Complete $0\hbar\omega$ Calculations of Gamow-Teller Strengths for Nuclei in the Iron Region

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(Received 3 February 1994)

Gamow-Teller strengths for selected nuclei in the iron region ($A \sim 56$) have been investigated via shell-model Monte Carlo calculations with realistic interactions in the complete fp basis. Results for all cases show significant quenching relative to single-particle estimates, in quantitative agreement with (n,p) data. The $T = 0$ residual interaction and the $f_{7/2}$-$f_{5/2}$ spin-orbit splitting are shown to play major roles in the quenching mechanism. Calculated $B(E2, 2_1^+ \to 0_1^+)$ values are in fair agreement with experiment using effective charges of $e_p = 1.1e$ and $e_n = 0.1e$.

PACS numbers: 21.10.Pc, 21.60.Cs, 21.60.Ka, 27.40.+z

Gamow-Teller (GT) transitions from the ground states of medium and heavy nuclei are important in both presupernova neutronization [1] and double β decay [2]. These transitions can be investigated experimentally through electron-capture–β-decay studies and through intermediate-energy (p,n) and (n,p) reactions. A longstanding puzzle has been that experiments [3] systematically yield total GT strengths several times smaller than single-particle estimates.

A number of explanations have been proposed for the observed quenching of the GT strength, including a depletion of strength by Δ excitations at about 300 MeV [4] and a reduction of the axial coupling constant to $g_A \cong 1$ in nuclear matter [5]. A less exotic cause would be the presence of multiparticle, multihole configurations, and in light nuclei, where complete $0\hbar\omega$ shell model calculations are possible, the GT strength generally decreases as the model space is enlarged [6]. However, an exponentially increasing computational difficulty limits similar studies in nuclei in mid-fp shell to the $2p$-$2h$ level, where calculations show a quenching only about half of that observed experimentally.

While full $0\hbar\omega$ calculations apparently do not recover the complete quenching of the GT strength for sd-shell nuclei [5], there are phenomenological indications that a complete treatment of the fp shell is both necessary and sufficient to describe GT quenching in the iron region [7], and a first calculation of ^{54}Fe in such a basis with a realistic interaction resulted in a quenching significantly larger than truncated estimates and comparable to experiment [8]. The purpose of this Letter is to present calculations for several nuclei in the iron region (^{54}Cr, ^{55}Mn, ^{54,56}Fe, and ^{56,58}Ni) aimed at exploring the universality of this quenching and its dependence upon the effective interaction.

Our calculations are performed in the complete set of $0f_{7/2,5/2}$-$1p_{3/2,1/2}$ configurations using the Monte Carlo (MC) methods described in Refs. [8,9]. As in previous truncated shell-model calculations of iron region nuclei [6], we have used for the bulk of our studies the Brown-Richter (BR) Hamiltonian [10] fitted to lower fp-shell nuclei, but we have also calculated ^{54}Fe with the Kuo-Brown (KB) interaction [11]. Calculations for ^{54,56}Fe, ^{56,58}Ni, and ^{54}Cr were performed at $\beta = 2$ MeV^{-1} and 32 time slices (both of which were checked to be sufficiently large to guarantee cooling to the ground state), while our ^{55}Mn results are at $\beta = 1$ MeV^{-1} and 16 time slices, evaluated using a weighted average of a ^{54}Cr ensemble. Each calculation involved some 3300 Monte Carlo samples at each of six values of the coupling constant g equally spaced between -1 and 0; extrapolation to the physical case ($g = 1$) was done by the method described in Ref. [8].

In Table I we give results for selected static observables. When the calculated binding energies are corrected for the Coulomb energy using the semiempirical formula $E_c = 0.717(Z^2/A^{1/3})(1 - 1.69/A^{2/3})$ MeV [12], all nuclei are overbound by about 1.5–2 MeV except ^{56}Ni (~ 3 MeV) and ^{58}Ni (~ 0 MeV). The $B(E2, 2_1^+ \to 0_1^+)$ values calculated with bare nucleon charges are typically within a factor of 2 of the experimental values if we assume that this transition saturates the total $0\hbar\omega$ strength. The agreement is improved if core polarization effects are simulated by introducing effective charges that account for coupling to 2^+ configurations involving other major shells. We find that adopting $e_p = 1.1e$ and $e_n = 0.1e$ for protons and neutrons, respectively, reproduces the observed $B(E2)$ values for ^{54}Fe, ^{56}Ni, and ^{58}Ni, while for the open-shell nuclei ^{54}Cr and ^{56}Fe slightly larger effective charges ($e_p \approx 1.2e$, $e_n \approx 0.2e$) are needed indicating a larger core polarization in the latter two than in the magic and semimagic nuclei of the $A \approx 56$ region. Of course, the $B(E2)$ values determine $e_p + e_n$ much better than either e_p or e_n separately, and we underestimate $e_p + e_n$ by some 10% by placing all of the $E2$ strength in the lowest transition. Nevertheless, our effective charges are smaller than those required ($e_p = 1.35e$, $e_n = 0.35e$) in truncated shell-model calculations [6], indicating that the complete $0\hbar\omega$ model space contains significant correlations absent in smaller model spaces. That our $e_p + e_n = 1.4e$ is significantly smaller than the value 1.7 estimated from admixture of configura-

0031-9007/94/72(26)/4066(4)$06.00

TABLE I. Static observables calculated for selected nuclei with $A \sim 56$.

Nucleus	^{54}Fe	^{54}Fe	^{56}Ni	^{54}Cr	^{55}Mn	^{56}Fe	^{58}Ni
Force	KB[a]	BR	BR	BR	BR	BR	BR
$-\langle H\rangle$ (MC)[b]	...	131.4 ±0.4	145.2 ±0.6	134.4 ±0.5	141.8 ±1.0	151.7 ±0.6	164.4 ±0.7
(expt)[b]	129.7	129.7	141.9	132.0	140.0	150.2	164.4
$\langle Q^2\rangle$ (fm^4)[c]	2560 ±83	1482 ±84	1572 ±13	1408 ±64	1447 ±55	1819 ±91	1674 ±18
$\langle Q_v^2\rangle$ (fm^4)[c]	368 ±31	381 ±34	380 ±3	424 ±36	384 ±24	416 ±41	520 ±7
$\langle Q_p^2\rangle$ (fm^4)[c]	718 ±29	478 ±5	487 ±3	420 ±23		542 ±32	528 ±6
$\langle Q_n^2\rangle$ (fm^4)[c]	749 ±26	454 ±30	487 ±3	496 ±31		582 ±37	569 ±7
$B(E2)$ (MC)[d]	144 ±6	96 ±1	98 ±1	84 ±5		108 ±6	106 ±1
	199 ±9	129 ±1	132 ±1	114 ±6		148 ±9	142 ±2
(expt)[d]	124 ±10	124 ±10	120 ±10	174 ±8		196 ±8	139 ±4
$\langle M1^2\rangle(\mu_N^2)$[e]	11.9 ±0.4	14.1 ±0.4	17.7 ±0.2	13.2 ±0.4	21.6 ±0.4	14.7 ±0.4	17.5 ±0.4

[a]The KB interaction has an undefined energy shift, so that $\langle H\rangle$ is meaningless.
[b]Binding energies (in MeV) relative to ^{40}Ca.
[c]Q_p and Q_n are the proton and neutron mass quadrupole moments, calculated with oscillator length $b = 1.97(A/56)^{1/6}$ fm, while $Q = Q_p + Q_n$ and $Q_v = Q_p - Q_n$.
[d]$B(E2, 2_1^+ \to 0_1^+)$ in units of e^2 fm^4 calculated with the bare charges (upper row) and effective charges $e_p = 1.1e$ and $e_n = 0.1e$ (lower row) and assuming that this transition saturates $\langle Q^2\rangle$.
[e]$M1$ is the magnetic moment operator assuming free nucleon g factors. μ_N denotes the nuclear magneton.

tions outside of the $0\hbar\omega$ model space [13] suggests slightly too much collectivity in the Brown-Richter interaction.

In Table II we list results for the Gamow-Teller strengths $B(\mathrm{GT}_+) = \langle(\sigma\tau_+)^2\rangle$, where τ_+ is the isospin operator changing a proton to a neutron. In general, the GT$_+$ strength is quenched significantly relative to the single-particle value, and is in good agreement with experiment in all cases except ^{58}Ni. Since the GT operators $\sigma\tau_+$ induce only $0\hbar\omega$ transitions, we do not expect a significant renormalization of the operators. Note that the quenching factors vary significantly from one nucleus to another and are not well approximated by a common constant value, as is conventional in astrophysical applications [14]. Compared to restricted ($2p$-$2h$) shell model approaches [6], our full fp-shell calculation recovers about twice the quenching for both ^{54}Fe and ^{56}Ni.

The energy centroids of the GT$_\pm$ strengths are also listed in Table II and can be compared with the experimental results from (n,p) and (p,n) reactions [3]. Since we use isospin-invariant Hamiltonians, analog states are exactly degenerate and the calculated GT$_-$ centroid is the energy of the GT resonance relative to the isobaric analog state, $\Delta E = E_{\mathrm{GT}_-} - E_{\mathrm{IAS}}$. Experimen-

TABLE II. Gamow-Teller strengths for various nuclei with $A \sim 56$. Upper section: the Monte Carlo (MC) results for the total GT$_+$ strengths are compared with the single-particle (SP) values and the experimental strengths extracted from (n,p) data. Statistical MC errors are quoted; detailed studies of ^{54}Fe indicate an additional 10% systematic error arising from the finite number of time slices and from the g extrapolation. The lower two sections give the calculated energy centroids of the GT strengths relative to the target ground state ($\bar{E}_{\mathrm{GT}}$) and in the daughter nucleus (E_x). The experimental data are from [3]. The quoted values for $\bar{E}_{\mathrm{GT}_+}$ assume isospin conservation.

Nucleus	^{54}Fe	^{54}Fe	^{56}Ni	^{54}Cr	^{55}Mn	^{56}Fe	^{58}Ni
Force	KB	BR	BR	BR	BR	BR	BR
$\langle \mathrm{GT}_+^2\rangle$ (SP)	10.3	10.3	13.7	6.9	8.6	10.3	13.7
$\langle \mathrm{GT}_+^2\rangle$ (MC)	2.2 ±0.3	4.3 ±0.2	7.4 ±0.3	1.4 ±0.1	2.2 ±0.2	2.73 ±0.04	5.6 ±0.3
$\langle \mathrm{GT}_+^2\rangle$ (expt)	3.5 ±0.7[a]	3.5 ±0.7[a]			1.72 ±0.2[b]	2.85 ±0.3[b]	3.76 ±0.4[b]
$\bar{E}_{\mathrm{GT}_+}$ (MC)	9.2 ±0.2	9.7 ±0.2	8.9 ±0.3		12.4 ±1.6	11.0 ±0.2	9.8 ±0.2
E_x (MC)	0.7 ±0.2	1.2 ±0.2	2.7		2.4 ±1.6	-0.4 ±0.2	1.2 ±0.2
E_x (expt)	2.8	2.8			4.1 ±0.5	2.7 ±0.5	3.5 ±0.5
ΔE (MC)	5.2 ±0.2	6.1 ±0.2	8.9 ±0.3			4.4 ±0.1	6.1 ±0.2
(syst)[c]	5.8	5.8	6.8	3.7	4.3	4.8	5.9
E_x (MC)	5.2 ±0.2	6.1 ±0.2				7.8 ±0.1	6.15 ±0.2
E_x (expt)	8.2	8.2					

[a]Summed to an excitation energy of 9 MeV.
[b]Summed to an excitation energy of 8 MeV.
[c]The systematics of Ref. [15] for $\bar{E}_{\mathrm{GT}_-} - E_{\mathrm{IAS}}$.

tal values for the latter are well parametrized by [15] $\Delta E = [6.8 - 27.9(N-Z)/A]$ MeV. Although $(N-Z)/A$ in our case is outside the range studied by Nakayama *et al.* [15], we find that the MC results in all of our cases agree with this parametrization to within 0.4 MeV, except for the double-magic nucleus ^{56}Ni where shell-closure effects apparently not considered in the empirical parametrization might be important.

To compare the $\mathrm{GT}_\pm$ centroids to the data, we calculate the excitation energy of the resonance E_x in the daughter nucleus either by using known analog states or from the experimental mass difference corrected by the Coulomb energy. Although the calculated centroids for the (n,p) reactions (GT_+) are systematically 1.5 or 2 MeV too low, they generally track the position of the GT resonance in the daughter nucleus well for all nuclei. In particular, the calculation places the GT strength for the odd-Z target ^{55}Mn at a higher excitation energy E_x than in the neighboring nuclei, in accord with experiment. A similarly high excitation energy is also observed for ^{51}V and ^{59}Co, which aside from ^{55}Mn, are the only odd-Z, mid-fp-shell nuclei experimentally studied thus far, suggesting an odd-even dependence of the excitation energy centroid. This might have an important consequence for the measurement of the $B(\mathrm{GT}_+)$ strength in (n,p) reactions, which can determine the strength reliably only up to daughter excitation energies of about 8 MeV. Given the odd-even dependence, experiments with odd-Z targets are therefore likely to "miss" a relatively larger fraction of the total strength with $E_x > 8$ MeV, an effect that must be taken into account if one wants to compare total strengths [7]. The odd-even dependence should also be quite important in astrophysical applications like presupernova calculations, but apparently has been neglected to date.

It is important to determine the causes of the large GT quenching. There is strong evidence that neutron-proton correlations in the ground state are the source of the quenching, e.g., Ref. [16]. Engel *et al.* have suggested that the GT quenching is particularly sensitive to the $T=0, J=1$ matrix element [17]. To investigate this point, we show in Fig. 1 $B(\mathrm{GT}_+)$ for ^{54}Fe in a calculation where all $T=0, J=1$ particle-particle matrix elements have been scaled by $0 \le g_{pp} \le 2$ (with $g_{pp}=1$ being the physical value). We show the results for $g=0$ only, but we expect the extrapolated results at $g=1$ to exhibit a similar behavior. There is a high sensitivity to g_{pp}, and, upon comparing the result at $g_{pp}=0$ (all $T=0, J=1$ matrix elements vanishing) to that at $g_{pp}=1$, we see that this component of the interaction causes about half of the total quenching, in good agreement with the phenomenological prediction of Ref. [17]. In a further calculation, we switched off *all* $T=0$ matrix elements and recovered about 90% of the single-particle estimate for $B(\mathrm{GT}_+)$. Hino *et al.* have argued that the increase of ground state correlations is accompanied by an increase of $\langle J_p^2\rangle$ and $\langle J_n^2\rangle$ as proton-neutron states with $J \neq 0$ will

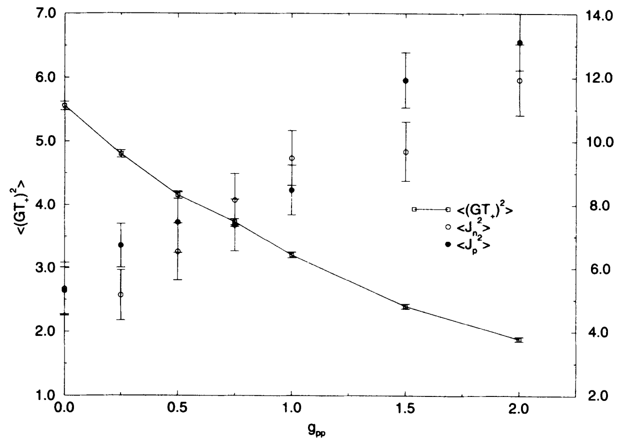

FIG. 1. The Gamow-Teller strength $B(\mathrm{GT}_+)$ and the expectation values of $\langle J^2\rangle$ for protons (full circles) and neutrons (open circles) as a function of the scaled strength of the $T=0, J=1$ interaction, g_{pp}, defined in the text. The calculation has been performed for ^{54}Fe at $\beta = 2\ \mathrm{MeV}^{-1}$ using the BR interaction and for the coupling constant $g=0$.

be admixed into the ground state by pn correlations [18]. The increase of $\langle J_{p,n}^2\rangle$ with increasing g_{pp} shown in Fig. 1 supports this argument.

The GT quenching is also expected to be very sensitive to the $f_{7/2}$-$f_{5/2}$ spin-orbit splitting. To investigate this effect, we have modified the BR interaction by decreasing the $f_{5/2}$ single-particle energy arbitrarily by 2 MeV, thus reducing $\epsilon_{5/2}$-$\epsilon_{7/2}$ from 6.49 to 4.49 MeV (this change defines the "MBR" interaction). $B(\mathrm{GT}_+)$ values calculated with this force are shown in Table III, where we also list effective spin-orbit splittings derived from the difference in the energy centroids of the neutron spectral functions, $\langle a_{7/2}^\dagger a_{7/2}\rangle$ and $\langle a_{5/2} a_{5/2}^\dagger\rangle$. The effective spin-orbit splitting generally tracks the single-particle energies, and is comparable to the expected single-particle splitting of 7.16 MeV. It is clear from these results that even modest changes in the single-particle energies can have large effects on the quenching, as was noted in Ref. [19]. Lowering the $f_{7/2}$-$f_{5/2}$ energy splitting decreases the total binding energy (which is overestimated by BR) significantly. However, it also decreases the centroids of the GT strengths which were already too low. Thus, the overbinding and the underestimation of the GT_+ excitation energy cannot be solved simultaneously by a shift of the $f_{7/2}$-$f_{5/2}$ energy splitting.

We have also calculated ^{54}Fe with the KB interaction. We find a GT strength about a factor of 2 smaller than for the BR interaction, indicating a strong, unanticipated sensitivity of the GT quenching to the effective interaction. A similar dependence is also observed in the $B(E2)$ values, for which the KB interaction predicts a value 50% larger than the BR interaction and in excess of the data. As the single-particle energies of the two interactions are nearly equal, the observed differences must stem from differences in the two-body interaction.

TABLE III. Selected properties of ^{54}Fe and ^{58}Ni calculated at $\beta = 2$ with the Brown-Richter (BR) interaction of Ref. [10] and its modification (MBR), where the $f_{5/2}$ single-particle energy has been lowered by 2 MeV.

Nucleus Force	^{54}Fe BR	^{54}Fe MBR	^{58}Ni BR	^{58}Ni MBR
$\langle GT_+^2 \rangle$	4.3 ±0.2	2.40 ±0.03	5.6 ±0.3	2.88 ±0.04
$\bar{E}_{GT_+}$	9.7 ±0.2	8.2 ±0.2	9.8 ±0.2	7.2 ±1.0
$-\langle H \rangle$	131.4 ±0.4	126.4 ±0.5	164.4 ±0.7	159.8 ±0.5
$\bar{E}_{7/2}$ [a]	11.77 ±0.08	12.36 ±0.03	11.73 ±0.09	10.40 ±0.03
$\bar{E}_{5/2}$ [b]	-3.45 ±0.08	-5.54 ±0.08	-3.36 ±0.16	-4.18 ±0.09
$\Delta \bar{E}_{LS}$ [c]	8.31 ±0.11	6.82 ±0.08	8.37 ±0.18	6.22 ±0.09

[a]Energy centroid in MeV of the neutron $f_{7/2}$ strength, obtained from the response function $\langle a^\dagger_{7/2}(\tau) a_{7/2} \rangle$.

[b]Energy centroid of the neutron $f_{5/2}$ strength, obtained from $\langle a_{5/2}(\tau) a^\dagger_{5/2} \rangle$.

[c]Effective spin-orbit splitting, $\bar{E}_{7/2} + \bar{E}_{5/2}$.

In summary, our complete fp-basis calculations of nuclei with $A \sim 56$ demonstrate that substantial quenching of the GT_+ strength is a general phenomenon for all of the nuclei calculated and that restricted shell model calculations miss a significant part of this quenching. Our calculations with the BR interaction give a quenching comparable to that observed in (n,p) reactions; a calculation of ^{54}Fe with the KB interaction gives an even greater quenching. Our results show that np correlations are a major contributor to this quenching, as is a small $f_{7/2}$-$f_{5/2}$ spin-orbit splitting. The binding energies and $B(E2, 2_1^+ \rightarrow 0_1^+)$ values calculated with the BR interaction are in reasonable agreement with experiment. In particular, the latter require significantly smaller effective charges than do previous, more restricted calculations.

Of course, all of our results depend upon the Hamiltonian used. The BR interaction has been fitted to the lower fp shell, and is probably not optimal for the present studies. In fact, we find some systematic shortcomings as the BR interaction tends to overbinding while placing the GT centroids at somewhat too low an excitation energy. Given these deficiencies and the strong sensitivity of the GT_+ strength to the effective interaction, it is premature to draw definite conclusions from the apparent good agreement between the experimental and calculated quenching of the GT_+ strength. A definite conclusion as to whether the quenching can be totally recovered in complete fp-basis calculations must wait until improved effective interactions are available. The new computational techniques we have used in this work would allow such an interaction to be determined in the complete fp or even $fp g_{9/2}$ basis.

This work was supported in part by the National Science Foundation, Grants No. PHY90-13248 and No. PHY91-15574, and by the Department of Energy, Grant No. DE-FG-0291ER-40608. W.E.O. acknowledges the Weingart Foundation for financial support. We are grateful to P. Vogel and B. A. Brown for helpful discussions. Computational cycles were provided by the Caltech Concurrent Supercomputing Consortium on the Intel DELTA parallel supercomputer.

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