

## Semiempirical Formulas for Single-Particle Energies of Neutrons and Protons

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The stepwise multiple linear regression technique has been used to analyze the single-particle energies of neutrons and protons in nuclei along the line of beta stability. Their regular and systematic trends lead to semiempirical model-independent formulas for single-particle energies of neutrons and protons in the bound nuclei as functions of nuclear parameters  $A$  and  $Z$  for given states specified by  $nl$ . These formulas are almost as convenient as the harmonic oscillator energy formulas to use. The single-particle energies computed from these formulas have been compared with the experimental data and are found in reasonable agreement.

### 1. INTRODUCTION

A computational method based on stepwise multiple linear regression technique is presented for generating formulas for nuclear single-particle separation energies. This work primarily concerns the application of computers to nuclear physics. A statistical computer program [1] has been used to obtain an analytical expression in a closed form for single-particle energies as a function of nuclear parameters  $A$ ,  $Z$ ,  $n$ ,  $l$  and  $j$ . The single-particle energies can be defined as the centers of gravity of the fragments (generally, they are fragmented by some residual interactions), weighted by the spectroscopic factors.

The extensive and useful information on the energies of the single-particle states has accumulated from many investigations with quasi free scattering and nucleon transfer and knockout reactions. In several theoretical efforts, various models have been used to obtain the energy levels of nuclei along the line of beta stability [2-12]. These works and others, specifying some procedure for calculating the nuclear single-particle states, yield information about many features of nuclear structure, for which it may be desirable to see to what extent their predictions show a systematic behavior through the periodic table in correlating energies of the bound single-particle states. Of course such a study cannot be concerned with the details of the fragmentation of the single-particle states, at least at the present time, for these are peculiar to each nucleus and thus would not be expected to show any systematic behavior. It is only the centroid energies that might show such behavior (although even for them it is quite possible that the differences in structure from one nuclide to the other might be

sufficient to destroy it). Taking the macroscopic view of the experimental data and calculated values of the centroid energies of single-particle states of neutrons and protons, one may, in general, observe a regular pattern followed by these energies.

To describe these patterns exactly by some simple formula [13] would be desirable from the point of view of its utility. Such a formula or formulas would be more convenient to use, for example, as an energy guess for calculations involving energy-dependent potentials [2].

The stepwise multiple linear regression analysis used in this work is briefly discussed in the following section. The regression analysis is a means of making an estimation of the value of one variable from the values of other given variables. In other words, regression analysis enables the effects of various factors to be evaluated from the data even when the data do not follow a simple pattern, or when the variables affecting the results cannot be controlled in such a manner as to make possible a designed experiment. [14] The description of the computation technique is given in Section 3.

## 2. STEPWISE MULTIPLE LINEAR REGRESSION TECHNIQUE

In some problem several variables are studied simultaneously to see how they are interrelated; in others there is one particular variable of interest, and the remaining variables are studied for their aid in throwing light on this particular variable. The latter class of problem is usually associated with a statistical technique called regression. Methods for dealing with problems of predicting one variable by means of several other variables, rather than by means of just one other variable such that the functional relation of the predicted variable with others is linearly dependent are called multiple linear regression methods. For example, if we were to predict the variable  $E$  in terms of variables  $x_1, x_2, x_3, \dots, x_n$  the problem would become one of best fitting equations

$$E = a_0 + a_1x_1 + a_2x_2 + \dots + a_nx_n, \quad (1)$$

in the sense of least squares, to a scatter diagram of points in  $n + 1$  dimensions. The problem is one of estimating the coefficients  $a_0, a_1, a_2, \dots, a_n$  by the method of least squares. This is done by mathematical methods in the same way as, for example, linear regression. It turns out that the least-squares values of  $a_0, a_1, \dots, a_n$  are obtained by solving the  $n + 1$  linear equations. Explicitly the equation

$$\sum_N E = a_0N + a_1 \sum_N x_1 + a_2 \sum_N x_2 + \dots + a_n \sum_N x_n \quad (2)$$

and other  $n$  equations of the type

$$\sum_N x_i E = \sum_N a_0 x_i + a_1 \sum_N x_1 x_i + \dots + a_i \sum_N x_i^2 + \dots + a_n \sum_N x_i x_n, \quad (3)$$

where  $i = 1, 2, \dots, n$ , are solved simultaneously to yield the coefficients  $a_0, a_1, \dots, a_n$ ; and  $N$  is the number of data points. In the ideal situation the choice of the type and

number of variables  $x$ 's and the calculation of the coefficients  $a$ 's must be such that the values of  $E$ 's calculated from Eq. (1) must be identical to the corresponding values of  $E$  used as input data for such analysis. This can be tested by calculating the multiple correlation coefficient  $R$  which is the positive value of the square root of the quantity  $R^2$  given by

$$R^2 = \frac{\sum_{i=1}^N (\hat{E}_i - \bar{E})^2}{\sum_{i=1}^N (E_i - \bar{E})^2} \quad (4)$$

where the  $\hat{E}_i$  are calculated from Eq. (1) and the  $E_i$  are the input data, and  $\bar{E}$  is the average value of  $E_i = ((1/N) \sum_{i=1}^N E_i)$ . For the ideal case, the value of  $R$  must be unity. In order to limit the number of variables  $x$ 's to a reasonable number (such that  $R \geq 0.9$ ) a stepwise multiple linear regression technique may be used in the analysis. This technique provides a method which adds one variable at a time to the regression equation in such a manner that the added variable is the most significant one among those not already in the regression equation.

### 3. COMPUTATIONAL PROCEDURE

The semiempirical formulas for single-particle energies are generated in terms of the nuclear parameters  $A$ ,  $Z$ ,  $n$ ,  $l$ , and  $j$  by the stepwise multiple linear regression analysis. The variables  $x$ 's occurring in Eq. (1) are linear. They correspond to various combinations of the nuclear parameters mentioned above. A certain number of combinations of nuclear parameters is formed by some physical and/or intuitive considerations. Others have been used just on a trial-and-error basis. For example, a constant term and  $A^{-1/3}$  are strongly suggested by mass formula. Similarly, the harmonic oscillator energy formula  $[2(n-1) + l + \frac{3}{2}] \hbar\omega$  leads to the inclusion of terms like  $A^{-1/3}$ ,  $nA^{-1/3}$ , and  $lA^{-1/3}$ . The spin-orbit doublet splitting proportional to  $l(l+1)$  suggests the inclusion of a term like  $j(j+1)A^{-2/3}$ . Terms proportional to  $A^{-1}$  and  $A^{-5/3}$  may be expected to be due to the consideration of pairing energy and deformation effects, respectively, if the input data are to have some effects of that nature. The terms discussed above serve merely as guidelines for constructing possibly relevant terms. It is not necessarily expected that each of the above terms will appear in the resulting formulas, but combinations of similar terms may appear. Besides these terms, many other terms have been constructed and treated as linear variables  $x$ 's. Such terms are limited to a total number of 80 variables, which is a sufficiently large number to account for all the possible nuclear parameters and their various combinations [1, 15]. Let these variables be denoted by  $n$ . This program computes a sequence of multiple linear equations in a stepwise manner. That is, at each step one variable is added to the regression equation. The variable added is the one which has the highest partial correlation with the difference in the dependent variable and the regression equation. In other words, it is the variable which, if it were added, would have the highest  $F$ -value, where the  $F$ -value has the  $F$ -distribution defined and computed later on. After a reasonably complete set of variables has been generated,

the problem is to find the coefficients of the significant variables. Coefficients for the most significant terms are computed first, followed by the next most significant terms in descending order of significance. The coefficients (including the constant term,  $a_0$ ) are reevaluated on the addition of each term until there are no more variables left, or until the significance of the remaining variables is below some specified value.

Single-particle energies of neutrons and protons in nuclei along the beta stable line and within the range  $10 < A < 300$  have been used as the input data in this regression analysis. These values were taken from the occupied states up to the Fermi level including 352 states for neutrons and 250 states for protons [2]. Each state of nuclei considered contributes one data point to the statistical program. Let these data points be called the number of cases and be denoted by  $N$ . These  $N$  cases are simply the input energy values used to generate the formulas in question consisting of a reasonable number of terms selected from a total number of  $n$  variables stored in the program. For the sake of convenience the computational procedure is divided into six stages in the order in which they appear.

Stage 1 primarily constructs a matrix from the input data. Let  $x_{ki}$  be the value of the  $i$ th variable for the  $k$ th case whose mean is computed from its definition

$$\bar{x}_j = \frac{1}{N} \sum_{k=1}^N x_{kj}, \quad j = 1, 2, \dots, n, \quad (5)$$

and a matrix  $A$  whose elements are given by

$$a_{ij} = \sum_{k=1}^N (x_{ki} - \bar{x}_i)(x_{kj} - \bar{x}_j), \quad i, j = 1, 2, \dots, n, \quad (6)$$

is constructed.

In Stage 2, from the matrix  $A$  thus constructed the quantities, namely, covariance  $s_{ij}$ , standard deviations  $s_i$ , and correlation  $r_{ij}$ , are computed from their following respective definitions for the whole population:

$$s_{ij} = \frac{1}{N-1} a_{ij}, \quad i, j = 1, 2, \dots, n, \quad (7)$$

$$s_i = (s_{ii})^{1/2}, \quad (8)$$

and

$$r_{ij} = \frac{s_{ij}}{s_i s_j}, \quad i, j = 1, 2, \dots, n \quad \left( = \frac{a_{ij}}{(a_{ii} a_{jj})^{1/2}} \right). \quad (9)$$

Stage 3 deals with each step in the stepwise regression procedure. The total number of variables  $n$  are divided into two disjoint sets. The first set consists of the independent variables being used in the regression equation in that particular step. They are designated by

$$x_{i1}, x_{i2}, \dots, x_{iq}.$$

The other set consists of the remaining variables including the dependent variable. (The dependent variable in this work is the energy,  $E = x_d$ , calculated by the regression formula for the step in progress.) Let this set of variables be denoted by

$$x_{j1}, x_{j2}, \dots, x_{jp}.$$

For the purpose of exposition assuming the set  $x_{j1}, x_{j2}, \dots, x_{jq}$  as the first  $q$  variables of the total  $n$ , the regression equation at a typical step then has the form:

$$E = a_0 + a_1x_1 + a_2x_2 + \dots + a_qx_q. \quad (10)$$

Next a partition matrix  $\mathbf{A}$  given by

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad (11)$$

is constructed where  $\mathbf{A}_{11}$  is a  $q \times q$  matrix and thus another matrix  $\mathbf{B}$  with elements  $b_{ij}$  is computed as

$$\mathbf{B} = \begin{bmatrix} A_{11}^{-1} & A_{11}^{-1}A_{12} \\ A_{21}A_{11}^{-1} & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{bmatrix}. \quad (12)$$

Since  $q$  independent variables have been used in this typical regression equation (10) the residual degrees of freedom  $df$  is thus given by

$$df = N - q - 1 \quad (13)$$

and the regression degrees of freedom  $q$  is denoted by

$$q = r \, df. \quad (14)$$

For this step and similarly for each step in the stepwise procedure the following quantities are defined, computed and stored:

For the residual degrees of freedom the sum of squares and the mean square are given by:

$$SS = b_{aa}, \quad (15)$$

and

$$MS = \frac{SS}{df} = \frac{b_{aa}}{N - q - 1}, \quad (16)$$

respectively.

For the regression degrees of freedom, the sum of squares and the mean square are given by:

$$RSS = a_{aa} - b_{aa}, \quad (17)$$

and

$$RMS = \frac{RSS}{rdf} = \frac{a_{aa} - b_{aa}}{q} \quad (18)$$

respectively.

From these terms, the  $F$ -value, the standard error of estimate, and the multiple correlation coefficient are computed, which are given by:

$$F = \frac{RMS}{MS} = \frac{a_{dd} - b_{dd}}{b_{dd}} \frac{N - q - 1}{q}, \quad (19)$$

$$S = (MS)^{1/2}, \quad (20)$$

and

$$R = \left( \frac{RSS}{a_{dd}} \right)^{1/2} = \left( 1 - \frac{a_{dd}}{b_{dd}} \right)^{1/2}, \quad (21)$$

respectively.

In Stage 4 for each independent variable  $x_i$  in the regression equation, the regression coefficient, its standard error, and  $F$ -value are computed. They are defined as:

$$a_i = b_{id} \quad \text{and} \quad a_0 = \sum_{i=1}^q a_i \bar{x}_i, \quad (22)$$

$$S_i = S(b_{ii})^{1/2}, \quad (23)$$

and

$$F_i = (a_i/S_i)^2, \quad (24)$$

respectively.

Stage 5 deals with each remaining independent variable  $x_i$  not included in the regression equation and computes for each of the variables the tolerance level, partial correlation coefficient, and  $F$ -value given by:

$$T_i = \frac{b_{ii}}{a_{ii}}, \quad (25)$$

$$R_i = \frac{b_{id}}{(b_{ii}b_{dd})^{1/2}}, \quad (26)$$

and

$$F_i = \frac{b_{id}^2(N - q - 2)}{b_{ii}b_{dd} - b_{id}^2}, \quad (27)$$

respectively.

The last stage, namely, Stage 6, actually executes a sequence of multiple linear regression equation in stepwise manner which are given in the Appendix A. In going from one step to the next an independent variable is added to or removed from the regression equation automatically until the final formula is obtained. In addition, variables can be forced into the regression equation if desired. In that case nonforced variables (i.e., free variables) are automatically removed according to the criteria set up for adding to and removing from the regression equation when moving from one step to the next. This movement is governed by the following three rules:

(i) If there are one or more independent variables in the regression equation that are not forced and whose  $F$ -value is less than the “ $F$ -to-remove” value specified in the input, the one with the least  $F$ -value will be removed.

(ii) If no variable is removed by (i) and there are one or more independent variables *not* in the regression equation which pass the tolerance test and are forced variables, the one with the highest forcing value and the highest  $F$ -value among all with the same forcing value will be added.

An independent variable  $x_i$  *not* in the regression equation is said to pass the tolerance test if its tolerance value  $T_i$  is greater than or equal to the “minimum tolerance value” specified in the input.

(iii) If no variable is removed by (i) or added by (ii) and there are one or more independent variables *not* in the regression equation which pass the tolerance test, are free variable, and have an  $F$  value greater than or equal to the “ $F$ -to-enter” value specified in the input, the one with the highest  $F$ -value will be added.

If no variable is added or removed by any one of the above three rules, the stepwise procedure is terminated yielding the final formula. These formulas are given by Eqs. (28) and (29) for single-particle energies of neutron and proton with their respective multiple correlation coefficients in the following section.

#### 4. RESULTS

Following the procedure, the stepwise multiple linear regression analysis, outlined in the preceding section, compact regression formulas are obtained readily with significantly large values of multiple correlation coefficients,  $R$  (very close to unity), and with a relatively small number of variables out of a large number generated from the nuclear parameters. In fact, the value of  $R$  goes immediately, to more than 0.9 as soon as a proper combination of  $n$ ,  $l$ , and  $A$  is included in the regression formulas. Some of the formulas for the single-particle energies for the occupied states of neutrons and protons are presented in the order of increasing  $R$  in the Appendix A. The formulas used for calculating the single-particle energies for neutrons and protons given in Table I and producing Figs. 1 and 2 are given here:

$$\begin{aligned}
 E_6(n) &= -94.905 + 70.836l/A^{1/3} + 89.992n/A^{1/3} + 17.956n \\
 &\quad - 18.037j(j+1)/A^{2/3} - 2.573n^2 + 43.290l(l+1)/A, \\
 R_6(n) &= 0.9938;
 \end{aligned}
 \tag{28}$$

$$\begin{aligned}
 E_6(p) &= -100.515 + 82.551l/A^{1/3} + 30.147n + 58.962n/A^{1/3} \\
 &\quad - 17.741j(j+1)/A^{2/3} - 3.722n^2 + 39.649Z/A^{4/3}, \\
 R_6(p) &= 0.9961.
 \end{aligned}
 \tag{29}$$

TABLE I  
Single-Particle Energies (MeV) for Neutrons and Protons in Some Finite Nuclei<sup>a</sup>

State	Neutrons			Protons		
	Input	Calc	Exp <sup>12</sup>	Input	Calc	Exp
<sup>16</sup> O						
1s <sub>1/2</sub>	46.76	45.94	47.00	44.94	45.75	44 ± 7 <sup>b</sup>
1p <sub>3/2</sub>	19.52	20.94	22.00	18.89	21.35	19.1 ± 1.4 <sup>b</sup>
1p <sub>1/2</sub>	12.54	12.41	15.70	11.77	13.06	12.7 ± 1.4 <sup>b</sup>
<sup>32</sup> S						
1s <sub>1/2</sub>	55.51	52.52		51.47	51.23	—
1p <sub>3/2</sub>	31.12	32.87		28.07	30.50	p 29.7 ± 6.1 <sup>?b</sup>
1p <sub>1/2</sub>	26.34	27.50		23.33	25.28	
1d <sub>5/2</sub>	15.45	14.09		12.91	13.26	16.2 ± 1.6 <sup>b</sup>
1d <sub>3/2</sub>		5.14			4.55	13.3 ± 1.6 <sup>b</sup>
2s <sub>1/2</sub>	14.26	13.93		11.92	12.05	9.5 ± 1.4 <sup>b</sup>
<sup>40</sup> Ca						
1s <sub>1/2</sub>	57.93	54.36		52.99	52.77	49.1 ± 12 <sup>b,c</sup> 58.4 ± 3.4 <sup>m</sup> , 56 <sup>n</sup> 77 ± 14 <sup>d</sup>
1p <sub>3/2</sub>	34.78	36.11		30.76	33.18	33.3 ± 6.5 <sup>c</sup> p 35.1 ± 0.6 <sup>m</sup>
1p <sub>1/2</sub>	30.74	31.49		26.73	28.68	32.4 ± 4 <sup>d</sup>
1d <sub>5/2</sub>	19.57	18.78	21.30	16.03	16.59	14.9 ± 2.5 <sup>b</sup> 19.0 ± 1.1 <sup>m</sup> 13.8 ± 7.5 <sup>c</sup>
2s <sub>1/2</sub>	16.78	17.81	18.10	13.98	15.31	10.6 ± 1.1 <sup>b</sup> 14.4 ± 0.3 <sup>m</sup> 12.1 ± 5.4 <sup>c</sup>
1d <sub>3/2</sub>	12.02	11.07	15.80	8.47	9.09	8.4 ± 0.5 <sup>e</sup> 10.9 ± 0.7 <sup>m</sup> 7.7 ± 2.6 <sup>d</sup>
<sup>46</sup> Sc						
1s <sub>1/2</sub>	57.70	55.29		55.66	53.55	53.6 ± 8.9 <sup>c</sup>
1p <sub>3/2</sub>	35.59	37.73		33.52	34.55	p 34.9 ± 8 <sup>c</sup>
1p <sub>1/2</sub>	31.99	33.45		29.89	30.39	
1d <sub>5/2</sub>	20.87	21.09		18.87	18.32	d 26.9 ± 8.9 <sup>c</sup>
2s <sub>1/2</sub>	18.16	19.75		16.43	16.94	13.2 ± 5.4 <sup>c</sup> 12.1 ± 1 <sup>e</sup> 11.87 <sup>f</sup>
1d <sub>3/2</sub>	13.93	13.96		11.90	11.38	11.17 <sup>f</sup>
1f <sub>7/2</sub>	7.66	5.39		5.59	4.86	
<sup>48</sup> Ca						
1s <sub>1/2</sub>	56.32	55.78		58.91	53.96	
1p <sub>3/2</sub>	34.87	38.58		36.53	35.28	
1p <sub>1/2</sub>	31.68	34.49		33.07	31.29	
1d <sub>5/2</sub>	20.70	22.31		21.63	19.25	
2s <sub>1/2</sub>	17.45	20.78		18.65	17.81	15.81 <sup>g</sup>
1d <sub>3/2</sub>	14.32	15.49		14.95	12.61	16.17 <sup>g</sup>
1f <sub>7/2</sub>	7.83	6.97		8.19	5.88	

(Table continued)



TABLE I (continued)

State	Neutrons			Protons		
	Input	Calc	Exp <sup>12</sup>	Input	Calc	Exp
<sup>51</sup> V						
1s <sub>1/2</sub>		56.24		54.34		59.8 ± 3.2 <sup>m</sup>
1p <sub>3/2</sub>		39.37		39.95		p 40.4 ± 0.7 <sup>m</sup>
1p <sub>1/2</sub>		35.44		32.13		
1d <sub>5/2</sub>		23.44		20.11		21.4 ± 2.5φ <sup>b</sup>
						19.5 ± 0.2 <sup>m</sup>
2s <sub>1/2</sub>		21.73		18.61		13.6 ± 0.5 <sup>e</sup>
						15.1 ± 0.2 <sup>m</sup>
						13.49 <sup>h</sup>
						15.7 ± 1.8 <sup>b</sup>
1d <sub>3/2</sub>		16.88		13.74		14.26 <sup>h</sup>
						11.8 ± 0.9 <sup>b</sup>
						10.3 ± 1.1 <sup>m</sup>
1f <sub>7/2</sub>		8.42			6.83	
2p <sub>3/2</sub>		4.87				
<sup>58</sup> Ni						
1s <sub>1/2</sub>	61.73	57.18		56.26	55.12	57.3 ± 7.5φ <sup>c</sup>
						63.7 <sup>n</sup>
1p <sub>3/2</sub>	40.00	40.99		35.46	37.35	p 37.6 ± 7.9 <sup>c</sup>
1p <sub>1/2</sub>	37.19	37.38		32.43	33.84	p 43.8 <sup>n</sup>
1d <sub>5/2</sub>	25.89	25.73		21.60	21.92	d 20.2 ± 9.8 <sup>b</sup> , 20.9 <sup>n</sup>
2s <sub>1/2</sub>	21.33	23.69		18.07	20.26	12.6 + 6.3 <sup>c</sup> 14.7 <sup>n</sup>
						11.19 <sup>f,h</sup>
1d <sub>3/2</sub>	20.08	19.71		15.57	16.07	11.72 <sup>f,h</sup>
1f <sub>7/2</sub>	12.90	11.38		8.76	8.84	10.1 ± 5.6 <sup>g,f</sup> 9.3 <sup>n</sup>
2p <sub>3/2</sub>	9.74	7.51			2.49	
<sup>90</sup> Zr						
1s <sub>1/2</sub>	63.86	60.11		60.26	57.59	
1p <sub>3/2</sub>	44.89	46.04		40.97	41.82	
1p <sub>1/2</sub>	43.00	43.34		38.94	39.20	
1d <sub>5/2</sub>	32.31	32.80		28.30	27.81	
2s <sub>1/2</sub>	27.03	29.80		22.84	25.41	
1d <sub>3/2</sub>	28.22	28.31		23.92	23.44	
1f <sub>7/2</sub>	20.61	20.39		16.30	15.54	
2p <sub>3/2</sub>	15.12	15.72	13.1 <sup>f</sup>	10.70	9.64	
1f <sub>5/2</sub>	13.64	14.11	12.6 <sup>f</sup>	8.96	9.42	
2p <sub>1/2</sub>	13.19	13.03	13.50 <sup>f</sup>	8.73	7.02	8.80 <sup>f</sup>
1g <sub>9/2</sub>	9.50	8.82			5.02	
1g <sub>7/2</sub>		0.74				
2d <sub>5/2</sub>		2.48				
3s <sub>1/2</sub>		4.62				
<sup>120</sup> Sn						
1s <sub>1/2</sub>	65.56	61.83		62.21	59.03	54.0 ± 8.1 <sup>?c</sup>
1p <sub>3/2</sub>	47.73	48.97		44.54	44.49	p 40.2 ± 7.2 <sup>?c</sup>
1p <sub>1/2</sub>	46.40	46.75		42.98	42.33	
1d <sub>5/2</sub>	36.24	36.38		32.44	31.39	d 30.0 ± 6.9 <sup>c</sup>
2s <sub>1/2</sub>	29.43	33.35		27.00	28.41	29.0 ± 6.8 <sup>a</sup>

(Table continued)

TABLE I (continued)

State	Neutrons			Protons		
	Input	Calc	Exp <sup>12</sup>	Input	Calc	Exp
$1d_{3/2}$	33.33	33.17		29.10	27.79	
$2p_{3/2}$	18.89	20.49		14.34	13.87	$2p$ $16 \pm 6.3^c$
$2p_{1/2}$	17.32	18.27		12.51	11.70	
$1f_{7/2}$	25.41	25.54		21.22	19.74	
$1f_{5/2}$	20.40	20.35		15.26	14.69	$f + g$ $16 \pm 6.8^c$
$1f_{3/2}$	14.86	14.97		10.09	9.52	
$1g_{7/2}$	7.32	8.29				
$2d_{5/2}$	10.30	8.39				
$2d_{3/2}$	7.64	4.69				
$3s_{1/2}$	9.80	10.01				
$1h_{11/2}$		5.15				
<sup>208</sup> Pb						
$1s_{1/2}$	69.04	64.72		63.03	61.45	
$1p_{3/2}$	53.16	53.89		48.31	49.05	
$1p_{1/2}$	52.43	52.35		47.38	47.55	
$1d_{5/2}$	43.54	43.67		38.05	37.64	
$2s_{1/2}$	36.52	39.29		31.96	33.42	
$1d_{3/2}$	41.88	41.10		35.96	35.14	
$1f_{7/2}$	34.34	34.06		28.24	27.24	
$1f_{5/2}$	31.34	30.46		24.46	23.74	
$2p_{3/2}$	26.35	28.46		20.01	21.02	
$2p_{1/2}$	25.62	26.92		18.55	19.52	
$1g_{9/2}$	25.35	25.07		18.53	17.83	
$1g_{7/2}$	20.76	20.44		12.53	13.33	11.45 <sup>k</sup>
$2d_{5/2}$	18.24	18.24		11.04	9.61	9.65 <sup>k</sup>
$1h_{11/2}$	16.44	16.68		8.72	9.42	9.30 <sup>k</sup>
$2d_{3/2}$	16.47	15.67		8.54	7.11	8.30 <sup>k</sup>
$3s_{1/2}$	16.15	19.01		10.75	11.30	7.95 <sup>k</sup>
						9.0
$1h_{9/2}$	9.75	11.03	10.70		3.92	3.8 <sup>c</sup>
$2f_{7/2}$	10.59	8.64	9.50			
$1i_{13/2}$	7.57	8.91	8.90		2.01	2.2 <sup>k</sup>
$3p_{3/2}$	9.77	8.18	8.20		+1.11	0.5 <sup>l</sup>
$2f_{5/2}$	7.87	5.04	7.80			0.8
$3p_{1/2}$	8.92	6.64	7.30			

<sup>a</sup> Question marks indicate uncertainty in level assignments.

<sup>b</sup> Quoted in Ref. [21].

<sup>c</sup> Reference [22].

<sup>d</sup> Reference [23].

<sup>e</sup> Quoted in Ref. [24].

<sup>f</sup> Reference [25].

<sup>g</sup> Reference [26].

<sup>h</sup> Quoted in Ref. [25].

<sup>i</sup> Reference [27].

<sup>j</sup> Reference [28].

<sup>k</sup> Quoted in Ref. [18].

<sup>l</sup> Quoted in Ref. [20].

<sup>m</sup> Reference [29].

<sup>n</sup> Reference [30].

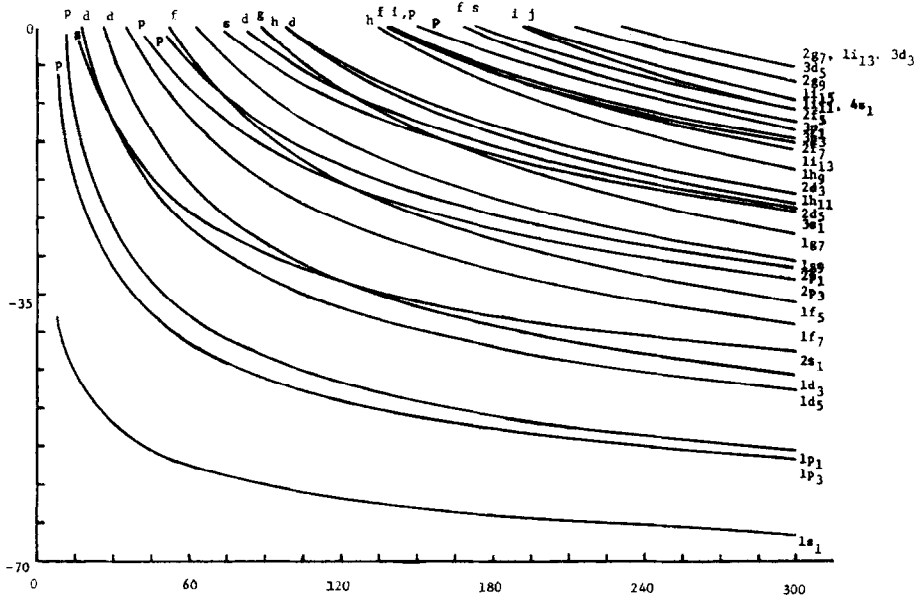


FIG. 1. Single-particle energies of neutrons computed from the semiempirical formula (28) for  $E(n)$  show a systematic variation as the mass number  $A$  varies. Subscripts to symbols for  $l$  refer to twice the values of  $j$ .

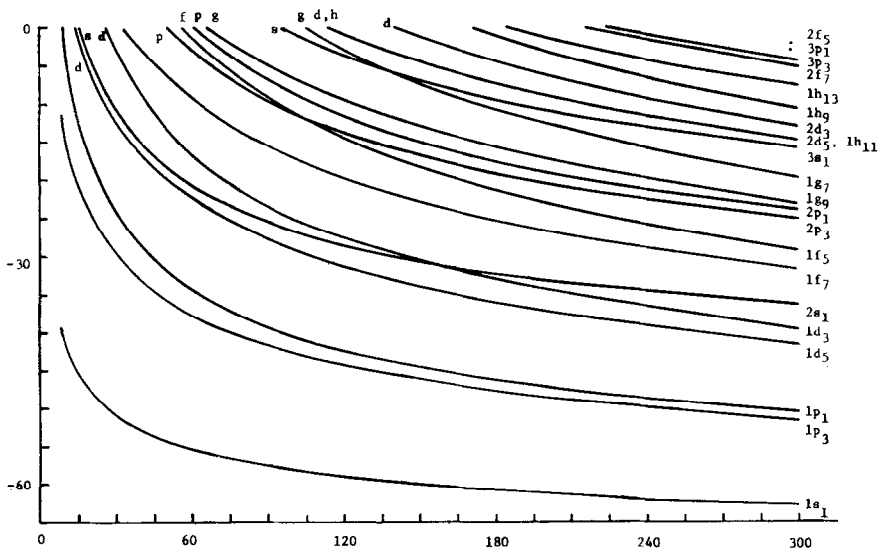


FIG. 2. Single-particle energies of protons computed from the semiempirical formula (29) for  $E(p)$  show a systematic variation as the mass number  $A$  varies. Subscripts to symbols for  $l$  refer to twice the values of  $j$ .

These formulas correspond to Eqs. (A1.6) and (A2.6), respectively, in Appendix A and have MeV units for energies. The last three formulas for  $E(n)$  and  $E(p)$  in Appendix A for which the value of  $R > 0.99$  include the most significant nuclear parameters  $A$ ,  $n$ ,  $l$ ,  $j$  in the expected combinations. On increasing the number of variables in the regression formulas beyond the number already in (28) and (29) the variation in the energy calculated from those formulas is insignificantly small. Such a precision is not desirable at this stage because of the lack of observed data available against which it could be tested and because of the large uncertainties involved in the presently available experimental data. If the number of terms were increased the formulas would become too unwieldy without increasing the value of  $R$  significantly. However, the truncation at this stage does not exhibit the effects due to pairing, deformation, etc., explicitly. These features may, however, be understood as being reflected in the values of the coefficients of the regression formulas. If the regression analysis is allowed to continue until all the variables fed in are used one will get all those terms representing directly such effects. This would simply increase the number of terms in the formulas without increasing any significant accuracy. Hence, in order to keep the formulas reasonably compact, the process should be stopped after an acceptable value of  $R$  (say, 0.9900–0.9990) is reached. In this analysis Eqs. (28) and (29) yield reasonably acceptable values of neutron and proton energies and also give the values of  $R$  greater than 0.99. It is desirable to truncate these formulas at this stage.

Examining the progression of the formulas given in Appendix A, namely, (A1.1) to (A1.6) and (A2.2) to (A2.6) for single-particle energies of neutron and proton, respectively, one finds a good deal of physical significance. It is, therefore, worth commenting here, rather than in Appendix A, on the structure of these formulas. The harmonic oscillator potential has been widely used in the shell model calculations, perhaps because of its simple treatment and also because of its close resemblance to the actual single-particle potential. Any deviation of a single-particle potential from the harmonic oscillator potential can be treated as a perturbation to the harmonic oscillator [16]. In other words, it can be shown that any single-particle potential can, in principle, be treated as a superposition of harmonic oscillator potentials [17]. This feature is reflected in the progression of the formulas in Appendix A. The first terms are considerably smaller in Eqs. (A1.1) and (A2.1) than in the remaining formulas. The corresponding correlation coefficients are also significantly smaller for the first formulas for the neutron and the proton. This is what one would naively expect, since the volume of the nucleus tends to increase the binding energy, as in the mass formula in the liquid-drop model, whereas the higher orbital states have decreasing energies. If we were to consider the single-particle energies based on its volume (i.e., the mass number  $A$ ) and orbital quantum number  $l$ , the only results that would be significantly wrong would be those exhibiting low values of  $R$ . However, should the principal quantum number  $n$  be included, then the results are expected to improve significantly, as is obvious by the large values of  $R$  in formulas (A1.2) and (A2.2). These two formulas depend on  $A$ ,  $n$ , and  $l$ , like the formula in the case of the harmonic oscillator in which the single-particle energy is  $(A + \frac{3}{2}) \hbar \omega$  or

$[2(n - 1) + l + \frac{3}{2}] \hbar\omega$  if  $A = 2n + l - 2$ . Formulas (A1.2) and (A2.2) should not be expected to give better results than the corresponding harmonic oscillator energy formula. In fact the difference in results of the second and third formulas should not be very significant as they both depend on the same number of parameters. This is evidenced from the values of  $R$  corresponding to these formulas. The additional  $n$ -dependent term is a slight perturbation to the harmonicity. There is also a difference in the order of appearance of  $nA^{-1/3}$ - and  $n$ -terms in formulas (A1.2, 3) and (A2.2, 3). The latter formulas belong to the proton, where the Coulomb correction manifests to the harmonic oscillator at the outset. The next major correction to the harmonic oscillator description is expected to be due to the spin-orbit interaction which appears in  $E_4(n, p)$ . Allowing more terms in  $E_5$  and  $E_6$  means including further perturbation (perhaps due to asymmetry, pairing effects, Coulomb potential, centrifugal term, etc.). Picturing the perturbation to the harmonic oscillator, one would expect the correction to the energy by terms proportional to  $n^2$ [16], which appears in  $E_5$ . Considering  $E_6$ , again neutron and proton formulas differ. Whereas the neutron formula,  $E_6(n)$ , prefers to exhibit the effect due to centrifugal force proportional to  $l(l + 1)$ , in the proton formula,  $E_6(p)$ , the Coulomb force proportional to  $Z$  appears explicitly in preference to the  $l(l + 1)$  term. Overall, formulas  $E_6(n, p)$  give a reasonable agreement with the observed data. Although the input data for the structure of these formulas was taken only from the occupied states of neutrons and protons, there are several interesting qualitative features of hole states which are apparent from Figs. 1 and 2 when these curves are projected. For example, an abnormally large spin-orbit doublet splitting occurs in cases where the  $j = l + \frac{1}{2}$  level is a particle state, while the  $j = l - \frac{1}{2}$  level is a hole state. For shell cases, the doublet splittings of neutrons and protons are in reasonably good agreement with the experiment [18]. In any one major shell the slopes of the level curves with smaller nodal numbers are steeper. In particular, the single-node levels  $1d$ ,  $1f$ , etc., are appreciably steeper than the other members of their shell, as is observed experimentally and is also concluded by other theoretical works [19, 20]. The nuclear systematics shown by formulas (28) and (29) arise from the input data, which are in turn derived from nuclear forces. The salient features of nuclear forces are thus inherited by these formulas from the input data. Hence, while these formulas are simple to use they have physical significance as far as the centroid energies of single particles in nuclear physics are concerned and exhibit the gross properties of nuclear forces.

Formulas (28) and (29) and the formulas in Appendix A were obtained when there was no preference for one variable over another. The program itself selects the variable which is most significant. However, a certain variable can be forced to appear with some priority. It turns out that if any number of variables is forced to appear in the formula with some priority then the resulting formula is no different from the one obtained without any bias as long as eventually the numbers of terms appearing in both formulas are identical. As an example of this effect two variables  $n(1 + A^{-1/3})$  and  $lA^{-1/3}$  were forced to appear in the regression formula soon after the constant term and after that the program could choose the variables according to its own

ordering. The resulting formula, having the same number of terms as Eq. (28), can be written as

$$\begin{aligned}
 E(n) &= -94.202 + 17.951n(1 + 1/A^{1/3}) + 70.838l/A^{1/3} \\
 &\quad + 72.049n/A^{1/3} - 18.038j(j + 1)/A^{2/3} \\
 &= -94.902 + 70.838l/A^{1/3} + 90.000n/A^{1/3} \\
 &\quad + 17.951n - 18.038j(j + 1)/A^{2/3} - 2.572n^2 \\
 &\quad + 43.385l(l + 1)/A,
 \end{aligned}$$

which is almost identical to Eq. (28) and its corresponding value of  $R$  is the same that belonging to Eq. (28). The energies calculated from these two equations have almost identical values and certainly cannot be distinguished on the scale on which Fig. 1 is drawn. Figures 1 and 2 represent the single-particle energies obtained using formulas (28) and (29) for neutrons and protons, respectively. Some of the single-particle energies of neutrons and protons have been compared with the experimental and input data [2] in Table I. The results of this work that enter this table have been obtained from Eqs. (28) and (29) with their corresponding values of  $R$  equal to 0.9938 and 0.9956. These numbers are large enough to obtain the output values of  $E(n)$  and  $E(p)$  computed from Eqs. (28) and (29), respectively, to match the input data closely, which in fact is observed in Table I.

## 5. DISCUSSION AND CONCLUSION

The constant terms of Eqs. (28) and (29) place the energies at a very negative value. The next three terms ( $+l/A^{1/3}$ ,  $+n$ , and  $+n/A^{1/3}$ ) can be attributed to harmonic oscillator effects and give the required increase (decrease in magnitude) in energy as  $n$  and/or  $l$  increase and the necessary decrease in energy as  $A$  increases. The term  $-j(j + 1)/A^{2/3}$  gives the spin-orbit splitting proportional to  $2l + 1$ , exhibiting the proper doublet sequence, and also shows the reduced spin-orbit effect as  $A$  increases. The  $n^2$  term illustrates a slight nonlinearity in the principal quantum number [16]. The  $l(l + 1)/A$  term in Eq. (28) accounts for a residual effect in the orbital angular momentum not taken care of by the  $l/A^{1/3}$  term. The neutron-proton differences are reflected in the values of the coefficients of Eqs. (28) and (29). The first two variables of these equations involving the terms  $l/A^{1/3}$  and  $n$  as the predominant terms are about equally significant and they account for the major effects, with their multiple correlation coefficient  $\simeq 0.92$ .

The nuclear systematics obtained from Eqs. (28) and (29) (see Figs. 1 and 2) show the distinctiveness of the single-particle states, the increase in binding energies as  $A$  increases, and the tendency to level off for deeply bound states in heavy nuclei, thus exhibiting the saturation property of nuclear forces. Both the neutron and proton systematics show gaps in the shell structure at all the observed magic numbers. Gaps are also exhibited for all the semi-magic numbers in the appropriate region. A gap

is seen for the semi-magic number 58, but because of level crossings, it does not occur at the Fermi level. The systematics seen in Figs. 1 and 2 thus satisfactorily reproduce the expected trends in the nuclear systematics.

Calculated and experimental single-particle energies are listed in Table I. There is generally a reasonable agreement with the experimental data[[21–30]. Nevertheless, it seems appropriate to make a few remarks on the discrepancies that one may observe in comparing the results of this work and the experimental data. They are partly due to the errors associated with the experimental data themselves. The experimental data available are rather imprecise and for deeply bound states they do not exist in most cases. Those data which are available have large errors and sometimes uncertainty in the existence of the states reported. The spin-orbit degeneracy is not removed in a good number of experiments. The single-particle energies obtained from various experiments for a given nucleus sometimes differ appreciably. For example, the  $1s$  proton state in  $^{40}\text{Ca}$  is reported to be  $49.1 \pm 12$  and  $77 \pm 14$ ,  $58.4 \pm 3.4$ ,  $56.0$  MeV in  $(p, 2p)$  [22] and  $(e, e'p)$  [23, 29, 30] reactions, respectively. Another example of the inconsistency in the experimental data is that the single-particle energy for a given state, as expected, does not increase, in general, as  $A$  increases in a good many cases. The  $p_{1/2}$  proton energies in  $^{12}\text{C}$  and  $^{16}\text{O}$  are  $15.9 \pm 1$  and  $12.7 \pm 1.4$  MeV, respectively [21]. A similar discrepancy is observed in  $^{58}\text{Ni}$  and  $^{120}\text{Sn}$  (see Table I) for  $1s$  protons and in  $^{28}\text{Si}$  ( $12.5 \pm 1.7$  MeV) and  $^{32}\text{S}$  ( $9.5 \pm 1.4$  MeV) for  $2s$  protons [21]. As to the calculated single-particle energies, they are generally too low for unoccupied or partially occupied levels and the  $2s_{1/2}$  calculated values are rather high for nuclei in the region  $44 < A < 65$ , which may be attributed to the input data which were used mostly for occupied bound states. As seen from the figures and tables, however, the model-independent, semiempirical, neutron and proton single-particle energy formulas, given by Eqs. (28) and (29), give a rather good description of the overall patterns observed in the bound-state spectrum. These formulas should not be expected to give realistic results for states above Fermi surface.

## APPENDIX A: REGRESSION EQUATION AND COEFFICIENTS

A sequence of multiple linear equations in a stepwise manner is given here along with the multiple correlation coefficient  $R$  of each equation. At each step, as a variable is added the value of the multiple correlation coefficient  $R$  is increased until the most significant set of nuclear parameters is included and/or a reasonable value of  $R$  (close to unity) is reached. First, the neutron energy formulas and their corresponding values of  $R$  are listed, and then those for protons. The coefficients of all terms in these formulas have units in MeV.

$$\begin{aligned} E_1(n) &= -36.335 + 29.545I/A^{1/3}, \\ R_1(n) &= 0.4870; \end{aligned} \tag{A1.1}$$

$$\begin{aligned} E_2(n) &= -83.800 + 59.166I/A^{1/3} + 120.647n/A^{1/3}, \\ R_2(n) &= 0.9552; \end{aligned} \tag{A1.2}$$

$$\begin{aligned} E_3(n) &= -85.919 + 59.622l/A^{1/3} + 88.039n/A^{1/3} + 8.207n, \\ R_3(n) &= 0.9795; \end{aligned} \quad (\text{A1.3})$$

$$\begin{aligned} E_4(n) &= -88.510 + 78.147l/A^{1/3} + 100.363n/A^{1/3} + 6.385n \\ &\quad - 16.103j(j+1)/A^{2/3}, \\ R_4(n) &= 0.9904; \end{aligned} \quad (\text{A1.4})$$

$$\begin{aligned} E_5(n) &= -94.474 + 76.933l/A^{1/3} + 97.753n/A^{1/3} + 14.789n \\ &\quad - 14.961J(J+1)/A^{2/3} - 2.090n^2, \\ R_5(n) &= 0.9926; \end{aligned} \quad (\text{A1.5})$$

$$\begin{aligned} E_6(n) &= -94.905 + 70.836l/A^{1/3} + 89.992n/A^{1/3} + 17.956n \\ &\quad - 18.037j(j+1)/A^{2/3} - 2.573n^2 + 43.290l(l+1)/A, \\ R_6(\hbar) &= 0.9938; \end{aligned} \quad (\text{A1.6})$$

$$\begin{aligned} E_1(p) &= -36.263 + 33.768l/A^{1/3}, \\ R_1(p) &= 0.5439; \end{aligned} \quad (\text{A2.1})$$

$$\begin{aligned} E_2(p) &= -74.454 + 55.772l/A^{1/3} + 23.768n, \\ R_2(p) &= 0.9116; \end{aligned} \quad (\text{A2.2})$$

$$\begin{aligned} E_2(p) &= -84.756 + 62.996l/A^{1/3} + 15.478n + 63.778n/A^{1/3}, \\ R_3(p) &= 0.9792; \end{aligned} \quad (\text{A2.3})$$

$$\begin{aligned} E_4(p) &= -87.843 + 83.036l/A^{1/3} + 13.568 + 78.331n/A^{1/3} \\ &\quad - 18.287j(j+1)/A^{2/3}, \\ R_4(p) &= 0.9941; \end{aligned} \quad (\text{A2.4})$$

$$\begin{aligned} E_5(p) &= -95.020 + 82.382l/A^{1/3} + 24.020n + 76.284n/A^{1/3} \\ &\quad - 17.540j(j+1)/A^{2/3} - 2.954n^2, \\ R_5(p) &= 0.9956; \end{aligned} \quad (\text{A2.5})$$

$$\begin{aligned} E_6(p) &= -100.515 + 82.551l/A^{1/3} + 30.147n + 58.962n/A^{1/3} \\ &\quad - 17.741j(j+1)/A^{2/3} - 3.722n^2 + 39.649Z/A^{4/3}; \\ R_6(p) &= 0.9961. \end{aligned} \quad (\text{A2.6})$$

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#### REFERENCES

1. Health Sciences Computing Facility, University of California, Los Angeles, UCLA (BMDO2R).
2. M. A. K. LODHI; M. A. K. LODHI, AND B. T. WAAK, *Phys. Rev. Lett.* **29** (1972), 301; *Ann. Phys.* **101** (1976), 1.
3. G. J. WAGNER, G. MAIRLE, U. SCHMIDT-ROHR, AND P. TURCK, *Nucl. Phys. A* **125** (1969), 80; G. J. WAGNER, *Bull. Amer. Phys. Soc. II* **14** (1969), 85; "Nuclear Structure Physics," p. 16, *Lecture Notes in Physics No. 23* (V. Similansky, I. Talmi, and H. A. Weidenmuler, Eds.), Springer, Berlin, 1973.



4. B. L. COHEN, *Amer. J. Phys.* **33** (1965), 1011.
5. K. TAKEUCHI AND P. MOLDAUER, *Phys. Lett. B* **28** (1969), 384.
6. R. K. BANSAL AND B. T. FRENCH, *Phys. Lett. II* (1964), 145; **19** (1965), 223; R. K. BANSAL, *Phys. Lett. B* **27** (1968), 184; **40** (1972), 189; B. J. FRENCH, in "Isospin in Nuclear Physics" (D. H. Wilkinson, Ed.), p. 260, Wiley, New York, 1969, and references therein.
7. D. J. MILNER AND P. E. HODGSON, *Phys. Lett. B* **35** (1971), 495; F. MALAGUTI AND P. E. HODGSON, *Nucl. Phys. A* **215** (1973), 243; P. E. HODGSON, *Rep. Progr. Phys.* **38** (1975), 847, and references therein.
8. C. V. VEJE, quoted in A. BOHR AND B. R. MOTTELSON, "Nuclear Structure," p. 239, Benjamin, New York, 1971.
9. H. W. MELDNER, *Ark. Fys.* **36** (1967), 593; *Phys. Rev.* **178** (1969), 1815.
10. H. W. MELDNER, M. W. WEISS, AND R. E. WRIGHT, *Phys. Rev. C* **14** (1976), 1615.
11. M. A. K. LODHI, *Phys. Rev.* **182** (1969), 1061; *Phys. Rev. C* **1** (1970).
12. D. VAUTHERIN AND D. M. BRINK, *Phys. Rev. C* **5** (1972), 626; J. W. EHLERS AND S. A. MOSZKOWSKI, *Phys. Rev. C* **6** (1972), 217; R. Y. CUSSON, H. TRIVEDI, AND D. KOLB, *Phys. Rev. C* **5** (1970), 2120; L. R. MILLER AND A. E. S. GREEN, *Phys. Rev.* **184** (1969), 1012; A. E. S. GREEN, G. DAREWYCH, AND R. BEREZDIVIN, *Phys. Rev.* **157** (1967), 929.
13. M. A. K. LODHI AND B. T. WAAK, *Phys. Rev. Lett.* **33** (1974), 431.
14. For example, see E. J. WILLIAMS, "Regression Analysis," Wiley, New York, 1959.
15. Texas Tech Computer Services, TTCS (BIMED-02R).
16. L. PAULING AND E. B. WILSON, "Introduction to Quantum Mechanics," p. 156, McGraw-Hill, New York, 1935.
17. S. S. WALD, private communication.
18. A. BOHR AND B. R. MOTTELSON, "Nuclear Structure, pp. 325, 328, Benjamin, New York, 1971.
19. K. TAKEUCHI AND P. A. MOLDAUER, *Phys. Lett. B* **28** (1969), 384, and references therein.
20. E. ROST, *Phys. Lett. B* **26** (1968), 184.
21. G. JACOB AND TH. A. J. MARIS, *Rev. Mod. Phys.* **45** (1973), 6; **38** (1966), 121.
22. A. N. JAMES, P. T. ANDREWS, P. KIRBLY, AND B. G. LOWE, *Nucl. Phys. A* **138** (1969), 145.
23. U. AMALDI, JR., *Phys. Lett.* **22** (1966), 593.
24. M. RIOU, *Rev. Mod. Phys.* **37** (1965), 375.
25. G. MAIRLE *et al.*, *Nucl. Phys. A* **134** (1969), 180.
26. A. N. JAMES, P. T. ANDREWS, P. BUTLER, N. COHEN, AND B. G. LOWE, *Nucl. Phys. A* **133** (1969), 89.
27. G. BASSANI *et al.*, *J. Phys. Soc. Japan, Suppl.* **24** (1968), 649, quoted in D. VAUTHESIN AND D. M. BRINK, *Phys. Rev. C* **5** (1972), 626.
28. A. J. WAPSTRA, *Physica* **21** (1955), 367, 389, quoted in K. A. BRUCKNER, A. M. LOCKETT, AND M. ROTENBERG, *Phys. Rev.* **121** (1961), 255.
29. K. NAKAMURA *et al.*, *Phys. Rev. Lett.* **33** (1974), 853; K. NAKAMURA, University of Tokyo Preprint No. UTPN-36 (1974).
30. M. BERNHEIM *et al.*, *Phys. Rev. Lett.* **32** (1974), 898.