Odd-Particle Systems in the Shell Model Monte Carlo Method: Circumventing a Sign Problem

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Odd-particle-number systems in the shell model Monte Carlo: circumventing a sign problem

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Application of the shell model Monte Carlo method to odd-particle-number systems has been hampered by the sign problem that originates from the projection on an odd number of particles. We introduce a novel method that avoids this sign problem by extracting the ground-state energy of a finite-size system with an odd number of particles from the asymptotic behavior of the imaginary-time single-particle Green's functions of the even-particle-number system. We apply this method to calculate pairing gaps of nuclei in the iron region. Our results are in good agreement with experimental pairing gaps.

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Introduction. The shell model Monte Carlo (SMMC) approach [1–4] has been used successfully to calculate statistical properties of nuclei [5–7] within the framework of the configuration-interaction shell model. Recently, this method has also been applied to trapped cold atom systems [8, 9]. The SMMC method enables calculations in model spaces that are many orders of magnitude larger than those that can be treated by conventional diagonalization methods.

For typical effective nuclear interactions, the SMMC method breaks down at low temperatures because of the so-called fermionic sign problem, leading to large statistical errors. In the grand-canonical ensemble, the sign problem can be avoided by constructing good-sign interactions that include the dominant collective components of effective nuclear interactions [10]. The remaining part of the effective interaction can be accounted for by using the method of Ref. 2.

In finite-size systems, such as nuclei, it is necessary to use the canonical ensemble, in which the number of particles is fixed. This particle-number projection gives rise to an additional sign problem when the number of particles is odd, leading to a rapid growth of statistical errors at low temperatures even for good-sign interactions. Consequently, it has been a major challenge to make accurate estimates of the ground-state energy of odd-particle systems in SMMC. Accurate ground-state energies are necessary for the calculation of level densities and pairing gaps (i.e., odd-even staggering of binding energies).

Here we develop a method based on the asymptotic behavior of the imaginary-time single-particle Green's functions of an even-particle system to calculate ground-state energies of neighboring odd-particle systems. This method is somewhat similar in spirit to a technique used in lattice quantum chromodynamics to extract hadron masses (see, e.g., in Ref. 11). We apply our Green's function method to calculate pairing gaps of nuclei in the iron region using the complete $fp + g_{9/2}$ shell model space.

Green's functions in SMMC. The SMMC method is based on the Hubbard-Stratonovich representation of the imaginary-time propagator, $e^{-\beta H} = \int D[\sigma] G(\sigma) U_\sigma(\beta)$, where β is the inverse temperature, H is the Hamiltonian, $D[\sigma]$ is the integration measure, $G(\sigma)$ is a Gaussian weight, and $U_\sigma(\beta)$ is the propagator of non-interacting nucleons moving in external auxiliary fields σ that depend on the imaginary time τ ($0 \le \tau \le \beta$). The canonical thermal expectation value of an observable $\hat{O}$ is given by $\langle \hat{O} \rangle = \int D[\sigma] G(\sigma) \mathrm{Tr}_{\mathcal{A}}[\hat{O} U_\sigma(\beta)] / \int D[\sigma] G(\sigma) \mathrm{Tr}_{\mathcal{A}} U_\sigma(\beta)$, where $\mathrm{Tr}_{\mathcal{A}}$ denotes a trace over the subspace of a fixed number of particles $\mathcal{A}$. In actual calculations we project on both proton number Z and neutron number N, and in the following $\mathcal{A}$ will denote (Z, N).

For a quantity X_σ that depends on the auxiliary fields σ, we define

$$\overline{X}_\sigma \equiv \frac{\int D[\sigma] |W(\sigma)| X_\sigma \Phi_\sigma}{\int D[\sigma] |W(\sigma)| \Phi_\sigma}, \tag{1}$$

where $W(\sigma) = G(\sigma) \mathrm{Tr}_{\mathcal{A}} U_\sigma$ and $\Phi_\sigma = W(\sigma)/|W(\sigma)|$ is the sign. With this definition, the above thermal expectation of an observable $\hat{O}$ can be written as $\langle \hat{O} \rangle = \overline{\langle \hat{O} \rangle}_\sigma$, where $\langle \hat{O} \rangle_\sigma = \mathrm{Tr}_{\mathcal{A}}[\hat{O} U_\sigma(\beta)] / \mathrm{Tr}_{\mathcal{A}} U_\sigma(\beta)$. In SMMC we choose M samples σ_k according to the weight function $|W(\sigma)|$, and estimate the average quantity in (1) by $\overline{X}_\sigma \approx \sum_k X_{\sigma_k} \Phi_{\sigma_k} / \sum_k \Phi_{\sigma_k}$.

For an even number of particles with a good-sign interaction, the average value of the sign Φ_σ remains close to 1. However, when the number of particles is odd, the average sign decays towards zero as the temperature is lowered. This leads to rapidly growing errors, hampering the direct application of SMMC at low temperatures for odd-particle systems.

For a rotationally invariant and time-independent Hamiltonian, we define the following scalar imaginary-time Green's functions [12]

$$G_\nu(\tau) = \frac{\mathrm{Tr}_{\mathcal{A}} \left[e^{-\beta H} \mathcal{T} \sum_m a_{\nu m}(\tau) a^\dagger_{\nu m}(0) \right]}{\mathrm{Tr}_{\mathcal{A}}\, e^{-\beta H}}, \tag{2}$$

where $\nu \equiv (nlj)$ labels the nucleon single-particle orbital

with radial quantum number n, orbital angular momentum l and total spin j. Here $\mathcal{T}$ denotes time ordering and $a_{\nu m}(\tau) \equiv e^{\tau H} a_{\nu m} e^{-\tau H}$ is an annihilation operator of a nucleon at imaginary time τ ($-\beta \le \tau \le \beta$) in a single-particle state with orbital ν and magnetic quantum number m ($-j \le m \le j$).

Using the Hubbard-Stratonovich transformation, the Green's functions defined in (2) can be written in a form suitable for SMMC calculations

$$G_\nu(\tau) = \begin{cases} \overline{\sum_m \left[\mathbf{U}_\sigma(\tau)(\mathbf{I} - \langle\hat{\rho}\rangle_\sigma\right]_{\nu m,\nu m}} & \text{for } \tau > 0 \\ \overline{\sum_m \left[\langle\hat{\rho}\rangle_\sigma \mathbf{U}_\sigma^{-1}(|\tau|)\right]_{\nu m,\nu m}} & \text{for } \tau \le 0 \end{cases}, \tag{3}$$

where we have used the notation in Eq. (1). Here $\mathbf{U}_\sigma(\tau)$ and $\mathbf{I}$ are matrices in the single-particle space representing the propagator $U_\sigma(\tau)$ and the identity, respectively. $\langle\hat{\rho}\rangle_\sigma$ is a matrix in the single-particle space whose $\nu m, \nu' m'$ matrix element $\langle\hat{\rho}_{\nu m,\nu' m'}\rangle_\sigma$ is defined in terms of the one-body density operator $\hat{\rho}_{\nu m,\nu' m'} = a^\dagger_{\nu' m'} a_{\nu m}$.

Assuming $\mathcal{A}$ is an even-even nucleus, $\mathcal{A}_\pm \equiv (Z, N \pm 1)$ are neighboring odd-even nuclei with odd number of neutrons. We denote by $E_J(\mathcal{A})$ the lowest energy eigenvalue of a given spin J for the $\mathcal{A}$-particle nucleus, and define $E_J(\mathcal{A}_\pm)$ similarly for the $\mathcal{A}_\pm$-particle nucleus. We also define $\Delta E_J(\mathcal{A}_\pm) = E_J(\mathcal{A}_\pm) - E_0(\mathcal{A})$. Assuming that the ground state of the even-even nucleus has spin zero [i.e., $E_{\rm gs}(\mathcal{A}) = E_0(\mathcal{A})$], the ground-state energy of the odd-even nucleus is given by, $E_{\rm gs}(\mathcal{A}_\pm) = E_{\rm gs}(\mathcal{A}) + \Delta E_{\rm min}(\mathcal{A}_\pm)$, where $\Delta E_{\rm min}$ is the minimum of $\Delta E_J(\mathcal{A}_\pm)$ over the possible values of J.

The energy $E_{\rm gs}(\mathcal{A})$ can be calculated directly from SMMC. In this work we show how $\Delta E_{\rm min}(\mathcal{A}_\pm)$ can be calculated accurately using the single-particle Green's functions of the $\mathcal{A}$-particle system, thereby enabling an accurate estimate of $E_{\rm gs}(\mathcal{A}_\pm)$

The neutron Green's function $G_\nu(\tau)$ that corresponds to an orbital with angular momentum j describes for $\tau > 0$ ($\tau \le 0$) a process that connects the $J = 0$ ground state of the even-even nucleus $\mathcal{A}$ to intermediate states in the odd-even nucleus $\mathcal{A}_+$ ($\mathcal{A}_-$) with spin $J = j$. It can be written as

$$G_\nu(\tau) = Z^{-1}(\beta) e^{-\beta E_{\rm gs}(\mathcal{A})} \left[R_\nu e^{-\Delta E_{J=j}(\mathcal{A}_\pm)|\tau|} + \delta G_{\rm ex} \right], \tag{4}$$

where the $+$ ($-$) subscript should be used for $\tau > 0$ ($\tau \le 0$), $Z(\beta)$ is the partition function of the $\mathcal{A}$-particle nucleus, and R_ν is proportional to the square of the reduced matrix element of a_ν between the ground state of the $\mathcal{A}$-particle nucleus and the lowest spin $J = j$ eigenstate of the $\mathcal{A}_\pm$-particle nucleus. The contribution from excited states is denoted by $\delta G_{\rm ex}$. Clearly, $\delta G_{\rm ex}$ is a sum of products of decaying exponentials which depend on excitation energies in the $\mathcal{A}_\pm$- and $\mathcal{A}$-particle systems, and squares of matrix elements of a_ν between the corresponding eigenstates.

When $\delta G_{\rm ex}$ is much smaller than the first term inside the square brackets on the r.h.s. of Eq. (4), the τ dependence of the Green's function can be well approximated by a single exponential, $G_\nu(\tau) \sim e^{-\Delta E_j(\mathcal{A}_\pm)|\tau|}$. In this asymptotic regime for τ, we can calculate $\Delta E_j(\mathcal{A}_\pm)$, and hence $E_{\rm gs}(\mathcal{A}_\pm)$ from the slope of $\ln G_\nu(\tau)$. This is the method we use here to calculate the ground-state energy of odd-A nuclei with odd number of neutrons. The ground-state energy of odd-A nuclei with odd number of protons can be similarly calculated using the proton Green's functions.

In principle, the asymptotic regime is accessed in the limit $\beta \to \infty$ and $|\tau| \to \infty$ with $|\tau| \ll \beta$. However, in a shell-model Hamiltonian with discrete, well separated energy levels, only a few transitions give significant contributions. If the relative contribution from $\delta G_{\rm ex}$ in Eq. (4) is less than a few percent, then (assuming that $|\tau| \sim 1$ MeV) the sensitivity of the slope of $\ln G_\nu(\tau)$ to this contribution is about a few tens of keV, which is comparable to our target accuracy. For low- and medium-mass nuclei, we expect the energy differences to be $\gtrsim 1$ MeV and the square matrix elements to be smaller than R_ν. Thus, calculations with β of a few MeV^{-1} and with an asymptotic regime of $\tau \sim 1$ MeV should be sufficient. This can be validated explicitly in *sd*-shell nuclei (see below), whose Hamiltonian can be diagonalized numerically. For larger model spaces, it is not possible to calculate explicitly the corrections in the sum of Eq. (4), and the asymptotic region has to be determined by the goodness of the linear fits to $\ln G_\nu(\tau)$.

Results. We first tested the Green's function method in *sd*-shell nuclei and then applied it to medium-mass nuclei in the complete $(pf + g_{9/2})$ shell. In these nuclei, we carried out calculations for several values of β in the range 3 MeV$^{-1} \le \beta \le 4$ MeV^{-1}. For each β, we calculated $G_\nu(\tau)$ for a range of values of τ in steps of 1/32 MeV^{-1}. The energy differences $\Delta E_J(\mathcal{A}_\pm)$ are then calculated by fitting straight lines to $\ln G_\nu(\tau)$ in the asymptotic region using generalized least squares regression.

We chose the asymptotic region such that the fits have χ^2 per degree of freedom ~ 1. We find a good asymptotic region to be 0.5 MeV$^{-1} \le \tau \le 2$ MeV^{-1}. For this choice the χ^2 per degree of freedom is between 0.8 and 1.2 for the cases we considered. The energies are calculated for each value of β and a weighted average of the energies at different values of β is then taken.

In a few selected cases, we also performed calculations for larger values of β (i.e., $\beta > 4$ MeV^{-1}), and found the corresponding values of $\Delta E_{\rm min}(\mathcal{A}_\pm)$ to be consistent with those obtained in the region 3 MeV$^{-1} \le \beta \le 4$ MeV^{-1}. This indicates that for the model spaces and particle numbers considered, the above chosen values of β are sufficiently large to isolate the ground state of the corresponding even-even nucleus.

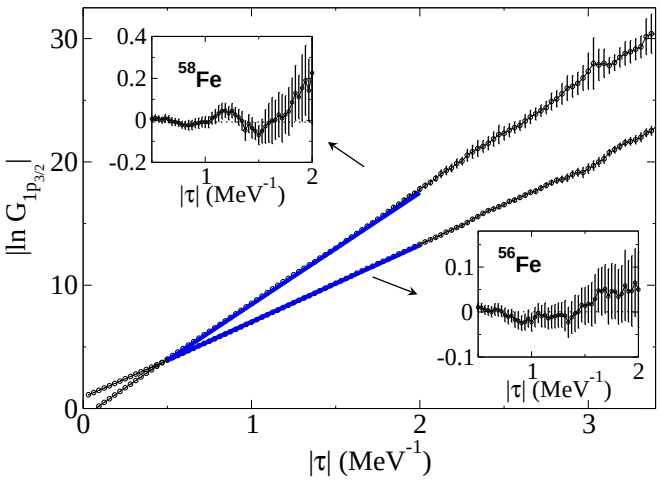

FIG. 1. The absolute value of logarithm of the Green's function (2) for the neutron orbital $\nu = 1p_{3/2}$ in ^{56}Fe (lower curve, $\tau > 0$) and ^{58}Fe (upper curve, $\tau \leq 0$) at $\beta = 4$ MeV^{-1}. The solid blue lines are linear fits for 0.5 MeV$^{-1} \leq |\tau| \leq 2$ MeV^{-1}. The slope of the fitted line in the lower (upper) curve provides the energy difference between the lowest $J = 3/2$ state in ^{57}Fe and the ground state of ^{56}Fe (^{58}Fe). The insets show the deviations from the linear fits.

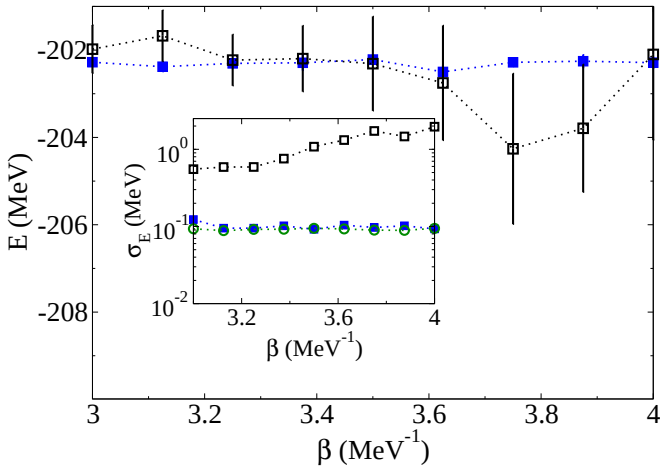

FIG. 2. The energy of the ^{57}Fe nucleus calculated from the present method and direct SMMC are shown by solid and open squares, respectively. The error bars describe the statistical errors. Inset: the statistical errors for the energy of ^{57}Fe in the present method (solid squares) and in direct SMMC calculations (open squares) are shown on a logarithmic scale. The statistical errors for the energy of ^{56}Fe using the same Hamiltonian are shown by open circles.

For a given odd system (an odd-even nucleus) there are two neighboring even systems (even-even nuclei), and our method can be used by starting from either of the even systems. The ground-state energies we get from these two calculations are consistent with each other, providing an independent validation of our method. Unless otherwise noted, the results we report here are the average of both of these calculations.

To test the validity and accuracy of our method, we performed calculations in the *sd* shell using a schematic good-sign Hamiltonian. In all cases, our results deviated no more than 0.1% from the exact ground-state energies, obtained by diagonalizing the Hamiltonian with the `OXBASH` code [13]. For example for ^{29}Si we found a ground-state energy of -133.98 ± 0.04 MeV compared with the exact result of -133.95 MeV. Our method also reproduced correctly the ground-state spin in all cases.

We applied our method to nuclei in the $(pf+g_{9/2})$ shell, using the isospin-conserving Hamiltonian of Ref. [5]. Typical results are demonstrated in Fig. 1, in which the absolute value of the logarithm of the Green's functions for the neutron orbital $\nu = 1p_{3/2}$ in ^{56}Fe ($\tau > 0$) and in ^{58}Fe ($\tau \leq 0$) are plotted versus $|\tau|$ for $\beta = 4$ MeV^{-1}. The linear fits (solid lines) were used in the calculation of the ground-state energy of ^{57}Fe. The deviations from the linear fits are shown in the insets of Fig. 1.

A direct application of the SMMC method to the odd-particle systems suffers from a sign problem which leads to very large statistical errors at low temperatures. In contrast, the method presented here does not have such problem. This is illustrated in Fig. 2 where we compare the energy and its statistical error for the ^{57}Fe nucleus in the present method (using the neutron Green's functions of ^{56}Fe) with the results obtained from the direct method. The errors in the present method remain roughly constant with β. At $\beta = 3$ MeV^{-1} the statistical error in the direct method is about 5 times larger than the present method while at $\beta = 4$ MeV^{-1} it is about 20 times larger. The inset shows the statistical errors on a logarithmic scale. For comparison we have also included the statistical error in the energy of the even-even nucleus ^{56}Fe using the same Hamiltonian. We note that the total computational time for a given value of β increases by less than a few percent when the Green's function calculations are included.

We applied our Green's function method for families of odd-neutron isotopes: $^{47-49}$Ti, $^{51-57}$Cr, $^{53-61}$Fe, $^{59-65}$Ni, $^{63-67}$Zn and $^{71-73}$Ge. The ground-state spins we determine are in agreement with experimental values in all cases except for ^{47}Ti, ^{57}Fe and ^{63}Ni. The anomalous ground-state spin of ^{57}Fe from the shell model perspective is well documented in the literature [14].

In our method we extract directly the odd-even ground state energy differences, and therefore this method is particularly suitable for accurate calculations of pairing gaps (i.e., odd-even staggering of masses).

When extracting an odd-even ground-state energy difference such as $\Delta E_{\rm min}(\mathcal{A}_+)$ we use the Hamiltonian of the $\mathcal{A}_+$ nucleus for both the $\mathcal{A}_+$ and $\mathcal{A}$ nuclei. Since the $fp+g_{9/2}$-shell Hamiltonian we use is nucleus-dependent [5], it is necessary to correct the ground-state energy of the $\mathcal{A}$ nucleus. As the latter is an even-even nucleus, this cor-

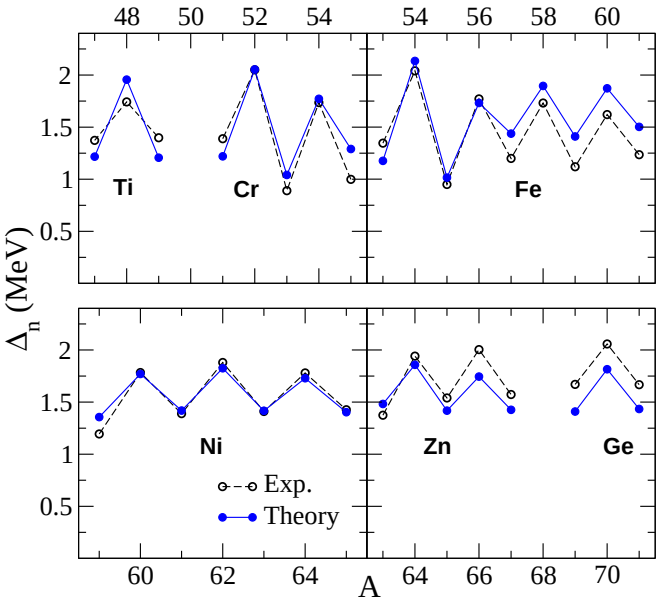

FIG. 3. Neutron pairing gaps Δ_n as a function of mass number A in $fp + g_{9/2}$-shell nuclei. The gaps calculated with the present Green's function method (solid circles connected by solid lines) are compared with the experimental gaps (open circles connected by dashed lines). The theoretical statistical errors are smaller than the size of the symbols.

rection can be found in direct SMMC calculations for the $\mathcal{A}$ nucleus. However, this correction can also be estimated as follows. The dependence of the interaction on the nucleus is rather weak; the strengths of the multipole-multipole interactions depend weakly on the mass number A ($\propto A^{-1/3}$) and the monopole pairing strength is constant through the shell. The largest variation among neighboring nuclei is that of the single-particle energies $\varepsilon_\mu(\mathcal{A})$ of the orbitals μ. Correcting for this variation, the neutron separation energy for the $\mathcal{A}_+$ nucleus is given by

$$S_n(\mathcal{A}_+) = -\Delta E_{\min}(\mathcal{A}_+) + \sum_\mu [\varepsilon_\mu(\mathcal{A}) - \varepsilon_\mu(\mathcal{A}_+)]\langle n_\mu\rangle_{\mathcal{A}} \ , \tag{5}$$

where $\langle n_\mu\rangle_{\mathcal{A}}$ are the average occupation numbers for the $\mathcal{A}$ nucleus using the Hamiltonian for the $\mathcal{A}_+$ nucleus. The second term on the r.h.s. of (5) approximates the difference between the ground-state energies of the $\mathcal{A}$ nucleus when calculated using the respective Hamiltonians for the $\mathcal{A}$ and $\mathcal{A}_+$ nuclei. We verified (in *sd*-shell nuclei) that this approximation is highly accurate and well within a typical statistical error. In our calculations we used (5) since the resulting statistical error is much smaller than the statistical error of direct SMMC calculations.

The neutron separation energy for the $\mathcal{A}$ nucleus is given by a similar expression. The neutron pairing gaps can then be calculated from the differences of separation energies $\Delta_n(\mathcal{A}) = (-)^N[S_n(\mathcal{A}_+) - S_n(\mathcal{A})]/2$, where $\mathcal{A}$ can now be either an even-even or an odd-even nucleus.

Our calculated pairing gaps are shown in Fig. 3 (solid circles), where they are compared with the experimental pairing gaps (open circles) as determined from odd-even staggering of binding energies. The statistical errors for the calculated pairing gaps (~ 0.01 MeV) are not visible in the figure. Our results agree quite well with the experimental values; in most cases the deviation of the theoretical pairing gaps from their experimental counterparts is less than 15%. Systematic deviations are observed for the iron isotopes above $A = 59$ and for the germanium isotopes. For the germanium isotopes the size of the model space might be insufficient, while the deviation for the iron isotopes indicates the necessity to refine our isospin-conserving Hamiltonian.

Conclusion. We have described a practical method that circumvents a sign problem for calculating the ground-state energy of odd-particle-number systems in the framework of the SMMC approach. We demonstrated the usefulness of the method by calculating pairing gaps of nuclei in the $fp + g_{9/2}$ shell. This method can also be applied to other finite-size many body systems such as trapped cold atoms. In principle, this method can be used more generally to calculate the lowest energy state for a given spin. Although the higher excited states typically have large statistical error, low-lying excitations can often be estimated quite accurately using this method. This problem could be addressed in future research.

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