First principles calculations for coefficients of the isobaric mass multiplet equation in the fp shell

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We present the first calculations for the coefficients of the isobaric mass multiplet equation (IMME) for nuclei from $A = 42$ to $A = 54$ based input from various nucleon-nucleon interactions. We show that there is clear dependence on the short-ranged charge-symmetry breaking (CSB) part of the strong interaction. There is a significant variation in the CSB part between the commonly used CD-Bonn, N^{3}LO and Argonne V18 nucleon-nucleon interactions. All of them give a CSB contribution that is too large compared to experiment.

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Charge symmetry breaking in nuclear systems is due to the difference between the masses of up and down quarks, reflected in slightly differing masses between neutrons and protons [1]. This leads to the assumption of the near charge symmetry and isospin symmetry independence of nuclear forces. When electromagnetic effects are taken out, observables like bulk properties and excited states should be nearly charge independent. In order to more text will be added...

We have performed a series of shell-model calculations using the program BIGSTICK to compute the c-coefficients of the IMME for $1p0f$-shell nuclei with $42 \leq$ A ≤ 54. The pertinent effective interactions for the degrees of freedom of the $1p0f$ shell were derived using many-body perturbation theory, see for example Ref. [4]. The two-body matrix elements where computed in two steps, first by renormalizing the nuclear two-body interactions using both a G-matrix approach and the so-called V$_{lowk}$ method. As models for the nuclear interactions, we employed the N^{3}LO [5], the AV18 [6] and the CD-Bonn [7] interaction models. These interaction models allow for a breaking of isospin symmetry and charge symmetry and include the isotensor and isovector components of the strong interaction. The renormalized nucleon-nucleon interactions were computed using a harmonic oscillator basis with an oscillator energy $\hbar\omega = 10.5$ MeV with an effective Hilbert space defined the twelve first oscillator shells. The V$_{lowk}$ interactions were obtained with a cut-off parameter of $\Lambda = 2.1$ fm^{-1}. For the N^{3}LO and the CD-Bonn interactions, the Coulomb interaction was added after the renormalization process. The second step consisted in obtaining an effective interaction tailored to a small shell-model space. This was achieved using many-body perturbation theory up to third-order in the renormalized nucleon-nucleon interactions, including so-called folded diagrams [4]. All codes used to generate these interactions are available online, see Ref. [8]. The renormalization was performed 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), defined in terms of the $T = 1$ components of the pp, neutron-neutron (nn) and proton-neutron (pn) interactions via

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

$$v^{(1)} = v_{pp} - v_{nn},$$

and

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

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. The GX1A interaction was used instead

FIG. 1: (color online) Results for the CD-Bonn potential in 1st, up to 2nd and up to 3rd order. The black circles are the experimental data. The solid lines show the Coulomb contribution, and the dashed lines show the CSB contribution.

FIG. 2: (color online) 1st 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.

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. The expectation value of the Coulomb, isovector, and isotensor interactions are then computed to give the full energy for each state,

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

and the c-coefficient is then

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

The A-dependence was properly accounted for by scaling the Coulomb component by $\sqrt{\hbar\Omega(A)/10.5}$, while the isovector and isotensor interactions were assumed to have the same A-dependence as the GX1A interaction. For each A-value, $\hbar\Omega(A)$ was determined by reproducing the rms radius obtained from a Hartee-Fock calculation using the SKX Skyrme interaction.

Figure 1 shows the results CD-Bonn in first, second and third order. The contributions are divided into Coulomb (full lines) and CSB (dashed lines). The J-dependence of these two contribution is very different. The long-range Coulomb has a relatively flat J-dependence with only a small rise at $J = 0$. The CSB contribution at $A = 42$ shows a peak at $J = 0$ with a sharp drop towards $J = 2$ that is characteristic of a short-ranged interaction. for $A = 42$ $J = 6$ is the maximum spin (for $T = 1$) in the $1p0f$ model space. For higher A values this sharp drop at $J = 2$ is replaced by a linear drop to $J = 6$ due to configuration mixing. CSB is very small for $J = 8$ and 10. The experimental data is from the compilation [2]. For A=46 we use the results from Fig. 2 of [3].

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 results in an enhancement of the overlapping proton and neutron density distributions.

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

FIG. 4: (color online) 1st order calculations for N^{3}LO with the CSB part multiplied by 0.8 and compared to experiment. See caption to Fig 2.

The CSB contribution turns out to be almost order independent. The Coulomb contribution is almost the same in 1st and 2nd order but increases 10-20% in 3rd order. It is remarkable that the experimental data are in rather good agreement with the 3rd order Coulomb result. There does not seem to be a need for CSB even though this component is known to be important in the NN scattering data that is incorporated into the potential models.

Figure 2 shows the results for the three potential models in 1st order. This shows that the CSB contribution is model dependent. There could be two reasons for this. The NN potential inputs for CSB are different. Or if they are the same the short range correlation effects taken into account in the V$_{lowk}$ renormalization are different. The results with N^{3}LO is in best agreement with experiment.

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

Our work guides future investigations in directions. For better first principles calculations, one should understand the origin of the different CSB contributions from three potentials. In particular in the spirit of using nuclear data to constrain the NN and NNN potentials (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 1st order Coulomb plus CSB is already close to the data. We can make it almost perfect by taking 1st order Coulomb and adding 80% of the N^{3}LO CSB part. This is shown in Fig. 4. The largest deviation from experiment comes for $J = 2$ at A=42. However, $A = 42$ is just at the beginning of the $1p - 0f$ model space and it is well know that admixtures from core excitations from the $0s - 1d$ shell are very important especially for $J = 0$ and $J = 2$. For example, the 2^+ to 0^+ B(E2) value for ^{42}Ca is about 10 times larger in experiment than compared to theory. The experimental fall off from $J = 0$ to $J = 6$ in A=42 looks like calculation for A=46. The theoretical wavefunctions for A=42 are dominated by $(f_{7/2})^2$ configurations and the wavefunctions for $A = 54$ are dominated by $(f_{7/2})^{-2}$ configurations. These two configuration have the same spectra (except for a small mass dependence). Compared to $A = 42$ the J dependence observed for $A = 54$ is closer that expected for a these pure configurations.

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