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^{41}Sc-^{41}Ca Coulomb displacement energy

N. Auerbach
*Department of Physics and Astronomy, Tel-Aviv University, Tel-Aviv, Israel**
and Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742

V. Bernard† and Nguyen Van Giai
Division de Physique Théorique, ‡ Institut de Physique Nucléaire, 91406 Orsay Cedex, France
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The Coulomb displacement energy in the ^{41}Sc-^{41}Ca system is calculated using three different methods. All three methods make use of Hartree-Fock densities at some stage. The Hartree-Fock calculations are performed with the SIII and SIV Skyrme-type forces. The results from all three methods are in agreement with each other. The resulting Coulomb displacement energy is less than 4 or less than 6 percent smaller than the experimental one depending on the force employed. Higher order Coulomb corrections are evaluated and it is found that they can be very large (of the order of 1 MeV) and depend on the approach taken. The use of the analog state defined with the T_- operator as a representation of the physical analog leads to an overestimate of the Coulomb displacement energy by more than 0.5 MeV. The inclusion of Coulomb distortion terms restores the result by reducing the Coulomb displacement energy. One can also conclude from the present study that the mechanism of treating higher order Coulomb corrections by taking the giant isovector monopole as the only important intermediate state is in fact the correct one and gives precise results.

[NUCLEAR STRUCTURE Coulomb displacement energy, ^{41}Sc-^{41}Ca system.]

I. INTRODUCTION

In this paper we examine the problem of Coulomb displacement (CD) energies[1,2] in nuclei emphasizing the case of mirror pairs. There are several methods to evaluate these energies in mirror nuclei. Each approach has its merits and shortcomings. We will explore three such methods and evaluate the CD energy using as a test case the CD energy in the ^{41}Sc-^{41}Ca pair. Each of the calculations presented makes use at some stage of Hartree-Fock (HF) proton and neutron densities. The density distributions are computed in the kind of HF calculations in which density-dependent forces of the Skyrme type[3] are employed.[4,5] These calculations reproduce quite well the experimental charge distributions.[5] The calculations of the proton and *neutron* densities are mutually dependent in an HF approach; it is therefore argued that since the proton density is correct one should have confidence in the neutron density distribution as well.

One of the important problems in the calculation of CD energies is higher order Coulomb corrections.[2,6,7] These corrections are essential in the precise evaluation of CD energies and their size depends crucially on the definition of an analog state. As we shall see, the question whether higher order corrections are large or small depends on the starting point of the calculation of CD energies, and therefore it is important to investigate several different approaches.

II. VARIOUS APPROACHES TO CD ENERGIES IN MIRROR NUCLEI

The CD energy is defined as the difference between the peak energy of the isobaric analog resonance (IAR) and the energy of the parent state $|\pi\rangle$, or in case of bound states the energy difference between the "physical" (measured) analog state and the parent state. For the simple case of a pair of mirror nuclei like ^{41}Sc-^{41}Ca the CD energy is the energy difference between the physical analog state which is the ^{41}Sc ground state and the parent state which is the ^{41}Ca ground state.

A. The total binding energy calculation

The problem of the CD energy in mirror nuclei seems to be relatively simple. All that one needs is to evaluate in the HF approximation the total binding energies of the two nuclei (^{41}Sc, ^{41}Ca) and subtract one from the other. In such a calculation the most important higher order Coulomb corrections are taken into account. Also core polarization effects of the type described first in Ref. 8 and discussed subsequently in other works[9-11] are included in this approach. The above core polarization corresponds to the excitation of the core monopole state by the nucleon which is outside the core. Other core polarization effects in which core states with higher multipolarity are excited are not taken into account

in the spherically constrained HF calculation of the total binding energies (BE) of the two mirror nuclei. The contribution of this type of core polarization effect to the CD energy is small although not negligible and can be estimated.[6,12]

The CD energy in this approach is given by

$$\Delta_{BE} = E_{HF}(^{41}\mathrm{Sc}) - E_{HF}(^{41}\mathrm{Ca}), \tag{1}$$

where E_{HF} denotes the total energy calculated in the HF approximation. The HF method is straightforward for closed shells. In the case of nonclosed shell nuclei one introduces a computational simplification by making the so-called filling approximation, in which one distributes the nucleons outside the closed shells in a uniform manner among all the states forming the next complete shell.[5,10] In this way, one introduces fractional occupation numbers. The expressions for the HF densities are given in the filling approximation by

$$\rho(\vec{r}) = \sum_i n_i |\phi_i(\vec{r})|^2 \tag{2}$$

with n_i being the occupation numbers and ϕ_i the HF wave functions. For mirror pairs with one nucleon outside the closed shells $n_l = 1/(2j_l+1)$ for the last orbital j_l. (In the ^{41}Sc-^{41}Ca case, $n_l = \frac{1}{8}$.) The filling approximation introduces a spurious Coulomb self-energy term. This term is simply due to the fact that the last proton in ^{41}Sc is replaced by eight $\frac{1}{8}$ protons which interact mutually. This self-interaction energy is

$$\Delta_S = \frac{1}{(2j_l+1)^2} \sum_{m,m'} \left\langle j_l m, j_l m' \left| \frac{e^2}{r_{12}} \right| j_l m, j_l m' \right\rangle \tag{3}$$

and must be subtracted from the CD energy obtained from Eq. (1) using the filling approximation.

Another difficulty in this method (as well as in the others) is the spurious isospin mixing introduced by the HF approximation for nuclei with $N \neq Z$. The spurious isospin mixing causes a spurious shift in the CD energy.[13] In the case of $T = \frac{1}{2}$ nuclei the spurious isospin mixing and shift are very small and we estimate this shift to be only a few keV in the $A = 41$ nuclei.

Yet, a more severe limitation in the method discussed is that it can only be used for mirror nuclei and cannot be applied to the case when the excess neutron number is large. In nuclei with $N - Z > 1$ the analog is not a ground state and one cannot use the HF approximation to compute its total energy. Moreover, even in the case of mirror nuclei ($T = \frac{1}{2}$) we must deal with the subtraction of two large numbers and hence there is *a priori* a possibility of introducing uncertainties in the evaluation of CD energies. In other words, instead of calculating directly the CD energy, which represents only a relatively small change in the total energy when going from the parent to the analog, we are dealing with the *total* energies themselves.

B. The $|A\rangle$ state approach

To avoid the above restrictions one attempts to calculate directly the energy difference between the isobaric analog state (or resonance) and the parent state by introducing model definitions of the analog state. In this case one must deal with higher order terms which correct for the fact that the starting point is a model state. The advantage is that we can apply this method to heavy nuclei where $N - Z > 1$ and where the analog is not the ground state (often unbound) and we avoid the step of calculating total binding energies.

One usually starts the description of the IAR by assuming that the parent state $|\pi\rangle$ is an eigenstate of the full Hamiltonian H which includes *the Coulomb potential*. This is a very convenient and natural starting point since one wants to use the available nuclear structure information and, in particular, the measured charge distribution. The next step is to define a model state for the isobaric analog[6]:

$$|A\rangle \equiv T_- |\pi\rangle \alpha^{-1/2}, \tag{4}$$

where $\alpha = \langle \pi | T_+ T_- | \pi \rangle$, and T_- is the usual isospin lowering operator $T_- = \sum_i t_-^{(i)}$, where $t_-^{(i)}$ changes the ith neutron into a proton leaving unaffected other quantum numbers. This state is not an eigenstate of the Hamiltonian but in the limit when the Coulomb force and other isospin violating forces are put to zero, it becomes an exact eigenstate of H. This is the intuitive reason why $|A\rangle$ is chosen as the starting point in describing the IAR. The energy difference between $|A\rangle$ and $|\pi\rangle$,

$$E_A \equiv \langle A|H|A\rangle - \langle \pi|H|\pi\rangle, \tag{5}$$

can be expressed as

$$E_A = \Delta_1 + \Delta_2, \tag{6}$$

where

$$\Delta_1 = \langle \pi | [T_+, [H, T_-]] | \pi \rangle \alpha^{-1} \tag{7}$$

and

$$\Delta_2 = \langle \pi | [H, T_-] T_+ | \pi \rangle \alpha^{-1}. \tag{8}$$

We must bear in mind, however, that the wave function of the IAR differs from that of $|A\rangle$ due

to the Coulomb distortion effects. The correction terms due to the distortion are given by the expression[6,7]:

$$\Delta_3 = \sum_q \frac{|\langle q|H|A\rangle|^2}{E_A - E_q}, \tag{9}$$

where the sum runs, in principle, over all states $|q\rangle$ orthogonal to $|A\rangle$. The full CD energy is then

$$E_{\mathrm{CD}}^A = \Delta_1 + \Delta_2 + \Delta_3 . \tag{10}$$

At this point one would immediately ask "Is the state $|A\rangle$ a good approximation of the real wave function as far as the CD energy is concerned?", or, in particular, "If $|\pi\rangle$ represents the ground state of ^{41}Ca, does $|A\rangle$ describe the ground state of ^{41}Sc so that the energy difference between ^{41}Sc and ^{41}Ca is well represented by E_A and Δ_3 may be neglected?" The answer to this question will be given in Secs. III and IV.

The term Δ_1 in Eq. (7) is the largest contribution to the CD energy and a proper treatment of it is crucial to the evaluation of E_{CD}^A. In an independent particle model such as, for example, the HF approximation for $|\pi\rangle$, the expression for Δ_1 is

$$\Delta_1 = \alpha^{-1} \int [\rho_n(\vec{r}_1) - \rho_p(\vec{r}_1)] \frac{e^2}{r_{12}} \rho_p(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 + \mathrm{exch}, \tag{11}$$

where ρ_n and ρ_p denote the neutron and proton densities in the parent nucleus, and "exch" means the exchange term.

We stress the following points concerning Eq. (11): (a) It is not a result obtained from a perturbation theory. The densities ρ_n and ρ_p are calculated in the presence of the Coulomb force and therefore Eq. (11) has contributions to all orders in e^2. Consequently, isospin mixing does contribute to Δ_1. (b) The difference $\rho_n - \rho_p$ involves the total densities and is *not* merely the neutron excess density $\rho_{\mathrm{exc}} = \sum_i |\phi_i|^2$, where the sum contains only the wave functions of the excess neutrons. The full density difference is $\rho_n - \rho_p = \rho_{\mathrm{exc}} + \Delta\rho$, where $\Delta\rho$ is the difference between the neutron core and proton densities.

In some calculations the definition of the analog as given in Eq. (4) was introduced, but in evaluating the density difference in Eq. (11) the approximation $\rho_n - \rho_p \simeq \rho_{\mathrm{exc}}$ was used[2,6]; hence the core term

$$\Delta_1^{\mathrm{core}} = \int \Delta\rho(\vec{r}_1) \frac{e^2}{r_{12}} \rho_p(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 + \mathrm{exch} \tag{12}$$

was discarded. This is conceptually inconsistent because the definition in Eq. (4) implies that $\rho_{\mathrm{exc}} + \Delta\rho$ be used in Eq. (12). However, as we shall see later, the neglect of all Δ_1^{core}, Δ_2, and Δ_3 leads to a numerically reasonable approximation of the CD energy in mirror nuclei.

The present HF calculations are able to provide the full density difference $\rho_n - \rho_p$. In Fig. 1(a) we show the $\rho_n - \rho_p$ density in ^{41}Ca and compare it with ρ_{exc}, i.e., the density of the $f_{7/2}$ neutron. We see that the isovector density $(\rho_n - \rho_p)$ in ^{41}Ca is very different from the excess neutron density ρ_{exc}. This should be kept in mind when various processes are considered which involve the difference of proton and neutron densities.

The origin of the difference between $(\rho_n - \rho_p)$ and ρ_{exc} is well understood by now.[2,6-11] The Coulomb force polarizes the core by expelling slightly the protons with respect to the neutrons. [The $\Delta\rho$ density can be derived[11] using the notion of the isovector monopole state and the results are in qualitative agreement with the HF calculations.] This causes $(\rho_n - \rho_p)$ to have a smaller radious than ρ_{exc} has. Therefore, one expects an increase in the Δ_1 term. In Fig. 1(b) we show the two densities multiplied by r^2 and the Coulomb potential $V_c(r)$ as they appear in the integrand of Eq. (12). We see that the effect in the densities is very pronounced. The quantity $r^2(\rho_n - \rho_p)$ is peaked at a radius 20% smaller than that of

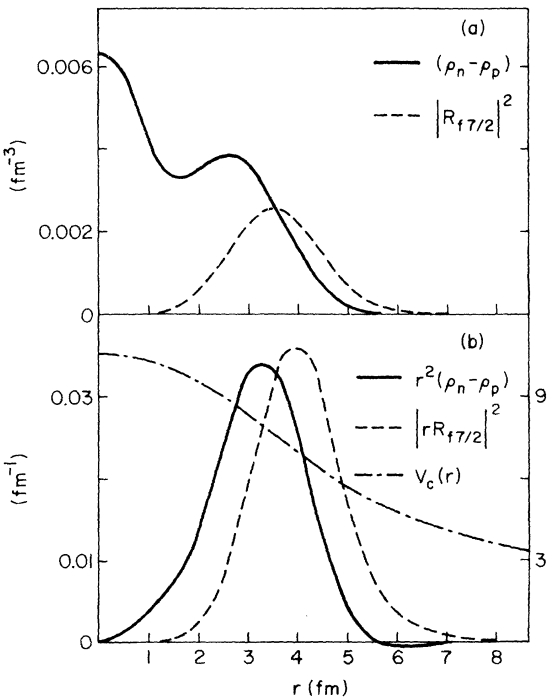

FIG. 1. (a) Densities $(\rho_n - \rho_p)$ and ρ_{exc} in ^{41}Ca calculated with interaction SIV. (b) The one-body Coulomb potential $V_c(r)$ and the above densities multiplied by r^2. The right-hand side scale refers to $V_c(r)$.

$|rR_{f_{7/2}}(r)|^2$. When evaluating the Δ_1 term we shall use the densities calculated in the ^{41}Ca system. This, as already discussed, introduces spurious isospin mixing which is, however, very small. The advantage is that the polarization correction[8-11] is included in this case. To check our results we performed the calculation of Δ_1 using the HF densities calculated in the ^{40}Ca system. We then added the core polarization correction evaluated separately. We found that the two results agreed within a few keV.

The term Δ_2 given by Eq. (8) is nonzero only when the parent state has admixed isospin. We must emphasize, however, and as already pointed out, that also the first term in Eq. (7) contains contributions from isospin mixing. The Δ_2 term can be evaluated directly by performing the integrals[6]:

$$\Delta_2 = \alpha^{-1} \int I(\vec{r}_1) \frac{e^2}{r_{12}} \rho_p(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 - \alpha^{-1} \int I(\vec{r}_1, \vec{r}_2) \frac{e^2}{r_{12}} \rho_p(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 , \quad (13)$$

where

$$I(\vec{r}_1, \vec{r}_2) = \rho_p(\vec{r}_1, \vec{r}_2) - \int \rho_n(\vec{r}_1, \vec{r}') \rho_p(\vec{r}', \vec{r}_2) d\vec{r}' , \quad (14)$$

with the notation $\rho_p(\vec{r})$ or $\rho_n(\vec{r})$ being the diagonal term of the density matrix, i.e., $\rho_{p(n)}(\vec{r}) = \rho_{p(n)}(\vec{r}, \vec{r})$ and $I(\vec{r}) = I(\vec{r}, \vec{r})$. The density matrices were obtained from the HF calculation.

Alternatively, one can calculate Δ_2 by using the notion of the isovector monopole state. Following Ref. 6 we expand the parent state $|\pi\rangle$ into states of good isospin denoted by $|T+n, T\rangle$,

$$|\pi\rangle = \sum_{n=0} \epsilon_{T+n} |T+n, T\rangle . \quad (15)$$

Substituting $|\pi\rangle$ into the expression for Δ_2 [Eq. (8)], we get

$$\Delta_2 = \alpha^{-1} \sum_{n=1} \langle \pi | [H, T_-] | T+n, T+1 \rangle \times [n(2T+n+1)]^{1/2} \epsilon_{T+n} . \quad (16)$$

Since H is approximately diagonal in states of good isospin, i.e.,

$$H|T+n, T+1\rangle \simeq E_{T+n, T+1} |T+n, T+1\rangle . \quad (17)$$

Then performing some algebra one obtains from Eq. (16)

$$\Delta_2 \simeq -\alpha^{-1} \sum_n n(2T+n+1) \epsilon_{T+n}^2 \delta E_n , \quad (18)$$

where the approximation is made $\delta E_n \equiv E_{T+n, T+1} - E_{T,T} \simeq E_{T+n, T+1} - E_{T,T}$.

We now assume that the sum in Eq. (18) is well approximated by a single state, the $T+1$ component of the giant isovector monopole state, denoted as $|M_{T+1}\rangle$. The fact that the giant isovector monopole exhausts most of the Coulomb strength is well known.[6,7,14-16] Thus, Eq. (18) can be put into the form

$$\Delta_2 = -2\epsilon_{T+1}^2 (T+1) \delta E_1 / \alpha , \quad (19)$$

where

$$\delta E_1 = E_{M_{T+1}} - E_{T,T} + E_{CD} . \quad (20)$$

In Eq. (20) $E_{M_{T+1}}$ is the energy of the $T+1$ component of the isovector monopole in the parent nucleus and E_{CD} is the Coulomb displacement energy. We also write

$$\alpha \equiv \langle \pi | T_+ T_- | \pi \rangle = 2T \left(1 + \epsilon_{T+1}^2 \frac{T+1}{T} \right) . \quad (21)$$

Leaving only terms linear in ϵ_{T+1}^2 we find

$$\Delta_2 = -\epsilon_{T+1}^2 \frac{T+1}{T} E_{M_{T+1}} . \quad (22)$$

In the last step, in going from Eq. (19) to Eq. (22) we dropped the term $-\epsilon_{T+1}^2 E_{CD}(T+1)/T$ since this term will be canceled by the same term in Δ_1 when the denominator α there is expanded. From now on, we shall refer to the Δ_1 term as *evaluated with* $\alpha = 2T$.

For large T

$$\Delta_2 \simeq -\epsilon_{T+1}^2 E_{M_{T+1}} , \quad (23)$$

but for $T = \frac{1}{2}$ mirror nuclei

$$\Delta_2 = -3\epsilon_{3/2}^2 E_{M_{3/2}} , \quad (24)$$

where $\epsilon_{3/2}^2$ denotes the admixture of the $T = \frac{3}{2}$ component of the isovector monopole and $E_{M_{3/2}}$ its energy, in the parent nucleus. Both numbers can be calculated using the HF and the RPA in which the residual particle-hole interaction V_{ph} is derived from the HF potential[17,18] U_{HF} with the prescription $V_{ph} = \partial U_{HF} / \partial \rho$. The estimate of Δ_2 using Eqs. (24) or (13) agree very well.

Finally, we must evaluate Δ_3. Since the states $|q\rangle$ in Eq. (9) are orthogonal to $|A\rangle$ one may rewrite Δ_3 in a form containing the commutator $[H, T_-]$, namely,[2,6]

$$\Delta_3 = \frac{1}{2T} \sum_q \frac{|\langle q | [H, T_-] | \pi \rangle|^2}{E_A - E_q} . \quad (25)$$

As in the treatment of Δ_2 we evaluate Δ_3 by exhausting the sum with the isovector monopole state. Since the states $|q\rangle$ are in the analog nucleus which has $T_z = T - 1$ we have (for nuclei

with $T \geq 1$) three possible components—$T+1$, T, and $T-1$ for the isovector monopole state. (In the case of $T=\frac{1}{2}$ nuclei the $T-1$ component does not exist.) We denote the corresponding states by

$$|M_{T+1}\rangle, \quad |M_T\rangle, \quad \text{and} \quad |M_{T-1}\rangle.$$

Taking only the isovector part of the commutator $[H, T_-]$ (essentially the isovector Coulomb potential $V_C^{(1)}$) we obtain[7,15]

$$\Delta_3 = \frac{1}{T}\left[\frac{|\langle M_{T-1}\|V_C^{(1)}\|\pi\rangle|^2}{E_A - E_{M_{T-1}}}\frac{2T-1}{2T+1} + \frac{|\langle M_T\|V_C^{(1)}\|\pi\rangle|^2}{E_A - E_{M_T}}\frac{1}{(T+1)} + \frac{|\langle M_{T+1}\|V_C^{(1)}\|\pi\rangle|^2}{E_A - E_{M_{T+1}}}\frac{1}{(T+1)(2T+1)}\right], \tag{26}$$

with

$$E_{M_{T'}} - E_A \simeq \bar{E}_M + \tfrac{1}{2}\xi[T'(T'+1) - T(T+1) - 2], \tag{27}$$

where $\bar{E}_M$ is some average position and $\xi \simeq 60$ MeV/A (see Refs. 7, 15, and 16). The reduced matrix elements satisfy

$$|\langle M_{T-1}\|V_C^{(1)}\|\pi\rangle| > |\langle M_T\|V_C^{(1)}\|\pi\rangle| > |\langle M_{T+1}\|V_C^{(1)}\|\pi\rangle|.$$

For large T the first term is the dominant one and we find

$$\Delta_3 \simeq -\frac{1}{T}\frac{|\langle M_{T-1}\|V_C^{(1)}\|\pi\rangle|^2}{\bar{E}_M - (T+1)\xi}. \tag{28}$$

In mirror nuclei, as already remarked, there are only two components: $T+1=\frac{3}{2}$ and $T=\frac{1}{2}$. The energy splitting between the two components is very small and the difference between the above reduced matrix elements is negligible.[15] Therefore to a good approximation:

$$\Delta_3 \simeq -\frac{|\langle M\|V_C^{(1)}\|\pi\rangle|^2}{\bar{E}_M}\frac{1}{T}, \tag{29}$$

where $|M\rangle$ is either the $\frac{3}{2}$ or $\frac{1}{2}$ component of the monopole. On the other hand,

$$\epsilon_{T+1}{}^2 \simeq \frac{1}{T+1}\frac{|\langle M\|V_C^{(1)}\|\pi\rangle|^2}{\bar{E}_M{}^2}. \tag{30}$$

Hence

$$\Delta_3 \simeq -\frac{T+1}{T}\epsilon_{T+1}{}^2\bar{E}_M, \tag{31}$$

and we finally obtain for $T=\frac{1}{2}$,

$$\Delta_3 \simeq -3\epsilon_{3/2}{}^2\bar{E}_M, \tag{32}$$

i.e., $\Delta_3 \simeq \Delta_2$ for mirror nuclei, and

$$\Delta_2 + \Delta_3 \simeq -6\epsilon_{3/2}{}^2\bar{E}_M. \tag{33}$$

Of course, Eqs. (22) and (26) are general and apply to any nucleus.

The method described in the present subsection makes up a consistent scheme to calculate the CD energies for both light nuclei with a small neutron excess and for heavier nuclei where the neutron excess is large. When applying the method one must be careful to treat all the higher order corrections Δ_1^{core}, Δ_2, and Δ_3 in a systematic manner. By ignoring some of these terms one can make considerable errors. The Δ_1^{core} correction has a positive sign and cancels a large portion of the negative corrections ($\Delta_2 + \Delta_3$). In some calculations of CD energies in heavy nuclei the correction Δ_1^{core} was not included but Δ_2 and Δ_3 were kept.[6,19] This led to a few hundred keV underestimate of the CD energy. And vice versa, as we shall see in Sec. III, the neglect of Δ_2 or Δ_3 and the inclusion of Δ_1^{core} leads to large errors for CD energies, especially in the case of a mirror pair.

C. The ρ_{exc} approach

In this approach one simply calculates the integral in Eq. (11) with $(\rho_n - \rho_p)$ replaced by ρ_{exc}, i.e.,

$$\Delta_{\text{exc}} = \frac{1}{2T}\int \rho_{\text{exc}}(\vec{r}_1)\frac{e^2}{r_{12}}\rho_p(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 + \text{exch}. \tag{34}$$

The understanding is that going from the parent state to the analog the change in energy is due only to the fact that an excess neutron becomes a proton and interacts with the field of the core protons. The ^{41}Ca and ^{41}Sc ground states differ only in their last nucleon which is changed from an $f_{7/2}$ neutron into an $f_{7/2}$ proton. The Coulomb energy from the proton core is unchanged and drops out when the differences are taken. This is why Δ_1^{core} and $\Delta_2 + \Delta_3$ defined in Sec. II B will essentially cancel each other. (All three corrections are connected with the core.) In addition to the term in Eq. (34), one must add the core polarization correction as given, for example, in Refs. 9–11, 20.

In nuclei with a large neutron excess (for example, in ^{90}Zr or ^{208}Pb, etc.) one cannot easily separate the contributions coming from the core and the excess neutrons. (When we refer to the core we have in mind the Z protons and the Z neutrons in the lowest orbitals, for example, in ^{208}Pb, the core consists of 82 protons and the corresponding 82 neutrons.) All higher order Coulomb effects or core polarization contributions involve expressions in which both the excess neutrons and core nucleons play a role and the contribution from each one cannot be separated. For example, when discussing higher

order terms one uses as the intermediate state, the collective isovector monopole. In the case of mirror nuclei this state is made up mainly of 1p-1h excitations from the core and the influence of the single nucleon outside the core may be neglected in the construction of the monopole. However, in a nucleus like ^{208}Pb the giant isovector monopole (its T and $T-1$ components) are made up of a coherent admixture of 1p-1h configurations in which the hole states are both in the core and in the excess neutrons. Therefore, in such cases one cannot rely on the argument as used in $T=\frac{1}{2}$ pairs that the influence of the core will cancel out.

We have already mentioned that, in many calculations of CD energies, correction terms to Eq. (34) were not included and when some were included thay were not treated consistently. For example, in some calculations one adds to $\Delta_{\rm exc}$ the Δ_2 and Δ_3 corrections derived in the $|A\rangle$ approach leaving out the $\Delta_1^{\rm core}$ term.[6,19]

A formal way to represent the present method and to derive Eq. (34) is to use the analog spin introduced by MacDonald.[21] Instead of using the T_- isospin lowering operator one defines a different operator $W_-=\sum_i w_-^{(i)}$, where $w_-^{(i)}$ changes a neutron occupying the ith *neutron state* $\phi_i^{(N)}$ into a proton occupying the ith *proton state* $\phi_i^{(P)}$. One then defines a new model analog state with T_- replaced by the W_- in Eq. (4), i.e.,

$$|W\rangle \equiv W_-|\pi\rangle/\langle\pi|W_+W_-|\pi\rangle^{1/2}. \tag{35}$$

With such a definition of the analog, the first order expression for the CD energy is the one given by Eq. (34). The contribution due to $\Delta\rho$ drops out because of the Pauli principle. The W_- operator will change a core neutron into a proton in a state which is already *fully* occupied by the core proton. Of course, an exact treatment of the CD in which the starting point is the w-analog state in Eq. (35) would also contain several additional correction terms (we shall not discuss them here).

III. RESULTS

We now present the results of CD energies calculated using each of the three methods discussed in Sec. II. The ^{41}Ca-^{41}Sc will be our test case.

A. General results

In addition to the terms we already discussed, one must add several small correction terms.[1,2,6,20] These are approximately the same for all three methods and they include: (1) the contributions from short range correlations, (2) dynamic proton-neutron mass difference, (3) vacuum polarization contribution to the Coulomb force, (4) the proton-neutron finite size correction, and (5) magnetic spin-orbit terms. In the case of ^{41}Sc-^{41}Ca the first three corrections are positive and the last two are negative so that the total correction (denoted δ) is approximately $\delta=0.01$ MeV within an accuracy of a few tens of keV.

TABLE I. The calculated HF rms radii and isospin admixtures in ^{41}Ca. The radii are in fm and ϵ^2 in percentage.

Force	r_p	r_{nc}	r_n	$r_{\rm exc}$	r_{n-p}	$\epsilon_{3/2}{}^2$
SIII	3.42	3.37	3.40	4.02	3.01	0.53
SIV	3.40	3.34	3.37	4.15	3.13	0.58

The calculations were performed in the HF approximation using the SIII and SIV forces,[5] which give good charge distributions and charge radii in the Ca region. In Table I we give some of the ground state quantities calculated for ^{41}Ca. The various rms radii are defined by

$$r_\alpha \equiv \langle r_\alpha{}^2\rangle^{1/2} = \left[\int \rho_\alpha(\vec{r}) r^2 \vec{d}r \Big/ \int \rho_\alpha(\vec{r}) d\vec{r}\right]^{1/2}, \tag{36}$$

where ρ_α stands for various density distributions; ρ_p is the proton density distribution, ρ_n the total neutron distribution, ρ_{nc} and $\rho_{\rm exc}$ the neutron core and neutron excess densities, and $\rho_{n-p}\equiv\rho_n-\rho_p$. The rms radii have the corresponding notations. We note that the neutron core rms radius r_{nc} is smaller by about 0.05 fm than the proton radius and that r_{n-p} is smaller by about 25% than $r_{\rm exc}$.

The amount of isospin mixing is calculated from the HF wave functions using the formula

$$\epsilon_{T+1}{}^2 = \frac{\langle\pi|T_+T_-|\pi\rangle - (N-Z)}{N-Z+2}, \tag{37}$$

where $|\pi\rangle$ is the HF wave function of the parent

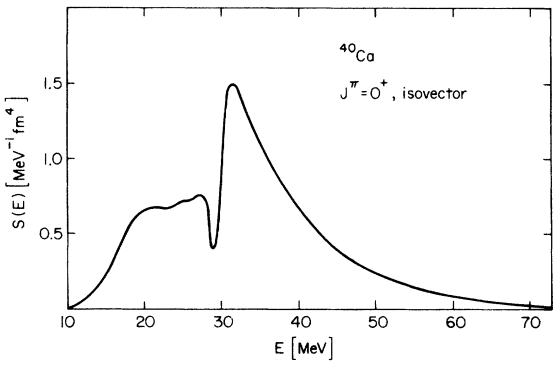

FIG. 2. Isovector monopole strength in ^{40}Ca calculated with interaction SIII.

TABLE II. Calculated CD energies for the ^{41}Sc-^{41}Ca case in the total binding energy approach. All the numbers are in MeV.

Force	Δ_{BE}	Δ_S	δ	E_{CD}^{BE}
SIII	7.17	0.17	0.01	7.01
SIV	7.01	0.17	0.01	6.85

ground state, which in our calculation is the ^{41}Ca ground state, and $N-Z=1$ in this case. The resulting number is $\epsilon_{3/2}{}^2 \simeq (0.5\text{–}0.6)\%$ (see Table I) for the isospin admixture in the ground state of ^{41}Ca. This corresponds to an isospin admixture in the ^{40}Ca core of $\epsilon_1{}^2 = \frac{3}{2}\epsilon_{3/2}{}^2 \simeq (0.7\text{–}0.9)\%$. In order to estimate the correction terms Δ_2 and Δ_3 we must know the energy of the isovector monopole $\bar{E}_M$ in ^{40}Ca. This was calculated in the RPA as described in Ref. 18. The distribution of the isovector monopole strength $r^2 t_z$ is shown in Fig. 2. The average energy of the distribution is $\bar{E}_M \simeq 35$ MeV.

B. Results from the total binding energy approach

Using the SIII and SIV forces, we obtain for the difference between the total binding energies of ^{41}Sc-^{41}Ca the numbers: $\Delta_{BE}=7.17$ MeV, and $\Delta_{BE}=7.01$ MeV, correspondingly. From these numbers we must subtract the self-interaction energy term [Eq. (3)] which we find to be $\Delta_S = 0.17$ MeV. The final results in this method,

$$E_{CD}^{BE} = \Delta_{BE} - \Delta_S + \delta\,, \tag{38}$$

are shown in Table II.

C. Results from the $|A\rangle$ state approach

The results are summarized in Table III. The main term Δ_1 is calculated with $\alpha = 2T$ and the other two terms Δ_2 and Δ_3 according to Eqs. (24) and (32). The superscript HF indicates that these were evaluated using the HF wave functions and the Coulomb force only was left in the commutator $[H, T_-]$. The total result in this approach is

$$E_{CD}^{A} = \Delta_1^{HF} + \Delta_2^{HF} + \Delta_3 + \delta\,. \tag{39}$$

TABLE III. Calculated CD energies for the ^{41}Sc-^{41}Ca case in the $|A\rangle$ state approach. All the numbers are in MeV.

Force	Δ_1^{HF}	Δ_2^{HF}	E_A^{HF}	Δ_3	δ	E_{CD}^{A}
SIII	8.11	−0.56	7.55	−0.56	0.01	7.01
SIV	8.02	−0.59	7.43	−0.59	0.01	6.84

TABLE IV. Calculated CD energies for the ^{41}Sc-^{41}Ca case in the ρ_{exc} approach. All the numbers are in MeV.

Force	Δ_{exc}	Δ_{pol}	δ	E_{CD}^{exc}
SIII	6.90	0.10	0.01	7.02
SIV	6.75	0.09	0.01	6.85

We have also indicated in the table the sum $E_A^{HF} = \Delta_1^{HF} + \Delta_2^{HF}$, which represents the CD energy (apart from δ) of the model analog state $|A\rangle$ in Eq. (4). Had the ground state of ^{41}Sc been the model analog then its energy would have been E_A^{HF}. We see that the state $|A\rangle$ does not give an accurate representation of the physical situation. The correction term due to distortions is more than −0.5 MeV large, i.e., 8% of the CD energy in ^{41}Ca. The final results E_{CD}^{A}, agree very well with the ones obtained in the previous method for both forces SIII and SIV.

D. Results from the ρ_{exc} approach

We evaluated the Δ_{exc} term, Eq.(34), with ρ_{exc} being the density distribution of the $f_{7/2}$ neutron in ^{41}Ca. The total CD energy in this approach is

$$E_c^{exc} = \Delta_{exc} + \Delta_{pol} + \delta\,, \tag{40}$$

where Δ_{pol} is the core polarization term.[8-11] The results are shown in Table IV and, as we see, the final result agrees very well with the values obtained in the previous two methods.

IV. SUMMARY AND CONCLUSIONS

One of the important points we note from the above results is that the higher order Coulomb corrections, as calculated in the analog state approach, are very large for the $A=40$ region. This was already noted in Ref. 7 where harmonic oscillator wave functions were used to estimate these effects. We find that also when realistic HF wave functions are used the corrections Δ_2 or Δ_3 are of the order of −0.5 to −0.6 MeV. Note that the Δ_1^{core} correction (which is second and higher order in the Coulomb interaction) is as large as 1.1 MeV in ^{41}Ca. It is therefore very important to treat these corrections consistently and systematically. This is, in particular, true for large neutron excess nuclei, where these corrections were not always evaluated in a systematic manner. In exploring the three methods of calculation we found that all of them give (when most of the important correction terms are introduced) nearly the same result. From the comparison of the results we learn that the mechanism of treating higher order Coulomb corrections by means of the giant isovector

monopole is the correct one.

Since the CD energies from all three methods agree it is meaningful to make a comparison with experiment. The experimental CD energy in the ^{41}Sc-^{41}Ca case is $E_{CD}^{exp} = 7.28$ MeV. The SIII force gives a CD energy 260 to 270 keV smaller than experiment. This is about a 3.5% discrepancy. For the SIV the discrepancy is 430 to 440 keV which is about 6% of the total CD energy in ^{41}Ca. Both forces, although somewhat different in their nature,[5] do give reasonable radii, charge distributions, and binding energies per nucleon. There is no obvious reason why to prefer one over the other.

In addition to all the corrections we included, there is a class of corrections not taken into account in our results. These are the contributions due to configuration mixing of 3p-2h states and some special types of 2p-1h states, namely, those 2p-1h states in which the particle couples to 1p-1h states not of isovector monopole character. Present estimates[12,22] of the contribution of 3p-2h and 2p-1h admixtures to the CD energy in $A = 41$ nuclei indicate that the corrections are positive and amount to about 50–150 keV. Thus, the SIII results, together with the above corrections, bring the discrepancy to less than 150 keV in ^{41}Ca. This is close to the limits of the theoretical uncertainties. The SIV force would give CD energies only 300 keV (4%) small than experiment.

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*Permanent address.
†Present address: Institut de Physique, Universite de Liege, Belgium.
‡Laboratoire Associe au CNRS.

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