Full configuration interaction quantum Monte Carlo in nuclear structure calculations

Authors: Shao-Liang Jin, Jian-Guo Li, Yuan Gao, Rong-Zhe Hu, Fu-Rong Xu, Fu-Rong Xu

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Abstract

The full configuration interaction quantum Monte Carlo (FCIQMC) method, originally developed in quantum chemistry, has also been successful in both molecular and condensed matter systems. Another natural extension of this methodology would be its application to nuclear structure calculations. We have developed the FCIQMC approach for studying nuclear systems. To validate the method, we applied FCIQMC to a small model space where standard shell model remain computationally feasible. Specifically, we performed calculations for Fe isotopes using pf-shell GXPF1A interaction and compared the results with those obtained from standard shell model calculations. To further demonstrate the capabilities of FCIQMC, we investigated its performance in systems exhibiting strong correlations, where conventional nuclear structure models are less effective. Using an artificially constructed strongly correlated system with a modified GXPF1A interaction, our calculations revealed that FCIQMC delivers superior results compared to many existing methods. Finally, we apply FCIQMC to Mg isotopes in the sdpf-shell model space, showing its potential to perform accurate calculations in large model spaces that are inaccessible to the shell model due to the limitations of current computational resources.

Full Text

Preamble

Full Configuration Interaction Quantum Monte Carlo in Nuclear Structure Calculations

S. L. Jin,[1] J. G. Li,[2,3,1] Y. Gao,[1] R. Z. Hu,[1] and F. R. Xu[1,3,*]

[1]School of Physics, and State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China
[2]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000,

China
[3]Southern Center for Nuclear-Science Theory (SCNT), Institute of Modern Physics, Chinese Academy of Sciences, Huizhou 516000, China

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The full configuration interaction quantum Monte Carlo (FCIQMC) method, originally developed in quantum chemistry, has also proven successful for both molecular and condensed matter systems. A natural extension of this methodology is its application to nuclear structure calculations. We have developed the FCIQMC approach for studying nuclear systems. To validate the method, we applied FCIQMC to a small model space where standard shell model calculations remain computationally feasible. Specifically, we performed calculations for Fe isotopes using the pf-shell GXPF1A interaction and compared the results with those obtained from standard shell model calculations.

To further demonstrate the capabilities of FCIQMC, we investigated its performance in systems exhibiting strong correlations, where conventional nuclear structure models are less effective. Using an artificially constructed strongly correlated system with a modified GXPF1A interaction, our calculations revealed that FCIQMC delivers superior results compared to many existing methods.

Finally, we apply FCIQMC to Mg isotopes in the sdpf-shell model space, demonstrating its potential to perform accurate calculations in large model spaces that are inaccessible to the shell model due to limitations of current computational resources.

Introduction

Atomic nuclei are self-bound quantum many-body systems, and a key goal in modern nuclear physics is to solve these systems from first principles. To achieve this, one can compute the ground-state and excited-state energies, along with their corresponding wavefunctions, either in coordinate space or within a specific basis, such as the harmonic oscillator basis.

Methods in coordinate space are typically represented by various quantum Monte Carlo (QMC) techniques, including diffusion Monte Carlo (DMC) and the related Green's function Monte Carlo (GFMC) [1–4]. These methods have proven successful for accurately solving the properties of light nuclei. However, a major obstacle for these methods is the Fermion sign problem: due to the antisymmetry property of the many-body wavefunction, the wavefunction necessarily contains both positive and negative amplitudes, which cannot be directly sampled using a probability distribution. To mitigate the sign problem, techniques such as the fixed-node approximation or the constrained-path method are often employed [2, 4]. A key challenge in these methods is the need for a trial wavefunction that approximates the true wavefunction as closely as possible.

The configuration interaction (CI) methods, including the configuration interaction shell model (CISM) [5, 6] and no-core shell model (NCSM) [7, 8], provide direct and accurate frameworks for solving quantum many-body systems in basis space. However, the configuration space grows exponentially with the number of particles, making it computationally infeasible to store all configurations in memory. To address this issue, one can truncate the configuration space using methods like particle-hole truncation or ω truncation. Despite these techniques, a large number of configurations is still required to achieve converged results, which is impossible for large-dimension systems [9].

An alternative approach is the post-Hartree-Fock methods, which offer polynomial complexity. These include perturbative approaches, such as many-body perturbation theory (MBPT) [10–13], and non-perturbative approaches, such as the in-medium similarity renormalization group (IMSRG) [14–16] and coupled cluster (CC) [17, 18]. However, all of these approaches rely on some kind of truncation scheme, which may introduce inaccuracies, particularly in strongly correlated systems. Efforts to improve accuracy by going to higher-order truncations [19, 20] are in progress, though computational cost remains a significant challenge.

In 2009, Booth et al. developed the full configuration interaction quantum Monte Carlo method for quantum chemistry calculations [21]. This method samples wavefunctions in the configuration space, allowing the storage of only a small subset of important configurations that is often several orders of magnitude smaller than those in the full configuration space. Moreover, by utilizing signed walkers and walker annihilation, FCIQMC can avoid the Fermion sign problem and converge to the exact wavefunction without requiring prior knowledge of its nodal structure.

FCIQMC has been successfully applied to a range of systems [21–23], including both molecular and condensed matter systems, and has proven particularly effective for strongly correlated systems [24, 25]. Given its strengths, it shows promise for nuclear structure calculations. In this study, we have developed a C++ code implementing FCIQMC, taking into account the symmetry properties of nuclear systems.

Several other quantum Monte Carlo methods also operate in configuration space, including the Monte Carlo shell model (MCSM) [26, 27], which constructs the basis by evolving in the auxiliary field and then diagonalizes the Hamiltonian using that basis; and the configuration interaction Monte Carlo (CIMC) [28, 29], which, despite its similar name to FCIQMC, uses a guiding wavefunction to perform a "fixed-node approximation" in configuration space. It is important to note that, although these methods share some similarities, they are fundamentally distinct from one another.

This article is organized as follows: In Sec. II, we introduce the theory and algorithm of FCIQMC and its enhanced variant. In Sec. III, we present benchmarking results with shell model calculations for Fe isotopes in the pf-shell, and

for an artificially constructed strongly correlated system. We have also tested large-space calculations with the examples of Mg isotopes in the full sdpf shell.

II. The Full Configuration Interaction Quantum Monte Carlo

The CI methods aim to solve the Schrödinger equation $\hat{H}\Psi_0 = E_0\Psi_0$ in a configuration space. A configuration is a Slater determinant constructed from the single-particle basis. Considering a system of N particles with M single-particle orbitals, $a_i^\dagger$ $(i = 1, 2, ..., M)$, we can express all possible configurations as $|D_i\rangle = a^\dagger ... a^\dagger|0\rangle$, where $|0\rangle$ is the particle vacuum state. The Lanczos algorithm is powerful for diagonalizing Hamiltonians in configuration space, as used in the computational codes of Bigstick [30] and kshell [31], obtaining the exact wavefunction $\sum C_i|D_i\rangle$.

The dimension of the full configuration space is on the order of $\binom{M}{N}$, which grows exponentially with the number of particles. This makes it impossible to store all the coefficients C_i in memory when the system is large.

The FCIQMC method, instead, samples wavefunctions in configuration space. To achieve this, we use the projection method rather than diagonalization to obtain the ground-state wavefunction Ψ_0, by the following operator:

$$\psi(\tau) = e^{-\tau(\hat{H}-E_0)}\psi(\tau = 0) \xrightarrow[\tau\to\infty]{} \Psi_0,$$

where E_0 is the ground-state energy, and τ indicates a time evolution. In this process, excited states are projected out, and only the ground state remains. This approach is achieved by the so-called imaginary time Schrödinger equation:

$$\frac{\partial\psi(\tau)}{\partial\tau} = -(\hat{H} - E_0)\psi(\tau).$$

Expanding this differential equation in the configuration space, we obtain:

$$\frac{\partial C_i}{\partial\tau} = -\sum_j (H_{ij} - S\delta_{ij})C_j.$$

Here, we replace the ground-state energy E_0 with a self-adaptive shift S because the ground-state energy is unknown before the calculation. The method of adapting the shift S will be explained later.

Similar to the QMC methods in coordinate space, the coefficient C_i can be either positive or negative, making it impossible to sample them directly as a probability distribution. In the FCIQMC method, this issue is addressed by introducing so-called walkers, which are distributed across various determinants.

The number of walkers in $|D_i\rangle$ is denoted by N_i. To represent negative coefficients, every walker is assigned a sign, allowing N_i to be either positive or negative. The total number of walkers is given by $\sum_i |N_i|$.

We expect the walker number in a given determinant to be proportional to the corresponding expanded coefficients. In this way, the imaginary time Schrödinger equation can be discretized as:

$$\frac{\Delta N_i}{\Delta \tau} = -\sum_j (H_{ij} - S\delta_{ij}) N_j.$$

A typical evolution of FCIQMC starts with a single determinant $|D_0\rangle$, which can be the Hartree-Fock ground state or a determinant with the particles filling the lowest orbitals of the basis used. We begin the evolution with N_0 walkers in $|D_0\rangle$, according to Eq. (7). The process of the imaginary time evolution can be split into three periods: warm-up, projection, and statistics.

In the warm-up period, we keep a constant shift $S = \langle D_0|\hat{H}|D_0\rangle > E_0$. The ground-state wavefunction will grow with $\exp[-(E_0 - S)\tau]$, causing the total walker number to increase exponentially. Once the total walker number reaches a certain number, we enter the projection period. During this period, the shift begins to vary according to the total walker number. The goal is to maintain the total walker number at a constant level.

The shift S is updated every A steps, as suggested in Ref. [21]:

$$S(\tau) = S(\tau - A\Delta\tau) - \frac{\zeta}{A\Delta\tau} \ln\left(\frac{N_w(\tau)}{N_w(\tau - A\Delta\tau)}\right).$$

In this paper, we adapt the shift S every $A = 10$ steps, and set $\zeta = 0.1$ for all calculations.

When the imaginary time evolution reaches equilibrium—which means that the total walker number is almost stable and the shift S fluctuates only slightly around the ground state—we begin the statistics period. We continue the equilibrium evolution for several steps and perform statistical analysis to evaluate the ground-state energy. The shift parameter S can be used to evaluate the ground-state energy, and we can also use the local time energy:

$$E(\tau) = \frac{\langle D_0|\hat{H}|\psi(\tau)\rangle}{\langle D_0|\psi(\tau)\rangle} = \sum_i \frac{N_i(\tau)}{N_0(\tau)} H_{0i},$$

where $N_0(\tau)$ is the walker number in the $|D_0\rangle$ determinant, and H_{0i} is for $\langle D_0|\hat{H}|D_i\rangle$.

Now, the remaining challenge is how to evolve the imaginary time Schrödinger equation (Eq. 7) stably and effectively, which is the key to the FCIQMC calculation. Every $\Delta\tau$ evolution is done in three steps [21] as follows.

The spawning step: For each walker in determinant $|D_i\rangle$, we select a connected $|D_j\rangle$ with a probability of $p_{\text{gen}}(j|i)$, and attempt to spawn walkers into $|D_j\rangle$ with the following probability:

$$p_{\text{spawn}}(j|i) = \frac{\Delta\tau|H_{ij}|}{p_{\text{gen}}(j|i)}.$$

The sign of the newly spawned walker is opposite to $\text{sign}(H_{ij}N_i)$. Spawning walkers with probability $p_{\text{spawn}}(j|i)$ means that we directly spawn $\lfloor p_{\text{spawn}} \rfloor$ walkers with a probability of 1, and spawn one walker with a probability of $p_{\text{spawn}} - \lfloor p_{\text{spawn}} \rfloor$.

Two determinants $|D_i\rangle$ and $|D_j\rangle$ are said to be connected if $H_{ij} \neq 0$ and $j \neq i$. For a system with only one-body and two-body interactions, there are two types of connected determinants: single excitations and double excitations.

For a single excitation, we first select an occupied orbital (labeled by a) from $|D_i\rangle$ with an equal probability of $1/N_a$ where N_a is the number of the occupied orbitals in $|D_i\rangle$. Next, we identify all unoccupied orbitals in $|D_i\rangle$ which have the same parity, same spin projection m and same isospin projection t_z as those of the a orbital. From this set of unoccupied orbitals, we randomly select one (labeled by b) with an equal probability of $1/N_b$ where N_b is the number of such unoccupied orbitals. The $|D_j\rangle$ is then constructed by removing the a orbital and adding the b orbital to $|D_i\rangle$. Finally, the generation probability $p_{\text{gen}}(j|i)$ is determined as the product of the two probabilities, i.e., equal to $1/(N_a N_b)$.

For a double excitation, we first select two occupied orbitals labeled by a and b. Similar to that in the single excitation discussed above, each selection of one pair of occupied orbitals has equal probability. Then, we identify all pairs of unoccupied orbitals which have the same parity, same total spin projection m, and same total isospin projection t_z as those of the two-body state formed by the a and b orbitals. From this set of unoccupied orbital pairs, we randomly select one pair with an equal probability. As in the single excitation case, the generation probability $p_{\text{gen}}(j|i)$ is determined by the product of the probabilities associated with selecting the pair of occupied orbitals and the pair of unoccupied orbitals.

In each spawning attempt, we perform either a single excitation or a double excitation, chosen with probabilities p_{single} and $p_{\text{double}} = 1 - p_{\text{single}}$, respectively. The final p_{gen} is multiplied by p_{single} when a single excitation is chosen, or multiplied by p_{double} when a double excitation is chosen. In the present work, we use $p_{\text{single}} = 1/2$ for all calculations. Our calculations have indicated that this choice of probability assignment does not have a noticeable impact on the outcomes.

The diagonal death/cloning step: For each walker in determinant $|D_i\rangle$, we calculate $p_{\text{death}}(i) = \Delta\tau(H_{ii} - S)$. If $p_{\text{death}}(i) > 0$, the walker will die with a probability of $p_{\text{death}}(i)$. If $p_{\text{death}}(i) < 0$, the walker will clone with a probability of $-p_{\text{death}}(i)$.

The annihilation step: Collect all the walkers in the same determinant (including the spawned walkers), and annihilate pairs of walkers with opposite signs until only walkers with the same sign remain in the determinant. This step is necessary for preventing the exponential growth of walkers [21].

This algorithm can be extended to a Hamiltonian with three-body interactions easily, although we have not incorporated it in the present computational code. The only modification would be that the spawning step should include triplet excitations.

The original FCIQMC [21], as described above, can work for some systems, but it requires a minimum walker number that can be very large in certain cases. For example, with our code we found that in sd and pf shells the converged evolution requires a walker number almost the same as the dimension of a full configuration calculation. This phenomenon is due to the sign problem. During the Monte Carlo evolution, some determinants may randomly acquire a small number of walkers with opposite signs to the main wavefunction [32]. These components of the wavefunction can spread in subsequent steps, which requires a large total walker number to suppress them adequately.

Deidre Cleland et al. showed that the walker number required for convergence can be dramatically reduced by using the initiator truncation [24]. In this method, one defines some important determinants as initiators, and restricts non-initiator walkers from spawning into unoccupied determinants. In this way, we align the sign of the walkers in the small walker-number determinants with those in the large walker-number determinants, which helps to suppress the sign problem. This method is referred to as the initiator FCIQMC (i-FCIQMC) [24]. Actually, it truncates the original Hamiltonian as follows:

$$\tilde{H}_{ij} = \begin{cases} 0 & \text{if } |D_j\rangle \text{ is not an initiator and } N_i = 0, \\ H_{ij} & \text{otherwise.} \end{cases}$$

In our calculations, we define initiators by the determinants $|D_i\rangle$ with $|N_i| > n_\alpha$, where n_α is called the initiator threshold. This prescription approaches the original FCIQMC algorithm when the total walker number goes to infinity. In the present work, we take an initiator threshold of $n_\alpha = 3$.

Another improvement to the original FCIQMC method is the use of floating-point walker numbers [33], which enhances the stability of the evolution and reduces the statistical error of the results. However, the floating-point walker approach can lead to a large number of determinants being occupied by a small number of walkers. To reduce memory usage, a walker number cutoff, N_{occ},

is introduced [33]. In this method, if the walker number N_i is less than N_{occ}, it is either replaced by N_{occ} with a probability of N_i/N_{occ} or removed with a probability of $1 - N_i/N_{\text{occ}}$. This same procedure is applied to the spawned walkers with a separate cutoff parameter κ. We use the floating-point walker number method in the present work, and we take $N_{\text{occ}} = 1$ and $\kappa = 0.1$ in all calculations.

The i-FCIQMC method can also be used to obtain excited states [34]. In this approach, several parallel imaginary-time evolutions are run. After each $\Delta\tau$ evolution, we use Gram-Schmidt orthogonalization to obtain the orthogonal components of the wavefunction.

III. Calculations and Discussions

We first benchmark our computations with standard shell model calculations for Fe isotopes with the pf-shell interaction GXPF1A [35] using the code kshell [31]. As a detailed example, the Monte Carlo evolution for ^{56}Fe is shown in Fig. 1 [Figure 1: see original paper]. In the warm-up period, the total walker number grows rapidly. When the total walker number reaches the preset limit (it is 10^7 in ^{56}Fe), the shift S starts to vary according to Eq. (8). In the present work, we have made a small modification based on that in Ref. [24], which is that we do not apply the initiator truncation in the warm-up period, while the initiator truncation is used in the subsequent periods. With the initiator truncation, the total walker number drops temporarily but grows up again. As time progresses, the system reaches equilibrium, and the shift S should be stable around the expected ground-state energy. After that, we continue the evolution for a few more steps and perform statistical analysis to extract the ground-state energy. In the ^{56}Fe calculation, we use $\Delta\tau = 5\times10^{-4}$ zs in the evolution. The projection period takes 3.5 zs, and the statistics period takes 1.5 zs.

The equilibrium walker number and evolution time can vary across systems, and there is no fixed ratio between the equilibrium walker number and the preset limit of the warm-up. The time required for the projection and statistical periods can also vary from system to system. The preset walker number and evolution time can be optimized through a trial run with a smaller walker number and some empirical judgment.

Table I presents our i-FCIQMC calculations of the Fe isotopes with the GXPF1A interaction, benchmarked against standard shell model calculations with the same interaction. The i-FCIQMC calculations give almost the same results as the full pf-configuration SM calculations, demonstrating the validity of i-FCIQMC when applied to nuclear structure calculations. In Table I, we have also shown the mean walker number in equilibrium, which is smaller than the dimension of the full configuration SM calculation. Using our current implementation, the i-FCIQMC method achieves these results with a memory requirement that is 1–2 orders of magnitude smaller than that of the SM calculations.

[Figure 1: see original paper]

FCIQMC is applicable to strongly correlated systems, while other methods would not work well. In Ref. [37], Horoi et al. demonstrated that for a strongly correlated system, the CC calculation may give significantly unbound energies compared to the full configuration SM calculation. In that work, the authors enhanced correlations in ^{56}Ni by decreasing the shell gap between $0f_{7/2}$ and $1p_{3/2}$ orbitals. We apply the i-FCIQMC method to the same systems, and the results are shown in Fig. 2 [Figure 2: see original paper], alongside results from CC methods, CISDTQ (configuration interaction singles, doubles, triplets, and quadruples), and full configuration SM. The calculated energies are given relative to the reference energy of -203.800 MeV, consistent with Ref. [37]. The statistical uncertainties arising in the i-FCIQMC calculations are negligible and are therefore not displayed in the figure. We use about 10^8 walkers for each state, which is the current limit of our computations.

In the CC methods, the ground state is expressed as $\exp(\hat{T})|D_0\rangle$, where the cluster operator $\hat{T}$ is defined as $\hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots$, and $\hat{T}_n$ is the n-particle-n-hole (np-nh) component of $\hat{T}$. In practice, $\hat{T}$ is typically truncated to $\hat{T}_1 + \hat{T}_2$, corresponding to the CCSD (CC singles and doubles) method. The completely renormalized (CR)-CC(2,3) method improves upon this by introducing a noniterative contribution from $\hat{T}_3$, thereby including additional correlations [37–39]. As illustrated in Fig. 2, the i-FCIQMC results for ^{56}Ni are close to the exact solutions from the pf-shell full configuration SM calculations, even in the strongly correlated case (i.e., with -2 MeV shell-gap shift). In contrast, both CCSD and CR-CC(2,3) give less bound energies, and the CR-CC(2,3) calculations approximate the CISDTQ (aka SM with 4p-4h truncation), indicating that they cannot account for correlations beyond the 4p-4h level in these systems [37]. The i-FCIQMC method allows walkers to explore all possible determinants within the full configuration space, enabling it to capture high-order correlations that are inaccessible to CC methods.

We have also extended our calculations to a larger model space of the sdpf shell. Using the sdpf-mu interaction [40], we have calculated Mg isotopes with a total walker number of $\approx 10^8$. The results are shown in Fig. 3 [Figure 3: see original paper]. Our present computing resources only allow us to perform the sdpf full configuration SM calculation for the light isotopes ^{24,26}Mg of the Mg chain. For heavier isotopes, the sdpf full configuration SM calculation exceeds our current computational capability. Therefore, we performed the SM calculation with an ω truncation in which an $N\,\omega$ truncation means that only the configurations with excitation energies $\leq N\,\omega$ are included in the SM calculation. In the present work, we truncate the configuration space with $2\,\omega$ and $4\,\omega$, as shown in Fig. 3. (Note that $4\,\omega$ calculations of isotopes heavier than ^{34}Mg remain beyond our current computational resources). We see that the SM calculations with the $2\,\omega$ truncation give unbound results compared to other methods, due to the truncation error. The i-FCIQMC and SM calculations with the $4\,\omega$ truncation provide similar results for the Mg isotopes, and are also in good agreement with the full configuration SM calculations in ^{24,26}Mg.

In i-FCIQMC calculations with approximately 10^8 total walkers, only 10–20 GB of memory is required, demonstrating its significant potential for nuclear structure calculations in configuration space. One of the major challenges of shell model calculations is the prohibitive memory cost in large model spaces. In contrast, i-FCIQMC requires a much smaller configuration space dimension compared to full configuration shell model calculations. Furthermore, unlike shell model calculations, i-FCIQMC does not require storing hundreds of Lanczos vectors, which significantly reduces memory usage. The current i-FCIQMC implementation is parallelized using OpenMP, and MPI parallelization has already been implemented for electron calculations [42]. We plan to further optimize the code with more efficient parallelization techniques in the future, enabling the calculation of larger total walker numbers. Studies of unstable nuclei at driplines and beyond [43–45] are attracting interest in current nuclear physics research. The extension to the complex-energy plane should be another valuable development of FCIQMC [46]. Furthermore, the calculation of other observables, such as β decays [47, 48], offers additional avenues for exploration.

IV. Summary

In this study, we applied the FCIQMC method to nuclear structure calculations, demonstrating its effectiveness in nuclear many-body systems. According to our code, the original FCIQMC method requires a large total walker number to converge, making it impractical for nuclear structure calculations. However, we show that the initiator FCIQMC method performs well in these calculations.

Our i-FCIQMC computations were benchmarked with full configuration shell model calculations, with a focus on Fe isotopes in the pf shell. The results confirm the validity of our i-FCIQMC computations. For ^{56}Ni, using the shell-gap-shifted GXPF1A interaction, the i-FCIQMC method produced more accurate results than those obtained with coupled cluster calculations, highlighting its strength in handling strongly correlated systems. Additionally, we performed large-space calculations for Mg isotopes in the sdpf shell, demonstrating the capability of i-FCIQMC to calculate large-space many-body systems.

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[Figure 2: see original paper]
[Figure 3: see original paper]

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