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Letter

Extension of the spectroscopic Monte Carlo method to realistic effective interactions

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Abstract. We propose an extension of the spectroscopic Monte Carlo method to realistic effective interactions. The scheme is applied to the recently introduced GXPF1 interaction for fp nuclei for the ground state of ^{60}Fe, ^{56}Ni, ^{64}Ni and ^{60}Zn. The method hinges on the use of Hartree-Fock-Bogoliubov wave functions (properly projected before variation) and on a reformulation of the effective interaction so that it is a sum of negative squares of Hermitian one–quasi-particle operators, so the application of the Hubbard-Stratonovich transformation to the elementary propagator $\exp[-\hat{H}]$ gives a functional integral over a Hermitian propagator. Limitations and difficulties encountered in the calculation are discussed.

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The shell model approach is the fundamental tool used in studying the structure of light nuclei. There are two ingredients which allow the feasibility of such studies. One is the knowledge of an effective nucleon-nucleon interaction among the valence particles. The other is the actual diagonalization of the large Hamiltonian matrix. With presently available computer resources, many fp shell nuclei seem to be reachable (for a recent review see, for example, ref. [1]). Whenever the size of the Hilbert space exceeds present-day computational capabilities, either a truncation of the Hilbert space is necessary or one uses variational approaches, with increasing degree of completeness. Among these latter, the most sofisticated are the FED VAMPIR approaches (along with the variant for the excited states) (refs. [2–4]). In these approaches the ground state is written as a sum of quasi-particle vacua properly projected to the exact quantum numbers before variation of the energy. In the quantum Monte Carlo diagonalization method the Hubbard-Stratonovich transformation (ref. [5]) is used to generate a many-body basis, which is then optimized, starting from the HF approximation (HFB is used for heavy nuclei) in which the Hamiltonian matrix is subsequently diagonalized (ref. [6]). Both approches tend to include increasingly more of the full Hilbert space as the basis is increased. From the point of view of the shell model Monte Carlo methods (refs. [7, 8]) instead, one encounters the so-called sign problem which prevents reasonable statistical accuracy from being reached, in the case one uses realistic effective interactions. In the past, in order to circumvent this problem, an extrapolation method was proposed (ref. [7]). In this method the original Hamiltonian is rewritten as a sum of a “good part” for which a Monte Carlo calculation can be performed and a “bad part”, $\hat{H} = \hat{H}_{\rm good} + g\hat{H}_{\rm bad}$. The original Hamiltonian has $g = 1$, but can be studied with Monte Carlo methods for any $g < 0$. The extrapolation method consists in performing a sequence of Monte Carlo calculations for several $g < 0$ values and extrapolating for $g = 1$. As shown in ref. [9], the method is reasonable for light systems in the fp region but it can give discrepancies as large as 2 Mev for the ground-state energy of ^{64}Ni using the KB3 effective interaction. Although there is no reason to believe that no extrapolation can reproduce the shell model results, one notices that there are no direct Monte Carlo calculations with realistic effective interactions, that is calculations performed exclusively with the Hamiltonian of choice, whithout resorting to auxiliary potentials and to extrapolation methods. The purpose of this Letter is to describe a few Monte Carlo calculations performed directly with the newly introduced GXPF1 effective interaction (ref. [10]) for the ground state of the fp shell nuclei ^{60}Fe, ^{56}Ni, ^{64}Ni and ^{60}Zn. The main idea is to modify the spectroscopic Monte Carlo method of ref. [11]. This method was used primarily with the pairing-plus-quadrupole model (which in the SMMC approach for

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the ground state does not necessitate the extrapolation method) and recently (ref. [12]) with the addition of the quadrupole pairing potential (which violates the sign prescription of ref. [7], and therefore necessitates the extrapolation method in the SMMC approach) and is based on the following idea. The imaginary time propagator $\exp(-\beta\hat{H})$ applied to reasonable accurate wave functions $|NZJM\rangle$ necessitates only small values of β in order to filter the ground state out of the approximate wave function. Good wave functions, such as the HFB wave functions, require projectors to good quantum numbers. When the Hubbard-Stratonovich transformation is applied to the evaluation of the numerator and denominator of the energy equation

$$E(\beta,N,Z,J) = \frac{\langle\psi NZ|\hat{P}_{JJ}\hat{H}\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}{\langle\psi NZ|\hat{P}_{JJ}\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}, \tag{1}$$

where $\hat{P}_{JJ}$ is the angular-momentum projector for $M = J$ (we included the cranking and the chemical-potential terms); the angular-momentum projector makes it prohibitively expensive to generate decorrelated Monte Carlo samples. Instead, with the proper choice of the cranking frequency (for $J > 0$) and of the chemical potentials, one generates integration points in the functional integral without the use of angular-momentum projectors. Only when a set of statistically independent integration points have been generated, the angular momentum is restored for the evaluation of eq. (1). It is crucial, in order to have reasonably low sign fluctuations, not only to work at not too large values of β, but also to apply the HS transformation to a sum of squares of Hermitian one-body (or one–quasi-particle) operators with negative coupling constants. Schematically, if the Hamiltonian, as we shall prove shortly, can be written as

$$\hat{H} = \hat{H}_0 - 1/2\sum_a k_a\hat{Q}_a^2\,, \tag{2}$$

where $\hat{H}_0$ is the single-particle Hamiltonian and the operators $\hat{Q}_a$ are one-particle (or quasi-particle) Hermitian operators with coupling constants $-k_a < 0$, the HS transformation applied to the infinitesimal imaginary time propagator $\exp(-\epsilon\hat{H})$ gives, for the propagator at finite β,

$$\exp{-\beta}(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p) = \int \mathrm{d}xG(x)\hat{W}(x)\,, \tag{3}$$

where x denotes the (multidimensional) integration variables, $G(x)$ is the Gaussian weight (inclusive of the various normalization constants) and $\hat{W}(x)$ is the propagator, usually of generalized quasi-particle type (as in refs. [11,12]), and is the time-ordered product of exponentials of Hermitian operators. For small values of β, the dominant part to the full functional integral is expected to be dominated by the static component (*i.e.* the imaginary time average of the time-varying integration variables $x(t)$). The necessary inclusion of the quantal fluctuations (*i.e.* the time dependence of the integration variables) and of the projector can change this. Explicitly, the energy of eq. (1) is evaluated as the ratio of the following two quantities:

$$\mathcal{E} = \frac{\mathrm{Re}\int \mathrm{d}xG(x)\langle\psi NZ|\hat{W}|\psi NZ\rangle\frac{\langle\psi NZ|\hat{P}_{JJ}\hat{H}\hat{W}(x)|\psi NZ\rangle}{\langle\psi NZ|\hat{W}|\psi NZ\rangle}}{\int \mathrm{d}x|\mathrm{Re}[G(x)\langle\psi NZ|\hat{W}|\psi NZ\rangle]|}, \tag{4}$$

$$\mathcal{O} = \frac{\mathrm{Re}\int \mathrm{d}xG(x)\langle\psi NZ|\hat{W}|\psi NZ\rangle\frac{\langle\psi NZ|\hat{P}_{JJ}\hat{W}(x)|\psi NZ\rangle}{\langle\psi NZ|\hat{W}|\psi NZ\rangle}}{\int \mathrm{d}x|\mathrm{Re}[G(x)\langle\psi NZ|\hat{W}|\psi NZ\rangle]|}, \tag{5}$$

where Re means real part. Both $\mathcal{E}$ and $\mathcal{O}$ are evaluated with the Metropolis Monte Carlo method using as a probability distribution the absolute value of the real part of $G(x)\langle\psi NZ|\hat{W}|\psi NZ\rangle$. We stress from the start that the resulting Monte Carlo calculation does have sign oscillations, but we are confining ourselves to small β values, where sign oscillations are irrelevant.

Before proceeding, let us prove eq. (2) for a general effective interaction. We can take as a starting point the results obtained in ref. [7] about the density decomposition of a general effective interaction. In ref. [7] the effective potential is first rewritten as

$$\begin{aligned}\hat{V} = 1/4\sum\sqrt{1+\delta_{ab}}\sqrt{1+\delta_{cd}}[W_{JT=0}(abcd)\\ +W_{JT=1}(abcd)]\hat{A}^\dagger_{JMTT_z}(ab)\hat{A}_{JMTT_z}(cd)\,,\end{aligned} \tag{6}$$

where a,b,c,d denote single-particle shells, $\hat{A}^\dagger_{JMTT_z}(ab)$ is the pair creation operator coupled to the angular momentum J, the third component M, and the isospin quantum numbers T and T_z. The sum extends over all possible single-particle shells and all possible values of $JMTT_z$. Using the anticommutation rules, the potential is written in terms of density-like operators as

$$\hat{V} = \hat{V}_1 - 1/2\sum_i\lambda_i[\hat{Q}_i(n)+\hat{Q}_i(p)]^2\,. \tag{7}$$

$\hat{V}_1$ is a one-body self-energy arising from the anticommutation rules and the operators (which can always be taken as Hermitian) $\hat{Q}_i(n,p)$ (for neutrons or protons) are of the type $\sum a^\dagger_{a,m_a}(q_i(n,p))_{a,m_a,b,m_b}a_{b,m_b}$. If all λ_i were positive, the application of the HS transformation would give, for the propagator inside the functional integral, a time-ordered product of Hermitian propagators. If some of the λ_i are negative, instead, the propagator inside the functional integral is the product of non-Hermitian propagators and we expect strong sign fluctuations in the Monte Carlo calculation even if a single time interval were used (*i.e.* a small value of β). Clearly, it is more desirable to have $\hat{V}$ written as a sum of negative squares of Hermitian operators, so that at least for small values of β the functional integral is dominated by positive contributions. For the GXPF1 interaction there are 400 operators $\hat{Q}_i$ of which 118 have a negative value of λ (the largest of which is a monopole with $|\lambda| \approx 0.67$). The Hamiltonian is conveniently rewritten by first extracting all traces out of the matrices q_i. If we denote explicitly by $\hat{\xi}_\tau = \sum_{rs} a_s^\dagger \xi_{sr} a_r$ the modes with negative λ_τ, we have

$$\hat{H} = C + \hat{H}_1 - \frac{1}{2}\sum_{\lambda_\mu > 0}[\hat{Q}_\mu(n) + \hat{Q}_\mu(p)]^2$$
$$-\frac{1}{2}\sum_{\lambda_\tau < 0}[\hat{\xi}_\tau(n) - \hat{\xi}_\tau(p)]^2 + \sum_\tau [\hat{\xi}_\tau(n)^2 + \hat{\xi}_\tau(p)^2]\,, \qquad (8)$$

where the absolute value of the λ_i has been reabsorbed in the definition of the various operators. The single-particle part (renamed $\hat{H}_1$) and the constant C are due to the extraction of the traces from the monopole part of the Hamiltonian. The positive terms in eq. (8) can be rewritten as

$$\sum_\tau \hat{\xi}_\tau^2 = \sum_\tau \sum_{rs} a_r^\dagger (\xi_\tau^2)_{rs} a_s + \sum_\tau \xi_{\tau,rs}\xi_{\tau,ij}\hat{P}_{ri}^\dagger \hat{P}_{sj}\,, \qquad (9)$$

where we introduced the destruction and creation pairing operators

$$\hat{P}_{sj} = a_s a_j, \qquad \hat{P}_{ri}^\dagger = a_i^\dagger a_r^\dagger\,. \qquad (10)$$

Using the superindices $\alpha = (ri), \beta = (sj)$ and the matrix $M_{\alpha,\beta} = \sum_\tau \xi_{\tau,rs}\xi_{\tau,ij}$ we arrive at the form

$$\sum_\tau \hat{\xi}_\tau^2 = \sum_\tau \sum_{rs} a_r^\dagger (\xi_\tau^2)_{rs} a_s + \sum_{\alpha,\beta} \hat{P}_\alpha^\dagger M_{\alpha,\beta} \hat{P}_\beta\,. \qquad (11)$$

It is easy to show that the matrix M is Hermitian. In the diagonal representation, let us set

$$M_{\alpha,\beta} = \frac{1}{2}\sum_\omega v_{\alpha,\omega}\Lambda_\omega v_{\beta,\omega}^*\,. \qquad (12)$$

The coeficient $1/2$ is for later convenience. The eigenvectors of M, $v_{\alpha,\omega}$ can be classified according to their symmetry properties under the exchange of the single-particle indices $\alpha = (ri) \to \alpha' = (ir)$. They can be either symmetric (which are appropriate for bosons) or antisymmetric (for fermions). Since the index α is to be summed in eq. (11), only the antisymmetric modes will contribute. There are $N_s(N_s - 1)/2$, where N_s is the number of single-particle states (that is, 190 antisymmetric modes in our case), some of them have negative Λ and some of them have positive Λ. In order to get rid of the positive Λ, we subtract and add to M the term $\frac{1}{2}g\delta_{\alpha,\beta}$. After some algebra, we obtain for sufficiently large g so that $\Lambda_\omega - g \le 0$,

$$\sum_\tau \hat{\xi}_\tau^2 = \sum_\tau \sum_{rs} a_r^\dagger (\xi_\tau^2)_{rs} - \frac{1}{2}\sum_\omega \hat{\Pi}_\omega^\dagger \hat{\Pi}_\omega + \frac{1}{2}g(N^2 - N), \qquad (13)$$

where

$$\hat{\Pi}_\omega = \sum_\beta \hat{P}_\beta v_{\beta,\omega}^* \sqrt{-\Lambda_\omega + g}, \qquad (14)$$

$\hat{\Pi}_\omega^\dagger$ being the Hermitian conjugate of the above. It should be noted that in eq. (13) there is still the positive square N^2; therefore our formalism cannot be applied for grand-canonical calculations. It is only in a particle-number–preserving subspace that the term $\frac{1}{2}g(N^2 - N)$ is a constant. Since these constants are competely irrelevant in the construction of the functional integral, they will be dropped. We can now proceed as usually done in the treatment of pairing potential. Introducing the quasi-spin operators

$$\hat{I}_{x\omega} = \frac{1}{2}(\hat{\Pi}_\omega^\dagger + \hat{\Pi}_\omega), \qquad \hat{I}_{y\omega} = \frac{i}{2}(\hat{\Pi}_\omega^\dagger - \hat{\Pi}_\omega) \qquad (15)$$

we arrive at, after evaluating the commutator $[\hat{\Pi}_\omega^\dagger, \hat{\Pi}_\omega]$

$$\sum_\tau \hat{\xi}_\tau^2 = -\frac{1}{2}\sum_\omega (\hat{I}_{x\omega}^2 + \hat{I}_{y\omega}^2) + c(N)\,, \qquad (16)$$

where $c(N)$ is a c-number function of the particle number. In obtaining this equation we used the property $\mathrm{tr}\xi_\tau = 0$. The term $a^\dagger \xi_\tau^2 a$ is cancelled by the commutator $[\hat{\Pi}_\omega^\dagger, \hat{\Pi}_\omega]$.

Finally, up to a constant, our original Hamiltonian becomes

$$\hat{H} = \hat{H}_1 - \frac{1}{2}\sum_{\lambda_\mu > 0}[\hat{Q}_\mu(n) + \hat{Q}_\mu(p)]^2$$
$$-\frac{1}{2}\sum_{\lambda_\tau < 0}[\hat{\xi}_\tau(n) - \hat{\xi}_\tau(p)]^2 - \frac{1}{2}\sum_\omega (\hat{I}_{x\omega}(n)^2 + \hat{I}_{y\omega}(p)^2), \qquad (17)$$

where we reintroduced the neutron and proton label (n, p). Also, in order to shorten the formula we assume that the cranking term and chemical-potential terms have already been included in the single-particle part $\hat{H}_1$. We shall call this expression the Hermitian decomposition of the Hamiltonian and stress that it can only be used in the subspace of the Hilbert space with a definite value of the particle number.

The Hubbard-Startonovich transformation applied to eq. (17) gives, apart a normalization constant

$$\exp[-\beta\hat{H}] = \int \mathrm{d}x G(x)\hat{W}(n)\hat{W}(p)\,, \qquad (18)$$

where the volume element $\mathrm{d}x$ is

$$\mathrm{d}x = \prod_{m=1}^{N_t}\left[\prod_\mu \mathrm{d}\sigma_{\mu m}\prod_\tau \mathrm{d}\eta_{\tau m}\prod_{t=n,p}\prod_\omega(\mathrm{d}\phi_{xmt\omega}\mathrm{d}\phi_{ymt\omega})\right] \qquad (19)$$

with N_t being the number of time intervals, $\sigma_{\mu m}$, $m = 1, \ldots, N_t$ the fields associated with the $\hat{Q}^2$ terms, $\eta_{\tau m}$, $m = 1, \ldots, N_t$ the fields associated with the $\hat{\xi}^2$ terms and $\phi_{xmt\omega}$ and $\phi_{ymt\omega}$ the fields associated with the $\hat{I}_x^2$ and $\hat{I}_y^2$ terms. The terms contained in the Gaussian weight are the following:

see eq. (20) below

with the single-particle matrices $K(n)$ and $K(p)$ (respectively for the neutrons and for the protons) given by eq. (22) below. The propagators in eq. (18) for the neutrons $\hat{W}(n)$ and for the protons $\hat{W}(p)$ are the time-ordered products $(t = n, p)$

$$\hat{W}(t) = \prod_{m=1}^{N_t}\exp\left[\frac{1}{2}(a^\dagger a)\begin{pmatrix} K & -\psi^* \\ \psi & -\tilde{K}\end{pmatrix}\begin{pmatrix} a \\ a^\dagger\end{pmatrix}\right]\,; \qquad (21)$$

$$G(x) = \mathrm{e}^{-1/2\sum_{m=1}^{N_t}\left[\sum_\mu \sigma_{\mu m}^2+\sum_\tau \eta_{\tau m}^2+\sum_{\omega,t=n,p}(\phi_{xmt\omega}^2+\phi_{ymt\omega}^2)\right]+1/2(\mathrm{tr}K(n)+\mathrm{tr}K(p)} \tag{20}$$

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here we have used a matrix notation so, for example, $(a^\dagger a)$ is the row vector $(a_r^\dagger, a_r)$ and

$$K = -\epsilon h_1 - \sqrt{\epsilon}\sum_\mu \sigma_{\mu m} q_\mu - \sqrt{\epsilon} s_t \sum_\tau \eta_{\tau m}\xi_\tau \tag{22}$$

with $s_t = +1, -1$ for $t = n, p$. h_1 is the single-particle Hamiltonian (after the addition of chemical potentials, cranking terms and rearrangements terms due to the extraction of the traces out of q_μ and ξ_τ appearing in $\hat{H}_1 = a^\dagger h_1 a$. The antisymmetric matrix ψ (one for the neutrons and one for the protons) is given by

$$\psi_{rs} = \sqrt{\epsilon}\sum_\omega v_{rs,\omega}^*[\phi_{xm\omega} + i\phi_{ym\omega}]\sqrt{-\Lambda_\omega + g}\,; \tag{23}$$

here we have replaced the superindex α by the pair of single-particle indices. Obviously only the antisymmetric modes are included in the sum over ω. The derivation of eqs. (18)-(23) parallels the one given in ref. [11] for the pairing + quadrupole model. These expressions are the ones appearing in eqs. (4) and (5).

In principle, the energies evaluated using eq. (1) are independent of the cranking frequencies and of the chemical potentials. However, the values of these parameters can affect the variances in the Monte Carlo evaluation of eqs. (4) and (5). While in our previous experience in the rare-earth region it was simple to determine their values using only the mean-field approximation to the functional integrals, in the case of the GXPF1 interaction we find that all gaps associated with the pairing terms in mean-field propagators are zero. This means that the mean-field propagators conserve the particle number, that is, the mean-field is insensitive to the values of the chemical potentials. Therefore, the recipe for the determination of the chemical potentials used in our previous work (ref. [11] and references therein) breaks down for this Hamiltonian. This is perhaps the strongest difficulty encountered in the calculations we shall discuss shortly. As a way out, we added a volume element of the type $\ln[\phi_{x\omega}^2]$ to the action exploiting the gauge symmetry of the pairing fields, and taking $\phi_{y\omega} = 0$. This prescription generates a strong chemical-potential dependence of the matrix elements of the propagator at the mean-field level. However, the chemical potentials obtained in this way are not always satisfactory (presumably weak pairing modes should not be included). This is a problem not completely understood. In the calculations, we took reasonable values not inconsistent with the single-particle energies.

The matrix elements of the GXPF1 potential are scaled according to the mass as done in ref. [10]. As trial wave functions, we have used VAMPIR-like wave functions (ref. [2]). We did not however project onto good isospin T, but rather, we took the wave function to be a product of a neutron and a proton wave functions. The VAMPIR wave functions are notoriously difficult to determine, and we stopped the variational calculation when the average absolute value of the energy gradient (the residual gradient) is of the order of 10^{-3} or smaller. We considered $\beta = 0.1$ MeV^{-1} and $\beta = 0.15$ MeV^{-1} (see footnote [1]). For the nuclei considered in this work, we obtained the following results (all energies and chemical potentials are in MeV, and all values of β are in MeV^{-1}).

For ^{60}Fe the ground-state energy of the VAMPIR wave function is -228.492 (the residual gradient is $4 \cdot 10^{-4}$), the Monte Carlo estimate of the energy is, at $\beta = 0.1$, $E(\beta) = -228.802 \pm 0.094$ (with 99 samples having a residual autocorrelation of 0.004), and at $\beta = 0.15$, $E(\beta) = -229.217 \pm 0.244$ (with 116 samples and a residual autocorrelation of -0.03). The exact shell model value (ref. [13]) is $E_{\mathrm{shm}} = -228.923$. At $\beta = 0.1$ the n and p chemical potentials are $-1.$ and -3.1. At $\beta = 0.15$ the chemical potentials were determined with the mean-field method as in ref. [11], taking into account the volume elements of the pairing fields; the values are 9 and -8.9 for neutrons and protons, respectively. Their value is hard to reconcile with the single-particle energy levels and it constitutes one of the difficulties previously mentioned. It should however be pointed out that the Hamiltonian of eq. (17) differs from the original Hamiltonian by a real function of the neutron and proton numbers that can affect the values of the chemical potentials. Although difficult to understand, they do not seem to affect the Monte Carlo result for the energy. For ^{64}Ni the energy of the VAMPIR wave function is -281.508 (residual gradient 0.0004). We performed the Monte Carlo calculation only at $\beta = 0.1$ and obtained $E(\beta) = -281.868 \pm 0.141$ with 103 samples (residual autocorrelation 0.02) using n and p chemical potentials equal to -3.1. This calculation was the first performed, before we added the volume element in the determination of the chemical potentials. After the recipe was modified, the calculation was repeated with the values 18.4 and -7.8 (for n and p, respectively), and we obtained $E(\beta) = -281.656 \pm 0.039$. The exact shell model value of ref. [13] is -281.780. For the much more studied nucleus ^{56}Ni, which closes the $f_{7/2}$ shell, the energy of the VAMPIR wave function is -206.058 (residual gradient 0.0035), the Monte Carlo calculation gave $E(\beta = 0.1) = -206.119 \pm 0.033$ and $E(\beta = 0.15) = -206.066 \pm 0.148$ (the number of samples and the residual autocorrelations are 94 and 123 and 0.12 and -0.09, respectively). The shell model value obtained with up to 7 excitations out of the $f_{7/2}$ shell is (ref. [13]) $E = -206.269$. In this case the

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[1] The variable β should not be confused with the inverse temperature, as we are not evaluating canonical partition functions, but it is rather a positive parameter which controls the quality of the wave function $\exp(-\beta\hat{H})|\psi NZ\rangle$. The better the trial wave function, the smallest the value of β necessary to converge to the ground state.

values we obtained are slightly higher than the shell model value. For the last case, ^{60}Zn, we had problems pointing out to a poor understanding of the chemical-potential problem, or perhaps to a not so good trial wave function for $N = Z$ (it should be recalled that we do not perform a T^2 projection). The VAMPIR wave function has an energy of -254.848 (residual gradient 0.0015), at $\beta = 0.1$ the Monte Carlo energy is -254.974 ± 0.219, at $\beta = 0.15$ the statistics was ruined by a single energy sample requiring probably several hundred samples to recover good statistics. The shell model ground-state energy, inclusive of up to 5 excitations of the $f_{7/2}$ shell, is -255.502. Because of this problem, we considered the value $\beta = 0.125$ instead. The Monte Carlo result for this value of β is $E(\beta = 0.125) = -255.356 \pm 0.164$ with 105 samples having a residual autocorrelation of -0.13. Although the shell model result does not include the full Hilbert space and despite the poorly understood problem of the chemical potentials (we took -0.9 and -0.9 at this value of β), the Monte Carlo result is quite satisfactory.

In conclusion, we generalized the Hermitian decomposition used in the spectroscopic Monte Carlo method of refs. [11] and [12] by modifying the decomposition of the Hamiltonian of ref. [7], and we were able to reproduce reasonably well the shell model energies of selected nuclei in the fp shell using the realistic GXPF1 effective interaction.

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