Effective-Interaction Calculation on the Energy Spectra of $1f$-$2p$ Nuclei. I*

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The energy spectra of normal-parity states of Ni isotopes are studied in the conventional shell model. The effective two-body interactions are determined by a least-squares fit between the calculated and observed low-lying energy levels. The agreement between the experimental and calculated energy spectra is quite remarkable. Single-nucleon spectroscopic factors for some low-lying states of odd-mass Ni isotopes are calculated. The resulting spectroscopic factors are similar to those calculated in other effective interaction calculations.

1. INTRODUCTION

In the past few years a considerable amount of theoretical work has been done on Ni isotopes. In the theoretical calculations an inert ^{56}Ni core was generally assumed. The neutrons outside the core was assumed to be distributed among the $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbitals. Since there is a large number of configurations available when the number of nucleons is large, many techniques were used to reduce the active model space. Hsu and French[1] studied the structure of even Ni isotopes using low-seniority, Tamm-Dancoff, and random-phase approximations. They found that they obtained the best agreement between their calculation and the exact shell-model calculation of Cohen *et al.*[2] when they used the low-seniority approximation. Plastino, Arvieu, and Moszkowski[3] examined the energy levels of even Ni isotopes by applying the Tamm-Dancoff approximation to the surface δ interaction. It was found that this approximation could give good results for ^{58}Ni but for the isotopes with higher mass number it worked relatively well for the first 2^+ and 4^+ states only. Gambhir showed[4] later on that the Tamm-Dancoff approximation could be improved by the inverse gap equation method proposed by Gillet and Rho.[5] Lawson, Macfarlane, and Kuo[6] studied the structure of Ni isotopes with the Hamada-Johnston potential in the shell model. The comparison with the experimental data showed that the Hamada-Johnston potential cannot describe the energy levels of Ni isotopes satisfactorily. It was shown later that the result of the Hamada-Johnston potential could be improved by using modified Tamm-Dancoff approximations.[7,8] The energy levels of Ni isotopes were analyzed by various potentials in the exact shell model.[9,10] They found that the agreement of the energy-level spectra with the experimental data, using Rosenfeld mixture, Serber exchange, and surface δ potentials, was similar to the agreement obtained when doing an effective-interaction calculation. When the Hamada-Johnston potential was used the agreement was not quite as good, and the calculation was even worse when the Tabakin potential was used. Glaudemans, De Voigt, and Steffens[11] carried out a rather complete calculation by using modified surface δ interaction and got quite good results. Recent calculations using Hartree-Fock-Bogoliubov wave functions also made some progress.[12,13] The most complete and successful study of the energy levels of Ni isotopes was given by the effective-interaction calculations carried out by Cohen *et al.*[14] and Auerbach.[15-17] In Cohen *et al.*'s calculation they fitted the energy levels with eight parameters: the four diagonal radial matrix elements of the central interaction in relative s states and the potential strengths of the central (single and triplet), the tensor, and the two-body spin-orbit parts. In Auerbach's calculation he computed the nondiagonal matrix elements by using the Kallio-Kolltveit potential[18] and determined the diagonal matrix elements by minimizing the difference between calculated and observed energy levels. The results of these effective-interaction calculations were very good. However, the meager experimental information in the earlier years prevented a direct parametrization with all two-body effective matrix elements. During recent years more experimental data of the energy levels of Ni isotopes have become available. Therefore, it is feasible to carry out an effective-interaction calculation with more parameters. It is the purpose of this work to investigate the structure of Ni isotopes in a model in which all of the two-body matrix elements are treated on an equal footing, i.e., as variable parameters. In Sec. 2 we describe our model in detail. In Sec. 3 we discuss the results of our calculation, and in the final section we present our conclusion.

2. MODEL

In this work an inert ^{56}Ni core is assumed. The success of previous effective-interaction-type

calculations supports the assumption that the core polarization effects can be absorbed by the effective residual interaction between valence nucleons. The low-lying energy specrra of ^{57}Ni suggest that the single-particle energy levels for $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbitals are 0, 0.78, and 1.08 MeV, respectively. The single-particle-state energy of $1g_{9/2}$ is estimated to be at least 3 MeV above the $2p_{3/2}$ level and higher than the $1f_{7/2}$ single-hole state. Therefore, for low-lying states its effect should be less than the core excitations and can be neglected. With this knowledge, we restrict our available configurations for the active model space to the form $(2p_{3/2}, 1f_{5/2}, 2p_{1/2})^n$. The two-body interactions within the configurations are determined by their matrix elements between the antisymmetric two-particle states of the single-particle orbits $2p_{3/2}$, $1f_{5/2}$ and $2p_{1/2}$. There are 30 such matrix elements. The abundant experimental data on Ni isotopes make it feasible to carry out a direct effective-interaction fit with all of the 30 matrix elements. For Ni isotopes from ^{58}Ni to ^{66}Ni there are about 100 low-lying levels with known spin-parity assignments. Out of the 100 levels we have selected 69 levels for which the J^π assignments are the most reliable and have used these levels in the least-squares-fit calculation. We used two sets of parameters in our calculation. In the first set we fixed the single-particle energies of the $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbitals at 0, 0.78, and 1.08 MeV and treated the 30 matrix elements as varying parameters (denoted by Set I hereafter). In the second set the single-particle energy spacings and the matrix elements are all treated as varying parameters (denoted by Set II hereafter). Since there are more than twice as many experimental levels as parameters, this parametrization seens to be credible. It is in-

TABLE I. Effective two-body matrix elements $\langle j_1 j_2 | V | j_3 j_4 \rangle_J$ determined in various theoretical calculations. The meaning of each column is explained in the text.

$2j_1$	$2j_2$	$2j_3$	$2j_4$	J	A	B	C	D	E
5	5	5	5	0	−1.25	−1.73	−1.74	−1.42	−1.41
5	5	5	5	2	−0.05	0.28	−0.40	−0.63	−0.64
5	5	5	5	4	0.46	0.17	0.32	0.58	0.58
5	5	5	3	2	0.14	0.54	−0.17	0.25	0.24
5	5	5	3	4	0.35	0.48	−0.25	0.42	0.43
5	5	5	1	2	−0.51	−0.64	−0.31	−0.17	−0.12
5	5	3	3	0	−1.26	−0.99	−1.12	−1.26	−1.21
5	5	3	3	2	−0.24	−0.25	−0.16	−0.55	−0.55
5	5	3	1	2	−0.46	−0.22	0.22	−0.27	−0.25
5	5	1	1	0	−0.95	−0.65	−0.56	−0.55	−0.58
5	3	5	3	1	0.40	1.06	1.10	0.33	0.33
5	3	5	3	2	0.30	0.57	0.30	0.15	0.15
5	3	5	3	3	0.37	0.65	0.80	0.79	0.79
5	3	5	3	4	−0.07	−0.39	−0.38	−0.25	−0.25
5	3	5	1	2	0.20	0.21	−0.39	0.03	0.04
5	3	5	1	3	0.12	0.02	0	−0.05	−0.08
5	3	3	3	2	0.14	0.15	−0.12	0.37	0.32
5	3	3	1	1	−0.04	0.06	0	0.18	0.21
5	3	3	1	2	0.17	0.10	0.18	0.24	0.29
5	1	5	1	2	−0.17	−0.28	−0.20	0.27	0.29
5	1	5	1	3	0.64	0.86	0.62	0.08	0.09
5	1	3	3	2	−0.06	−0.21	−0.23	−0.09	−0.15
5	1	3	1	2	−0.33	−0.23	0.33	−0.22	−0.21
3	3	3	3	0	−0.88	−1.04	−0.92	−0.65	−0.64
3	3	3	3	2	−0.25	0.37	0.24	0.42	0.42
3	3	3	1	2	−0.27	−1.10	0.83	−0.57	−0.57
3	3	1	1	0	−0.96	−1.03	−0.97	−0.84	−0.87
3	1	3	1	1	0.06	0.71	1.24	0.59	0.64
3	1	3	1	2	−0.36	−0.41	−0.60	0.12	0.10
1	1	1	1	0	−0.24	−0.31	−0.89	−0.76	−0.64

TABLE II. Experimental and calculated single-nucleon stripping spectroscopic factors for some of the low-lying levels of odd-mass Ni isotopes.

Residual nuclei	E (MeV)	Experimental l	j	$(2j+1)S$	Calculated Set I	Set II
^{59}Ni	0.00	1	$\frac{3}{2}$	2.77	1.68	1.69
	0.34	3	$\frac{5}{2}$	5.19	4.32	4.37
	0.47	1	$\frac{1}{2}$	1.24	1.56	1.60
	0.88	1	$\frac{3}{2}$	0.31	0.27	0.27
	1.31	1	$\frac{1}{2}$	0.56	0.26	0.19
^{61}Ni	0.00	1	$\frac{3}{2}$	1.67	1.09	1.11
	0.07	3	$\frac{5}{2}$	3.37	2.09	2.12
	0.29	1	$\frac{1}{2}$	1.21	1.49	1.47
	0.66	1	$\frac{3}{2}$	0.04	0.08	0.08
	0.91	3	$\frac{5}{2}$	0.23	0.00	0.00
	1.11	1	$\frac{3}{2}$	0.18	0.08	0.08
	1.13	3	$\frac{5}{2}$	0.27	0.06	0.06
	1.19	1	$\frac{3}{2}$	0.25	0.01	0.01
^{63}Ni	0.00	1	$\frac{1}{2}$	0.75	1.26	1.24
	0.09	3	$\frac{5}{2}$	2.39	0.93	0.93
	0.16	1	$\frac{3}{2}$	1.07	0.81	0.82
	0.52	1	$\frac{3}{2}$	0.31	0.01	0.01
	1.00	1	$\frac{1}{2}$	0.66	0.01	0.01
^{65}Ni	0.00	3	$\frac{5}{2}$	1.49	0.42	0.40
	0.06	1	$\frac{1}{2}$	1.23	0.86	0.90
	0.31	1	$\frac{3}{2}$	0.17	0.56	0.56
	0.69	1	$\frac{3}{2}$	0.62	0.00	0.01

teresting to mention that although some of the low-lying levels with known J^π assignment are not included in the least-squares calculation, when the calculation was carried out, calculated levels were found which agreed quite remarkably with the experimental levels that had not been included. The detailed results will be discussed in the next section.

3. RESULTS

A. Effective-Interaction Matrix Elements

The effective-interaction matrix elements are determined by the least-squares calculation. The resulting matrix elements are presented in Table I. In column A the reaction matrix elements including a perturbative single-nucleon core excitation correction[6] are listed. The effective two-body matrix elements calculated by Cohen *et al.*[14] and Auerbach[17] are listed in columns B and C, respectively. In columns D (Set I) and E (Set II) the matrix elements determined in this work are presented. The $(2p_{1/2}$-$2p_{3/2})$ and $(1f_{5/2}$-$2p_{3/2})$ single-particle spacings corresponding to the matrix elements in column E are found to be 0.96 and 0.79 MeV, respectively. Such values are quite consistent with the single-particle energies determined by the pickup experiments. From Table I

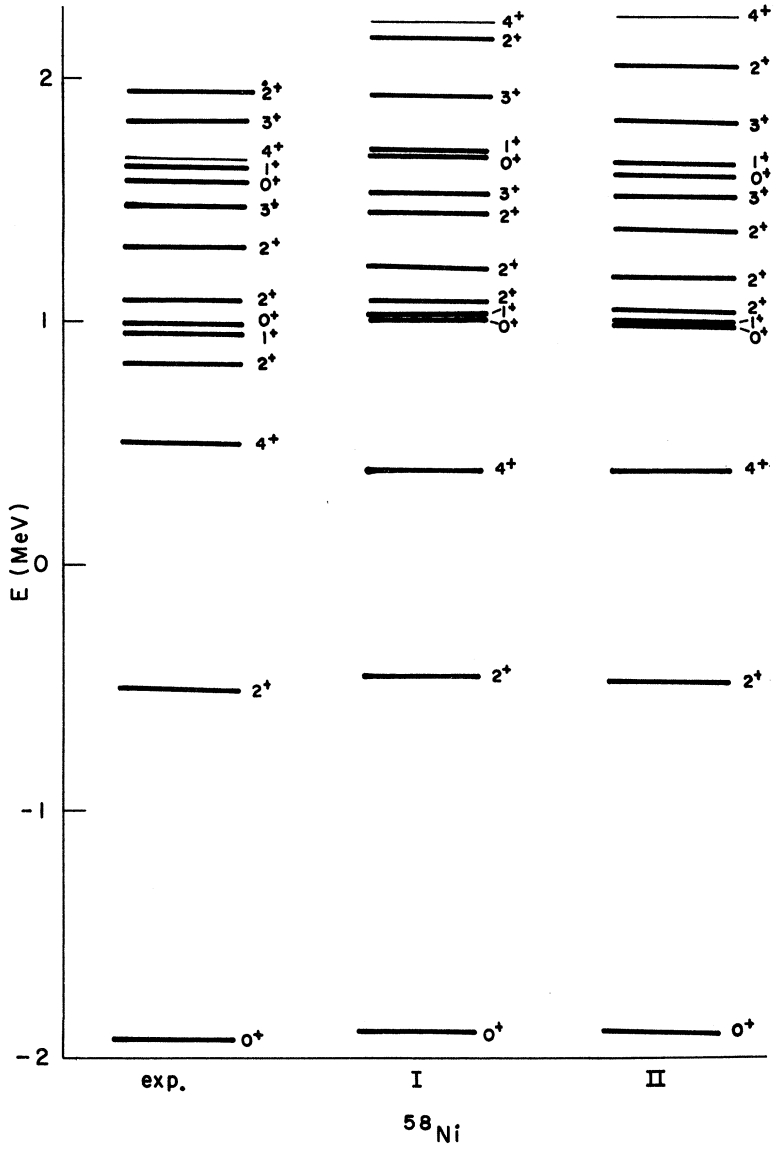

FIG. 1. Experimental and calculated energy levels of ^{58}Ni.

we see that the matrix elements in all effective-interaction calculations are quite similar. The matrix elements determined from the Hamada-Johnston potential (column A) differ slightly from the other four sets. Since the energy levels depend on the matrix elements rather sensitively, the resulting energy levels calculated from the matrix elements in column A are quite different from those determined by the other effective-interaction matrix elements. It was shown that the interactions in column A produce large discrepancies in the energy spectra when the number of valence nucleons increases. This is reasonable since the interactions in column A are determined from the free nucleon-nucleon interaction force. However, the qualitative agreement between the interactions in column A and other effective interactions clearly indicates that a qualitative guide can be drawn from the realistic nucleon-nucleon interactions.

B. Energy Levels

The comparison between calculated energy levels and the experimental levels is shown in Figs. 1–9. The experimental ground-state binding energies are calculated in a standard way as in Refs. 6 and 14. The levels that are included in the least-squares calculation are indicated by heavy lines while the levels that are excluded are indicated by light lines. The over-all rms deviations are 0.13 and 0.12 MeV for Set I and Set II calculations, respectively. From the figures we can notice the following features:

(i) The calculated ground-state binding energies agree quite well with the experimental values. Starting from ^{61}Ni the ground-state binding energies become positive. This result indicates that the interactions between identical shells are repulsive[14,19] and agrees with the results of other effective-interaction calculations.

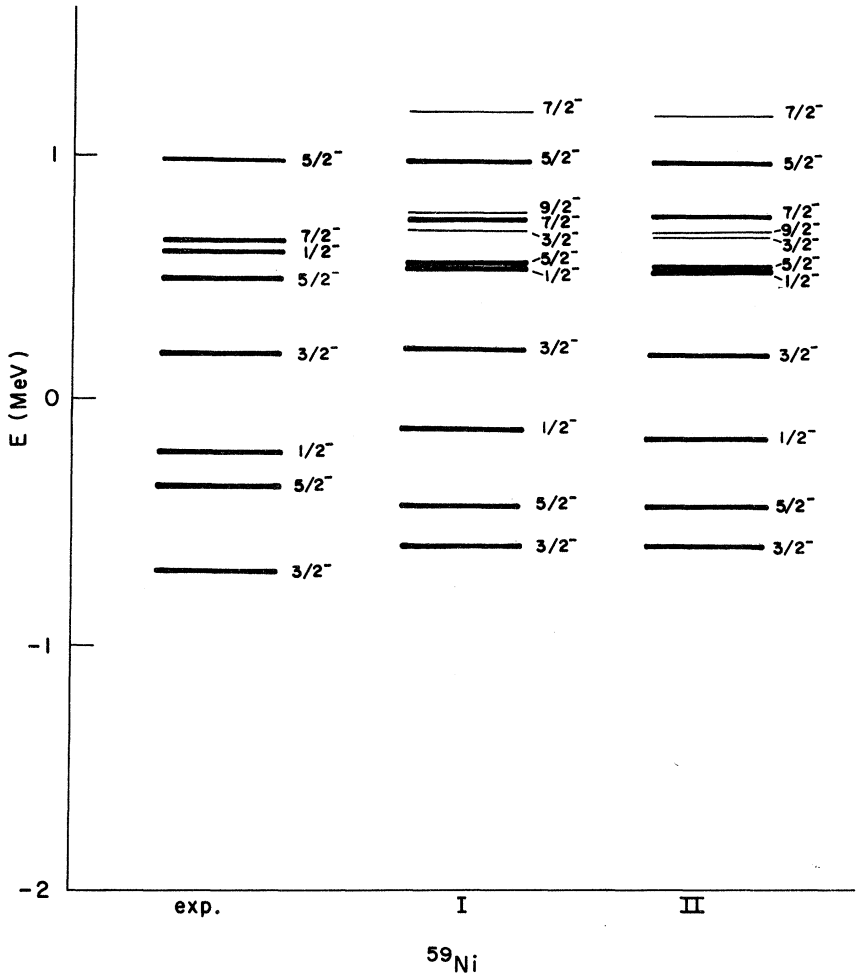

FIG. 2. Experimental and calculated energy levels of ^{59}Ni.

(ii) In general, the result of the even-mass isotopes is quite good. The first 2^+ state is very well reproduced. The excitation energy of the first 2^+ level starts at 1.45 MeV for ^{58}Ni then drops to 1.38 MeV for ^{60}Ni, and to 1.37 MeV for ^{62}Ni. After ^{64}Ni the excitation energy for this level rises again to 1.45 MeV for ^{64}Ni and to 1.5 MeV for ^{66}Ni. This tendency is favored by the experimental data. In earlier effective-interaction calculations the excitation energies for these levels were almost constant, the value being 1.5 MeV.

The so-called "vibration-like" spectra with a triplet of states $J=0^+$, 2^+, 4^+ lying about twice the energy of the first excited 2^+ state is evident in our calculation. However, this seems to be less obvious for ^{58}Ni and ^{66}Ni, the first and the last nucleus in our model space.

(iii) The general result for odd-mass isotopes seems to be, relatively speaking, slightly poorer than those for the even-mass isotopes. At present, the experimental energies, parities, and spins of the levels in the region above the second $\frac{1}{2}^-$ level

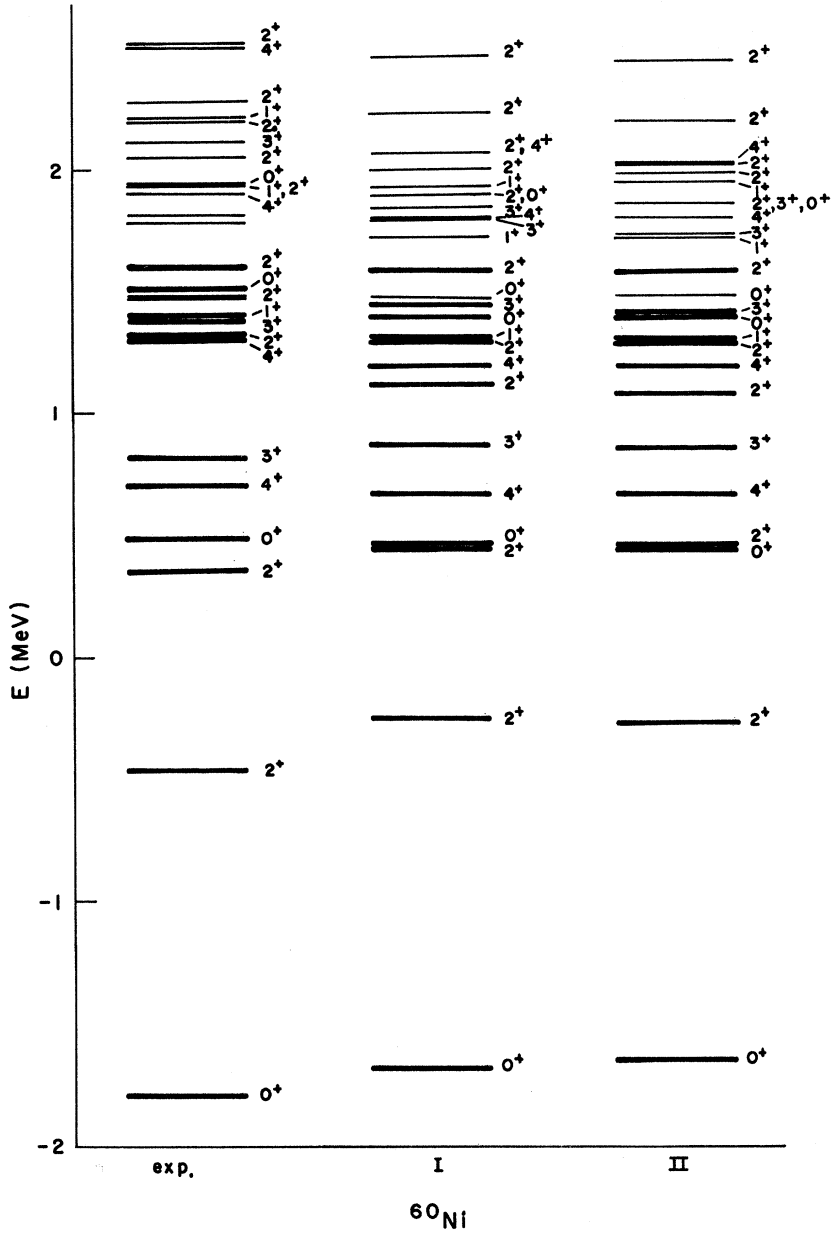

FIG. 3. Experimental and calculated energy levels of ^{60}Ni.

(4.73 MeV) of ^{63}Ni and in the region above the second $\frac{3}{2}^-$ level (9.15 MeV) of ^{65}Ni are not well known. Our model seems to predict a larger level density than that of the known experimental levels.

(iv) In the energy spectra of ^{58}Ni a 1^+ level is predicted at 1.04 MeV. This level was not detected experimentally since its position was very close to the second 0^+ (1.00-MeV) level. Start *et al.*[20] made a rather detailed analysis of the ^{58}Ni energy spectra. They detected the 41-keV γ ray resulting from the 1.00-MeV (corresponding to excitation energy 2.943 MeV) to 0.96-MeV (corresponding to excitation energy 2.902 MeV) transition and determined the J^π assignment of the latter level to be 1^+. It is interesting that this level was missed both experimentally and theoretically in the earlier works.

(v) In the energy spectra of ^{59}Ni a $\frac{9}{2}^-$ level is predicted at about 0.80 MeV. This level was also predicted in other effective-interaction calculations but so far it has not been found experimentally. However, it is interesting to notice that the predicted position of this level in our model lies higher than that of previous effective-interaction calculations. In fact the predicted position of this level is near the region in which the experimental situation of the energy spectra of ^{59}Ni is not well known. Therefore the calculation of our model suggests that this level may be sought experimentally in the region above the first $\frac{7}{2}^-$ (0.67-MeV) level.

(vi) In the spectra of ^{61}Ni the level at 1.66 MeV (corresponding to excitation energy 1.02 MeV) is detected by many experiments but its J^π assignment and origin are highly uncertain.[21-24] The calculation in this work suggests that the most probable assignment is $\frac{1}{2}^-$.

(vii) The low-lying energy spectra of ^{64}Ni is very interesting. The J^π assignment of the level at 6.60 MeV (corresponding to excitation energy 2.27 MeV) is rather controversial. Some of the experimental data favor a 2^+ assignment while some others favor a 0^+ assignment.[25-27] When either assignment is taken in theoretical calculations, the agreement between the calculated and experimental energy levels is poor.[14,18] In Cohen

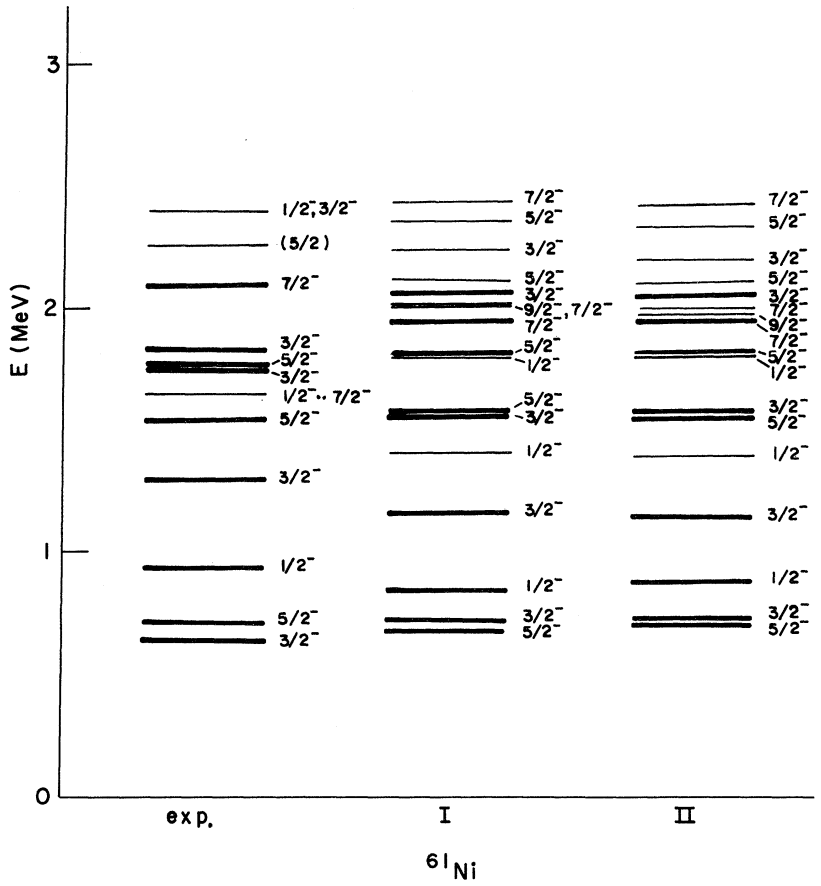

FIG. 4. Experimental and calculated energy levels of ^{61}Ni.

et al.'s calculation a 2^+ assignment was chosen and as a result they found a rather large discrepancy at the first 0^+ excited state. In Auerbach's calculation a 0^+ assignment was chosen and the agreement between the calculated and the measured 2^+ states became poor. Our calculation, however, suggests that the level at 6.60 MeV may be a $(0^+, 2^+)$ doublet. In our calculation we found that a large discrepancy cannot be avoided if either of the assignments is selected. However, if we treat the level as a $(0^+, 2^+)$ doublet, the discrepancy is greatly reduced. Since there are different experiments supporting each assignment, we believe that it is reasonable to assume the doublet structure for this level. The level at 6.81 MeV (corresponding to excitation energy 2.48 MeV) is not certain in the sense that only very few experiments have detected this level.[21] The calculation in this work suggests that the most probable J^π assignment is 2^+ if it really exists.

C. Spectroscopic Factors

The corresponding wave functions are used to calculate the single-nucleon spectroscopic factors. The experimental and calculated (d,p) spectroscopic factors for some low-lying states in the odd-mass Ni isotopes are displayed in Table II for comparison. There are two general features. (i) The agreement between the calculated and experi-

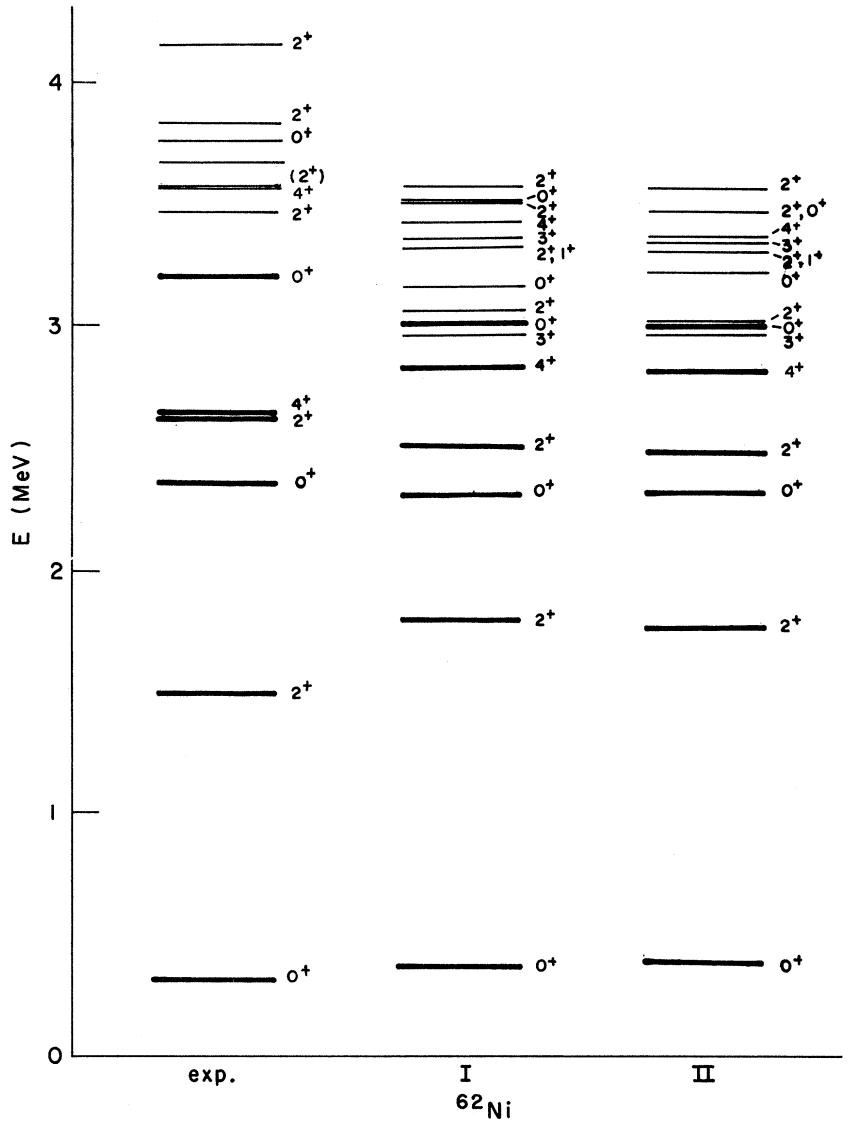

FIG. 5. Experimental and calculated energy levels of ^{62}Ni.

mental values is better for lighter isotopes (^{59}Ni, ^{61}Ni) but poorer for heavier isotopes (^{63}Ni, ^{65}Ni). (ii) The calculated strength is concentrated in the lowest $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states. In fact, except for ^{59}Ni the strength for the higher $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ levels is negligible. The experimental spectroscopic strength is also concentrated in the lowest $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states but the strength for higher states is not negligible.[22,28] Furthermore, the experimental value of the spectroscopic factor for the $\frac{3}{2}^-$, 0.69-MeV state of ^{65}Ni is considerably larger than that for $\frac{3}{2}^-$, 0.32-MeV state while the calculation in this work predicts the reverse order. The discrepancies may come from the contributions of the higher configurations omitted in this work. When these configurations are included, they may cause considerable seniority mixing which, in turn, will effect the spectroscopic factor calculation. On the other hand, the contribution of these configurations to the low-lying levels will still be small since the single-particle energies of the higher orbitals are considerably higher than energies of the low-lying levels.

4. CONCLUSIONS

The properties of low-lying levels of Ni isotopes are studied by a shell model within the identical nucleon configurations $(2p_{3/2}, 1f_{5/2}, 2p_{1/2})^n$. All of the 30 two-body matrix elements and the single-particle level spacings are treated as varying parameters. The parameters are determined by a least-squares fit with 69 most reliable low-lying levels. The resulting effective two-body interaction matrix elements are similar to those determined by other effective interaction calculations.

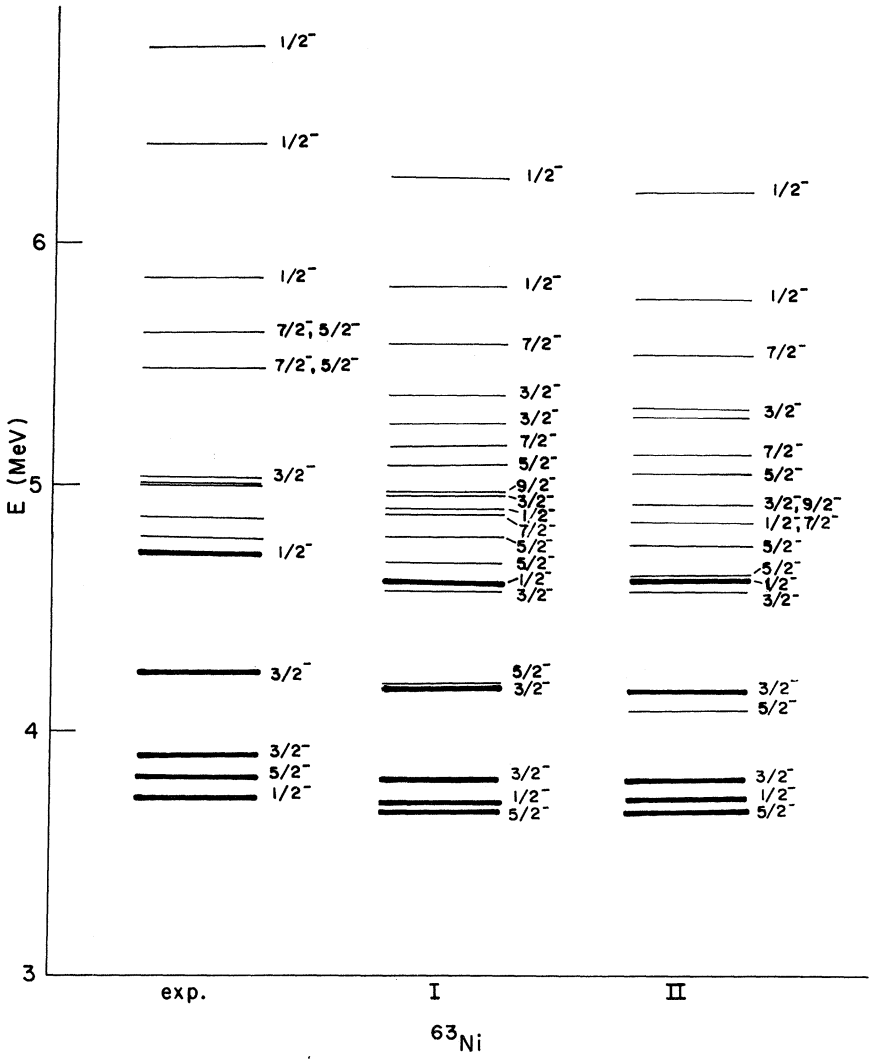

FIG. 6. Experimental and calculated energy levels of ^{63}Ni.

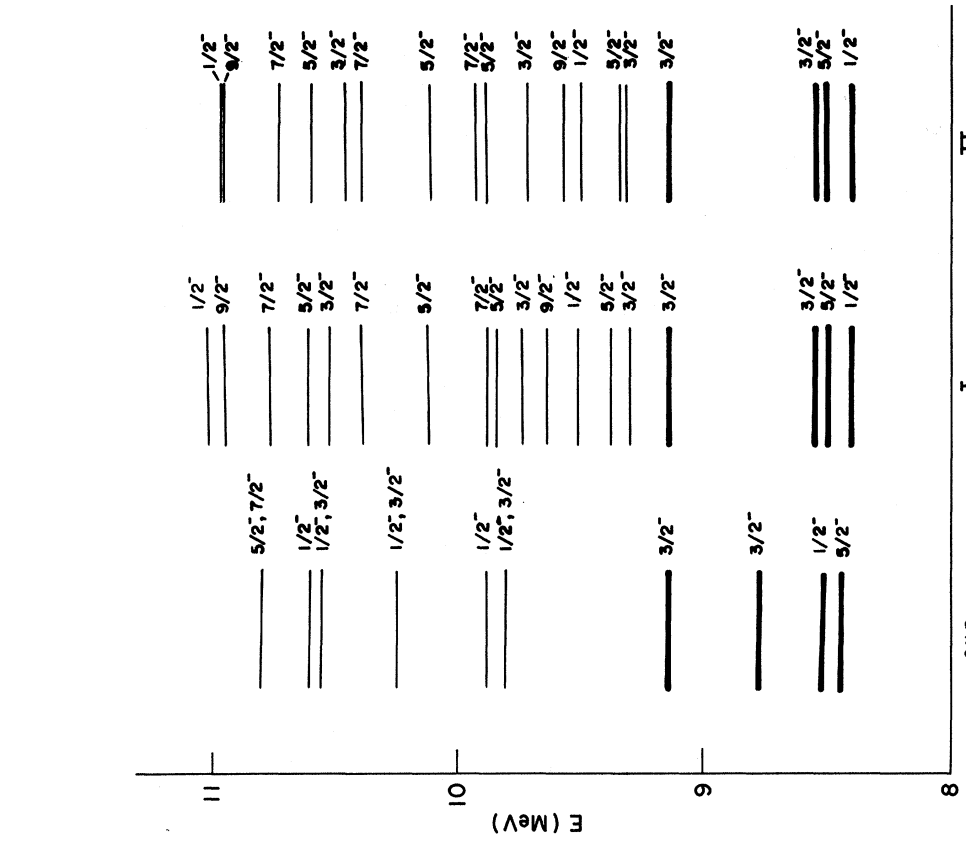

FIG. 8. Experimental and calculated energy levels of ^{65}Ni.

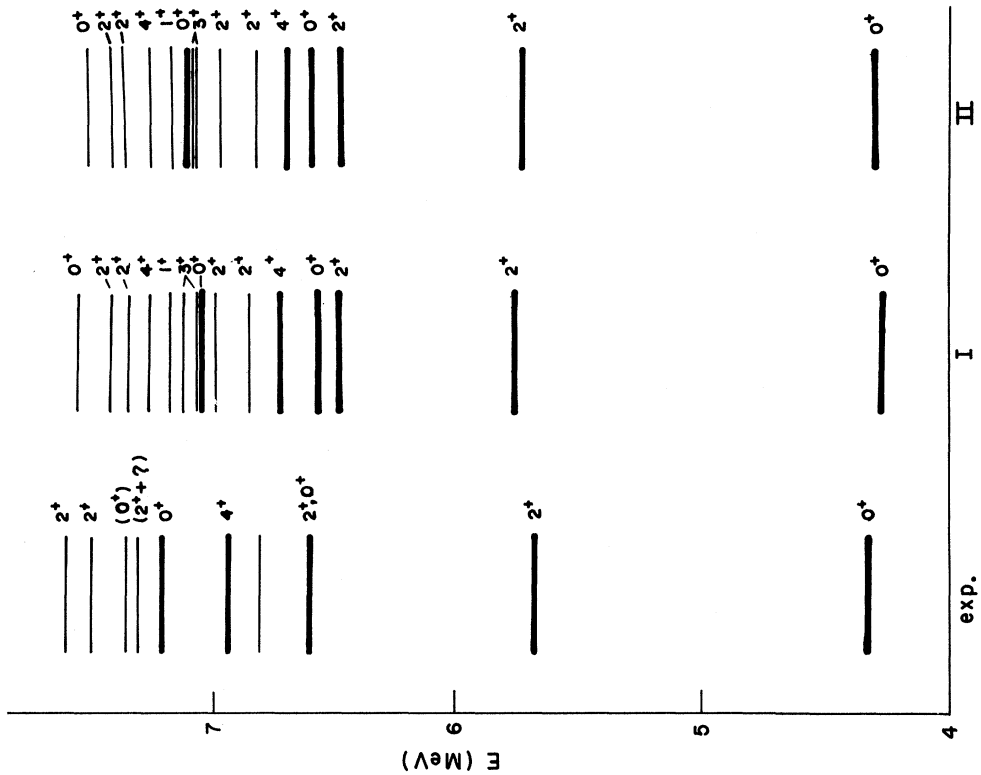

FIG. 7. Experimental and calculated energy levels of ^{64}Ni.

However, since the energy spectra are rather sensitive to the two-body matrix elements, the resulting energy spectra in this calculation show considerable improvement when compared with previous effective-interaction calculations. The resulting wave functions are used to calculate the single-nucleon stripping spectroscopic factors. The results of the spectroscopic factors are very similar to those calculated by previous effective-interactions calculations.[14,18] The fact that there are considerable discrepancies between the experimental and calculated spectroscopic factors suggests that the resulting wave functions are not adequate to compute those quantities that depend on wave functions sensitively. Therefore we expect that the calculations of transition rates and magnetic moments within the present configurations will also have rather large discrepancies unless the neglected configurations are taken into account. Cohen *et al.*[14] calculated the $E2$ transition rates

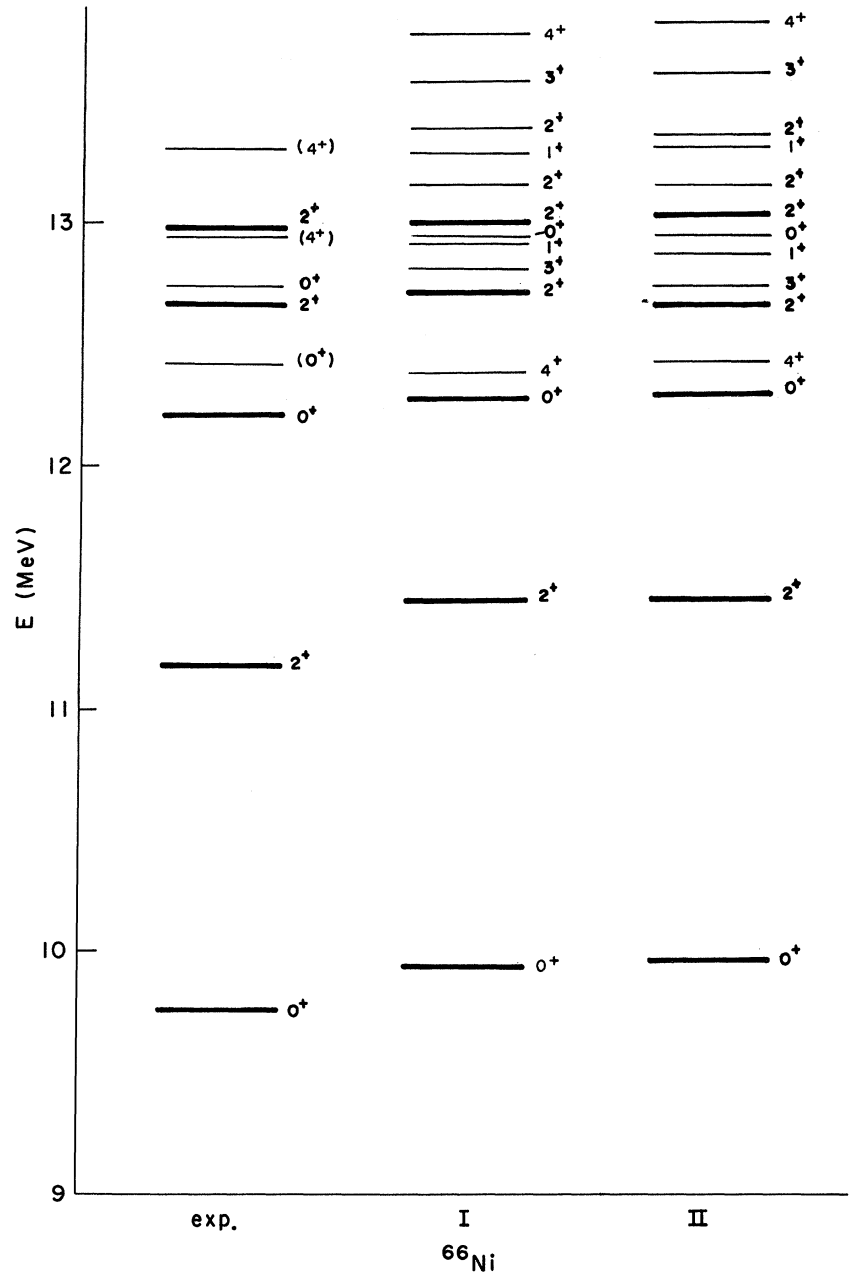

FIG. 9. Experimental and calculated energy levels of ^{66}Ni.

and magnetic moments of Ni isotopes by introducing an effective $E2$ operator which absorbs the influence of the neglected configurations explicitly. It will be interesting to investigate the effect of the neglected configurations explicitly. The calculation of Arvieu, Salusti, and Verneroni[29] suggested that the contributions of $1g_{9/2}$ configuration mixing were not important in light Ni isotopes and Cohen *et al.*[14] pointed out that the contributions from $1g_{9/2}$ orbit configuration mixing may be more important for heavier Ni isotopes. The fact that in all effective-interaction calculations the agreement of heavier Ni isotopes is relatively poorer than that of light Ni isotopes really supports their point of view. However, a calculation that is similar to this work and expands the model space to include $1g_{9/2}$ orbit or core excitations will be too massive. A possible feasible approach is to expand the model space to include $1g_{9/2}$ orbit or core excitations but restrict the basis states with low seniorities. The analyses of previous effective-interaction calculations indicate that it is a good approximation to consider seniority up to 4 for even-mass Ni isotopes and to 3 for odd-mass Ni isotopes. When the result of such a calculation is compared with the result of this work, useful information about the contributions from core excitations and $1g_{9/2}$ orbit can be drawn.

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