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Effective interactions and charges in ^{58}Ni

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Abstract. The structure of the low-lying states of ^{58}Ni has been calculated in shell model by assuming an inert ^{56}Ni core plus two valence nucleons in the $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbitals. The two-body matrix elements are first expressed in terms of seven radial matrix elements and these are then parametrized to give best fit between the computed and the observed energies of the levels below 4 MeV. The wavefunctions obtained using these two-body matrix elements are used to study the concept of effective charges. It is found that a single effective charge is not sufficient to predict the B(E2) rates equally well for the thirteen known transitions for which experimental values are available. Assumption of state-dependent effective charges gives a far better agreement. An analysis using wavefunctions obtained with Kuo's two-body matrix elements also gives a similar result.

Keywords. ^{58}Ni; shell model; effective operators; nuclear spectroscopy; E2 transition rates.

1. Introduction

Shell model calculations are severely restricted in the number of valence nucleons and the extent of configuration space they can handle. The truncation of configuration space generally involves ignoring an assumed core-configuration as well as other configurations higher in energy than a stipulated limit. Such truncation raises many interesting problems regarding effective interactions and effective electromagnetic moments to be associated with these valence nucleons. It is not easy to calculate from first principles the effective nuclear operators to be used in any given configuration space. Often one resorts to an empirical analysis of some experimental data on the energy spectra and electromagnetic transitions in suitable nuclei to deduce information on the effective operators. Such an analysis can sometimes yield valuable information on the concealed core-excitation effects and the nature of the assumed core.

We report here an analysis of the presently available data on ^{58}Ni to obtain the effective interactions as well as effective charges associated with E2 transitions in this nucleus. The analysis is made possible now because a rather large amount of data—14 energy levels and 13 B (E2) values—have become available recently (Start *et al* 1971).

Previously, quite a few shell model calculations have been carried out for Ni-isotopes, generally assuming an inert ^{56}Ni core plus valence nucleons in the $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbitals (Cohen *et al* 1967, Auerbach 1967, Arvieu *et al* 1970, Plastino *et al* 1966, Glaudemans *et al* 1972, Hsieh *et al* 1973, Lawson *et al* 1966, Kuo 1967 and Hsu and French 1965). Empirically determined effective interactions (in the first six of the references cited above), as well as interactions deduced from realistic nucleon-nucleon potentials (Lawson *et al* 1966 and Kuo 1967) have given equally good fits to the energy spectra of low lying states. The empirical methods of estimating the effective interaction have varied with authors. Cohen *et al* (1967) fitted the energy levels with eight parameters—the four potential interaction strengths and four radial integrals modifying the interaction in relative s-states of two nucleons. The eight parameters were estimated through a least squares fit to 24 observed levels in ^{58}Ni, ^{59}Ni, ^{60}Ni, ^{61}Ni and ^{62}Ni. Auerbach (1967) in his calculations used Kallio-Kolltveit (1964) potential to get the non-diagonal matrix elements and for the diagonal matrix elements made a least squares fit to the observed levels. Arvieu *et al* (1970) and Plastino *et al* (1966) applied effective surface delta interaction (SDI) and later Glaudemans *et al* (1972) used modified surface delta interaction (MSDI) to estimate the effective interaction parameters through a fit to the known energy levels of several Ni-isotopes taken together.

Methods outlined above were followed, since for a long time information on the energy levels of Ni-isotopes was limited and a direct estimation of all the 30 two-body matrix elements (TBME) was not possible. However, recently enough information has become available to make such a direct estimate possible. Hsieh *et al* (1973) have evaluated the 30 TBME through a minimization programme where the square of difference between the calculated and known energies of 69 levels of Ni-isotopes of mass numbers 58 to 66 is minimized. In this calculation and all others where a simultaneous fit to the energy levels of all Ni-isotopes is made, the agreement between calculated and observed spectra is relatively poorer for heavier isotopes. Cohen *et al* (1967) attribute this to the possible contribution from the configurations arising out of the neglected $1g_{9/2}$ orbit. This should become important for heavier isotopes. Also Macfarlane (1972) points out that the " calculations done for more than two particles clearly show that many-body effects are sizeable ". In view of the above two comments, we have tried to calculate the structure of low-lying states of ^{58}Ni, using the observed energy levels of ^{58}Ni only.

Our second and rather the main motivation has been to study the state dependence of effective charges in a truncated configuration. It has been found that the wave functions deduced from shell model calculations with reasonable values of effective charges ($e_n \approx 1{\cdot}0$–$2{\cdot}0$) fail to give good agreement with observed B(E2) values (Start *et al* 1971). This encourages us to carry out a somewhat more flexible analysis of the observed data. The B(E2) rates (Start *et al* 1971) are analysed to give effective matrix elements of the quadrupole operator for the single particle states of the configuration space. We hope to take into account the effect of the possible core excitations on transition rates through the effective reduced single-particle transition matrix elements.

The estimation of TBME's is discussed in the next section, where we have also compared them with the well-known Kuo (1968) matrix elements and with those estimated by Hsieh *et al* (1973). Section 3 contains the details of computations of the effective charges and the B(E2) rates, and section 4 the conclusion.

2. Effective interaction

Although there now exists a considerable body of experimental evidence (Jaffrin 1969) showing that low-lying states of ^{58}Ni involve a sizable amount of core-excitation, we shall attribute the properties of the low-lying states of ^{58}Ni to the two valence neutrons moving in $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbits around the doubly closed-shell core of ^{56}Ni. We shall show in this section that the effect of core-excitation on level energies can be included in an appropriately chosen effective two-body interaction. From the experimentally observed data on states of ^{57}Ni we take (like everybody else) for the energies of the single particle states

$$E(p_{3/2}) = 0{\cdot}0; \quad E(f_{5/2}) = 0{\cdot}78; \quad E(p_{1/2}) = 1{\cdot}08 \text{ MeV}.$$

The one-hole two-particle $7/2^-$ state in ^{57}Ni occurs at about 2·6 MeV excitation. However, in keeping with our philosophy of effective operators we do not take into account any hole-configurations. The single-particle $g_{9/2}$ state lies at least 3 MeV above the $p_{3/2}$ state, and its admixture into the states of ^{58}Ni considered by us is presumably unimportant.

The configuration space $(p_{3/2}, f_{5/2}, p_{1/2})^2$ gives 14 different states, and one can identify all of them with states observed in ^{58}Ni below 4 MeV excitation.

We shall assume the effective interaction to be central. The 30 TBME's $\langle J_1 J_2 J \mid V \mid J_1 J_2 J) \rangle$ (we have only $T = 1$ interaction) can be effectively parametrized as follows. The matrix elements are transformed to L–S coupling scheme, and the orbital part of the wave functions is further analysed in relative and centre-of-mass motions using the Brody-Moshinsky transformation (Brody and Moshinsky 1960). The procedure is the same as described in Shah and Pandya (1962), Pandya (1963) and Pandya and Green (1964). One then sees that apart from all the geometrical factors, the interaction potential V enters the matrix elements only through the radial matrix elements

$$I_{nl} = \int_0^\infty R_{nl}^2(r)\, V_{ls}(r)\, r^2\, dr$$

where $R_{nl}(r)$ is the oscillator wavefunction of relative coordinate r, in relative orbital angular momentum state with quantum numbers nl. The $T = 1$ restriction allows the total spin S to take $S = 0$ for even l and $S = 1$ for odd l values. Past experience as well as simple qualitative arguments suggest that most of the contribution to the matrix elements comes from interaction between two nucleons in relative $l = 0$ (s) or $l = 1$ (p) states. Geometry of the f-p shell shows that for $l = 0$ we obtain $n = 0, 1, 2, 3$ and for $l = 1$, $n = 0, 1, 2$. We treat the seven radial matrix elements I_{0s}, I_{1s}, I_{2s}, I_{3s}, I_{0p}, I_{1p} and I_{2p} as independent parameters and take all other $I_{nl} \equiv 0$. It may be noted that the assumption of central interaction is necessary to avoid further off-diagonal radial matrix elements. All the thirty $T = 1$ TBME's are now linear combinations of the seven parameters described above.

In our procedure the seven parameters are obtained through a least squares fitting procedure. The parameters are optimized to give the best agreement between the calculated and the observed energies (relative to the ground state) of the thirteen excited states below 4 MeV excitation energy. Optimization techniques have been discussed at many places, a recent reference being *Function Minimizations* by James (1972). (This reference has a complete bibliography of the various methods.) From the various methods discussed in this text we selected Newton's method for

Table 1. The strength of radial matrix elements (I_{nl}) in MeV

I_{nl}	I_{0s}	I_{1s}	I_{2s}	I_{3s}	I_{0p}	I_{1p}	I_{2p}
(in MeV)	−5·12	−3·05	−3·0	−3·79	−0·14	−1·21	0·39

Table 2. Effective two-body matrix elements $\langle J_a J_b | V | J_c J_d \rangle_J$

$2J_a$	$2J_b$	$2J_c$	$2J_d$	J	Kuo	Present calculations	Hsieh *et al* (set D)
3	3	3	3	0	−0·65	−1·60	−0·65
		5	5	0	−1·07	−0·81	−1·26
		1	1	0	−0·81	−1·08	−0·84
5	5	5	5	0	−1·58	−1·46	−1·42
		1	1	0	−0·83	−0·28	−0·55
1	1	1	1	0	−0·14	−0·83	−0·76
3	5	3	5	1	0·31	−0·14	0·33
		3	1	1	−0·06	0·0	−0·18
3	1	3	1	1	0·06	−0·06	0·59
3	3	3	3	2	−0·24	−0·41	0·42
		3	5	2	−0·16	−0·10	−0·37
		3	1	2	−0·26	−0·49	−0·57
		5	5	2	−0·19	−0·22	−0·55
		5	1	2	−0·11	−0·18	−0·09
3	5	3	5	2	0·21	−0·19	0·15
		3	1	2	−0·16	−0·14	−0·24
		5	5	2	−0·14	−0·12	−0·25
		5	1	2	−0·23	−0·24	−0·03
3	1	3	1	2	−0·38	−0·76	0·12
		5	5	2	−0·38	−0·16	−0·27
		5	1	2	−0·38	−0·26	−0·22
5	5	5	5	2	−0·14	−0·51	−0·63
		5	1	2	−0·49	−0·21	−0·17
5	1	5	1	2	−0·23	−0·45	0·27
3	5	3	5	3	0·32	−0·06	0·79
		5	1	3	0·10	−0·01	−0·05
5	1	5	1	3	0·53	−0·12	0·08
3	5	3	5	4	−0·17	−0·72	−0·25
		5	5	4	−0·33	−0·19	−0·42
5	5	5	5	4	0·35	−0·18	0·58

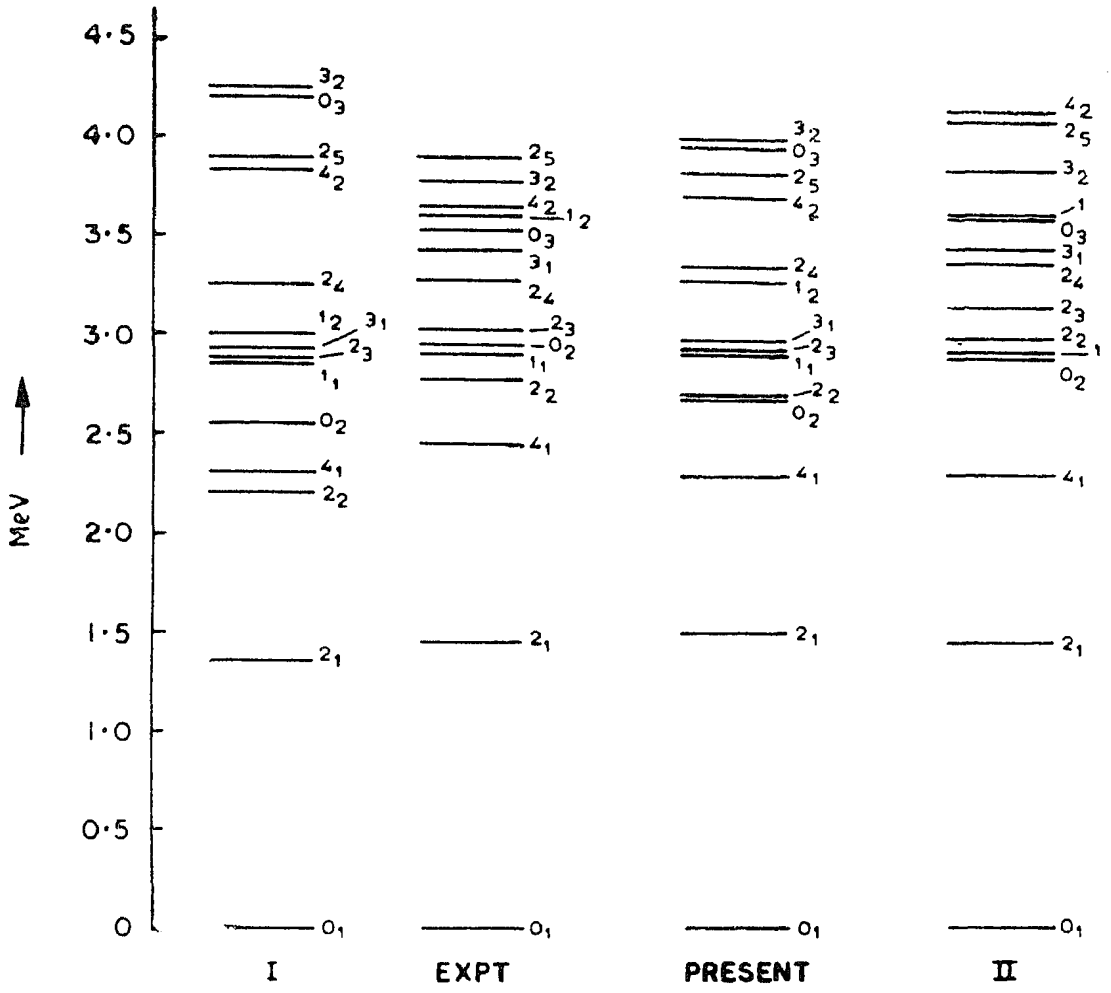

Figure 1. The observed experimental energy levels of ^{58}Ni are compared with our calculations in columns 2 and 3. The columns marked I and II show energy levels calculated with Kuo (1968) matrix elements, and those of Hsieh *et al* (1973) respectively.

the speed. The details of the method are given in the Appendix. First, derivatives at an initial estimated point $(I_{nl})_0$ are calculated and then we linearize the problem to estimate corrections $\triangle I_{nl}$. The parameters $(I_{nl})_0$ are updated by a fraction of the estimated corrections $\triangle I_{nl}$, and the cycle is repeated to reach a minimum.

The radial matrix elements thus obtained are listed in table 1. Figure 1 shows the calculated energy spectrum and its comparison with the observed one. The energy levels calculated with Kuo (1968) matrix elements and the spectrum obtained by Hsieh *et al.* (1973) are also shown in figure 1. Our calculation reproduces beautifully the observed level densities at different excitation energies. The root-mean-square deviation between the observed and calculated energies is about 810 KeV ($\approx$ 58 KeV per level). The TBME's calculated with these I_{nl} are compared with TBME's of Kuo (1968) and of Hsieh *et al.* (1973) in table 2.

We observe that the seven radial matrix elements in relative $l = 0$ and $l = 1$ states are adequate to represent the effective interaction; the relative magnitudes of these matrix elements (table 1) already justify our neglect of interaction in higher l ($l \geqslant 2$) states. The effective interaction is predominantly an s-state interaction,

3. Effective quadrupole charge matrix elements

The phenomenological interaction of the previous section gives a good account of the energy spectrum of ^{58}Ni in spite of the neglect of considerable amounts of core-excited configurations which are surely present in these states. Similarly, one should expect that an adequate account of the electromagnetic properties of these states should require use of effective matrix elements of the corresponding electromagnetic operators. In the earlier shell model calculations this is attempted by assigning an effective charge to each of the valence nucleons. Thus one takes, for example, an effective E2 operator as:

$$Q_{2\mu} = e_t \sum_i r_i^2 \, Y_{2\mu}(\theta_i, \phi_i)$$

evaluates the matrix elements of this operator with standard harmonic oscillator wavefunctions, and then fits the value of e_t to obtain best possible agreement with the observed B(E2) data. Such a procedure has not achieved much success in ^{58}Ni (Start *et al* 1971). Effective charges $e_t \sim 2$ are required, and even then the agreement between calculated and observed values is rather poor. Start *et al* use wavefunctions obtained with Kuo matrix elements, and effective charge $e_t = 1$. Their results show agreement for barely three out of the observed thirteen B(E2) values. Glaudemans *et al* (1972) in their shell model calculation get an effective charge $e_t = (1{\cdot}70 \pm 0{\cdot}08)$. They made a least squares fit to 33 B(E2)'s and 3 quadrupole moments in various Ni-isotopes. However, they conclude that the electromagnetic properties of third and higher states of a given spin and parity in general show poor agreement.

When dealing with the TMBE's of the effective interaction, we isolated various geometrical factors, and considered as free parameters only the radial matrix elements which explicitly contain the potential operator V. One can similarly see that the electric quadrupole operator enters the calculation of B(E2) values only through matrix elements such as (see the Appendix for details):

$$\langle j_1 \,||\, Q_2 \,||\, j_2 \rangle = e_{j_1 j_2} \langle j_1 \,||\, r^2 \, Y_2(\theta, \phi) \,||\, j_2 \rangle$$

$|j_1\rangle$, $|j_2\rangle$ are standard single-particle spherical shell model wavefunctions and the double-barred matrix elements are defined by De-Shalit and Talmi (1963).

Our calculations for ^{58}Ni will involve the matrix elements containing the effective charges e_{55}, e_{53}, e_{51}, e_{33} and e_{31}. For convenience of notation we write $e_{55} \equiv e_{5/2,5/2}$ etc. ($e_{11} \equiv 0$). These five e_{j_1, j_2} are treated as free parameters defining the effective electric quadrupole operator in our configuration space. This provides a much greater flexibility for interpreting the B(E2) data, than if we have only a single parameter. Of course, there is enough reason to believe that 'core-excitation' effects may not be so simple as to be compensated for by a single free parameter.

We take the experimental data of Start *et al* (1971) for the thirteen B(E2) rates and use the wavefunctions obtained with the TBME's calculated in the last section to compute these transition rates with a knowledge of the five parameters defining the effective charge. These five parameters were chosen by a least squares fit procedure (Details are given in the Appendix). All experimental data were weighted by including a weight function defined as 1/(Standard Deviation)^2. Standard deviation for $2_5 \to 2_1$ transition was taken as 1·0. The best parameters

Table 3. Value of effective charges ($e_{J_1J_2}$)

J_1	J_2	I_{nl}-wave-functions (No restriction)	Kuo-wave-functions (No restriction)	I_{nl}-wave-functions (Restricted fit)	Kuo-wave-functions (Restricted fit)
3/2	3/2	2·05	1·24	1·88	1·23
3/2	5/2	−1·52	1·62	−0·90	1·58
3/2	1/2	1·93	−0·48	1·86	−0·72
5/2	5/2	4·04	1·35	2·0	1·36
5/2	1/2	2·43	2·24	1·9	1·99

Table 4. Experimental and theoretical B(E2) rates in ^{58}Ni expressed in units of $e^2\,fm^4$

Transition $J_i \to J_f$	Experimental values	Root-mean-square fit value				Kuo with all charges = 1·0
		(I_{nl}) no restriction	(Kuo) no restriction	I_{nl} charges restricted	Kuo charges restricted	
$2_1 \to 0_1$	140^{+10}_{-11}	147	32·5	118	27·3	33·7
$2_2 \to 0_1$	$0{\cdot}36^{+0{\cdot}12}_{-0{\cdot}10}$	0·52	2·0	0·72	0·32	11·4
$2_3 \to 0_1$	23^{+4}_{-3}	23·3	16·8	18·7	19·2	0·15
$2_4 \to 0_1$	38^{+7}_{-6}	37·1	29·5	6·4	31·9	0·52
$2_5 \to 0_1$	6·6±1·0	6·6	7·7	5·1	5·1	0·10
$2_2 \to 2_1$	199^{+61}_{-63}	92·1	8·7	60·4	4·0	23·9
$2_3 \to 2_1$	20^{+10}_{-8}	17·3	1·9	27·0	0·98	13·7
$2_4 \to 2_1$	104 ±31	14·9	8·7	7·4	11·5	4·0
$2_5 \to 2_1$	2·5	3·6	7·0	0·29	6·6	3·3
$0_2 \to 2_1$	0·004 ±0·0006	0·09	2·4	12·1	2·0	15·6
$0_2 \to 2_2$	231±29	61·5	180	18·2	183	33·7
$0_3 \to 2_1$	71^{+21}_{-16}	23·8	1·2	17·9	4·7	4·6
$4_2 \to 2_1$	18^{+14}_{-8}	14·4	0·18	4·0	0·20	0·002

Experimental values are taken from Start *et al* (1971)

so obtained are listed in column 2 of table 3 and the corresponding B(E2) rates in column 3 of table 4.

The effective charge e_{55} appears to be rather large. Similarly the negative value for the off-diagonal effective charge e_{53} appears to be surprising at first sight. We have tried to see if there is a particular subset of experimental B (E2) data that forces such abnormal values for these two parameters. This is done by first restricting $e_{55} = 2{\cdot}0$ and varying only the other four parameters. This gives very low values, $1{\cdot}54 e^2$ fm^4 for $(2_4 \rightarrow 0_1)$; $7{\cdot}7$ e^2 fm^4 for $(2_4 \rightarrow 2_1)$ and $1{\cdot}06$ e^2 fm^4 for $(0_3 \rightarrow 2_1)$ transitions and rather a high value of $1{\cdot}05$ e^2 fm^4 for $(0_2 \rightarrow 2_1)$ transition. Similarly the results obtained with restricting $e_{53} = 2{\cdot}0$ and varying only the other four parameters are enhanced values of $41{\cdot}3$ e^2 fm^4 for $(2_2 \rightarrow 0_1)$; 114 e^2 fm^4 for $(2_3 \rightarrow 2_1)$ transition; $28{\cdot}4$ e^2 fm^4 for $(2_5 \rightarrow 2_1)$ transition and a lower value of $11{\cdot}3$ e^2 fm^4 for $(2_4 \rightarrow 2_1)$ transition. However, more generally we modified the programme to restrict the charges in the range $-1{\cdot}0$ and $2{\cdot}0$ and the best fit with this imposed restriction is also listed in column 4 of table 3 and the corresponding B(E2) rates in column 5 of table 4. The fit deteriorates for $2_4 \rightarrow 0_1$, $2_5 \rightarrow 2_1$, $0_2 \rightarrow 2_1$ and $4_2 \rightarrow 2_1$ transitions.

A similar calculation has also been performed with Kuo's TBME's. The effective charges that give best fit with and without the restrictions mentioned above are listed in columns 3 and 5 of table 3 and the B(E2) rates they give are tabulated in columns 4 and 6 of table 4. In column 7 of this table we also list the B(E2) rates obtained with $e_t = 1{\cdot}0$. (They are same as reported by Start *et al* 1971.) A comparison of columns 1, 6 and 7 of table 4 clearly shows the improvement when one uses state-dependent effective charges.

The estimated errors on the effective charges obtained here are about 10%. The most serious discrepancy is found in the $0_2 \rightarrow 2_1$ transition. However, the general agreement is very satisfactory, and far better than anything that can be obtained by using only a single charge parameter. It will be interesting to mention that Oberlechner and Richert (1972) who have included particle-hole space in the shell model calculation of ^{58}Ni report that 0_2 and 2_1 states have a large 4p–2h component and this may explain the poor agreement of the $0_2 \rightarrow 2_1$ transition.

We would like to point out that if a good measurement of E2 transitions amongst the lowest three states of ^{57}Ni and the quadrupole moments becomes available, it would furnish an excellent test of the effective charges deduced in this section.

4. Conclusion

We have shown that the two-body matrix elements deduced from phenomenological or from realistic nucleon-nucleon interactions are equally good for calculating energy levels. However, the effect of the neglected configurations (in particular core excitation) is rather complex on effective charges. This is evident from the fact that some of the diagonal terms attain a very high value and the off-diagonal matrix elements are modified to an extent that in one case they become negative. The change is very sensitive to the wavefunctions. Our procedure gives negative e_{53} when we use the wavefunctions of our TBME's and a negative e_{31} with wavefunctions calculated with Kuo's TBME's.

The state dependence of effective charges is justified since the B(E2)'s calculated with single effective charges are found to show much poorer fit. Similar state

dependence of M1 reduced single-particle matrix elements has been found by Glaudemans *et al* (1972) in Ni-isotopes. However, in their fitting of B(E2) rates they found that " an independent adjustment of five reduced single-particle matrix elements for E2 operator did not reproduce the experimental data much better than the one-parameter fit of the neutron charge ". This may be due to the difference in their and our approach. Whereas we used transitions only in ^{58}Ni to estimate the effective charges, Glaudemans *et al.* (1972) used transitions in several Ni-isotopes. Their value for $e_t = (1{\cdot}70 \pm 0{\cdot}08)$ is quite close to the majority of the values we obtained.

State dependence of effective charges have been calculated for ^{17}O and ^{17}F nuclei by Siegel and Zamick (1970) and for 2p–1f nuclei by Federman and Zamick (1969). In both these calculations strong state dependence is found. However, Siegel and Zamick (1970) emphasize that one needs a good estimate of $\langle j \,||\, r^2 \,||\, j' \rangle$ to compare the theoretical estimate of e_t with that estimated from experiment and the accuracy of $\langle j \,||\, r^2 \,||\, j' \rangle$ is tied to the accuracy with which the parameters for Saxon-Woods potential can be estimated. More recent calculations are by Osnes (1973) for $A = 17$ and $A = 41$ and by Kirson (1974) for $A = 17$. These results also show a strong state dependence for effective charges. It would be of interest to calculate the effective charges for ^{58}Ni in a microscopic formulation, to see how they compare with what we obtain in this work. As a word of precaution we may quote Kirson (1974): " Present calculations (microscopic) are, of course, far from perfect ".

It will be of interest to do similar calculations for other nuclei near doubly closed shells and check the state dependence of effective charges. It would also be of theoretical interest to calculate them from a microscopic description. The large deviation found in ^{58}Ni shows (i) the existence of interference phenomena from the various components, and (ii) that even the low lying states of ^{58}Ni have a complex structure. Another interesting extension of the prescription we adopted here will be to follow the same procedure for higher mass members of Ni-isotopes and study how the effective interactions and effective charges vary with mass numbers.

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Appendix

The reduced transition rate B(E2) for electric quadrupole radiation is given by (De Shalit and Talmi 1963)

$$B(\mathrm{E2};\ J \to J') = \frac{1}{2J+1} \left| \langle (J' \,\|\, \sum_i e_i r_i^2\ Y_2\ (\theta_i \phi_i) \,\|\, J \rangle \right|^2 \qquad \text{(A–1)}$$

The state functions $|\, J' \rangle$ and $|\, J \rangle$ are known in the form;

$$\left.\begin{aligned} |J'\rangle &= \sum_{J_1'J_2'} a(J_1'J_2';\ J')\,|J_1'J_2';\ J'\rangle \\ \text{and} \\ |J\rangle &= \sum_{J_1J_2} a(J_1J_2;\ J)\,|J_1J_2;\ J\rangle \end{aligned}\right\} \qquad \text{(A–2)}$$

where $a(J_1'J_2';\ J')$ and $a(J_1J_2;\ J)$ stand for the amplitudes of the various components $|J_1'J_2';\ J'\rangle$ and $|J_1J_2;\ J\rangle$ respectively. The state vector $|J_1J_2;\ J\rangle$ denotes an antisymmetrised state with total angular momentum J formed by coupling two particle states $|J_1\rangle$ and $|J_2\rangle$ and a similar definition holds true for $|J_1'J_2';\ J'\rangle$.

Putting (A–2) in (A–1) we get

$$B(\mathrm{E2};\ J\to J') = \frac{1}{2J+1}\Big[\sum_{J_1'J_2'J_1J_2} a(J_1'J_2';\ J')\,a(J_1J_2;\ J) \times \{\langle J_1'J_2';\ J' \,||\, \sum_i e_i r_i^2\, Y_2(\theta_i\phi_i) \,||\, J_1J_2;\ J\rangle\}\Big]^2 \qquad \text{(A–3)}$$

To evaluate the reduced matrix element appearing within curly brackets of eq. (A–3) use was made of the relation (Thankappan and Pandya 1962, Rose and Brink 1967).

$$\begin{aligned} &\langle J_1'J_2';\ J'T' \,||\, T_L(1)+T_L(2) \,||\, J_1J_2;\ JT\rangle \\ &= (-)^{L+J_1-J'_2}(2J+1)^{1/2} \times \tfrac{1}{2}\{[1+\delta_{J_1'J_2'}][1+\delta_{J_1J_2}]\}^{-\frac{1}{2}} \\ &\quad \times (\delta_{J_2'J_2}(-)^{J'}\sqrt{2J_1'+1}\,W(J_1'J_1J'J;\ LJ_2')\,M(J_1'J_1) \\ &\quad + \delta_{J_1'J_1}(-)^{J+T+T'}\sqrt{2J_2'+1}\,W(J_2'J_2J'J;\ LJ_1')\,M(J_2'J_2) \\ &\quad + \delta_{J_1'J_2}(-)^{T'+1}\sqrt{2J_2'+1}\,W(J_2'J_1J'J;\ LJ_1')\,M(J_2'J_1) \\ &\quad + \delta_{J_2'J_1}(-)^{J'+J+T+1}\sqrt{2J_1'+1}\,W(J_1'J_2J'J;\ LJ_2')\,M(J_1'J_2) \end{aligned} \qquad \text{(A–4)}$$

In the above equation we have introduced the following notations.

$$T_L(i) = e_i\, r_i^2\, Y_L(\theta_i\phi_i)$$

and

$$M(J_1J_2) = [\langle J_1 \,||\, T_L(1) \,||\, J_2\rangle + (-1)^{T+T'}\langle J_1 \,||\, T_L(2) \,||\, J_2\rangle] \qquad \text{(A–5)}$$

Equation (A–4) is written in the most general form. The isospin of the initial and final states are T and T'. For our purpose $T = T' = 1$. Also L, which stands for the rank of the operator T_L, is 2 for an E2 operator.

The evaluation of B (E2) using equation (A–3) reduces to the estimation of the reduced matrix elements of the operator T_L (i), *i.e.*

$$\begin{aligned} \langle J_1 \,||\, T_L(\mathrm{i}) \,||\, J_2\rangle &= \langle J_1 \,||\, e_i r_i^2\, Y_2(\theta_i\phi_i) \,||\, J_2\rangle \\ &= \mathrm{e}_{J_1J_2}\langle r_i^2\rangle_{n_1l_1n_2l_2}\langle l_1J_1 \,||\, Y_2(\theta_i\phi_i) \,||\, l_2J_2\rangle \end{aligned} \qquad \text{(A–6)}$$

The values of $\langle r_i^2\rangle_{n_1l_1,\ n_2l_2}$ are taken as:

$$\langle r^2\rangle_{1\mathrm{f},\ 1\mathrm{f}} = \langle r^2\rangle_{2\mathrm{p},\ 2\mathrm{p}} = \tfrac{9}{2}\,b^2$$

and

$$\langle r^2 \rangle_{2p,\,1f} = \langle r^2 \rangle_{1f,\,2p} = -\sqrt{14}\, b^2$$

with $b^2 = 1{\cdot}03\, A^{1/3}\,\mathrm{fm}^2$ (McGrory *et al* 1971).

We do not assign any fixed value for the charge $e_{J_1J_2}$. Rather it is treated as an adjustable parameter and its best value is chosen so as to make the calculated values agree to measured values as closely as possible with the method of least squares. The function minimised is:

$$F = \sum_k \omega_k [B(\mathrm{E2})_{\mathrm{obs}} - B(\mathrm{E2})_{\mathrm{cal}}]_k^2 \qquad \text{(A–7)}$$

ω_k defines the weight function and is taken as the $1/\sigma_k^2$ where σ_k is the standard deviation of the observed value.

The method discussed below minimizes the function F of eq. (A–7). To make the notation simpler, and the description more general, we rewrite (A–7) as:

$$F(x) = \sum_k \omega_k [Y_k - T_k(x)]^2 \qquad \text{(A–8)}$$

Here Y_k are the measured values of the quantity being fitted and T_k the values predicted by the model. The x's are the unknown parameters to be evaluated.

The minimization techniques are discussed at many places, a recent reference is *Function Minimizations* by James (1972). (This reference contains a complete bibliography of the common methods.) We used Newton's method. In this method the first derivatives of the model functions $T_k(x)$ are needed. It is rather complicated to calculate these analytically for the two minimizations discussed here. The dependence of T_k's (energy levels and E2 rates) on x's (I_{nl} and $e_{J_1J_2}$) is too complex to allow an analytical expression for their derivatives with respect to x's. A numerical method (the method of finite differences) is thus used to evaluate $\partial T_k/\partial x_i$. Better results follow if derivatives at a point x_{0i} are calculated through the difference of $T_k(x_{0i})$ evaluated at points chosen symmetrically on either side of x_{0i} (James 1972 and Stewart 1967), *i.e.*

$$\frac{\partial T_k}{\partial x_{0i}} = [T_k(x_{0i} + d) - T_k(x_{0i} - d)]/2d \qquad \text{(A–9)}$$

These derivatives are then used to linearize $F(x)$. Let us assume that an initial guess of x, say x_0, can be made. Then we write

$$x = x_0 + \triangle x$$

Making a Talylor's series expansion of (A–8), we write

$$F(x) = \sum_k \omega_k \left[Y_k - T_k(x_0) - \sum_{i=1}^{n} \left(\frac{\partial T_k}{\partial x_{0i}}\right) \triangle x_i \right]^2 \qquad \text{(A–10)}$$

In the above equation $x_{01}, x_{02} \ldots\ldots x_{0n}$ are the initial values of the n parameters x_0. We select the n variables $\triangle x_i$ such as to minimize $F(x)$. This is achieved by putting the condition

$$\frac{\partial F}{\partial_{\omega}(\triangle x_i)} = 0 \qquad \text{(A–11)}$$

for each of the unknown $\triangle x_i$. What we get by doing this is that instead of estimating x_i directly we estimate first $\triangle x_i$'s the correction to an initial guess x_0.

The conditions (A–11) lead to n linear equations in n unknown $\triangle x_i$'s and this is called 'linearization' of the problem. Written in a matrix form, the n equations which follow from conditions (A–11) are:

$$[A]\,[B] = [C] \tag{A–12}$$

$[A]$ is an $(n \times n)$ matrix and $[B]$ and $[C]$ are column matrices of dimension (n), with elements:

$$A_{ij} = \sum_k \omega_k \left(\frac{\partial T_k}{\partial x_{0i}}\right)\left(\frac{\partial T_k}{\partial x_{0j}}\right)$$

$$B_j = \triangle x_j$$

$$C_i = \sum_k \omega_k (Y_k - T_k)\left(\frac{\partial T_k}{\partial x_{0i}}\right)$$

In the last equation for T_k we take its value at x_0. Equation (A–12) is solved to get $\triangle x_1$, $\triangle x_2$,..... $\triangle x_n$. These may not be exact increments, for we have neglected higher order terms in the Taylor series expansion (A–10). The usual practice then is to start a new iteration after the first one by updating the old x_{0i} with a fraction of $\triangle x_{0i}$. The cycle is then repeated till a minimum is reached.

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