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Realistic calculations for c-coefficients of the isobaric mass multiplet equation in $1p0f$ shell nuclei

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We present calculations for the c-coefficients of the isobaric mass multiplet equation for nuclei from $A = 42$ to $A = 54$ based on input from three realistic nucleon-nucleon interactions. We demonstrate that there is a clear dependence on the short-ranged charge-symmetry breaking (CSB) part of the strong interaction and that there is significant disagreement in the CSB part between the commonly used CD-Bonn, N^{3}LO, and Argonne V18 nucleon-nucleon interactions. In addition, we show that all three interactions give a CSB contribution to the c-coefficient that is too large when compared to experiment.

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Isospin is a powerful spectroscopic tool in nuclear physics that can be used to label and characterize states not only in a specific nucleus, but also corresponding states in an analog nucleus. Isospin, denoted by T, is an additive quantity similar to the intrinsic spin of the proton and neutron [1]. The charge, Q, of the particle is defined by the z-component via $Q = \frac{1}{2} + T_z$. Thus, a nucleus with Z protons and N neutrons has $T_z = (Z-N)/2$ and may have isospin states with $T_z \leq T \leq (Z+N)/2$. Isospin symmetry is broken by components in the nuclear Hamiltonian that treat protons and neutrons differently. The most obvious, and significant, component is the Coulomb interaction acting only between protons due to their electric charge. There are, however, weaker isospin-symmetry breaking components in the nucleon-nucleon interaction itself caused by differences in the masses of up and down quarks and their intrinsic electric charges, which is reflected in the slightly different masses exhibited by neutrons and protons [2] and the slightly different strong-interaction scattering lengths observed in the proton-proton (pp), neutron-neutron (nn), and the $T = 1$ proton-neutron (pn) channels [3–7].

Important signatures of isospin-symmetry breaking interactions are differences in the binding energy of nuclei within the same isospin multiplet with fixed nucleon number A. These mass splittings, or Coulomb-displacement energies, offer a sensitive probe of the properties of isospin-symmetry breaking in nuclei. The three $T = 1$ nucleon-nucleon channels can be decomposed into three isospin components: isoscalar (rank 0), isovector (rank 1), and isotensor (rank 2), defined in terms of the pp, nn, and pn interactions via

$$v^{(0)} = \frac{1}{3}(v_{pp} + v_{nn} + v_{pn}) \quad (1)$$

$$v^{(1)} = (v_{pp} - v_{nn}) \quad (2)$$

$$v^{(2)} = v_{pn} - \frac{1}{2}(v_{pp} + v_{nn}). \quad (3)$$

With these three components, the masses for a set of states within a multiplet with isospin T may be described by the isobaric mass multiplet equation (IMME) [8]

$$M(T_z) = a + bT_z + cT_z^2, \quad (4)$$

where the coefficients a, b, and c are dependent on the isoscalar, isovector, and isotensor components of the nuclear Hamiltonian, respectively. The linear and quadratic dependence on T_z is due to the application of the Wigner-Ekart theorem and the appropriate Clebsch-Gordan coefficients arising for the isovector and isotensor components of the Hamiltonian, respectively. For $T = 1$ states, the b- and c-coefficients are equivalent to half the mirror-energy displacement (MED) and triple-energy displacement (TED), respectively, discussed in Refs. [9, 10]. In these two references, the angular momentum, or J-dependence of these quantities; where it was concluded that the observed J-dependence in the MED and TED was explained within the context of the underlying two-body matrix elements (TBME), and that overall, an empirically determined correction relative to the Coulomb TBME was needed. In earlier empirical studies of isospin-nonconserving interactions for $0s1d$ and $1p0f$-shell nuclei, it was found that globally c-coefficients are well reproduced if the $T = 1$ pn interaction is 2% more attractive than the average of pp and nn [11].

Here, we compute c-coefficients (TED) as a function of excitation energy and angular momentum for nuclei in the mass range $42 \leq A \leq 54$ using the Coulomb interaction and isospin-symmetry breaking interactions derived from three realistic nucleon-nucleon interactions utilizing well-known renormalization procedures [17]. We calculate the effect of charge-symmetry breaking in the strong force on the c-coefficients and demonstrate that effective two-body CSB interactions derived from state-of-the art nucleon-nucleon interactions each fail to describe experimental data. Further, we demonstrate that at this level, that the CSB interactions derived from the three realistic interactions are in significant disagreement with each other. This signifies either: 1) a deficiency

in our understanding of isospin-symmetry breaking in the nucleon-nucleon interaction, 2) significant isospin-symmetry breaking in the initial three-nucleon interaction, or 3) large contributions to isospin-symmetry breaking in three-nucleon interactions induced by the renormalization procedure.

We performed a series of shell-model calculations using the program BIGSTICK [14, 15] to compute the c-coefficients of the IMME for odd-odd $N = Z$ nuclei and their $T = 1$ analogs in the $1p0f$ shell with $42 \leq$ A ≤ 54. Calculations were performed with the full $1p0f$-shell model space, except for $A = 54$ where up to five particles excited from the $0f_{7/2}$ orbit were permitted with M-scheme dimensions ~ 500 M [16]. The c-coefficients were computed with CSB-interactions derived from each realistic nucleon-nucleon interactions using renormalization techniques and many-body perturbation theory as described in Ref. [17]. The two-body matrix elements were computed in two steps. In the first step, the nuclear two-body interaction was renormalized using either the G-matrix approach [18–20] or the $V_{low\ k}$ method [21]; both schemes give almost indistinguishable effective interactions. The second step consisted in obtaining an effective interaction tailored to a small shell-model space using many-body perturbation theory up to 3$^{\rm rd}$ order with the renormalized nucleon-nucleon interaction, which includes the so-called folded diagrams [17]. All codes used to generate these interactions are publicly available [22].

To derive the nuclear CSB interactions, we employed the realistic N^{3}LO [24], AV18 [25] and CD-Bonn [5] nucleon-nucleon interactions. These interaction models include breaking of isospin symmetry and charge symmetry in the strong interaction. We note that the AV18 interaction also includes detailed electromagnetic corrections and the full interaction potential was used in the first step, whereas Coulomb was included for the N^{3}LO and CD-Bonn interactions after renormalization. The two-body matrix elements of the Coulomb and nucleon-nucleon interactions were computed using a harmonic oscillator (HO) basis with an oscillator energy $\hbar\omega = 10.5$ MeV with an effective Hilbert space defined by the first twelve oscillator shells. The $V_{low\ k}$ interactions were obtained with a cut-off parameter of $\Lambda = 2.1$ fm^{-1}. The model-space effective interaction was computed with and without the Coulomb interaction, and the Coulomb two-body matrix elements were obtained from the difference between these proton-proton (pp) matrix elements. The renormalized interaction computed without Coulomb was then decomposed into the three isospin components: isoscalar (rank 0), isovector (rank 1), and isotensor (rank 2), as defined in Eqs. (1)-(3).

The validity of the use of harmonic-oscillator radial wave functions for the Coulomb interaction was tested by performing an energy-density functional (EDF) calculation for ^{48}Cr with the SkX Skyrme functional [23]. From this, we obtained the $\hbar\omega$ needed to reproduce the calculated rms charge radius (10.72 MeV). We then calculated the Coulomb two-body matrix elements (TBME) with the EDF and HO radial wave functions for the $1p0f$ orbitals. The average difference for the diagonal TBME for all orbitals was about 1 keV. The difference for the most important $0f_{7/2}$ orbital was (13,10,8,8) keV for $J =$ (0,2,4,6) TBME. For our application, we conclude that it is sufficient to use the HO basis for the Coulomb matrix elements as long as $\hbar\omega$ is scaled according to the total rms radius. Here, the A-dependence was properly accounted for by scaling the Coulomb matrix elements by $\sqrt{\hbar\omega(A)/10.5}$, where $\hbar\omega(A)$ was determined from the rms radius obtained from a spherical EDF calculation for $42 \leq A \leq 54$ nuclei using the SkX Skyrme functional.

The c-coefficients of the IMME were obtained utilizing first-order perturbation theory. The base for each calculation was the eigenstate, E_0, for each member of the $T = 1$ triplet, $|T_z\rangle$, obtained using the isoscalar GX1A Hamiltonian [26]. The GX1A interaction was used instead of the $v^{(0)}$ interaction obtained from the realistic interaction described above because of well-known extensions that must be included to properly capture the behavior of higher-order components and the three-body interaction in the traditional configuration-interaction shell model for atomic nuclei, see for example Refs. [27, 28]. The TBME for the derived isovector and isotensor interactions were assumed to have the same A-dependence as the GX1A interaction. The expectation value of the Coulomb, isovector, and isotensor interactions are then computed to give the full energy for each state,

$$E(T_z) = E_0 + \langle T_z | v^{\rm Coul} + v^{(1)} + v^{(2)} | T_z \rangle$$

the c-coefficient is then computed from

$$c = [E(T_z = 1) - 2E(T_z = 0) + E(T_z = -1)]/2.$$

Figure 1 shows the typical dependence on the order of many-body perturbation theory as demonstrated by the CD-Bonn interaction. In the left-hand panel, the contribution from Coulomb is shown for each order, while in the right-hand panel, the dashed lines show the CSB contribution from the CD-Bonn interaction, while the solid lines show the full value obtained by adding the Coulomb and CSB components for each order. The figure demonstrates that the J-dependence of the Coulomb- and CSB-contributions is quite different. The long-range Coulomb has a relatively flat J-dependence with only a small rise at $J = 0$. On the other hand, the CSB contribution at $A = 42$ shows a peak at $J = 0$ with a sharp drop towards $J = 2$, which is characteristic of a short-ranged interaction. This same pattern is also observed with a simple δ-function interaction model and the empirical CSB interaction in Refs. [9, 11]

For $A = 42$, $J = 6$ is the maximum angular momentum (for $T = 1$) in the $1p0f$ model space. For higher values of A, this sharp drop at $J = 2$ is replaced by a linear drop to $J = 6$ due to configuration mixing. We note that for $J = 8$ and 10, the effect of charge-symmetry breaking is small. The experimental data is taken from

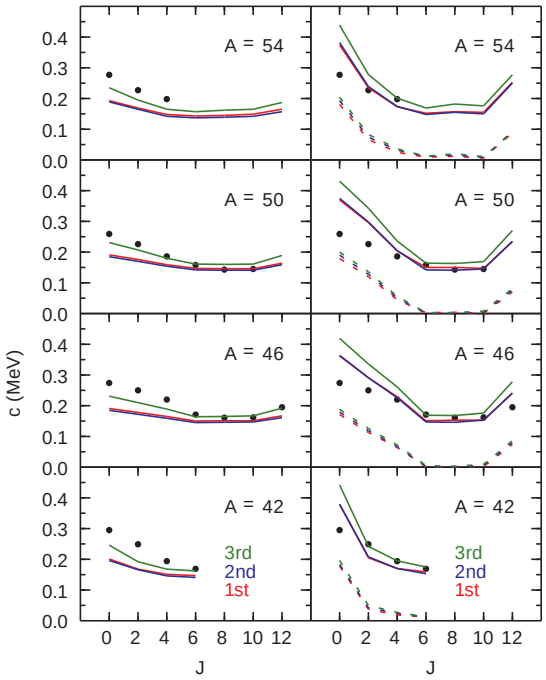

FIG. 1. (color online) Results for the CD-Bonn potential up to 1st (red), 2nd (blue), and 3rd (green) order. The black circles are the experimental data. The solid lines in the left-hand panel show the Coulomb contribution to the c-coefficients. In the right-hand panel, the dashed lines show the CSB contribution from CD-Bonn, while the full line represents the full calculation, CSB + Coulomb.

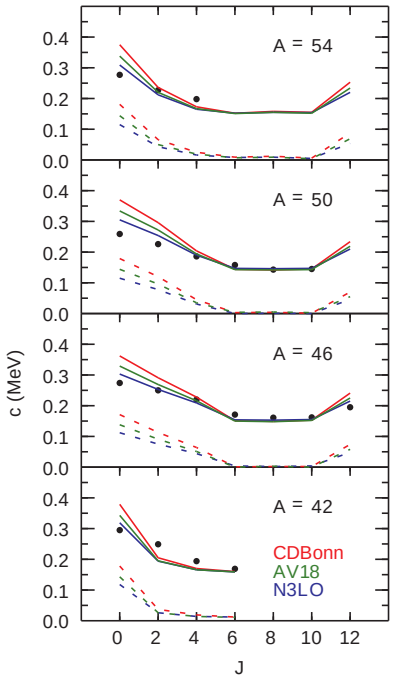

FIG. 2. (color online) first-order calculations compared to experiment. The black circles are the experimental data. The solid lines show the sum of Coulomb and CSB contributions. The dashed lines show only the CSB contribution.

the compilation [12], except for $A = 46$, where we use the results from Fig. 2 of [13].

Both Coulomb and CSB have a small increase at $J = 12$. The reason for this is that protons with $J = 6$ and neutrons with $J = 6$ are maximally aligned, resulting in an enhancement of the overlapping proton and neutron density distributions.

The CSB contribution turns out to be almost order independent, while the Coulomb contribution is almost the same at 1st and 2nd order in many-body perturbation theory, but increases by 10-20% at 3rd order. This suggests that the CSB interaction is substantially short-ranged in nature, and the G-matrix and $V_{low\ k}$ treatment may be sufficient. A simple analysis of all $J = 0$ two-body matrix elements, using Eqs. (1)-(3), shows that for the core-polarization contribution at 2nd order, the correction to c-coefficient is about ten times smaller than that for the a-coefficient. This applies to most two-body matrix elements that define Eqs. (1)-(3).

It is remarkable that the experimental data are in rather good agreement with the third-order Coulomb result, where there seems to be no need for CSB even though this component is well known to be important in nucleon-nucleon (NN) scattering data that is incorporated into the potential models.

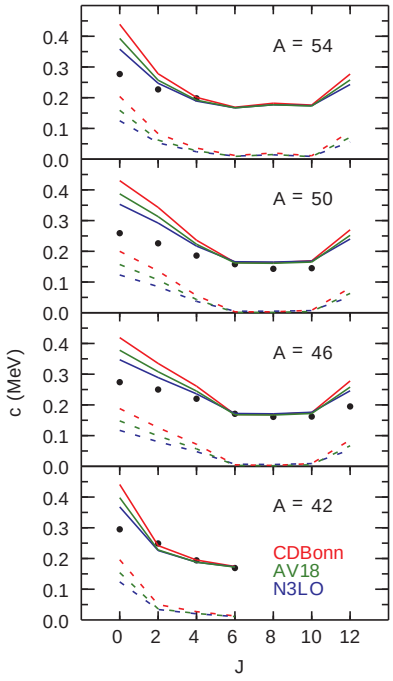

FIG. 3. (color online) Calculations up to 3rd order compared to experiment. See caption to Fig 2.

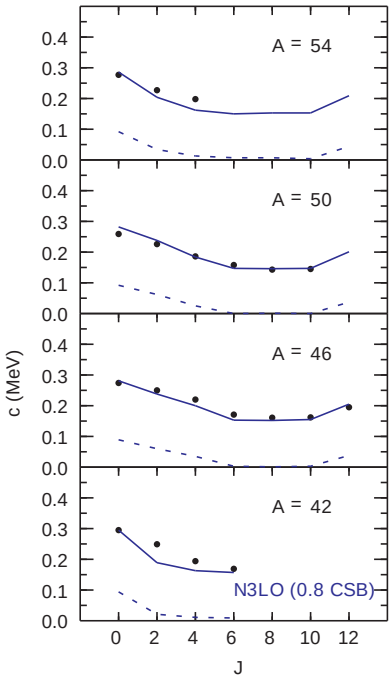

FIG. 4. (color online) first-order calculations for N^{3}LO with the CSB part multiplied by 0.8 and compared to experiment. See caption to Fig 2.

Figure 2 shows the results for the three potential models to 1st order in many-body perturbation theory. This shows that the CSB contribution is model dependent. There could be a few reasons for this. While the NN interactions are all fit to scattering data and reproduce the nucleon-nucleon scattering length equally well, there could be differences in the underlying treatment of the CSB components. For example, while AV18 is a purely local potential, both N^{3}LO and CD-Bonn are non-local, albeit in different ways. The short-range correlation effects taken into account in the G-matrix and V$_{low\ k}$ renormalizations could have different effects on this small component of the NN interactions, which may be corrected when induced three-nucleon terms are included. We note that the results obtained with N^{3}LO are in best agreement with experiment, although all three interactions over predict the c-coefficients. The fact that all three interactions significantly over predict experiment might also be an indication of charge-symmetry breaking in the initial three-nucleon interaction.

Figure 3 shows the results for the three potentials at 3rd order.

Our work suggests future investigations to discover the full extent of the nature of charge symmetry breaking in the nuclear force. For better first principles calculations, one should understand the origin of the different CSB contributions from these three realistic potentials. In particular, in the spirit of using nuclear data to constrain the NN and three-nucleon ($3N$) interactions (in addition to NN scattering data) one should use the c-coefficient as a constraint on the CSB part. From a practical point of view, we start with the fact that first-order Coulomb plus CSB is already close to the data. We can make it almost perfect by taking the first-order Coulomb contribution and add 80% of the N^{3}LO CSB part. This is shown in Fig. 4.

The largest deviation between our calculations and experiment is for $J = 2$ in $A = 42$. In $A = 42$, the experimental data for $J = 0 - 6$ fall off in a manner that is similar to that exhibited in the calculation for $A = 46$, while the calculated fall off is more similar to that calculated for $A = 54$. This is explained by noting that the theoretical wave functions for $A = 42$ are dominated by $(0f_{7/2})^2$ configurations, while the wave functions for $A = 54$ are dominated by $(0f_{7/2})^{-2}$ configurations, thus, the calculated J-dependence between $A = 42$ and 54 is similar. However, the experimental J dependence for $A = 42$ is far more similar to that of $A = 46$. The reason for this is that $A = 42$ is not well described in the $1p0f$ model space alone due to mixing with configurations involving nucleons excited from $1s0d$ orbits to the $1p0f$ shell, as is exhibited by the fact that the B(E2) value for the $J = 2^+ \rightarrow 0^+$ transition in ^{42}Ca is about 10 times larger than that calculated in the $1p0f$ model space [29].

The overprediction of the c-coefficient for CD-Bonn was also noted in Ref. [30] which performed *ab initio* calculations for $A = 10$ nuclei within the framework of the No-core Shell Model using the CD-Bonn interaction. The calculated c-coefficient was 535 kev, which is substantially larger than the experimental value of 362 keV.

In conclusion, we have presented the first calculations for the c-coefficients of the IMME for nuclei from $A = 42$ to $A = 54$, based on input from three state-of-the-art realistic nucleon-nucleon interactions and their pertinent shell-model effective interactions. The CSB contribution is almost independent of the order of renormalization in many-body perturbation theory, suggesting that the charge-symmetry breaking part of the interaction is, to a large extent, short-range in nature. In effective field theory, this might indicate two-pion, or even higher-order excitations that probe the short-range nature of the CSB interaction. In addition, we find that the three state-of-the art interactions yield different results, and are in disagreement. This suggests that either: 1) the charge-symmetry breaking in the nucleon-nucleon interaction is poorly known, 2) there is strong charge-symmetry breaking in the three-nucleon interaction, or 3) there are significant induced three-nucleon interaction arising from the renormalization procedure.

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