Isospin-breaking interactions studied through mirror energy differences

M. A. Bentley,[1,*] S. M. Lenzi,[2] S. A. Simpson,[1] and C. Aa. Diget[1]
[1]*Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom*
[2]*Dipartimento di Fisica e Astronomia dell'Università and INFN, Sezione di Padova, I-35131 Padova, Italy*
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Background: Information on charge-dependent (i.e., isospin-non-conserving) interactions is extracted from excited states of mirror nuclei.
Purpose: Specifically, the purpose of the study is to extract effective isovector ($V_{pp} - V_{nn}$) interactions which, in general, can either be of Coulomb or nuclear origin.
Methods: A comprehensive shell-model description of isospin-breaking effects is used to fit data on mirror energy differences in the $A = 42$–54 region. The angular-momentum dependence of isospin-breaking interactions was determined from a systematic study of mirror energy differences.
Results: The results reveal a significant isovector term, with a very strong spin dependence, beyond that expected of a two-body Coulomb interaction.
Conclusions: The isospin-breaking terms that are extracted have a J dependence that is not consistent with the known CSB properties of the bare nucleon-nucleon interaction.

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I. INTRODUCTION

The charge symmetry of the nuclear force, the formal statement that $V_{pp} = V_{nn}$, is one of the fundamental building blocks of modern physics and led, in part, to the powerful concept of isospin in nuclear physics [1]. In the special case of a pair of mirror nuclei, where the number of pp interactions in one nucleus equals the number of nn interactions in the other, charge symmetry leads to remarkable symmetries in nuclear behavior with pairs of analog states characterized by virtually identical wave functions. Electromagnetic interactions lift the degeneracy of the analog states, but do not generally affect the underlying symmetry. It is well known, from nucleon-scattering data [2], that isospin symmetry is slightly broken, although the size of the charge-symmetry breaking (CSB) effect is sufficiently small for it to be considered negligible for most calculations of nuclear structure phenomena. However, in considering differences in behavior of analog states, such as mass differences between analog nuclei [Coulomb displacement energies (CDE)], consideration of CSB will become important. There have been suggestions (e.g., [3,4]) that CSB effects are responsible for the well-known Nolen-Schiffer anomaly [5] in which predictions of CDE failed to match experimental data, and CSB effects are routinely included in nuclear mass models where CDE are calculated (e.g., [6–9]).

However, the details of how CSB contributes to the *effective* two-body interaction in the nuclear medium, such as the J-dependent residual interactions in the shell model (where J is the angular-momentum coupling of a pair of nucleons), are not straightforward to establish, but are nevertheless important in studies relating to isospin symmetry in nuclei. This is especially the case for determination of the crucial isospin-mixing terms required in the modeling of super-allowed Fermi decays [10]—one of the most important applications of the concept of isospin in contemporary physics. In general, extracting detailed information on the effective $V_{pp} - V_{nn}$ (*isovector*) interaction can *only* be achieved through detailed analysis of analog states across a multiplet. To date, the approach was restricted to modeling of CDE (i.e., with nuclear binding energies as the input) and fitting to experimental data to extract sets of empirical isovector matrix elements (e.g., [11–13]). A complementary, potentially very sensitive, approach is to extract numerical information on isovector interactions from systematics of *excitation energies* of mirror nuclei, which are extremely sensitive to the angular-momentum (J) dependence of the interaction. In this paper we present such an analysis.

The present work is motivated by the large body of data that was obtained in the last two decades on differences in excitation energy between analog states in mirror nuclei [mirror energy differences (MED)] in the $f_{7/2}$ shell (e.g., [14–21]). There have been parallel efforts to develop a shell-model-based approach to reproduce the MED in terms of electromagnetic and other isospin-breaking effects (e.g., [15,16,22]). This was extremely successful in the $f_{7/2}$ shell—see recent reviews [14,23]. Out of this analysis has emerged a phenomenon, known as the $J = 2$ *anomaly*, in which it was found necessary to include in the model a significant isovector interaction, in addition to the two-body Coulomb interaction, for $J = 2$ couplings of $f_{7/2}$ particles [22,24]. This pointed initially to a CSB effect [22], though such an interpretation is clearly questionable without better information on the phenomenon.

A number of important questions arise out of the observation of the $J = 2$ anomaly, which are addressed here. Most important is the need to develop an understanding of the origin of the effect and how it relates, if at all, to the known CSB properties of the bare nucleon-nucleon interaction. It is also necessary to try to reconcile the $J = 2$ phenomenon to recent published work [25] that have indicated, through an analysis of CDE, the need for inclusion of an isospin-breaking term

*michael.bentley@york.ac.uk

of isovector origin at $J = 0$. Both these results, in which only *one* specific matrix element (for a particular coupling J) is considered, indicate that there is likely to be a strong J dependence of the isovector isospin-nonconserving effect, whatever its origin. It is in the study of the J dependence of these isovector effects that the use of excited states (i.e., MED) can yield particularly sensitive information, for the following reasons. First, the difference in energy between mirror nuclei is a purely isovector effect, with isoscalar and isotensor contributions canceling in the subtraction. Secondly, it is well known (e.g., [5,11]) that attempting to reproduce the difference between ground-state *binding energies* of mirror pairs (CDE, of the order of 10 MeV) in terms of isovector effects can be challenging, requiring very careful evaluation of the absolute sizes of monopole and multipole Coulomb terms, and their mass dependence; see, e.g., [11] for a comprehensive study. MED, however, are measured in relation to the ground state and are mainly sensitive to the angular-momentum dependence of these isovector phenomena, not their absolute magnitude. For example, it will be shown later in this paper that in a shell-model analysis, the MED are largely insensitive to the absolute values of isospin-non-conserving matrix elements, but directly dependent on the J dependence of these matrix elements.

The purpose of the analysis presented here, therefore, is to bring together the large body of MED data that have been gathered to date in the $f_{7/2}$ shell and evaluate them in the context of a single shell-model prescription with a fixed parametrization [14]. From this we seek to determine the J dependence of the isospin-nonconserving matrix elements required to reproduce the experimental data and establish the consistency of the effect as a function of mass and isospin. This was done through extracting effective isovector two-body interactions in the $f_{7/2}$ shell through fitting the shell model to the full set of experimental MED. It is demonstrated here that the additional isovector isospin-non-conserving interaction (beyond the two-body Coulomb term) required to account for the data is statistically significant, remarkably consistent across the shell, and has a clear and measurable J dependence.

II. MODEL AND PROCEDURE

The calculations used here are based entirely on the prescription of Ref. [14] which was shown to provide an extremely reliable description of MED in the $f_{7/2}$ region. In addition to the Coulomb interaction, it is the isovector part of the two-body interaction (i.e., $V_{pp} - V_{nn}$) which contributes to the MED (and breaks isospin). As introduced in Ref. [22], this is taken into account in the calculation of the MED, by including an additional operator V_B^J, to account for missing isovector effects beyond the usual two-body Coulomb interaction, such as CSB of the nucleon-nucleon interaction. It was long assumed, in the analysis of MED, that V_B would be close to zero if the electromagnetic effects are properly accounted for in the model. Nevertheless, additional isospin-breaking terms of this kind would need to be accounted for here, especially if they possessed a strong J dependence. Indeed, as stated earlier, it was found to be necessary [15,16,22,24] to consider a large $J = 2$ component for V_B. In fact, isovector terms of the order of 100 keV for two nucleons in the $f_{7/2}$ shell coupled to $J = 2$ have been used successfully in the previous analysis [14,22]. In addition to these *multipole* effects, MED are also sensitive to electromagnetic *monopole* effects such as shifts of single-particle energies and changes in radius or deformation as a function of spin. The shell-model prescription for the MED, described in Ref. [14] and based on the method introduced by Zuker *et al.* [22] consists for four "terms" each separately describing physical effects contributing to the MED. A calculation of the states of interest in each member of the mirror pair is performed, with each of these terms included, and the two calculations subtracted to determine the theoretical MED.

Term 1: Multipole Coulomb term. This term consists of the Coulomb interaction within the model space determined in a harmonic oscillator basis. It accounts for changes in Coulomb energy resulting from the recoupling of angular momentum J of pairs of protons with increasing excitation energy.

Term 2: Monopole single-particle term. This accounts for the fact that the relative single-particle shell-model energies, between different orbitals, is different for a proton or a neutron. Two effects are included: The first is the Coulomb energy stored in a single-proton orbital, because of the overlap of its wave function with the protons in the core. This varies with orbital angular momentum l and is accounted for using the prescription of Ref. [22]. The second is the electromagnetic spin-orbit interaction—a relativistic effect associated with the interaction between the spin moment of the nucleon and the Coulomb field of the nucleus with which it interacts [5]. These two contributions combine to yield differences between neutron and proton single-particle levels of up to around 100–200 keV, and these modifications were made directly to the single-particle levels used as input to the shell-model calculations.

Term 3: Monopole radial term. Changes in mean nuclear radii and/or deformation as a function of spin will contribute to the MED through changes in the bulk Coulomb energy from the difference in Z between the mirror pair. This is accounted for in the same way as Refs. [16,22] with the parametrization of Ref. [14], in which the total occupation of the $p_{\frac{3}{2}}$ orbit is tracked as a function of spin, as this orbital is expected to have a larger mean radius. The MED that results is proportional to the difference in Z between the mirrors.

Term 4: Isospin-breaking term. This term is the subject of the current paper, and represents any additional isospin breaking isovector term, beyond the usual two-body Coulomb interaction. It is accounted for by computing the expectation value of the V_B^J interaction and taking the difference between the two mirror nuclei. As introduced in Ref. [22], a single V_B^J matrix element was used to date, in the $T = 1$ channel, for two nucleons coupled to angular momentum J. As stated earlier, it was found that a strength of 100 keV for $J = 2$ couplings was required to properly account for the data, and this was included in the standard parametrization of Ref. [14]. The model, based on these four terms, has proved to be extremely successful in reproducing the MED results, without any adjustment of parameters between nuclei; see Ref. [14] for details.

In the current work, we seek to extract best-fit values of V_B^J, and so a modified approach is necessary. We determine the theoretical MED for a given state α—an analog state in the two mirror nuclei—using

$$\mathrm{MED}^{\mathrm{th}}_{\mathrm{tot}}(\alpha) = \mathrm{MED}^{\mathrm{th}}_{C}(\alpha) + \mathrm{MED}^{\mathrm{th}}_{B}(\alpha). \quad (1)$$

$\mathrm{MED}^{\mathrm{th}}_{C}(\alpha)$ contains the contribution to the MED of Terms 1–3, as described above, which account for the Coulomb multipole and radial effects and the contributions from the single-particle terms. $\mathrm{MED}^{\mathrm{th}}_{C}(\alpha)$ can therefore be thought of as containing all the electromagnetic effects in the model. The second term in Eq. (1) represents the contribution to the MED of the additional isovector terms V^J_B. Here, this is determined using a perturbative approach, as follows:

$$\mathrm{MED}^{\mathrm{th}}_{B}(\alpha) = \sum_{J=0,2,4,6} \Delta c^J_B(\alpha) V^J_B, \quad (2)$$

where $c^J_B(\alpha)$ is the expectation value of the operator,

$$\left[(a^\dagger a^\dagger)^{T=1,J}_{\pi f_{7/2}} (aa)^{T=1,J}_{\pi f_{7/2}}\right],$$

which provides a coefficient that effectively "counts" pairs of $f_{7/2}$ protons coupled to angular momentum J. $\Delta c^J_B(\alpha)$ is the difference of this value between the analog states of the mirror pair, relative to the ground state. The restriction of V^J_B to the $f_{7/2}$ shell is a pragmatic one—the wave functions are dominated by $f_{7/2}$ configurations, and the changes in occupation of the $f_{7/2}$ levels as a function of spin are small for the states concerned. Hence, the dominant multipole effects will be associated with the $f_{7/2}$ orbital.

The ANTOINE shell-model code was used [26], with the KB3G interaction [27], and the calculations are performed for nuclei in the range $A = 42$–54, i.e., ensuring that there are at least two active $f_{7/2}$ particles and holes in the wave functions, because the sd shell is closed. The full fp valence space is exploited for all nuclei, with no restrictions on the total number of excitations from $f_{7/2}$ to the higher-lying fp orbits. Large-scale shell-model calculations in this basis have been shown (e.g., [27]) to reproduce spectroscopic data on excitation energies and transition strengths in the upper $f_{7/2}$ shell with excellent reliability.

The data points fitted corresponded to all the known MED values for all yrast natural-parity excited states of mirror pairs in the $A = 42$–54 range (i.e., from two particles to two holes in the $f_{7/2}$ shell). This corresponds to 17 pairs of nuclei and 93 excited analog states. The data used are listed in Table I, and labeled by A, J^π, and T. The latter value corresponds to the value of $|T_z| = |N - Z|/2$ because the analog states concerned all have the lowest possible isospin. The references used for the MED data are also quoted. The only data points excluded from the fit are states beyond the terminating spin for the $f_{7/2}$ space. The value of $\mathrm{MED}^{\mathrm{th}}_{C}$ (i.e., the model without the inclusion of the V^J_B terms, is shown in Table I. All the data points are published with the exception of new results on the excited analog states of the odd-odd mirror pair ^{52}Co $-^{52}$Mn [35] (seven excited states with $J^\pi = 4^+ - 11^+$) and the $J^\pi = \frac{3}{2}^-$ state in ^{53}Ni/^{53}Mn [36].

The coefficients V^J_B were then allowed to vary freely, for the $f_{7/2}$ interactions only, and the best fit was obtained. Here, the experimental errors on MED are small compared with the theory "error," denoted σ_{th}. To arrive at the final errors on V^J_B,

TABLE I. The experimental and theoretical MED data used in this analysis. Each row corresponds to a pair of analog states J^π of isospin $T = |T_z|$, in a mirror pair of mass number A with proton numbers $Z = \frac{A}{2} \pm T$. The theoretical MED values have been obtained using the method described in the text, with isospin-non-conserving parameters V^J_B derived from the fit; see numbers highlighted in bold in Table II.

Data points			Model (keV)			Expt. (keV)
A,T	J^{π} [a]	Ref.	$\mathrm{MED}^{\mathrm{th}}_C$	$\mathrm{MED}^{\mathrm{th}}_B$	$\mathrm{MED}^{\mathrm{th}}_{\mathrm{tot}}$	$\mathrm{MED}_{\mathrm{expt.}}$
42, 1	0^+	[28]	g.s.	g.s.	g.s.	0
42, 1	2^+		−98	97	−1	31
42, 1	4^+		−130	75	−55	−76
42, 1	6^+		−143	55	−88	−146
43, $\frac{1}{2}$	$\frac{7}{2}^-$	[29]	g.s.	g.s.	g.s.	0
43, $\frac{1}{2}$	$\frac{11}{2}^-$		−54	43	−11	28
43, $\frac{1}{2}$	$\frac{15}{2}^-$		−78	29	−49	−35
43, $\frac{1}{2}$	$\frac{19}{2}^-$		−89	16	−73	−57
44, 1	2^+	[30]	g.s.	g.s.	g.s.	0
44, 1	4^+		−11	−11	−22	−15
44, 1	5^+		−34	6	−28	17
45, $\frac{1}{2}$	$\frac{3}{2}^-$	[31]	−18	15	−3	21
45, $\frac{1}{2}$	$\frac{5}{2}^-$		−8	19	11	16
45, $\frac{1}{2}$	$\frac{7}{2}^-$		g.s.	g.s.	g.s.	0
45, $\frac{1}{2}$	$\frac{9}{2}^-$		−6	−9	−15	−29
45, $\frac{1}{2}$	$\frac{11}{2}^-$		−3	−12	−15	−6
45, $\frac{1}{2}$	$\frac{13}{2}^-$		18	−13	5	−30
45, $\frac{1}{2}$	$\frac{15}{2}^-$		5	−20	−15	−11
45, $\frac{1}{2}$	$\frac{17}{2}^-$		57	−9	48	3
45, $\frac{1}{2}$	$\frac{19}{2}^-$		75	−31	44	48
45, $\frac{1}{2}$	$\frac{23}{2}^-$		33	−7	26	44
45, $\frac{1}{2}$	$\frac{27}{2}^-$		26	−23	3	16
46, 1	0^+	[32]	g.s.	g.s.	g.s.	0
46, 1	2^+		−43	22	−21	2
46, 1	4^+		−69	36	−33	−23
46, 1	6^+		−44	23	−21	−73
46, 1	8^+		−44	30	−14	−80
46, 1	10^+		−22	31	9	−65
46, 1	12^+		−10	1	−9	−55
47, $\frac{1}{2}$	$\frac{3}{2}^-$	[15]	g.s.	g.s.	g.s.	g.s.
47, $\frac{1}{2}$	$\frac{5}{2}^-$		18	−5	13	10
47, $\frac{1}{2}$	$\frac{7}{2}^-$		26	7	33	28
47, $\frac{1}{2}$	$\frac{11}{2}^-$		12	28	40	37
47, $\frac{1}{2}$	$\frac{15}{2}^-$		−3	44	41	39
47, $\frac{1}{2}$	$\frac{19}{2}^-$		−42	38	−4	7
47, $\frac{1}{2}$	$\frac{23}{2}^-$		−36	26	−10	4
47, $\frac{1}{2}$	$\frac{25}{2}^-$		−25	21	−4	−20
47, $\frac{1}{2}$	$\frac{27}{2}^-$		0	12	12	30

TABLE I. (*Continued.*)

Data points			Model (keV)			Expt. (keV)
A,T	$J^{\pi\,a}$	Ref.	MED_C^{th}	MED_B^{th}	$\text{MED}_{\text{tot}}^{\text{th}}$	$\text{MED}_{\text{expt.}}$
47, $\frac{1}{2}$	$\frac{31}{2}^-$		−31	30	0	21
48, 1	4^+	[17]	g.s.	g.s.	g.s.	g.s.
48, 1	5^+		−4	8	4	3
48, 1	6^+		23	−2	21	10
48, 1	7^+		35	−2	33	29
48, 1	8^+		16	0	16	0
48, 1	9^+		30	3	33	28
48, 1	11^+		39	−1	38	36
48, 1	13^+		42	8	50	49
49, $\frac{1}{2}$	$\frac{5}{2}^-$	[33]	g.s.	g.s.	g.s.	g.s.
49, $\frac{1}{2}$	$\frac{7}{2}^-$		10	−14	−4	−10
49, $\frac{1}{2}$	$\frac{9}{2}^-$		13	−29	−16	−25
49, $\frac{1}{2}$	$\frac{11}{2}^-$		20	−31	−11	−22
49, $\frac{1}{2}$	$\frac{13}{2}^-$		49	−48	1	−20
49, $\frac{1}{2}$	$\frac{15}{2}^-$		72	−51	21	−3
49, $\frac{1}{2}$	$\frac{17}{2}^-$		110	−42	68	29
49, $\frac{1}{2}$	$\frac{19}{2}^-$		126	−41	85	77
49, $\frac{1}{2}$	$\frac{23}{2}^-$		117	−23	94	91
49, $\frac{1}{2}$	$\frac{27}{2}^-$		73	−17	56	70
49, $\frac{1}{2}$	$\frac{31}{2}^-$		114	−36	78	20
49, $\frac{3}{2}$	$\frac{7}{2}^-$	[20]	g.s.	g.s.	g.s.	g.s.
49, $\frac{3}{2}$	$\frac{11}{2}^-$		−26	28	2	4
49, $\frac{3}{2}$	$\frac{15}{2}^-$		−39	25	−14	-69
50, 1	0^+	[16]	g.s.	g.s.	g.s.	g.s.
50, 1	2^+		−22	0	−22	−18
50, 1	4^+		0	−21	−21	−29
50, 1	6^+		29	−13	16	−4
50, 1	8^+		67	3	70	42
50, 1	10^+		27	−20	7	28
50, 1	11^+		35	−8	27	45
51, $\frac{1}{2}$	$\frac{5}{2}^-$	[34]	g.s.	g.s.	g.s.	g.s.
51, $\frac{1}{2}$	$\frac{7}{2}^-$		4	14	18	16
51, $\frac{1}{2}$	$\frac{9}{2}^-$		−25	31	6	6
51, $\frac{1}{2}$	$\frac{11}{2}^-$		−2	34	32	27
51, $\frac{1}{2}$	$\frac{13}{2}^-$		-57	45	−12	−7
51, $\frac{1}{2}$	$\frac{15}{2}^-$		-25	46	21	21
51, $\frac{1}{2}$	$\frac{17}{2}^-$		−121	11	−110	−94
51, $\frac{1}{2}$	$\frac{19}{2}^-$		−93	42	−51	−45
51, $\frac{1}{2}$	$\frac{21}{2}^-$		−50	14	−36	−35
51, $\frac{1}{2}$	$\frac{23}{2}^-$		−10	19	9	17
51, $\frac{1}{2}$	$\frac{27}{2}^-$		32	37	69	90
51, $\frac{3}{2}$	$\frac{7}{2}^-$	[21]	g.s.	g.s.	g.s.	g.s.

TABLE I. (*Continued.*)

Data points			Model (keV)			Expt. (keV)
A,T	$J^{\pi\,a}$	Ref.	MED_C^{th}	MED_B^{th}	$\text{MED}_{\text{tot}}^{\text{th}}$	$\text{MED}_{\text{expt.}}$
51, $\frac{3}{2}$	$\frac{9}{2}^-$		17	−55	−38	−36
51, $\frac{3}{2}$	$\frac{11}{2}^-$		71	−60	11	15
51, $\frac{3}{2}$	$\frac{15}{2}^-$		144	−51	93	102
52[b], 1	See [35]		See Ref. [35]			See Ref. [35]
52, 2	0^+	[21]	g.s.	g.s.	g.s.	g.s.
52, 2	2^+		42	−74	−32	−37
52, 2	4^+		78	−89	−11	15
52, 2	6^+		149	−44	105	133
53, $\frac{1}{2}$	$\frac{7}{2}^-$	[24]	g.s.	g.s.	g.s.	g.s.
53, $\frac{1}{2}$	$\frac{9}{2}^-$		47	−41	6	−1
53, $\frac{1}{2}$	$\frac{11}{2}^-$		83	−42	41	28
53, $\frac{1}{2}$	$\frac{13}{2}^-$		113	−29	84	85
53, $\frac{1}{2}$	$\frac{15}{2}^-$		125	−27	98	118
53, $\frac{1}{2}$	$\frac{17}{2}^-$		119	−13	106	110
53, $\frac{1}{2}$	$\frac{19}{2}^-$		130	−13	117	138
53[b], $\frac{3}{2}$	$\frac{3}{2}^-$	[36]	See Ref. [36]			See Ref. [36]
53, $\frac{3}{2}$	$\frac{5}{2}^-$	[20]	10	−70	−60	−58
53, $\frac{3}{2}$	$\frac{7}{2}^-$		g.s.	g.s.	g.s.	g.s.
53, $\frac{3}{2}$	$\frac{11}{2}^-$		56	−41	15	15
54, 1	0^+	[19]	g.s.	g.s.	g.s.	g.s.
54, 1	2^+		68	−81	−13	−16
54, 1	4^+		129	−63	66	82
54, 1	6^+		143	−47	96	122

[a]In the quoted literature, some of the J^π values are listed in parentheses where assignments were made on the basis of mirror symmetry arguments rather than spectroscopic measurement. For the sake of clarity, the parentheses are omitted here.
[b]Eight of the MED data points included in the fit, and the associated theoretical calculations, are not yet published and so have not been explicitly listed in the table. These are the $J^\pi = \frac{3}{2}^-$ state in ^{53}Ni and seven states in ^{52}Co with $J^\pi = 4^+ - 11^+$. Details are found in Refs. [35,36].

σ_{th} was adjusted, for each fit, such that $\sqrt{2\chi^2} \approx \sqrt{2n_d - 1}$ where n_d is the number of degrees of freedom. For the fit across the $A = 42$–54 region, for example, $\sigma_{\text{th}} \approx 23$ keV.

III. RESULTS

The results of fitting Eq. (1) to the experimental data are shown in Table II, for three ranges of nuclei in the $f_{7/2}$ shell, corresponding to, approximately, the full $f_{7/2}$ shell ($A = 42$–54), the top two-thirds of the shell ($A = 47$–54), and the top third ($A = 51$–54). This was done as it is known that the reliability of the model calculation in this space, and with this interaction, improves towards the top of the $f_{7/2}$ shell. Hence

TABLE II. The isospin-breaking matrix elements, V_B^J, for $f_{7/2}$ pairs, extracted from the fits for various mass ranges (see text). The final columns indicate the final rms deviation between the data and the model (using the fitted parameters) compared with the calculations assuming $V_B^J = 0$.

Range	$f_{7/2}$ matrix elements V_B^J (keV)				rms deviation	
	V_B^0	V_B^2	V_B^4	V_B^6	fit	No V_B
One-parameter fit						
$A = 42$–54	–	68(6)	–	–	32	41
$A = 42$–54	−79(6)	–	–	–	26	41
$A = 47$–54	–	71(5)	–	–	27	38
$A = 47$–54	−83(5)	–	–	–	22	38
$A = 51$–54	–	61(3)	–	–	28	40
$A = 51$–54	−71(3)	–	–	–	23	40
Full fit						
$A = 42$–54	−79(16)	25(13)	1(12)	−19(12)	23	41
$A = 47$–54	−56(15)	46(11)	9(10)	2(11)	16	38
$A = 51$–54	13(16)	82(10)	64(11)	39(11)	9	40
Full fits: centroid-subtracted						
$A = 42$–54	**−72(7)**	**32(6)**	**8(6)**	**−12(4)**	23	41
$A = 47$–54	−66(7)	36(5)	−1(5)	−8(4)	17	38
$A = 51$–54	−41(6)	28(3)	10(4)	−15(2)	18	40

these ranges were chosen to examine how sensitive the results are to the different regions of the shell.

Initially, fits were performed allowing only one of the four possible V_B^J terms to vary, keeping the other terms fixed at zero. The results are listed in the one-parameter fit section of Table II, and the results listed are those for fits where only the term at $J = 2$ or $J = 0$ (i.e., V_B^2 and V_B^0) was allowed to vary. It is immediately clear that either a large positive $J = 2$ term, or a large negative $J = 0$ term emerge from these results. This is consistent across all the three regions. The r.m.s. deviation from the data for the fits with, and without, the inclusion of the V_B terms are shown in the final two columns of Table II. The r.m.s. deviation improves with the inclusion of the terms. It is noteworthy that there is not very much difference in the fit quality following the addition of a positive $J = 2$ term, or a negative $J = 0$ term, although the latter seems marginally favored. The key point, however, seems to be that the best fit is obtained when the $J = 2$ term has a significantly more positive value than the $J = 0$ term, by 70–80 keV.

Next, fits were performed where all four terms were allowed to vary freely. An immediate point to note from our analysis is that the four terms appear to be strongly correlated. This is a natural consequence of the fact that MED are largely insensitive to the absolute values of the isovector multipole terms and, at least for V_B^J values of the order of ±100 keV, the fit quality here depends on the J dependence of the V_B^J values included. The r.m.s. deviation improves in all ranges, when all parameters are included.

The four-parameter fits again clearly indicate, in all ranges, that a positive rise from V_B^0 to V_B^2 is required, now at around 100 keV. It is now also clear that a better fit is obtained, in all ranges, when the values of V_B^4 and V_B^6 are also more positive than V_B^0. The comparison of the r.m.s. deviation values also indicates that the fit improves dramatically as more restricted ranges of nuclei at the upper end of the shell are considered. This may not be surprising as it is well known that in the upper part of the $f_{7/2}$ shell, the fp-shell space and KB3G interaction combine to give an excellent description of nuclear properties in terms of energies, transition rates, GT strengths, and nuclear moments (see, e.g., [27,37,38])—and nuclei near ^{56}Ni are especially well described [39]. In the lower part of the shell, the missing particle-hole excitations from the sd shell reduces the reliability of the model.

The difference between the absolute values of the three sets of fits, shown in the central section of Table II, is not meaningful, as discussed above. It is more convenient, therefore, to plot these values relative to a *centroid* which, for a two-body multipole interaction with matrix elements V^J can be written,

$$V^{\mathrm{cent}} = \frac{\sum_J (2J+1)V^J}{\sum_J (2J+1)}. \tag{3}$$

In the final section of Table II the centroid-subtracted values, $V_B^J - V_B^{\mathrm{cent}}$ are listed. The errors on the centroid-subtracted values have been calculated accounting fully for the correlations between the parameters. The reduced error bars result from the fact that, as expected, the correlation between the centroid-subtracted parameters is much reduced. For example, the $V_B^0 - V_B^2$ correlation coefficient for the full fit in the $A =$ 42–54 range, changes from 0.86 to 0.21 once the centroid is subtracted. We see immediately that all three fits have a very similar J dependence, relative to a centroid. The r.m.s. deviation for these centroid-subtracted values are largely unchanged, except for the uppermost part of the shell, again highlighting that there is little sensitivity in the MED to the absolute values of the matrix elements. The values in bold in Table II (the fits across the whole $f_{7/2}$ shell, with the centroid subtracted) are therefore taken as the definitive values from this analysis, and used as the key result for the purpose of this paper.

The results of the full four-parameter fits, with centroid subtraction, are shown in Fig. 1(a). The results for the three ranges are clearly consistent, and the J dependence does not seem dependent on how much of the $f_{7/2}$ shell is included in the analysis. Having established these four best-fit parameters for V_B^J, the individual isospin-non-conserving contribution, $\mathrm{MED}_B^{\mathrm{th}}$, can be determined using these parameters for each of the 93 states. These values are listed in Table I, along with the total resulting total theoretical MED, for all states.

The fit results can also be examined as a function of isospin and location in the shell, and so fits were performed both for individual mirror pairs and for pairs of specific isospin T. Because of small numbers of data points following this restriction, it is not possible to perform a full fit, hence either the V_B^2 or V_B^0 term can be used, as this accounts for the most significant effect. Figure 2(a) shows the extracted V_B^0 term for each of the 17 mirror pairs individually in the shell. For each of these, the fit is compared to the value [solid line] and error [dashed line] for the fit of V_B^0 across the whole shell. Across

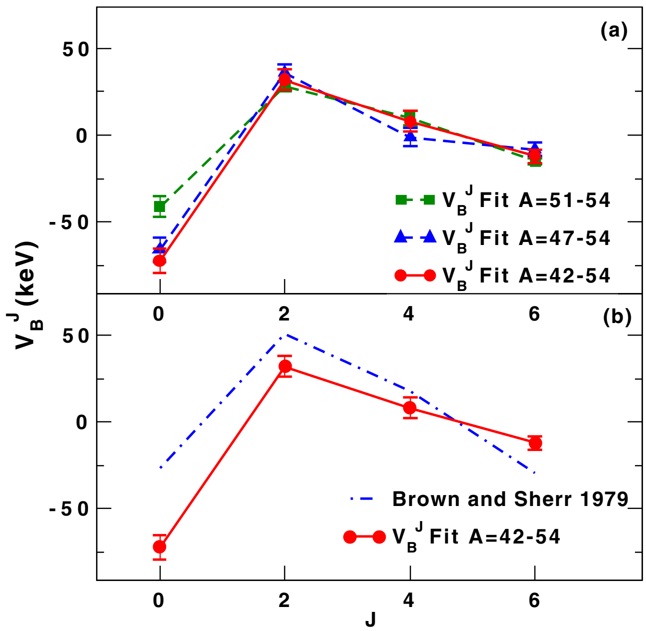

FIG. 1. (Color online) (a) The centroid-subtracted V_B^J coefficients in the $f_{7/2}$ shell derived from the fits presented in this paper; see text for details. Fits across three mass ranges are shown: $A = 42$–54 (red circles), $A = 47$–54 (blue triangles), and $A = 51$–54 (green squares). (b) The results of the fit across the whole shell, $A = 42$–54 [red circles, same data as (a)], compared with (blue dot-dashed line) the results of Ref. [11] based on a CDE analysis.

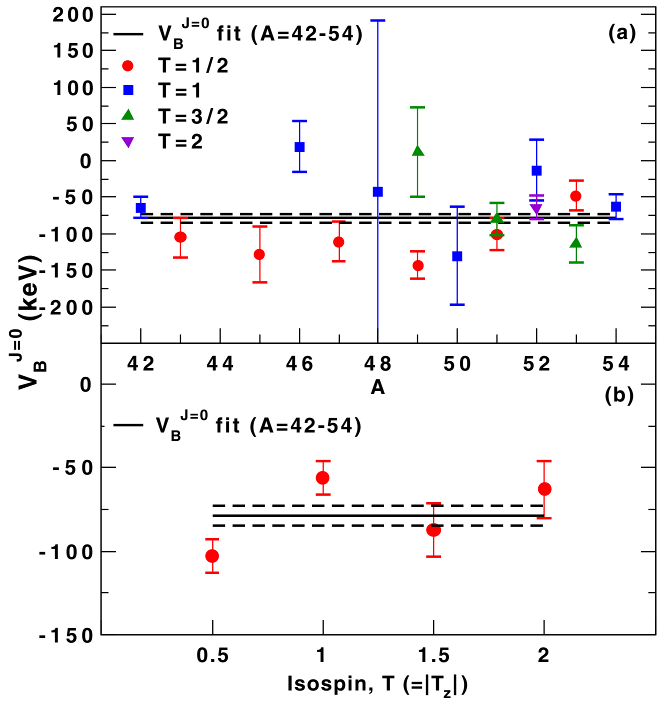

FIG. 2. (Color online) The extracted value of V_B^0 from a single-parameter fit for (a) each mirror pair individually, with different symbols and colors corresponding to the isospin (T) of the analog states, and (b) for sets of mirror pairs grouped according to the isospin $T = |T_z| = \Delta Z/2$. The best-fit value of $V_B^0 = -79(6)$ keV, from a single-parameter fit across the whole shell, is indicated in (a) and (b), and $\sigma_{\rm th} = 23$ keV was assumed. In (a), the data point of $-440(210)$ for $T = 1$, $A = 44$, for which there are only two data points, is not included in the plot for clarity.

the mass range, the value of V_B^0 is consistently negative and largely consistent with the whole-shell value of $-79(6)$ keV, with no obvious trend with $A(Z)$. The large error for $T = 1$, $A = 48$ arises from the fact that, as was shown in Ref. [17], cross-conjugate symmetry within the $f_{7/2}$ shell means that multipole effects of any origin make very little contribution to the MED for a mirror pair with $A = 48$. The fitted V_B^0 values are also insensitive to the value of the isospin of the analog states, as shown in Fig. 2(b). Monopole contributions to the MED are expected to scale directly with ΔT_Z (and hence T) and so this analysis points firmly toward the effect identified as being associated with the two-body interaction.

The effect of the inclusion of the V_B^J terms is shown in Fig. 3 which shows MED data for four example mirror pairs with a range of masses and isospin. The dashed lines show the MED results using only the first term in Eq. (1), i.e., with no V_B^J terms. The solid line shows the effect of including the best-fit, centroid-subtracted values of $V_B^{0,2,4,6}$. The need for inclusion of the isovector V_B^J terms in the interaction is compelling.

IV. DISCUSSION

The data in Table II show that a positive isovector V_B term of around 70 keV, for $J = 2$ couplings in the $f_{7/2}$ shell yields an improved agreement with the experimental data. This effect, previously known as the $J = 2$ anomaly, was well established in a number of recent papers, e.g., [14,19,21]. However, Table II also shows clearly that a *negative* V_B term of around 80 keV, for $J = 0$ couplings, has essentially the same effect. This is in contrast to the conclusions drawn from analysis of the ^{54}Ni/^{54}Fe ($T = 1$) and ^{52}Ni/^{52}Cr ($T = 2$) mirror pairs [19,21] in which some states near the band termination seemed to favor the $J = 2$ solution over the $J = 0$ one. However, the more complete fit here, which includes all 93 published analog states in the shell, indicates that there is little difference between them, when the whole shell is considered. This confirms the key result, i.e., that the V_B value for the $J = 2$ coupling is significantly more positive than the $J = 0$ value. When all four V_B terms are included in the fit, a rise of about 100 keV from $J = 0$ to $J = 2$ is observed, with an additional J dependence identified for the $J = 4$ and $J = 6$ coupling.

As stated earlier, information on the two-body isovector interaction can be extracted from nuclear masses through shell-model predictions of the Coulomb displacement energies (CDE)—differences in *total* binding energy between isobaric analog states in neighboring nuclei. This was done in the $f_{7/2}$ shell in 1979 by Brown and Sherr [11] using only a single-j shell-model calculation in which all the isovector and isotensor interactions were allowed to vary. The extracted isovector ($V_{pp} - V_{nn}$) interactions, having had the Coulomb part (V_C^J) subtracted, were -31 keV, 46 keV, 13 keV, -34 keV for the $J = 0,2,4$, and 6 couplings, respectively. These numerical values are equivalent to the V_B^J terms extracted here.

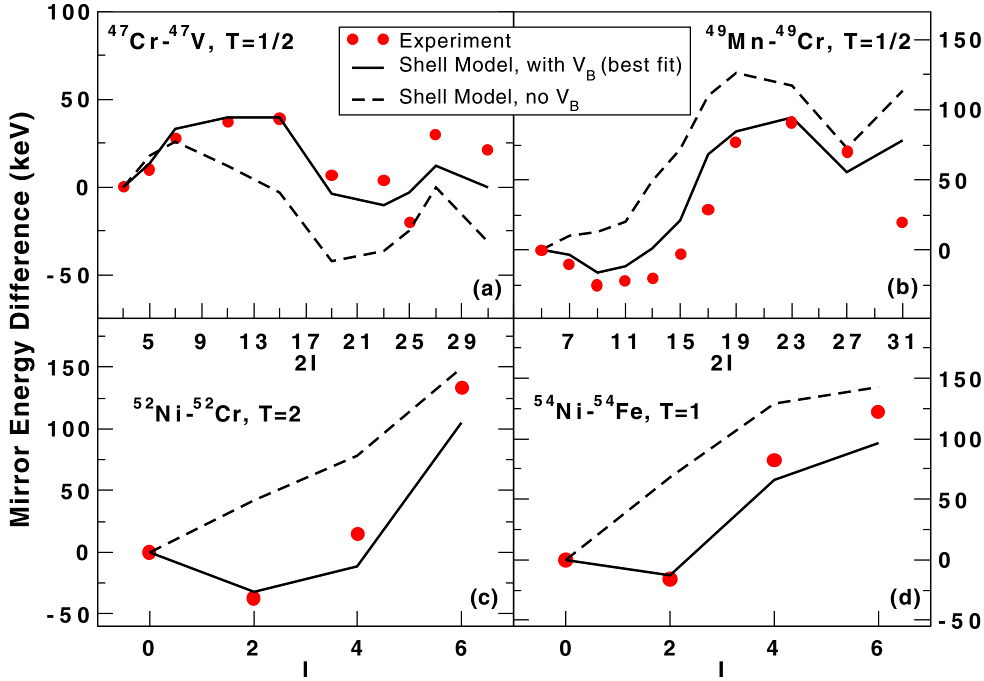

FIG. 3. (Color online) The experimental and predicted mirror energy differences for four mirror pairs in the $f_{7/2}$ shell of various masses and isospins as a function of total angular momentum I. The dashed line shows the result of the first term of Eq. (1) and the solid line shows the full calculation including the best-fit V_B^J parameters shown in bold in Table II.

The values from Brown and Sherr [11], now with the centroid subtracted, are plotted using the dot-dashed line in Fig. 1(b), and are compared with the results of the current work. In comparing these two sets of results, it is important to note that Brown and Sherr fitted absolute binding energies and our work fits MED data (which only involve *excitation energy*). Thus the two approaches are complementary and, moreover, there is almost no overlap of the data sets used. Of course, the shell-model interaction and valence space are now much more developed. Nevertheless, the agreement between these two independent approaches, especially the detail of the J dependence, is remarkable, and the same effect is obviously at play.

The magnitude of the variation of the V_B^J terms is significant. For example, for $f_{7/2}$ particles re-coupling from $J = 0$ and $J = 2$, the change in V_B is larger than (and the opposite sign to) the change in the two-body Coulomb interaction. The key point therefore is that the total *isovector* interaction ($V_{pp} - V_{nn} = V_C^J + V_B^J$) has a J dependence that is not consistent with a two-body Coulomb interaction alone.

In the recent shell-model study of Kaneko *et al.* [25], isospin-non-conserving nuclear interactions were considered in detailed systematics of CDE across a range of nuclei. Only $J = 0$ isospin-non-conserving terms were considered in that work, and it was found that for the $f_{7/2}$ shell an isovector term of -100 keV (i.e., protons more attractive than neutrons) was required to explain some of the systematics. In effect, including an isovector term of -100 keV only for $J = 0$, and not for $J = 2,4,6$, introduces some J dependence of the same magnitude as extracted here. The analysis of Ref. [25] does not specifically consider the J dependence but is presumably more sensitive to the absolute values of the isovector terms. Nevertheless, there are therefore strong indications that these two independent approaches, using different experimental information, are highlighting some aspects of the same phenomenon.

An isovector, isospin-non-conserving interaction can be either Coulomb or nuclear in origin, and any J-dependent effects associated with charge-symmetry breaking of the nuclear interaction might be expected to appear in the extracted V_B^J term. In nucleon-nucleon scattering analysis [2] the $^1S_0$ scattering lengths are -17.3 ± 0.4 fm for pp and -18.8 ± 0.3 fm for nn, having corrected for the electromagnetic effects, thus indicating that the nn interaction is slightly stronger in the $^1S_0$ channel. Henley [40] estimated that for potentials of the Yukawa type, the fractional difference in scattering length corresponds to $\sim$14 times the fractional difference in effective nucleon-nucleon potential. Thus, we find that V_{nn} is approximately $0.6 \pm 0.2\%$ stronger than V_{pp}. Even though this is only an estimate, we can consider how this might translate into a shell-model effective interaction for $f_{7/2}$ particles. If we were to restrict this CSB contribution to the $J = 0$ channel, then for the KB3G interaction, this corresponds to an isovector term of $V_B^0 \sim +11$ keV (and zero for the $J = 2,4,6$ matrix elements). This introduces only a weak J dependence and, crucially, of opposite sign to our observation. If the CSB effect were introduced proportionally into the other matrix elements, as was done in previous work (e.g., [6,12]), the net effect would be even smaller. It is therefore clear that the J dependence we observe here is not consistent, neither in sign nor magnitude, with the known CSB observations from free-nucleon scattering.

This analysis points to other electromagnetic contributions missing in the model. Attempts have been made, for example, at a re-normalization of the two-body Coulomb matrix elements to account for missing core interactions [16] but the required J dependence could not be reproduced. In general terms, we must also consider how in-medium effects modify the effective nucleon-nucleon interaction in such a way that isovector effects might be introduced. For example, it was long predicted (e.g., [41]) that the Coulomb-induced difference in the effective total potential depths for protons and neutrons yields a different pairing strength from the different nucleon relative momenta. Thus, the possible influence of this kind of phenomenon on, for example, monopole and quadrupole pairing interactions, needs to be investigated.

In summary, we have presented a systematic analysis of isospin-non-conserving interactions from mirror energy differences. The results reveal that a consistently large set of isospin-non-conserving interactions are required in the $f_{7/2}$ shell and that these have an exceptionally strong J dependence. The J dependence of the isovector interactions extracted is not consistent with charge-symmetry-breaking interactions observed in free nucleon-nucleon scattering. Theoretical work that examines Coulomb-induced in-medium effects, as well as consideration of fundamental CSB interactions, is required to investigate the source of the very large effects seen.

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