Practical Solution to the Monte Carlo Sign Problem: Realistic Calculations of ^{54}Fe

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We present a practical solution to the "sign problem" in the auxiliary field Monte Carlo approach to the nuclear shell model. The method is based on extrapolation from a continuous family of problem-free Hamiltonians. To demonstrate the resultant ability to treat large shell-model problems, we present results for ^{54}Fe in the full fp-shell basis using the Brown-Richter interaction. We find the Gamow-Teller β^+ strength to be quenched by 58% relative to the single-particle estimate, in better agreement with experiment than previous estimates based on truncated bases.

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Recent publications [1,2] have described quantum Monte Carlo methods for exact solution of the nuclear shell model. The methods are based on the Hubbard-Stratonovich (HS) representation [3] of the imaginary-time many-body propagator in terms of one-body propagators of noninteracting nucleons moving in a fluctuating field. Thermal averages can be calculated, as can ground-state properties; errors arise only from discretization and statistical sampling, both of which can be controlled. As these computations scale much more gently with the number of single-particle orbits (N_s) and/or the number of valence nucleons (N_v) than do direct diagonalization techniques, they hold great promise for treating very large model spaces.

Unfortunately, the applicability of shell-model Monte Carlo calculations has heretofore been limited by the "sign problem" generic to all fermionic Monte Carlo techniques [1,2,4,5]. The sign of the integrand may vary from sample to sample and the net integral results from a delicate cancellation that is difficult to reproduce with a finite number of samples. The problem is well documented (and as yet unsolved) in simulations of correlated electron systems [4]. Except for an important, yet schematic, class of nuclear interactions [2], we have found that all realistic nuclear shell-model Hamiltonians suffer from a sign problem.

In this Letter, we report a practical solution to the sign problem and present the first realistic calculation of a mid-fp-shell nucleus, ^{54}Fe [6]. Our method is based on an extrapolation of observables calculated for a "nearby" family of Hamiltonians whose integrands have a positive sign. Success depends crucially upon the degree of extrapolation required. We have found that, for all of the many realistic interactions tested in the sd and fp shells, the extrapolation required is modest, amounting to a factor of 2 variation in the isovector monopole pairing strength.

A general time-reversal invariant Hamiltonian with two-body interactions can be brought to the form

$$H = \sum_\alpha \left(\epsilon_\alpha^* \bar{\mathcal{O}}_\alpha + \epsilon_\alpha \mathcal{O}_\alpha\right) + \frac{1}{2}\sum_\alpha V_\alpha \left\{\mathcal{O}_\alpha, \bar{\mathcal{O}}_\alpha\right\} , \quad (1)$$

where the $\mathcal{O}_\alpha$ are a convenient set of one-body operators and $\bar{\mathcal{O}}$ denotes the time reverse of $\mathcal{O}$. For real V_α, H in Eq. (1) is manifestly time-reversal invariant. The auxiliary field Monte Carlo approach utilizes the HS representation of the imaginary-time many-body propagator $U = \exp(-\beta H)$ as a path integral over one-body propagators in fluctuating auxiliary fields. Upon introducing N_t time slices of duration $\Delta\beta = \beta/N_t$ and complex c-number auxiliary fields $\sigma_{\alpha n}$ ($n = 1, \ldots, N_t$), we can write the canonical expectation value of an observable $\mathcal{O}$ as

$$\langle \mathcal{O} \rangle \equiv \frac{\mathrm{Tr}\,(\mathcal{O} e^{-\beta H})}{\mathrm{Tr}\,(e^{-\beta H})} \approx \frac{\int D[\sigma] W(\sigma) \Phi(\sigma) \langle \mathcal{O} \rangle_\sigma}{\int D[\sigma] W(\sigma) \Phi(\sigma)} . \quad (2)$$

Here, the approximation becomes exact as $N_t \to \infty$ and the metric is $D[\sigma] = \Pi_{\alpha,n} [d\sigma_{\alpha n} d\sigma_{\alpha n}^* \Delta\beta |V_\alpha|/2\pi]$. The non-negative weight is $W(\sigma) = \zeta(\sigma) \exp(-\sum |V_\alpha| \times |\sigma_{\alpha n}|^2 \Delta\beta)$, where $\zeta(\sigma) \equiv \mathrm{Tr}\, U_\sigma$ is the canonical partition function of the one-body evolution operator $U_\sigma \equiv U_{N_t} \cdots U_1$, where $U_n = \exp(-\Delta\beta h_n)$, and the one-body Hamiltonian for the nth time slice is $h_n = \sum_\alpha (\epsilon_\alpha^* + s_\alpha V_\alpha \sigma_{\alpha n}) \bar{\mathcal{O}}_\alpha + (\epsilon_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}^*) \mathcal{O}_\alpha$, with $s_\alpha = \pm 1$ for $V_\alpha < 0$ and $s_\alpha = \pm i$ for $V_\alpha > 0$. The "sign" is $\Phi(\sigma) \equiv \zeta(\sigma)/|\zeta(\sigma)|$ and $\langle \mathcal{O} \rangle_\sigma \equiv \mathrm{Tr}\,(\mathcal{O} U_\sigma)/\zeta(\sigma)$. Both $\zeta(\sigma)$ and $\langle \mathcal{O} \rangle_\sigma$ can be evaluated in terms of the $N_s \times N_s$ matrix $\mathbf{U}_\sigma$ that represents the evolution operator U_σ in the single-particle space.

The sign problem arises because the one-body partition function $\zeta(\sigma)$ is not necessarily positive, so that the Monte Carlo uncertainty in the denominator of Eq. (2) (the W-weighted average sign, $\langle \Phi \rangle$) can become comparable to or larger than $\langle \Phi \rangle$ itself. In most cases $\langle \Phi \rangle$ decreases exponentially with β or with the number of time slices [5].

An important class of interactions free from the sign problem [i.e., $\Phi(\sigma) \equiv 1$] was found in Ref. [2]. This occurs when $V_\alpha < 0$ for all α in Eq. (1). In that case, $s_\alpha = 1$ for all α, so that both h_n and U_σ are time-reversal invariant. The eigenvectors of $\mathbf{U}_\sigma$ then occur as time-reversed pairs with complex conjugate eigenvalues λ_i, λ_i^* ($i = 1, \ldots, N_s/2$), the grand canonical partition function $\zeta(\sigma) = \Pi_i |1 + \lambda_i|^2$ is positive definite, and the canonical partition function for even N_v is also positive definite.

Based on the above observation, it is possible to decompose H into its "good" and "bad" parts, $H = H_G + H_B$, with

$$H_G = \sum_\alpha (\epsilon_\alpha^* \bar{\mathcal{O}}_\alpha + \epsilon_\alpha \mathcal{O}_\alpha) + \frac{1}{2} \sum_{V_\alpha < 0} V_\alpha \{\mathcal{O}_\alpha, \bar{\mathcal{O}}_\alpha\},$$
$$H_B = \frac{1}{2} \sum_{V_\alpha > 0} V_\alpha \{\mathcal{O}_\alpha, \bar{\mathcal{O}}_\alpha\} . \quad (3)$$

The "good" Hamiltonian H_G includes, in addition to the one-body terms, all the two-body interactions with $V_\alpha < 0$, while the "bad" Hamiltonian H_B contains all interactions with $V_\alpha > 0$. By construction, calculations with H_G alone have $\Phi(\sigma) \equiv 1$ and are thus free of the sign problem.

We define a family of Hamiltonians H_g that depend on a continuous real parameter g as $H_g = H_G + gH_B$, so that $H_{g=1} = H$. If the V_α that are large in magnitude are "good," we expect that $H_{g=0} = H_G$ is a reasonable starting point for the calculation of an observable $\langle \mathcal{O} \rangle$. One might then hope to calculate $\langle \mathcal{O} \rangle_g = \mathrm{Tr}\,(\mathcal{O} e^{-\beta H_g})/\mathrm{Tr}\,(e^{-\beta H_g})$ for small $g > 0$ and then to extrapolate to $g = 1$, but typically $\langle \Phi \rangle$ collapses even for small positive g. However, it is evident from our construction that H_g is characterized by $\Phi(\sigma) \equiv 1$ for any $g \leq 0$, since all the "bad" $V_\alpha (> 0)$ are replaced by "good" $gV_\alpha < 0$. We can therefore calculate $\langle \mathcal{O} \rangle_g$ for any $g \leq 0$ by a Monte Carlo sampling that is free of the sign problem. If $\langle \mathcal{O} \rangle_g$ is a smooth function of g, it should then be possible to extrapolate to $g = 1$ (i.e., to the original Hamiltonian) from $g \leq 0$. We emphasize that $g = 0$ is not expected to be a singular point of $\langle \mathcal{O} \rangle_g$; it is special only in the Monte Carlo evaluation.

In the nuclear shell model, the two-body interaction can be written in a density decomposition as [2]

$$\frac{1}{2} \sum_{abcd} \sum_{KT\pi} E^\pi_{KT}(ac, bd) \sum_M (-)^M \rho_{KMT}(ac) \rho_{K-MT}(bd) .$$

Here $\rho_{KMT} = \rho^p_{KM} + (-)^T \rho^n_{KM}$ $(T = 0, 1)$, $\rho^{(p,n)}_{KM}(ac) = (a^\dagger_a \times \tilde{a}_c)_{KM}$ is the one-body density operator for the pair of proton or neutron orbits (a, c) coupled to angular momentum K and its z projection M, and $\pi = (-)^{l_a + l_c} = (-)^{l_b + l_d}$ is the parity. The matrices E^π_{KT} are constructed from the two-body matrix elements $V^\pi_{JT}(ab, cd)$ of good angular momentum J, isospin T, and parity π through a Pandya transformation. For interactions that are time-reversal invariant and conserve parity, the $E^\pi_{KT}(i, j)$ are real symmetric matrices that can be diagonalized by a real orthogonal transformation. The eigenvectors $\rho_{KM}(\alpha)$ play the role of $\mathcal{O}_\alpha$ in Eq. (1), and the eigenvalues $\lambda_{K\pi}(\alpha)$ are proportional to V_α. In the Condon-Shortley [7] convention $\bar{\rho}_{KM} = \pi(-)^{K+M} \rho_{K-M}$ so that the "good" eigenvalues satisfy sign $[\lambda_{K\pi}(\alpha)] = \pi(-)^{K+1}$ [8]. To minimize the number of auxiliary fields required, we use the freedom to add an arbitrary symmetric interaction to H [2] and choose $V^S_{JT=1} = V^A_{JT=0}$ so that $E_{KT=1} \equiv 0$. $E_{KT=0}$ is then uniquely determined by the antisymmetric part of the interaction through the combination $(V^A_{JT=0} + V^A_{JT=1})$.

To demonstrate the viability and utility of the method, we have applied it to the mid-fp-shell nucleus ^{54}Fe using the realistic Brown-Richter interaction [9]. The number of m-scheme Slater determinants describing the 6 valence protons and 8 valence neutrons moving among the $N_s = 20$ single-particle states of the $0f_{7/2,5/2}$ and $0p_{3/2,1/2}$ orbitals is $\binom{20}{6}\binom{20}{8} \approx 5 \times 10^9$. For comparison, the largest model space treated by standard diagonalization techniques is currently ^{48}Ti [10] where the m-scheme dimension is $\approx 7 \times 10^6$.

Figure 1 (upper) shows the eigenvalues $V_{K\pi\alpha} = \pi(-)^K \lambda_{K\pi}(\alpha)$ of the Brown-Richter interaction; only about half of the eigenvalues are negative. However, those with the largest magnitude are all "good." It is possible to use an inverse Pandya transformation to calculate the usual two-body matrix elements $V^\pi_{JT}(ab, cd)$ for the "good" and "bad" interactions, allowing the ma-

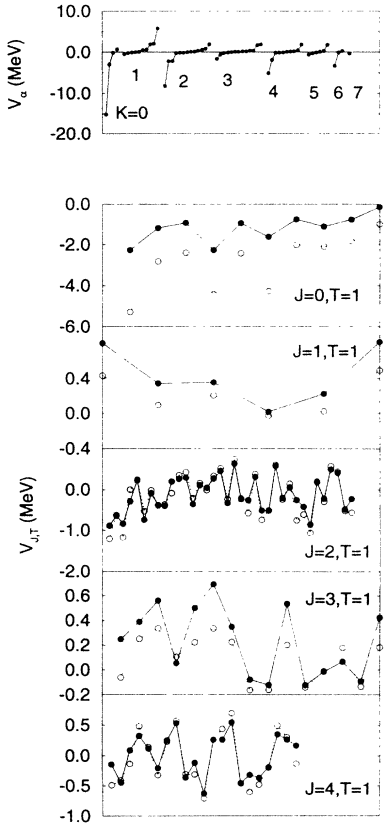

FIG. 1. Upper: The eigenvalues V_α of the Brown-Richter interaction in the fp shell. Eigenvalues for each particle-hole angular momentum K are plotted in increasing order. Bottom: The two-body matrix elements $V_{JT=1}(ab, cd)$ of the Brown-Richter interaction (solid circles) and its "good" part (open circles), for $J \leq 4$. The ordering for each J is arbitrary. Plots of the $V_{JT=0}$ and the remaining $T = 1$ matrix elements (not shown) are similar to those shown for $J \geq 1$.

trix elements of H_G to be compared in Fig. 1 (lower) with those of the full interaction. The greatest deviation is for $J = 0, T = 1$ (the monopole pairing interaction), where H_G is about twice as attractive as the physical H. In all other channels, H_G and H are quite similar.

We have performed Monte Carlo calculations for $\beta = 2\ \mathrm{MeV}^{-1}$ using $N_t = 32$ (so that $\Delta\beta = 0.0625\ \mathrm{MeV}^{-1}$). For $g = -1, -0.8, -0.6, -0.4, -0.2$, and 0, we took approximately 3300 uncorrelated samples. The computations were performed on the Intel Touchstone DELTA 512-node parallel computer, where each node is an Intel i860 processor. Each node produced and analyzed a sample in about 4 min, so that each value of g took about 25 min in total. Selected calculations for larger values of β or N_t show that we have converged to the true ground-state properties.

The results for various observables are shown in Fig. 2. The extrapolations to the physical Hamiltonian ($g = 1$) are done by least-squares polynomials. For each observable except $\langle H\rangle$, the degree of the polynomial is chosen to be the lowest for which χ^2 per degree of freedom is less than 1; linear or quadratic extrapolations are almost always sufficient. For $\langle H\rangle$, the variational principle implies the additional constraint of vanishing derivative at $g = 1$, in which case a quadratic or cubic polynomial is used. We have also calculated response functions $R(\tau) = \langle \mathcal{O}^\dagger(\tau)\mathcal{O}(0)\rangle$ by polynomial extrapolation of our calculations of $\ln[R_g(\tau)/R_g(0)]$ for $g \le 0$. Fitting $\ln[R_1(\tau)/R_1(0)]$ to a polynomial in τ allows us to determine moments of the normalized strength function $f_{\mathcal{O}}(E)$, such as $\bar{E} \equiv \int E f_{\mathcal{O}}(E) dE$. Our overall method was checked in detail [11] by comparison with direct diagonalization in the *sd* shell using the Brown-Wildenthal interaction [12] and in the lower *fp* shell (^{44}Ti) using the Brown-Richter interaction [9].

Table I summarizes the extrapolated results for various observables. Note that the statistical uncertainty in these values is proportional to the uncertainties in the Monte Carlo results for $g \le 0$, and so can be reduced by increasing the number of samples. The calculated first

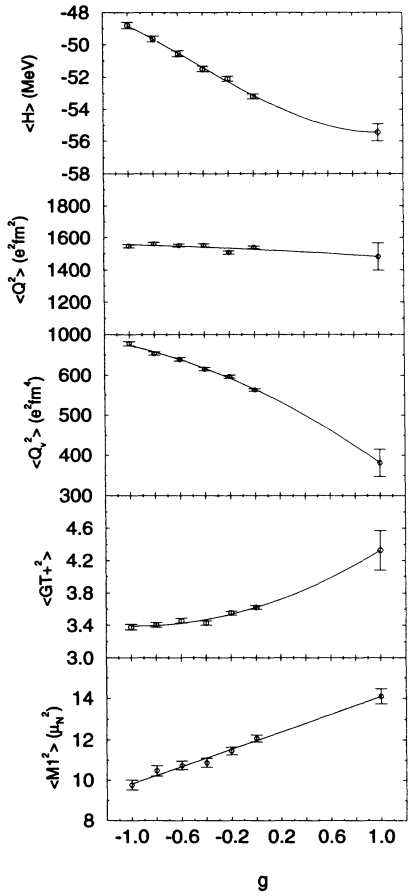

FIG. 2. The results of the Monte Carlo calculations for ^{54}Fe at $\beta = 2\ \mathrm{MeV}^{-1}$ for several observables as a function of $g \le 0$. $Q = Q_p + Q_n$ is the isoscalar quadrupole, $Q_v = Q_p - Q_n$ is the isovector quadrupole, GT_+ is the Gamow-Teller operator changing a proton to a neutron, and $M1$ is the magnetic moment operator using the free-nucleon g factors. The lines are polynomial extrapolations; the extrapolated values and corresponding uncertainties are shown at $g = 1$. The extrapolation is linear for $\langle M1^2\rangle$, but quadratic for $\langle Q^2\rangle$, $\langle Q_v^2\rangle$, and $\langle \mathrm{GT}_+^2\rangle$. For $\langle H\rangle$, the extrapolation is cubic with the constraint of vanishing derivative at $g = 1$.

TABLE I. Monte Carlo results for ^{54}Fe.

$\langle H\rangle = -55.5 \pm 0.5$ MeV		
	Total strength	$\bar{E}$ (MeV)
Isoscalar quadrupole	$\langle Q^2\rangle = 1482 \pm 84\ \mathrm{fm}^4$	1.25 ± 0.16
Isovector quadrupole	$\langle Q_v^2\rangle = 381.3 \pm 33.8\ \mathrm{fm}^4$	12.7 ± 0.2
Gamow-Teller (p,n)	$\langle(\mathrm{GT}_-)^2\rangle = 10.32 \pm 0.24$	6.13 ± 0.17
Gamow-Teller (n,p)	$\langle(\mathrm{GT}_+)^2\rangle = 4.32 \pm 0.24$	9.7 ± 0.2
$M1$	$\langle(M1)^2\rangle = 14.1 \pm 0.4\mu_N^2$	8.6 ± 0.7
Occupation numbers		
Protons		Neutrons
$\langle a^\dagger a\rangle_{f_{7/2}} = 4.92 \pm 0.03$		$\langle a^\dagger a\rangle_{f_{7/2}} = 6.35 \pm 0.03$
$\langle a^\dagger a\rangle_{p_{3/2}} = 0.56 \pm 0.02$		$\langle a^\dagger a\rangle_{p_{3/2}} = 0.86 \pm 0.02$
$\langle a^\dagger a\rangle_{p_{1/2}} = 0.11 \pm 0.01$		$\langle a^\dagger a\rangle_{p_{1/2}} = 0.17 \pm 0.01$
$\langle a^\dagger a\rangle_{f_{5/2}} = 0.41 \pm 0.01$		$\langle a^\dagger a\rangle_{f_{5/2}} = 0.61 \pm 0.01$

moment of the isoscalar quadrupole strength function, 1.25 ± 0.16 MeV, should be compared with the empirical excitation energy of the first 2^+ state, 1.408 MeV. Our estimate for the $B(E2)$ for the decay of this state assuming free nucleon charges (and that this transition has all of the strength) is $96 \pm 1\ e^2\ \mathrm{fm}^4$, while effective charges $(e_p, e_n) = (1.1, 0.1)e$ would be required to reproduce the experimental value of $126\ e^2\ \mathrm{fm}^4$. These charges are significantly smaller than the $(1.35, 0.35)e$ used in truncated calculations [13] or the $(1.33, 0.64)e$ used in the lower fp shell [9]. The total mass quadrupole strength, $\langle Q^2 \rangle = 1482 \pm 84\ \mathrm{fm}^4$, is significantly larger than the simple single-particle estimate of $380\ \mathrm{fm}^4$. The total $M1$ strength $\langle (M1)^2 \rangle = (14.1 \pm 0.4)\mu_N^2$ is quenched relative to the single-particle estimate of $42.55\mu_N^2$. It is also interesting to note that the occupation numbers of the single-particle orbits are smeared across the Fermi surface.

Of particular physical interest are the Gamow-Teller operators. Our calculations exactly satisfy the sum rule $\langle (\mathrm{GT}_-)^2 \rangle - \langle (\mathrm{GT}_+)^2 \rangle = 3(N - Z) = 6$. The single-particle estimate for $\langle (\mathrm{GT}_+)^2 \rangle$ corresponding to the $f_{7/2}$ proton $\rightarrow$ $f_{5/2}$ neutron transition is 10.28 [14], so the shell-model Monte Carlo value of 4.32 ± 0.24 is quenched by 58%. This value is comparable to the experimental result of 3.1 ± 0.6 [15], but significantly smaller than previous estimates of 6.40 or 6.70 based on truncated bases [13]. The additional quenching on the full space correlates with the enhanced $B(E2, 2_1^+, \rightarrow 0_1^+)$ (i.e., smaller effective charge), as was surmised in [13].

Direct comparison with experimental Gamow-Teller strength functions requires that we know the energy of the daughter ground state relative to ^{54}Fe. Since the ^{54}Co ground state is the isobaric analog state (IAS) of the ^{54}Fe ground state, we find a mean (p, n) excitation energy of $\bar{E}_x = 6.13 \pm 0.17$ MeV. This is in agreement with the systematics of Nakayama *et al.* [16], which give $E_{\mathrm{GT}^-} - E_{\mathrm{IAS}} = 5.81$ MeV, but is somewhat low relative to the experimental value of 8.2 MeV [15]. When our calculations of the mean (n, p) excitation energy are corrected for the Coulomb energy (including exchange) and the nucleon mass difference, we find $\bar{E}_x = 1.24 \pm 0.2$ MeV, to be compared with the experimental centroid of 3 MeV [15]. A more consistent theoretical value of $\bar{E}_x$ can be obtained by calculating the mass differences of the $A = 54$ isobars within the shell-model Monte Carlo [11].

The method presented in this Letter is a practical solution to the sign problem for realistic shell-model interactions. A full-basis calculation of ^{54}Fe with the Brown-Richter interaction shows the feasibility of the method, with significant quenching of the Gamow-Teller β^+ strength. Systematic studies of the temperature, nuclide, and interaction dependence of these calculations will be reported elsewhere. Our techniques also enable the determination of an optimal effective interaction and effective operators in a greatly enlarged model space.

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