely, $\nu=0.16832$. This ν was determined by the fit to the work of Kearsley[2] for Pb^{206} (Sec. IV. 1). This leads to a spectrum very similar to Fig. 2 (e), but shifted upward, with $E(0a)=-1.14$ MeV. The $2a$ level lies at −0.249 MeV, which is too high. For the second calculation the exact parameters of Kearsley were used. The maximum absolute energy difference between corresponding levels in the two calculations is 14 keV.

Figure 2 (f) shows the levels for the same SE Yukawa interaction and ν as in Fig. 2(d), but the central + tensor TO interaction (7). Its strength is $-\frac{1}{2}$ times that of the Feshbach-Schwinger TE interaction. The level schemes of Fig. 2 (e) and (f) are similar for the lowest five levels, but they differ qualitatively for some higher levels. For example, in Fig. 2 (f) the state $1a$ almost coincides with $10a$ and $0b$; in Fig. 2 (e) it lies about 0.5 MeV higher.

It does not seem possible to exclude either this interaction or a central TO interaction at the present time. Nor can a Yukawa shape for the SE interaction be excluded. The Gaussian SE interaction does, however, lead to the best agreement with the data now available, of all the interactions investigated so far. Further details will be given for the results with this interaction.

3. Results for the Gaussian SE Interaction

For this section the SE interaction is just (3) with the parameters of Sec. III; the TO interaction equals zero, and $\nu=0.20539$. The level diagrams of Fig. 2 (a) and (b) are extended to higher energies in Fig. 3. There are several groups of levels, with gaps between them. The first group, levels $0a$ to $8a$, belongs predominantly to the configuration $(2g_{9/2})^2$, the next, levels $10a$ to $1a$ except $0b$, belongs to $2g_{9/2}1i_{11/2}$. The next higher group of levels, $2d$ to $7b$ together with the levels $0b$, $2c$, and 3^-a, belongs predominantly to three configurations; these are: $2g_{9/2}3d_{5/2}$, $(1i_{11/2})^2$, and $1j_{15/2}2g_{9/2}$.

[29] The calculations of True and Ford (Ref. 5) and Kearsley (Ref. 2) did not, however, include all of the configurations of the $N=83$ to 126 main shell. Calculations by the present methods indicate that the inclusion of all these configurations leads to agreement similar to that of True and Ford, provided that a value of ν approximately 8% lower than that given by them is used.

TABLE I. Energies of excited states in MeV, calculated for a singlet-even Gaussian interaction (3) with $V_0=-31.61$ MeV and $r_n=1.7765$ F, and harmonic-oscillator parameter $\nu=0.20539$ F^{-2}. Each energy is given relative to the energy of the ground state; it is: $E(Jx)-E(0a)$. The label x ahead of each energy indicates the order of the state; a is the state with lowest energy for given J. All energies below 4.25 MeV are given, and also a few of the higher ones. The energies are listed by the configuration which has the largest amplitude a_{max} in the corresponding wave function. If $a_{max}>0.99$, the energy is given in italics.

	$J=0$	1	2	3	4	5	6	7	8	9	10
Parity +											
$(2g_{9/2})^2$	*a* 0		*a* 0.802		*a* 1.041		*a 1.123*		*a 1.153*		
$(1i_{11/2})^2$	*b* 1.651		*d* 2.345		*d* 2.596		*d* 2.681		*c* 2.693		*b 2.741*
$2g_{9/2}1i_{11/2}$		*a 2.024*	*b* 1.964	*a 2.007*	*b* 1.966	*a 2.001*	*b* 1.938	*a 1.993*	*b* 1.873	*a 1.983*	*a 1.613*
$2g_{9/2}3d_{5/2}$			*c* 2.101	*b 2.694*	*c* 2.398	*b 2.769*	*c* 2.564	*b 2.814*			
$2g_{9/2}4s_{1/2}$					*e* 3.053	*c 3.284*					
$2g_{9/2}2g_{7/2}$		*b 3.724*	*e*[a] 3.625	*d 3.724*	*g* 3.620	*e 3.724*	*g* 3.632	*d 3.724*	*d* 3.089		
			f[a] 3.728								
$2g_{9/2}3d_{3/2}$				*e 3.759*	*h* 3.723	*f 3.735*	*e* 3.331				
$(1j_{15/2})^2$	*d* 3.649		(a)		*i* 3.855		*i* 3.949		*f* 3.974		*c 3.996*[b]
$1i_{11/2}3d_{5/2}$				*c 3.584*	*f* 3.517	*d 3.567*	*f* 3.519	*c 3.558*	*e* 3.412		
$1i_{11/2}4s_{1/2}$						*g 4.054*	*h* 3.914				
$1i_{11/2}2g_{7/2}$			*h* 4.093	*f 4.338*	*l* 4.432	*h* 4.424	*j* 4.386	*e 4.463*	*g 4.440*	*b 4.485*	
$1i_{11/2}3d_{3/2}$					*k* 4.236	*i* 4.514	*k* 4.507	*f 4.536*			
$(3d_{5/2})^2$	*c* 3.359		*g* 3.915		*j* 4.155						
Parity −											
$1j_{15/2}2g_{9/2}$				*a 2.157*	*a 2.517*	*a 2.439*	*a 2.598*	*a 2.512*	*a 2.629*	*a 2.546*	*a 2.648*[b]
$1j_{15/2}1i_{11/2}$			*3.428*	*b 3.408*	*b 3.427*	*b 3.381*	*b 3.429*	*b 3.349*	*b 3.430*	*b 3.300*	*b 3.430*[b]
$1j_{15/2}3d_{5/2}$						*c 3.930*	*c 4.183*	*c* 4.069	*c 4.208*	*c* 4.134	*c 4.224*

	$J=11$	12	13	14
$(1j_{15/2})^2$		*4.008*		*4.019*
$1j_{15/2}2g_{9/2}$	*a* 2.565	*a 2.664*		
$1j_{15/2}1i_{11/2}$	*b* 3.191	*b 3.430*	*2.672*	

[a] Both states $2e$ and $2f$ have the largest amplitude for $2g_{9/2}2g_{7/2}$. The $(1j_{15/2})^2$ amplitude is only slightly smaller for both of them.
[b] Continued for $J>10$ at bottom of table.

In Table I the energies of excitation $E(Jx)-E(0a)$ are given for all levels up to 4.25-MeV excitation and for a few higher ones. They are listed by that configuration which has the largest amplitude a_{max} in the wave function of the state. Many states are rather pure, with $a_{max}>0.99$. The energies of these states are italicized in the table. It must be emphasized that even though $a_{max}>0.99$, the amplitudes of other configurations may still be rather large. For example, the wave function for 5^-a has amplitudes 0.9908 and 0.1177 for $1j_{15/2}2g_{9/2}$ and $1j_{15/2}3d_{5/2}$, respectively.

The wave functions for all states with $E(Jx)<2.15$ MeV (excitation <3.40 MeV) and parity + except those with $a_{max}>0.99$ are given in Table II. Only two states with parity − and $E(Jx)<2.15$ MeV have $a_{max}\leq 0.99$. Their wave functions are specified by the amplitudes of the following table:

J^-x	$E(J^-x)$ in MeV	$1j_{15/2}2g_{9/2}$	$1j_{15/2}1i_{11/2}$	$1j_{15/2}2g_{7/2}$
11^-a	1.311	−0.9868	0.1376	0.0850
11^-b	1.937	0.1450	0.9855	0.0880

Configuration interaction plays an important part in determining the energies of some states. For example, the state $(2g_{9/2})^2$ with $J=0$ has energy −0.805 MeV; configuration interaction leads to a state $0a$ with −1.254 MeV. The wave functions generally do not vary greatly with ν, or with an additional TO interaction.

Comparison with experimental data. The energy of the ground state, $E(0a)$, was already compared with data in Part 1 of this section. Four excited states have been at least tentatively identified; their energies of excitation, $E(Jx)-E(0a)$, from theory and from experiment[11] are given below.

State	$2a$	$4a$	$6a$	$4c$
Theory	0.802	1.041	1.123	2.398 MeV
Experiment	0.795	1.09	1.17	2.40 MeV

Comparison of the experimental and theoretical schemes of Fig. 2 (a), (b), and Fig. 3 suggests the identification of several other states primarily on the basis of the proximity of one or two possible theoretical states to an experimental one. More experimental information is needed, however, before one can trust such identifications. The excited state at 2.93 MeV with $E=1.68$ MeV [Fig. 3 (a)] does not lie close to any calculated level. Possibly it is one of the first core-excited states.

Interchange of $1i_{11/2}$ and $1j_{15/2}$ single-particle states. As mentioned in Sec. II, it is not entirely certain from experiment that the order of these two states in Pb^{209} is correct. The SE Gaussian interaction calculations

TABLE II. The wave functions of the states with energy $E(Jx)$ <2.15 MeV [excitation energy $E(Jx)-E(0a)$ <3.40 MeV], parity +, and maximum amplitude $a_{max}\leq 0.99$. For all remaining states in this energy interval except $11^{-}a$ and $11^{-}b$ the largest amplitude exceeds 0.99. The energy $E(Jx)$ is given in MeV. The remaining entries in each column are amplitudes.

Jx	$0a$	$0b$	$0c$	$2a$	$2b$	$2c$	$2d$	$4a$	$4b$	$4c$	$4d$	$4e$	$6b$	$6c$	$6d$	$6e$	$8b$	$8c$	$8d$
$E(Jx)$	−1.254	0.398	2.106	−0.452	0.710	0.848	1.091	−0.213	0.712	1.144	1.342	1.799	0.684	1.310	1.428	2.077	0.619	1.439	1.835
$(2g_{9/2})^2$	0.8909	−0.4019	−0.1751	0.9549	0.1803	−0.2140	−0.0080	0.9846	0.0692	0.1404	0.0068	−0.0304	0.0581	−0.0892	0.0095	−0.0682	0.0659	−0.0386	0.1031
$(1i_{11/2})^2$	0.3050	0.8265	−0.3226	0.1267	−0.2682	0.4538	−0.7779	0.0577	−0.0914	−0.4741	0.8509	−0.0695	−0.0682	0.5277	0.8322	−0.1113	−0.0615	0.9789	0.1804
$(1j_{15/2})^2$	−0.2280	−0.3872	−0.3511	−0.0874	0.1170	−0.1731	0.2033	−0.0386	0.0460	0.1261	−0.1138	−0.0276	0.0380	−0.0908	−0.0670	−0.1136	0.0374	−0.0780	0.0763
$(3d_{5/2})^2$	0.1526	0.0569	0.7869	0.0550	−0.0522	0.0788	0.0364	0.0247	−0.0158	−0.0643	−0.0188	0.0516							
$(4s_{1/2})^2$	0.0663	0.0235	0.2448																
$(2g_{7/2})^2$	0.1613	0.0315	0.1163	0.0710	−0.0268	0.0393	0.0020	0.0351	−0.0101	−0.0365	−0.0022	0.0150	−0.0074	0.0254	−0.0031	0.0391			
$(3d_{3/2})^2$	0.0866	0.0273	0.2221	0.0273	−0.0222	0.0326	0.0143												
$2g_{9/2}1i_{11/2}$				−0.0383	0.8463	0.5291	−0.0003	−0.0403	0.9810	−0.1786	0.0194	0.0243	0.9882	0.1232	0.0159	0.0610	0.9878	0.0829	−0.1002
$2g_{9/2}3d_{5/2}$				0.1924	−0.3747	0.6315	0.5871	0.0892	−0.1012	−0.7240	−0.4780	−0.4448	−0.0652	0.7641	−0.5373	−0.3177			
$2g_{9/2}4s_{1/2}$								0.0640	−0.0667	−0.3414	−0.1658	0.8742							
$2g_{9/2}2g_{7/2}$				−0.0558	0.0275	−0.0423	−0.0024	−0.0591	0.0212	0.0915	0.0061	−0.0616	0.0294	−0.1332	0.0172	−0.4771	0.0624	−0.1525	0.8421
$2g_{9/2}3d_{3/2}$								−0.0361	0.0296	0.1366	0.0551	−0.0919	0.0499	−0.2530	0.1044	−0.5947			
$1i_{11/2}3d_{5/2}$								0.0173	−0.0236	−0.0452	−0.0083	0.0484	−0.0417	0.0610	−0.0124	0.4509	−0.0953	0.0600	−0.4783
$1i_{11/2}4s_{1/2}$													−0.0343	0.0546	−0.0172	0.2057			
$1i_{11/2}2g_{7/2}$				0.0647	−0.1026	0.0873	−0.0002	0.0257	−0.0501	−0.0712	0.0131	0.0388	−0.0435	0.0450	0.0075	0.0894	−0.0419	0.0227	−0.0560
$1i_{11/2}3d_{3/2}$								0.0319	−0.0377	−0.0637	−0.0108	0.0440	−0.0263	0.0314	−0.0060	0.0940			
$3d_{5/2}4s_{1/2}$				0.0572	−0.0576	0.0848	0.0447												
$3d_{5/2}2g_{7/2}$				−0.0244	0.0271	−0.0400	−0.0265	−0.0264	0.0183	0.0738	0.0274	−0.0337	0.0289	−0.1186	0.0462	−0.1422			
$3d_{5/2}3d_{3/2}$				−0.0306	0.0264	−0.0392	−0.0175	−0.0383	0.0226	0.0865	0.0245	−0.0598							
$4s_{1/2}2g_{7/2}$								−0.0272	0.0208	0.0807	0.0323	−0.0669							
$4s_{1/2}3d_{3/2}$				−0.0377	0.0352	−0.0513	−0.0264												
$2g_{7/2}3d_{3/2}$				0.0604	−0.0632	0.0922	0.0599	0.0238	−0.0157	−0.0613	−0.0223	0.0260							

have been repeated with the assumption that these two single-particle levels are interchanged. The changes in the energies of the lowest five levels are only of the order of 20 keV. There is now a state $4b$ at 2.357 MeV excitation; this leads to somewhat worse agreement with a state identified as (4^+) than the $4c$ state of Table I. The changes in energy for those states which are rather pure ($a_{max}>0.99$) are consistent with the expectation that states of configurations with one $1i_{11/2}$ state would be raised by approximately 0.64 MeV, with a corresponding lowering of configurations with one $1j_{15/2}$ state. For example, the states $1a$, $3a$, $5a$, $7a$, and $9a$, which are predominantly $2g_{9/2}1i_{11/2}$ (see Table I), should now have energies approximately 2.66, 2.65, 2.64, 2.63, and 2.62 MeV, respectively. These predictions are correct within 0.02 MeV. At present, neither these nor other states whose energies change substantially with the exchange of the $1i_{11/2}$ and $1j_{15/2}$ single-particle states have been identified experimentally. Therefore it is not possible now to draw a conclusion from Pb^{210} about the order of these states.

Remarks about γ-ray transition probabilities. When more experimental data on Pb^{210} become available, it may be useful to calculate estimates of γ-ray transition probabilities with the wave functions of the present investigation. Such calculations must be made in the scheme of Refs. 24, 25, and 20, because this scheme was used in the calculation of the wave functions. If the phase conventions are not followed strictly, some calculated transition probabilities may be incorrect by a factor of a few orders of magnitude. Therefore, details of such calculations will be given in the Appendix. The γ-ray transition probabilities are, however, much more sensitive to details of the wave functions than are the energies. They may depend strongly upon very small admixtures of core-excited states. Also, it is usually necessary to make a more or less arbitrary assumption about an "effective" neutron charge in the calculation of these transition probabilities.

VI. DISCUSSION OF THE RESULTS

It has been known for a long time that the nucleon-nucleon scattering data at low energies are consistent with simple effective interactions in the singlet and triplet states with relative angular momentum zero (^1S and ^3S states). To account also for the properties of the ground state of the deuteron, a somewhat more complicated effective interaction is needed, and its parameters are not uniquely specified.[17] Even this interaction, however, is much simpler than those which appear to be necessary to account for nucleon-nucleon scattering at high energies.[16]

At the present time there is no indication that any of the simpler interactions can account for the properties of nuclei due to the inner nucleons, for example, for the total binding energy of the ground state of Pb^{208}. However, the results for Pb^{206} and Pb^{210} suggest the possibil-

ity that a simple effective interaction which gives agreement for ^1S proton-proton scattering at low energies leads to approximately correct matrix elements for not only ^1S, but also ^1D, ^1G, $\cdots$ states of relative angular momentum of two *outer neutrons* of these two heavy nuclei. At present, the agreement appears to be somewhat better with a Gaussian shape for this effective interaction than with a Yukawa shape.

Although the SE Gaussian and Yukawa interactions (3) and (4) are equivalent for low-energy p-p scattering, they are not accurately equivalent for the outer neutrons of Pb^{210}. A value of the harmonic-oscillator parameter ν of about 0.205 F^{-2} gives the best fit for the Gaussian interaction (3) in Pb^{210}, whereas $\nu \approx 0.185$ F^{-2} or still less for best fit with the Yukawa interaction (4). Even for these parameters, the energies of corresponding states differ somewhat.

For many states, the main contribution to the binding energy of the outer nucleons calculated here comes from the SE interaction. Even a substantial TO interaction will make only a small contribution to their matrix elements. This is especially true for the lowest five states. It is not surprising, therefore, that it does not seem possible at present to draw any detailed conclusions about the effective TO interaction. It seems probable, however, that the strength of its central part lies in the interval from $-1/2$ to $+1/2$ times that of the SE interaction. A more complete level scheme for Pb^{210} may yield information on this strength. A central +tensor TO interaction (7), with $-1/2$ times the strength of the TE interaction (6), has a large effect only on the energy of the state $1a$, among the low states of Fig. 2 (f). It may be noted that high-energy nucleon-nucleon scattering experiments suggest a weak TO interaction.[16]

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APPENDIX. ON THE CALCULATION OF γ-RAY TRANSITION PROBABILITIES

This Appendix will be based upon de-Shalit and Talmi,[25] Chapter 17, and True and Ford[3] (TF), Sec. IV. B. 1. The notation of TF will be used. Equations TF (13) to (17) fit into the framework of the present paper without changes. Equation TF (18) for

$$\langle jj'I\|M_\lambda\|jj''I'\rangle = (jj'I\|[M_\lambda(1)+M_\lambda(2)]\|jj''I')_a \quad (19)$$

also fits, and has been checked. The subscript a in (19) indicates that the wave functions for both the initial and the final states are antisymmetric.

The operator for an $M1$ transition, from Ref. 25, Eq. (17.10), is given by

$$[M_1(i)]_m = g_l l_m^{(1)}(i) + g_s s_m^{(1)}(i), \quad (20)$$

where $l^{(1)}$ and $s^{(1)}$ are the operators for orbital and spin angular momentum, in the usual irreducible tensor form. The diagonal reduced matrix element is given by TF (19), but the off-diagonal reduced matrix element, for $j \neq j'$, is

$$\langle j\|M_1\|j'\rangle = (\tfrac{1}{2}nlj\|M_1\|\tfrac{1}{2}nlj')$$
$$= (-1)^{j-l+\frac{1}{2}}(g_l-g_s)\left[\frac{3}{4\pi}\times\frac{2l(l+1)}{(2l+1)}\right]^{1/2}\frac{e\hbar}{2Mc}. \quad (21)$$

Equation (21), for the present scheme [see Eq. (17)], differs from TF (20) by a factor of -1.

The operator for an $E\lambda$ transition, from Ref. 25, Eq. (17.9), is given by

$$[Q_\lambda(i)]_m = e_{\text{eff}}\,(r_i)^\lambda\, Y_m{}^\lambda(\theta_i,\phi_i), \quad (22)$$

where $Y_m{}^\lambda$ is a spherical harmonic, and the coordinates of the ith particle are (r_i,θ_i,ϕ_i). The reduced matrix elements of Q_λ are

$$\langle j\|Q_\lambda\|j'\rangle = (\tfrac{1}{2}nlj\|Q_\lambda\|\tfrac{1}{2}n'l'j') = e_{\text{eff}}(nl|r^\lambda|n'l')(\tfrac{1}{2}lj\|Y_\lambda\|\tfrac{1}{2}l'j') \quad (23a)$$

$$= e_{\text{eff}}(nl|r^\lambda|n'l')\left[\frac{[\lambda][j][j']}{4\pi}\right]^{1/2}(-)^{j-\frac{1}{2}}\begin{pmatrix} j & j' & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\delta_{l,\lambda,l'} \quad (23b)$$

$$= e_{\text{eff}}(nl|r^\lambda|n'l')\left[\frac{[\lambda][j]}{4\pi}\right]^{1/2}(-)^{j'-j}C(j\lambda j';\tfrac{1}{2}0)\,\delta_{l,\lambda,l'}, \quad (23c)$$

where Y_λ is the irreducible tensor operator for the spherical harmonics (Ref. 25, p. 521), $[x]\equiv 2x+1$, and

$$\delta_{l,\lambda,l'} = \begin{cases} 1, & \text{if } l+\lambda+l' \text{ is even} \\ 0, & \text{otherwise.}\end{cases}$$

The formula for the reduced matrix element contains a 3-j symbol in (23b), and a vector-addition coefficient in (23c). Formula (23c) for $\lambda=2$ differs from TF (21) by a factor of $(-1)^{j'-j}$, because of the phase convention used here.