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LETTER TO THE EDITOR

Quadrupole moments of ^{35,37}Cl in the overlap representation

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Abstract. For ^{37}Cl there is close agreement between the quadrupole moment measured by atomic methods and that deduced from proton pick-up spectroscopic factors, but there is probably some discrepancy in the case of ^{35}Cl where the pick-up data are more ambiguous. The agreement casts doubt on the use of 'effective charges' for these nuclei.

In the overlap representation (Clement 1973b) the quadrupole moment is expressed explicitly in terms of single-particle quadrupole integrals and the spectroscopic factors extracted from single-proton transfer reactions. For ^{35,37}Cl the moments given in the Nuclear Data Tables (Fuller and Cohen 1969) have been determined fairly accurately by atomic means. Pick-up and stripping spectroscopic factors for these nuclei have recently been subjected to a partial sum rule analysis (Clement and Perez 1974) which has enabled their absolute magnitudes to be determined within quoted errors. Thus a comparison between calculated and experimental quadrupole moments can be made for ^{35,37}Cl which will check the value of the overlap representation with its method of calculation and underlying assumptions. The latter mainly consist in the assumption that shells are completely closed or open in which case their contribution to the quadrupole moment is zero. The contributions of non-valence shells are included in shell-model calculations by the introduction of 'effective charges' whose values are often determined from fits to data. There can be no effective charges in the overlap representation where small contributions to moments are explicit but possibly not seen experimentally. If we find agreement with the existing pick-up data, in which there is no evidence for non-valence shell contributions, the result would lead us to question the use of effective charges in this region of the periodic table and the wavefunctions with which they are used.

The overlap representation (Clement 1973b) gives the following explicit form for the quadrupole moment of 2s–1d shell nuclei with spin $J = \frac{3}{2}$

$$
\begin{aligned}
Q = -\tfrac{2}{5}e\Big[& Q(1\mathrm{d}_{3/2}, 1\mathrm{d}_{3/2})[S_0^-(\tfrac{3}{2}) + \tfrac{1}{5}(S_1^-(\tfrac{3}{2}) + S_3^-(\tfrac{3}{2})) - \tfrac{3}{5}S_2^-(\tfrac{3}{2})] \\
& + Q(1\mathrm{d}_{5/2}, 1\mathrm{d}_{5/2})[-\tfrac{2}{7}S_4^-(\tfrac{5}{2}) + \tfrac{22}{35}S_3^-(\tfrac{5}{2}) + \tfrac{4}{35}S_2^-(\tfrac{5}{2}) - \tfrac{4}{5}S_1^-(\tfrac{5}{2})] \\
& + Q(1\mathrm{d}_{5/2}, 1\mathrm{d}_{3/2})\left(-\frac{4\sqrt{6}}{35}\theta_3^-(\tfrac{5}{2}, \tfrac{3}{2}) + \tfrac{2}{5}(\tfrac{3}{7})^{1/2}\theta_2^-(\tfrac{5}{2}, \tfrac{3}{2}) + \tfrac{2}{5}\theta_1^-(\tfrac{5}{2}, \tfrac{3}{2})\right) \\
& + Q(1\mathrm{d}_{3/2}, 2\mathrm{s}_{1/2})\left(-\tfrac{4}{5}\theta_2^-(\tfrac{3}{2}, \tfrac{1}{2}) + \frac{4}{\sqrt{5}}\theta_1^-(\tfrac{3}{2}, \tfrac{1}{2})\right)
\end{aligned}
$$

$$+Q(1d_{5/2},2s_{1/2})\left(-\frac{(21)^{1/2}}{5}\theta_2^-(\tfrac{5}{2},\tfrac{1}{2})-\frac{1}{\sqrt{5}}\theta_1^-(\tfrac{5}{2},\tfrac{1}{2})\right)\Bigg], \tag{1}$$

where

$$S_{J_\alpha}^-(jl)=\sum_{\alpha,J_\alpha\,\text{fixed}} S'_\alpha(jl),$$

$$\theta_{J_\alpha}^-(j_1l_1;j_2l_2)=\sum_{\alpha,J_\alpha\,\text{fixed}} \pm[S'_\alpha(j_1l_1)S'_\alpha(j_1l_2)]^{1/2}.$$

The spectroscopic factor (including any isospin factor) for the pick-up of a proton in orbit (jl) to final state α, spin J_α is $S'_\alpha(jl)$ and the quadrupole integrals, expressed in terms of the corresponding overlap functions, $\phi_\alpha(x;jl)$, are

$$Q_\alpha(j_1l_1;j_2l_2)=\left(\frac{A-1}{A}\right)^2\int\phi_\alpha(x;j_1l_1)\phi_\alpha(x;j_2l_2)x^4\,dx,$$

where for a target nucleus of mass number A, $x=|\boldsymbol{r}_A-\boldsymbol{R}_{A-1}|$.

In the above expression these integrals have been assumed to be independent of α. They were previously (Clement 1973b) given values obtained from harmonic oscillator wavefunctions whose parameter is given by $\hbar\omega=40\,A^{-1/3}$ MeV. Although this procedure gives the overall size of the nucleus correctly it is becoming apparent that oscillator functions so specified are poor approximations for valence nucleons (Abdulmomen *et al* 1973). We therefore used overlap functions calculated in a potential of Batty and Greenlees (1969) consisting of a real Saxon–Woods potential ($r_N=1{\cdot}28$ fm, $a_N=0{\cdot}76$ fm), a spin–orbit potential ($V_{so}=5{\cdot}78$ MeV, $r_{so}=1{\cdot}09$ fm and $a_{so}=0{\cdot}60$ fm) and the Coulomb potential ($r_C=1{\cdot}20$ fm). The central well-depth V_N was adjusted to fit the observed separation energies. The potential results in proton densities whose RMS radii are in good agreement with experiment over a range of nuclei so that we expect the resulting quadrupole integrals to be much more realistic. The relevant results are

$^{36}S_{gs}$: $Q_\alpha(d_{3/2},d_{3/2})=13{\cdot}5\,\text{fm}^2$,

$^{34}S_{gs}$: $Q_\alpha(d_{3/2},d_{3/2})=13{\cdot}9\,\text{fm}^2$,

$^{34}S_{2{\cdot}13\,MeV}$: $Q_\alpha(d_{3/2},d_{3/2})=13{\cdot}2\,\text{fm}^2$, $\quad Q_\alpha(d_{3/2},s_{1/2})=12{\cdot}1\,\text{fm}^2$.

A better procedure might be to adjust the well depth V_N to give the mean separation energy for stripping and pick-up spectroscopic strength (Clement 1969). It has been checked that this would make negligible difference to the results obtained.

The values for the quadrupole integrals are almost 20% larger than the harmonic oscillator values. Thus the latter, which are widely used in shell-model calculations, can seriously underestimate quadrupole moments.

The above expression for Q has been given explicitly so that the relative size of the various terms can be seen. The single-particle $d_{3/2}$ value is given by putting $S_0^-(\frac{3}{2})=1$ and all the other spectroscopic sums equal to zero. The only other term with a coefficient greater than or equal to unity is the $\theta_1^-(\frac{3}{2},\frac{1}{2})$ term whose coefficient is 1·79 numerically and to which, therefore, Q is sensitive.

There is no evidence of any considerable departure from closure of the $d_{5/2}$ shell either theoretically (Wildenthal *et al* 1971) or experimentally. Stripping experiments by Moistener and Alford (1970) show only extremely small $d_{5/2}$ transfers to 4^+ states. The partial sum rule analysis carried out by us on low excitation energy transfer data (Clement and Perez 1974) is also consistent with this assumption. In order to fit the

sum rules the absolute magnitudes of the pick-up spectroscopic factors obtained by Puttaswamy and Yntema (1969) had to be reduced by factors of $0{\cdot}81 \pm 0{\cdot}06$ for ^{37}Cl and $0{\cdot}92 \pm 0{\cdot}06$ for ^{35}Cl. This brought them into close agreement with spectroscopic factors obtained by Gray *et al* (1970) for ^{37}Cl and by Wildenthal and Newman (1968) for ^{35}Cl. The only question of dispute between the experiments is then the amount of $d_{3/2}$ strength mixed in to the $2s_{1/2}$ transfers to the 2^+ states of ^{34}S at 2·13 and 3·30 MeV and to the 1^+ state at 4·07 MeV. Wildenthal and Newman (1968) set upper limits on this strength whereas it is given as zero by Puttaswamy and Yntema (1969) except for the 2·13 MeV state.

Because of this ambiguity in $d_{3/2}$, $2s_{1/2}$ mixing we have used the Puttaswamy and Yntema (1969) data to calculate the quadrupole moments given in table 1. For ^{37}Cl we obtain perfect agreement with the Nuclear Data Tables value (Fuller and Cohen 1969). For ^{35}Cl there is a discrepancy of $-0{\cdot}028$ b if the appropriate sign for θ_2 is chosen. However, because of the sensitivity to $\theta_1^-(\frac{3}{2},\frac{1}{2})$, this discrepancy would be removed by a $d_{3/2}$ spectroscopic factor of only 0·19 to the 4·07 MeV ^{34}S state whereas the upper limit quoted by Wildenthal and Newman (1968) is 0·28. The ambiguity in θ_2^- is less important as it tends to be cancelled by the S_2^- contribution.

Table 1. Quadrupole moments, Q_{OR}, from the overlap representation as compared to their atomic values. Except as stated, the spectroscopic sums are obtained from the data of Puttaswamy and Yntema (1969) renormalized by factors of $0{\cdot}81 \pm 0{\cdot}06$ for ^{36}Cl and $0{\cdot}92 \pm 0{\cdot}06$ for ^{35}Cl (Clement and Perez 1974).

Nucleus	$S_0^-(\frac{3}{2})$	$S_2^-(\frac{3}{2})$	$\theta_2^-(\frac{3}{2},\frac{1}{2})$	$\theta_1^-(\frac{3}{2},\frac{1}{2})$	Q_{OR} (b)	Q_{atomic} (b)
^{37}Cl	1·06	—	—	—	$-0{\cdot}057 \pm 0{\cdot}005$†	−0·062
^{35}Cl	0·92	0·34	+0·28	—	$-0{\cdot}051 \pm 0{\cdot}005$†	−0·079
			−0·28	—	$-0{\cdot}029 \pm 0{\cdot}005$†	
				+0·34‡	−0·028	

† Errors deduced from the above errors in the renormalization constants.
‡ Additional possible contribution to the quadrupole moment arising from the data of Wildenthal and Newman (1968) which would remove the discrepancy between Q_{OR} and Q_{atomic}.

Alternatively, the representation in terms of the pick-up spectroscopic amplitudes θ_1^-, θ_2^- can be transformed into one in terms of the corresponding stripping amplitudes θ_1^+, θ_2^+ using partial sum rules (Clement 1973a). The only change is to multiply the appropriate term in (1) by $(-1)^{j_1+j_2}$ which is 1 in our case. Thus we can look at the stripping spectroscopic factors for ^{35}Cl found by Moistener and Alford (1970). For the 4·44 MeV 2^+ state in ^{36}Ar their spectroscopic factors give $\theta_2^+ = \pm 0{\cdot}15$. There is also various fragmentary strength of indeterminate spin which could total at most $\theta^+ \simeq \pm 0{\cdot}1$. These values are inconsistent with a θ_1^- as large as 0·34 and could give at most a contribution of $-0{\cdot}016$ b to the quadrupole moment. An overall discrepancy of $-0{\cdot}012$ b between Q_{OR} and Q atomic would remain.

To sum up, the situation for ^{35}Cl is that the pick-up data are not inconsistent with giving the correct value of Q, whereas the stripping data suggest there is a residual discrepancy of at least 18% in that Q_{OR} is too small numerically. To resolve the situation experiments giving improved values of θ^- would be highly desirable.

The use of effective charges in nuclear physics is unsatisfactory in that it hides an ignorance of actual wavefunctions and also it brings only qualitative agreement between theory and experiment. The shell-model calculations of Wildenthal *et al* (1971) for $A = 30$–35 have $\tilde{e}_p = 1{\cdot}5e$ and $\tilde{e}_n = 0{\cdot}5e$. Their theoretical quadrupole moment for ^{35}Cl is

$$Q_{th} = -0{\cdot}090 \text{ b}.$$

However, we have seen that the harmonic oscillator quadrupole integrals involved probably underestimate the actual integrals by about 20%. This criticism also applies to the survey of electromagnetic properties for $A = 30$–34 nuclei carried out by Glaudemans *et al* (1971). With realistic integrals Q_{th} would be too large by nearly 40% which raises the question of whether effective charges are needed at all.

In the overlap representation we use what is in effect the experimentally determined single-particle density matrix. The use of partial sum rules (Clement and Perez 1973, 1974) enables us to assert that spectroscopic factors can be determined to an accuracy of within 10% which is considerably better than has been generally supposed. We find very good agreement with experiment for ^{37}Cl and conflicting results for ^{35}Cl where there is probably some residual discrepancy.

No effective charges are involved. Collective E2 effects will enter the overlap representation through the interference terms, $\theta^{-}_{J_\alpha}(j_1, j_2)$. For example there could be $1g_{7/2}$ occupancy in Cl to interfere with $1d_{3/2}$. The measurement of spectroscopic factors for two (lj) values in a single transfer reaction is required. Whilst light-ion transfer reactions are reasonably successful in finding a small $l_<$ component mixed with a large $l_>$ component the converse is impossible. To determine experimentally whether effective charges are really needed in shell-model calculations we need to detect this converse situation, for example $1g_{9/2}$ interference with $1d_{5/2}$ in the lower part of the s–d shell. It is possible that heavier-ion transfer experiments might provide an answer and we stress the importance for shell-model calculations and the use of effective charges of an investigation of the subject.

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