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Effective charge in the large A limit

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The isoscalar effective charge correction $e^0 = e_n + e_p$ is calculated for a series of $N = Z$ closed shell plus one nucleon from $A = 4$ to $A = 480$. The results are then extrapolated to large A. A delta interaction $-G\delta(\vec{r}_{12})$ is used, with the strength G chosen by the "quadrupole condition" that the mean single particle–single hole splitting for the quadrupole state be $2\hbar\omega$. The effective charge is calculated in first order, in the Tamm-Dancoff and the random phase approximation. The value of e^0 varies from about 0.5 for mass 4 to 1 for $A \to \infty$. The value of *one* is the Bohr-Mottelson result for an $N = Z$ closed shell. We see that in our model this result holds only asymtotically.

[NUCLEAR STRUCTURE Effective charge theory.]

In this work we study how the quadrupole effective charge changes as we vary the mass number A, and in particular we examine the large A behavior. There are several reasons for such a study.

In previous calculations it was seen that the $E2$ effective charge was larger for ^{40}Ca plus an $f_{7/2}$ nucleon, than it was for ^{16}O plus a $d_{5/2}$ nucleon. We may well wonder, then, if the effective charge increases beyond bound as A goes to infinity or if it levels off. Another point is whether we can make any contact with the simple results of Bohr and Mottelson,[1] which we shall shortly discuss, and the results of Noya, Arima, and Horie.[2] There is a common thread—the latter authors use a delta interaction to calculate the core polarization, but using a Hamiltonian with a zero range interaction, yields, in a restricted variational calculation, the well known Mottelson conditions[3] from which the effective charges can also be calculated.

We make life as simple as possible by considering only $N = Z$ closed shells plus one nucleon. The A values of the closed shells for which we perform calculations are 4, 16, 40, 80, 140, 224, 336, and 480. These are the shells that are obtained by ignoring the spin orbit splitting. We consider the valence nucleon with no nodes:

$$|nlj\rangle = |0\ l_{\max}\ j = l_{\max} + \tfrac{1}{2}\rangle\,,$$

$$\text{e.g., } 0p_{3/2}, 0d_{5/2}, 0f_{7/2}, \cdots$$

Of course most nuclei are not stable. In this sense the calculation is not realistic. We can regard this calculation as more of a mathematical study in which we attempt to reach an infinite nuclear matter result by the easiest route through finite nuclei. Nevertheless, we shall find a systematic trend which could have empirical relevance.

We will consider mainly the isoscalar quadrupole effective charge correction. By this we mean the sum of the corrections when a neutron is added to the closed shell and when a proton is added. The popular prescription (not necessarily correct) is to use a neutron effective charge of $\frac{1}{2}$ and a proton effective charge of 1.5. In that case $e^n = \frac{1}{2}$, $e^p = \frac{1}{2}$, and $e^0 = 1$. (Note that the full isoscalar effective charge is $1 + e^0$.)

Under the conditions considered here ($N = Z$), Bohr and Mottelson[1] would also predict $e^0 = 1$, provided "loose binding effects" are ignored. This is a special case of their more general formula for $N \neq Z$ (see page 515 of Ref. 1):

$$e_{\rm pol}(E2) \approx e\{Z/A - 0.32(N-Z)/A + [0.32 - 0.3(N-Z)/A]\tau_z\}\,.$$

The result $e^0 = 1$ can be obtained in a restricted variational calculation using a *zero range interaction*. The restriction is that the trial Slater determinant consist of deformed harmonic oscillator wave functions in which the deformed oscillator length parameters $b_x = b_y \neq b_z$ are the same for all orbits. For the zero range interaction the expectation value of the potential energy is a function only of $(b_x b_y b_z) = b_0^3$ and hence does not depend on b_z. The entire dependence on b_z resides in the expectation value of the kinetic energy

$$\langle T\rangle = \frac{\hbar^2}{2m}(\Sigma_x/b_x^2 + \Sigma_y/b_y^2 + \Sigma_z/b_z^2)\,,$$

where Σ_x is the sum of $(N_x + \frac{1}{2})$ with N_x being the number of quanta in the x direction for a particular orbit.

Thus the expectation value of the Hamiltonian is

$$\langle H\rangle = \frac{\hbar^2}{2m}\left[(\Sigma_x+\Sigma_y)b_z/b_0^3+\Sigma_z/b_z^2\right]+V(b_0)\,.$$

The equilibrium condition $\partial\langle H\rangle/\partial b_z = 0$ yields the Mottelson conditions[3] $b_z^2/b_x^2 = 2\,\Sigma_z/(\Sigma_x+\Sigma_y)$. From these conditions Mottelson was able to derive the simple result for the effective charge, which for $N=Z$ nuclei can be expressed as $e^0 \simeq 1$. More precisely the isoscalar effective charge can be broken up into a core part and a valence part (e_c, e_v). The values for $A=4$, 16, and 40 are respectively (0.71, 0.24), (0.91, 0.06), and (0.96, 0.02).

However, the restricted assumption that all nucleons have the same parameters b_x, b_y, and b_z has been shown to be unreasonable. For example, a valence proton of spin up cannot interact with a core proton of spin up with zero range interaction; two spin-up fermions cannot be at the same point in space. Thus in first order perturbation theory, the spin-up protons in the core will not be deformed; on the other hand, the spin-down protons will be deformed. One should therefore use a trial solution in which different orbits have different deformations and this will lead to values of e^0 which are in general different from one.

If we go beyond first order perturbation theory there may be a tendency for the deformations to equalize, i.e., spin-up proton and spin-down proton deformations come closer together.

Here we shall take the simplest of all zero range interactions—the two-body delta interaction. (More complicated zero range interactions are combinations of two- and three-body delta interactions; these form part of the Skyrme interactions,[4] for example.) We assume harmonic oscillator wave functions throughout. Thus we lose the sometimes physically important effect of loose binding, i.e., a loosely bound valence particle cannot polarize the core as well as a tightly bound one. This leads to small effective charges.

The delta interaction is written $-G(1+xP^\sigma)\,\delta(\vec{r}_1-\vec{r}_2)$, where P^σ is the spin exchange operator. However, the isoscalar effective charge for an $N=Z$ closed shell is independent of x, so we need only consider $-G\delta(\vec{r}_i-\vec{r}_j)$. The delta interaction was of course used by Noya, Arima, and Horie[2] in their pioneering calculations of $E2$ effective charge. Our calculation will differ from theirs in the manner by which we choose G, and that we extend the calculation beyond first order to the Tamm-Dancoff approximation (TDA) and random phase approximation (RPA).

Also the motives are somewhat different. They were rightly concerned with trying to understand the experimental results which seemed to demand effective charge renormalization. Here we are more concerned with establishing a connection between different approaches.

One problem with an attractive delta interaction is that it does not yield nucleon saturation. The nucleons want to collapse to a point. That is why the additional repulsive terms in the Skyrme interaction[4] are needed. However, here we are dealing with a quadrupole property of a nucleus rather than monopole, and feel that sensible results can be obtained. We apply a consistency condition on G.

For some fixed value of b, the oscillator length parameter, we choose G so that the single particle–single hole splitting for the giant quadrupole state (QS) is $2\hbar\omega$. The definition of the QS state is

$$|\mathrm{QS}\rangle = N\sum_i r^2(i)Y_{2,M}(\Omega_i)\,|0\rangle$$

$$= N\sum_{\mathrm{ph}} |(\mathrm{ph}^{-1})^{L=2}\rangle\langle(\mathrm{ph}^{-1})^{L=2}_M \sum r^2 Y_{2,M}|0\rangle\,,$$

where N is a normalization factor. We call this procedure the "quadrupole condition" on G. See Fig. 1.

Note that with such a choice of G, the effective charge is independent of b, the oscillator length parameter. To see this we note that the effective charge in first order is

$$\delta e = -\sum_{\mathrm{ph}} \frac{\langle jVj(\mathrm{ph}^{-1})^{L=2\;T=0}\rangle}{\Delta E = 2\hbar\omega}\,\frac{\langle(\mathrm{ph}^{-1})^{L=2}Q0\rangle}{\langle jQj\rangle}\,.$$

Using the oscillator length parameter as the only scale of length in the problem, we note that $2\hbar\omega$ goes as $1/b^2$. The matrix element of the delta interaction is proportional to $1/b^3$. Thus when G/b^3 is equated to a constant times $2\hbar\omega$ (which goes as $1/b^2$), then G must be proportional to b. Thus we have the matrix element

$$\langle jG\delta(\vec{r}_i-\vec{r}_j)j(\mathrm{ph}^{-1})^{L=2\;T=0}\rangle$$

scaling as $b\times 1/b^3 = 1/b^2$. This cancels out the behavior of $\Delta E = 2\hbar\omega$ which also varies as $1/b^2$.

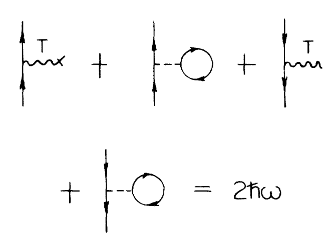

FIG. 1. Single particle–single hole splitting for the giant quadrupole state is equated to $2\hbar\omega$, the so called "quadrupole condition."

Thus, as previously stated, the effective charge correction e^0 is independent of b. This result is encouraging because it means that the quadrupole effective charge is insensitive to the radius.

After the first order calculation is done we can easily perform a TDA calculation. This means simply changing the energy denominator from $\Delta E = 2\hbar\omega$ to $\Delta E = 2\hbar\omega + \overline{V}_{\text{ph}}^{L=2\ T=0}$, which we call $\eta\hbar\omega$, as in Fig. 4. We plot η as a function of j in Fig. 5. In the above $\overline{V}_{\text{ph}}$ is the particle-hole interaction averaged over the various particle-hole states which comprise the isoscalar quadrupole state. In calculating $\overline{V}_{\text{ph}}$ we use the same interaction $-G\delta(\vec{r}_{12})$ which was used to obtain the effective charges, and to obtain the single particle–single hole splittings.

Once we have e^0_{First} and e^0_{TDA} we obtain e^0_{RPA} as follows. We define σ by $e^0_{\text{TDA}}/e^0_{\text{First}} = 1/(1-\sigma/2)$. From this we obtain σ. The RPA result for the effective charge is

$$e_{\text{RPA}}/e_{\text{First}} = 1/(1-\sigma)\,.$$

As was previously mentioned we have performed the calculation only up to $j=\frac{17}{2}$. But the curves vary in a sufficiently smooth way so we are reasonably confident that we can extrapolate the results to large A.

The method of extrapolation is to make the assumption that the effective charge correction varies as

$$e^0 = C_0 + C_1/j + C_2/j^2$$

for large j where C_0, C_1, and C_2 are constants.

The constants C_0, C_1, and C_2 are fitted in two different ways. First we fit the calculated effective charges for all j, $\frac{3}{2}$ up to $\frac{17}{2}$. A surprisingly good fit is thus obtained. However, since this is supposed to be a large j expansion, we then make a second fit in which only the four largest values of j ($\frac{11}{2}$, $\frac{13}{2}$, $\frac{15}{2}$, and $\frac{17}{2}$) are used. Of particular interest is C_0 which we interpret as the value of e^0 as $A\to\infty$.

The extrapolation procedure described above is also applied to the strength G and to the average particle-hole interaction. Concerning the strength G, we already mentioned that it was chosen so that the mean single particle–single hole splitting for the giant quadrupole state is $2\hbar\omega$ as in Fig. 1.

We also consider an alternate method of obtaining the strength G—we call this the "dipole condition." Here we demand that the mean energy of the single particle–single hole splitting for the giant dipole state is $1\hbar\omega$. The values of G for various nuclei are shown for both the "quadrupole condition" and the dipole condition in Fig. 2. However, since we are dealing with quadrupole effective charges, we then stick to the quadrupole condition for the rest of the paper.

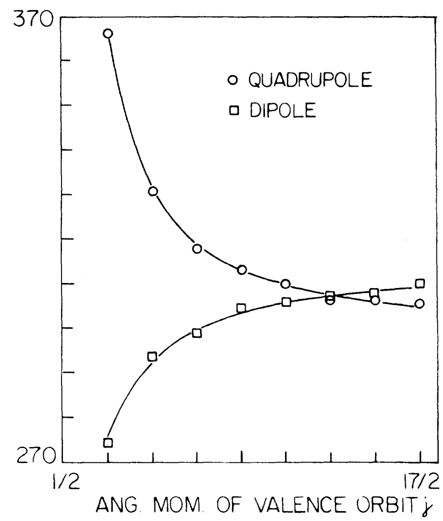

FIG. 2. The values of G for both the quadrupole condition and the dipole condition.

RESULTS

A. Some details of the calculation

In doing the calculation we take $\hbar\omega = 41/A^{1/3}$ MeV and $\nu = m\omega/\hbar = 1/b^2 = 0.9887/A^{1/3}$ fm^2.

In Table I we first show the isoscalar effective charge correction in first order perturbation theory for $G = 500$ MeV fm^3.

In calculating the effective charge we have to evaluate radial integrals

$$\int R_{n_1 l_1}(r) R_{n_2 l_2}(r) R_{n_3 l_3}(r) R_{n_4 l_4}(r) r^2 dr\,,$$

where $R_{nl}(r)$ is a harmonic oscillator radial wave function. These integrals can be evaluated analytically but this is very tedious. Therefore we evaluate the integrals numerically using a 24 point Gaussian quadrature.

How accurate are the integrals? We cannot answer this definitively. However, we performed the "*dipole test*" in mass 4. The mean energy of the spurious 1^- $T=0$ dipole state should be $\hbar\omega/2$ in a TDA calculation. This means that the potential energy part of the single particle–single hole splitting plus the particle-hole shift, when averaged over the spurious state, should be zero. (Referring to Fig. 4, and changing from the quadrupole state to the $L=1$ spurious state, this means that the sum of all the diagrams should be $\hbar\omega/2$.)

We verified that when the radial integrals are evaluated analytically this is exactly true. However, when we use the Gaussian quadrature to

TABLE I. Effective charge versus A.

A	e^0 [a]	G [b] MeV fm^3	e^0_{First} [a]	e^0_{TDA} [c]	e^0_{RPA} [c]	η
0						
4	0.453	366.24	0.332	0.398	0.497	1.668
16	0.629	330.68	0.416	0.515	0.676	1.614
40	0.723	317.73	0.460	0.576	0.770	1.597
80	0.778	312.79	0.487	0.613	0.827	1.588
140	0.814	309.57	0.504	0.637	0.865	1.584
224	0.843	306.04	0.516	0.653	0.889	1.581
336	0.858	305.98	0.525	0.665	0.907	1.579
480	0.871	305.35	0.532	0.675	0.923	1.577

[a] First order effective charge for $G = 500$ MeV fm^3 and $\nu = 0.9887/A^{1/3}$ fm^{-2}, $\Delta E = 2\hbar\omega = 82/A^{1/3}$ MeV.

[b] The strength G determined by the quadrupole condition, see Fig. 1.

[c] Effective charge using strength G given in 3rd column of this table.

evaluate the radial integrals there is about a 2% deviation from this result for mass 4. This deviation is acceptable although it will introduce a bit of noise when we attempt to extrapolate our results to $A \to \infty$. We mention again that the value of e^0 calculated with the quadrupole condition will be independent of that chosen for b.

B. The strength of the interaction

The results that we obtain are quite interesting. First of all there are no divergences as A goes to infinity for any of the quantities that we calculate—G, e^0_{First}, e^0_{TDA}, e^0_{RPA}, or η.

The strength of the interaction $G[V = -G\delta(\vec{r}_{ij})]$ is plotted in Fig. 2 for both the quadrupole and dipole conditions. The behavior as a function of A is quite different. In the $L = 2$ case, G is decreasing as a function of A, but for $L = 1$ it is increasing. For large A G levels off in both cases to values which are close to each other but not identical.

The solid line passing through the points, is not merely to aid the reader, but is actually a fit with the formula

$$G = G_0 + G_1/j + G_2/j^2 .$$

When all points $j = \frac{3}{2}$ to $j = \frac{17}{2}$ are included in the fit, the formula becomes

$$L = 2, \quad G = (297.97 + 47.47/j + 82.50/j^2)\ \mathrm{MeV\,fm}^3,$$

$$L = 1, \quad G = (314.58 - 44.51/j - 24.09/j^2)\ \mathrm{MeV\,fm}^3.$$

The results for $L = 2$ are given both in Table I and Fig. 2. The results for $L = 1$ are contained only in Fig. 2.

C. The effective charge

By far the most interesting result in this paper is that we are able to make contact with the Bohr-Mottelson formula.[1] However, this is achieved only in the limit of large A. In the RPA calculation the isoscalar effective charge correction e^0 does indeed approach close to 1 as $A \to \infty$. We must allow of course for uncertainties in the extrapolation procedure and the fact that the radial integrals are evaluated numerically. But the result seems solid, and if we were more clever we could probably show it analytically.

Before discussing the results in more detail we note that the RPA value of the effective charge correction e^0 is about 0.5 for mass 4 and increases steadily to about 1 as $A \to \infty$. This may well correspond to what is really happening, and therefore would constitute an improvement on the Bohr-Mottelson formula. Indeed the authors remark on page 518 of Ref. 1 "the observed rather small polarization charge in the region of ^{16}O may indicate that the coupling has been overestimated for these light nuclei."

We try to fit the effective charge to the formula

$$e^0 = C_0 + C_1/j + C_2/j^2 .$$

We first give the results, when all values $j = \frac{3}{2}$ to $\frac{17}{2}$ are included, as follows.

First order $0.578 - 0.419/j + 0.065/j^2$
TDA $0.741 - 0.598/j + 0.114/j^2$
RPA $1.043 - 1.057/j + 0.356/j^2$

We note that the solid lines in Fig. 3 are not aids to the eye, but rather are the above formulas. The fits are very good.

We next give the results when only the last 4 points, $j = \frac{11}{2}, \frac{13}{2}, \frac{15}{2}$, and $\frac{17}{2}$ are included.

First order $0.588 - 0.499/j + 0.204/j^2$
TDA $0.743 - 0.600/j + 0.708/j^2$
RPA $1.062 - 1.372/j + 1.574/j^2$

Yet another method of extrapolation was used. We use the asymptotic value of e^0_{First} and e^0_{TDA}. We obtain σ by

$$e^0_{\mathrm{TDA}}/e^0_{\mathrm{First}} = 1/(1 - \sigma/2) .$$

We then obtain

$$e^0_{\mathrm{RPA}} = e^0_{\mathrm{First}}/(1 - \sigma) .$$

The results we now obtain are the following.

	e^0_{RPA} $(A \to \infty)$
All points included	1.033
Only last four points	1.008

D. The energy of the isoscalar quadrupole state

Using the quadrupole condition for G we plot the energy of the isoscalar quadrupole state by sum-

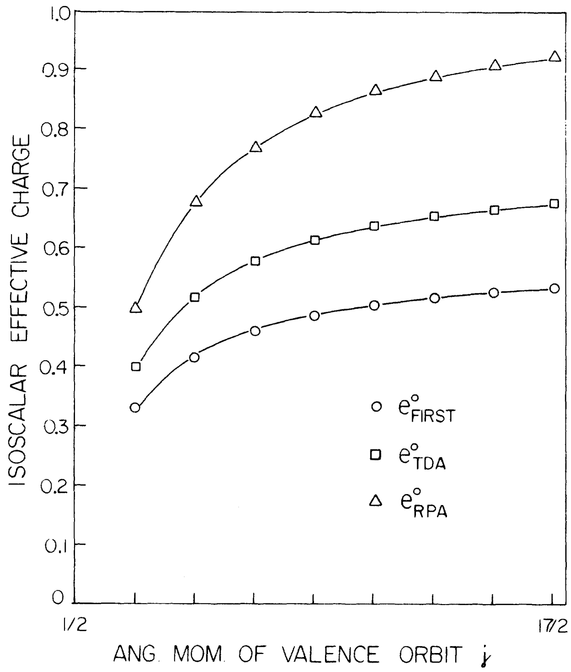

FIG. 3. Isoscalar effective charges; $e^0_{\rm First}$, $e^0_{\rm TDA}$, and $e^0_{\rm RPA}$ for various nuclei.

ming the diagrams in Fig. 4. We equate the sum to $\eta\hbar\omega$ and list η in Table I and plot it in Fig. 5.

We express η in terms of the previously mentioned $1/j$ expansion for 2 cases.

All points included $\eta = 1.568 + 0.062/j + 0.132/j^2$
Only last four points $\eta = 1.571 + 0.019/j + 0.246/j^2$

We can compare this with the value of η obtained in a very simple schematic model in which the first order effective charge is $\frac{1}{2}$ and σ is $\frac{1}{2}$. In this model

$$e^0_{\rm TDA} = \frac{0.5}{1-0.25} = \tfrac{2}{3} \quad e^0_{\rm RPA} = \frac{0.5}{1-0.5} = 1 \, .$$

From this we could infer that the energy of the isoscalar quadrupole state in TDA is $1.5\hbar\omega$ and in RPA is $\sqrt{2}\,\hbar\omega$.

We see that our delta interaction result does not

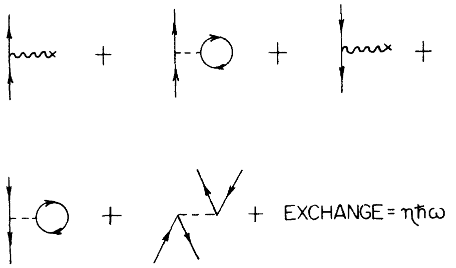

FIG. 4. The energy denominator in the expression for the effective charge is equal to $\eta\hbar\omega$ for the TDA case.

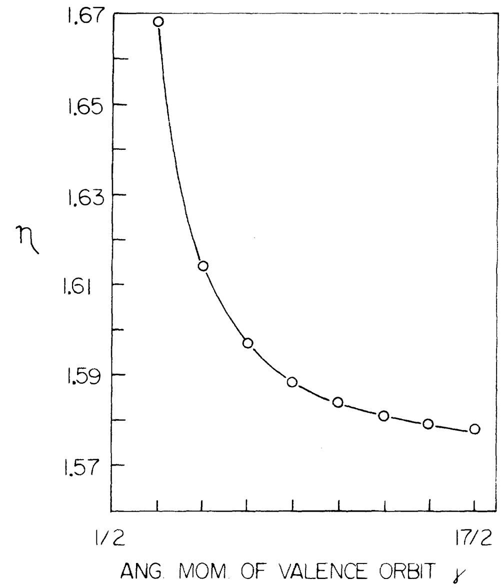

FIG. 5. η as defined in Fig. 4 is plotted as a function of j.

quite go to this schematic model result. The asymptotic energy of the quadrupole state is $1.57\hbar\omega$ instead of $1.5\hbar\omega$. The asymptotic value of $e^0_{\rm First}$ is 0.58 instead of 0.5 and the corresponding value of σ is 0.44.

However, the combination of $e^0_{\rm First} > 0.5$ and $\sigma < 0.5$ conspires to yield $e^0_{\rm RPA} \approx 1$ (allowing for a certain amount of noise in the numerical integrals and in the extrapolation).

Referring to Fig. 3, one amusing point concerns the extrapolation to small j, in particular $j=\frac{1}{2}$. We could well imagine that if the curve for, say, $e^0_{\rm RPA}$ were extended in this direction it might pass through zero. This result might seem reasonable since $j=\frac{1}{2}$ corresponds to a $0s_{1/2}$ particle and no core. However, we are also dividing by the quadrupole moment of a $0s_{1/2}$ nucleon. That is, the expression is zero over zero.

CONCLUDING REMARKS

We have shown that if the strength of a delta interaction is chosen in a sensible way (the quadrupole condition), then all the relevant quantities pertaining to the quadrupole properties of the nucleus, namely, the effective charge in first order, in the TDA and in the RPA, and the energy of the isoscalar quadrupole state in units of $\hbar\omega$, approach a constant finite value in the limit of large A.

In the RPA the isoscalar effective charge correction varies from about 0.5 for mass 4 to about 1 as $A \to \infty$. The energy of the isoscalar quadrupole state approaches $1.57\hbar\omega$. The strength of the interaction itself approaches a constant ~300 MeV

fm^3.

We can obtain a remarkably good fit to all the above quantities if we assume that they vary as $C_0 + C_1/j + C_2/j^2$, where j is the value of the angular momentum of the valence nucleon.

Our principal motive was to try to gain a better understanding of the remarkable formulas of Bohr and Mottelson.[1] These authors are able to obtain wide sweeping results without explicit reference to detailed nuclear forces. Our efforts to reconcile their methods with the usual nuclear force methods have been modest, but nevertheless instructive, and we hope that further work in this direction will be undertaken.

In this work we have shown that the simple result $e^0 = 1$ which the above authors obtained, holds only asymptotically ($A \to \infty$) in our model. We attribute the difference, at least in part, to the assumption that when a nucleus deforms, all nucleons have the same deformation parameters (b_x, b_y, and b_z). This is in conflict with the Pauli principles in first order perturbation theory. However, as $A \to \infty$ it may be that because of higher order effects the assumptions of Bohr and Mottelson[1] are fulfilled. For light nuclei the RPA may be at fault for not including the effects of valence polarization.

In this work we have considered a special case of the zero range interaction, the delta interaction $-G\delta(\vec{r}_i - \vec{r}_j)$. As mentioned in the text, there are other zero range interactions, such as the combination of two- and three-body delta interactions of Skyrme, and Vautherin and Brink[4]:

$$-t_0\delta(\vec{r}_i - \vec{r}_j) + t_3\delta(\vec{r}_i - \vec{r}_k)\delta(\vec{r}_j - \vec{r}_k)\,.$$

The parameters t_0 and t_3 are chosen to obtain the correct binding energy and mean square radius for a given nucleus. Calculations of the isoscalar effective charge correction e^0 have been calculated for mass 4, 16, and 40 with this zero range Skyrme interaction by Zamick, Golin, and Moszkowski.[5] The RPA results were respectively 0.76, 1.16, and 1.71. The corresponding results in *this* work are 0.50, 0.68, and 0.77. We see that the results are quite different for these two different sets of zero range interactions, although in both cases the values increase with increasing A. It is not clear whether the Skyrme results will approach a finite value as $A \to \infty$.

Clearly then, a more systematic study of the Skyrme interactions as a function of mass number, is in order. We hope to carry this out in the near future.

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