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Novel extrapolation method in the Monte Carlo shell model

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We propose an extrapolation method utilizing energy variance in the Monte Carlo shell model to estimate the energy eigenvalue and observables accurately. We derive a formula for the energy variance with deformed Slater determinants, which enables us to calculate the energy variance efficiently. The feasibility of the method is demonstrated for the full pf -shell calculation of ^{56}Ni , and the applicability of the method to a system beyond the current limit of exact diagonalization is shown for the $pf + g_{9/2}$ -shell calculation of ^{64}Ge .

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The shell model (SM) calculation has been very successful in understanding the nuclear structure on the basis of nucleons interacting via the nuclear force. The conventional, standard solver for SM calculations is the exact diagonalization of Hamiltonian matrix in a given model space. Recently, the SM calculation has played an indispensable role especially in studying neutron-rich exotic nuclei, including β -decay properties on r -process nuclei (e.g., Refs. [1,2]). For such studies, the model space of the SM calculation should contain some intruder orbits in addition to one major shell. In this case, the dimension of its Hilbert space is often explosively large and the practical calculation is infeasible. Overcoming such a difficulty is a crucial challenge for modern SM calculations, where much effort has already been directed (e.g., Refs. [3–7]). The Monte Carlo shell model (MCSM) [3] is one of the methods that aim at surpassing the limit of the conventional diagonalization [8] and have succeeded in realistic applications.

The MCSM has been formulated by combining auxiliary-field quantum Monte Carlo and diagonalization methods [9]. The MCSM yields the resulting wave function as a linear combination of a relatively small number of deformed-basis wave functions. While the convergence pattern of the energy eigenvalue as a function of the basis number suggests the validity of the approximation, the convergence is, in many cases, not fast enough to estimate the exact energies accurately. This is a long-standing problem in the MCSM. The same problem also occurs in the conventional SM calculations when the model space is truncated.

In the case of the conventional SM calculations with truncation, the approximated eigenvalue seems to decrease exponentially as a function of the basis number. As an empirical trial, the exact energy can be guessed by an exponential extrapolation [10], though this technique cannot be applied directly to the MCSM. In this article, to estimate the exact energy eigenvalue, we consider another novel method free from such convergence patterns.

Recently an extrapolation method utilizing energy variance to estimate exact energy eigenvalue has been developed [11].

Because this method is expected to be valid independently of the representation of the basis function, its application to the SM is of interest. Despite efforts for such applications [12,13], its full-scale application has been infeasible due to the limitation of computer resources. In the present work, by deriving a new formula for the expectation value of the Hamiltonian squared, such an extrapolation is made feasible.

First, we briefly review the framework of the MCSM. We use a general two-body interaction as

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k, \quad (1)$$

where c_i^\dagger denotes a creation operator of single-particle state i . In the present work, the MCSM wave function is given as a linear combination of angular-momentum-projected, parity-projected deformed Slater determinant wave functions,

$$|\Psi_N\rangle = \sum_{n=1}^N \sum_{K=-J}^J f_{n,K}^{(N)} P_{MK}^{J\pi} |\psi_n\rangle, \quad (2)$$

where $P_{MK}^{J\pi}$ is the angular-momentum and parity projector and N is called the MCSM dimension. Each $|\psi_n\rangle$ is a deformed Slater determinant,

$$|\psi_n\rangle = \prod_k \left(\sum_l D_{lk}^{(n)} c_l^\dagger \right) |-\rangle, \quad (3)$$

where $|-\rangle$ denotes an inert core. The coefficient $D^{(n)}$ is selected from many (roughly 1000) candidates generated stochastically utilizing the auxiliary field Monte Carlo technique. The coefficient $f_{n,K}^{(N)}$ is determined by the diagonalization of the Hamiltonian matrix in the subspace spanned by projected Slater determinants, $P_{MK}^{J\pi} |\psi_n\rangle$. This diagonalization also determines the energy, $E_N \equiv \langle \Psi_N | H | \Psi_N \rangle$, as a function of N . In principle, we increase N until E_N becomes converged.

Next, we introduce the energy-variance extrapolation into the MCSM (MCSM-extrapolation method) following the idea of Ref. [12]. The MCSM provides us with a successive sequence of the wave functions $|\Psi_1\rangle, |\Psi_2\rangle, \dots, |\Psi_N\rangle, \dots$ For

each N , we evaluate the energy variance as

$$\langle \Delta H^2 \rangle_N \equiv \langle \Psi_N | H^2 | \Psi_N \rangle - \langle \Psi_N | H | \Psi_N \rangle^2, \quad (4)$$

and we plot the energy E_N as a function of its variance. As we increase N and improve the approximation, the resulting energy approaches the exact energy, and the corresponding energy variance approaches zero. These values are fitted by a second-order polynomial, and the energy is extrapolated to the limit of $\langle \Delta H^2 \rangle \rightarrow 0$ in the same manner as other applications of energy-variance extrapolation [12].

$$\frac{\langle \phi | H^2 | \psi \rangle}{\langle \phi | \psi \rangle} = \sum_{i < j, \alpha < \beta} \left(\sum_{k < l} v_{ijkl} [(1 - \rho)_{k\alpha} (1 - \rho)_{l\beta} - (1 - \rho)_{l\alpha} (1 - \rho)_{k\beta}] \right) \left(\sum_{\gamma < \delta} v_{\alpha\beta\gamma\delta} (\rho_{\gamma i} \rho_{\delta j} - \rho_{\delta i} \rho_{\gamma j}) \right) + \text{Tr}[(t + \Gamma)(1 - \rho)(t + \Gamma)\rho] + \left(\text{Tr} \left[\rho \left(t + \frac{1}{2} \Gamma \right) \right] \right)^2, \quad (5)$$

with $\Gamma_{ik} = \sum_{jl} v_{ijkl} \rho_{lj}$. The trivial summations and their indices for the matrix products are omitted. The first term in Eq. (5) is written as a product of two matrices as the first term on the right-hand side. This factorization reduces the eightfold loop into a sixfold loop and decreases the computation time drastically.

Now, we apply the MCSM-extrapolation method to ^{56}Ni with the pf -shell and the FPD6 interaction [14]. The m -scheme dimension of ^{56}Ni reaches 1.0×10^9 . The present work was performed using the newly developed MCSM code [15], which enables us to run it on the latest supercomputers.

Figure 1 shows the MCSM results of the ground-state ($J^\pi = 0^+$) and the first-excited-state ($J^\pi = 2^+$) energies as functions of the MCSM dimension. These energies show good convergences, but slight differences from the exact values remain. We show how these gaps are filled by the extrapolation method later. The energy by the current MCSM calculation is -203.161 MeV with $N = 150$, while the past results of the

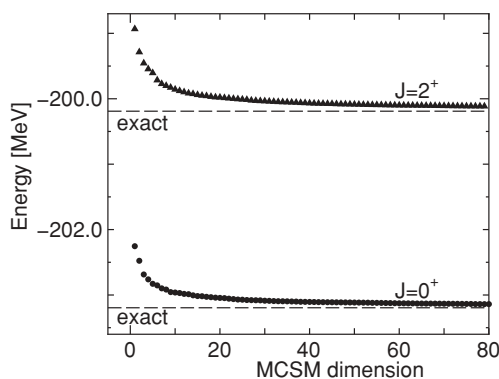


FIG. 1. Convergence patterns of the ground and first excited states of ^{56}Ni in the pf -shell. The solid circles and triangles denote the MCSM results of $J = 0^+$ and $J = 2^+$, respectively. The dashed lines show the exact values by the diagonalization method.

The obstacle in the implementation of the MCSM-extrapolation method was the large amount of computation needed to evaluate $\langle \phi | H^2 | \psi \rangle$, where $|\phi\rangle$ and $|\psi\rangle$ are deformed Slater determinants. If we regard H^2 as a general four-body operator, the evaluation of the matrix element consists of the eightfold-loop summation of the 24 terms of products of four generalized one-body density matrices, $\rho_{ij} = \langle \phi | c_j^\dagger c_i | \psi \rangle / \langle \phi | \psi \rangle$. In the present work, thanks to the separability of H^2 , the evaluation of the matrix element is formulated as

MCSM were -203.100 MeV in 1998 [16] and -203.152 MeV in 2001 [3]. Over a decade, progress in the method and in computational power has gradually improved the precision of the MCSM. Nevertheless, we still find 37 keV error from the exact energy, -203.198 MeV. Note that the MCSM error of the 2_1^+ state is the same order of magnitude.

Figure 2 shows the E_N as a function of $\langle \Delta H^2 \rangle_N$ provided by the MCSM wave function. We fit the MCSM points of E_N against $\langle \Delta H^2 \rangle_N$ with $10 \leq N \leq 150$ by quadratic curve and extrapolate the MCSM results to $\langle \Delta H^2 \rangle \rightarrow 0$. The extrapolated energy is -203.198 MeV, which agrees with the exact one within 1 keV. Here, we excluded the first nine points of E_N for the quadratic fit because the extrapolation method assumes that approximated wave functions are sufficiently

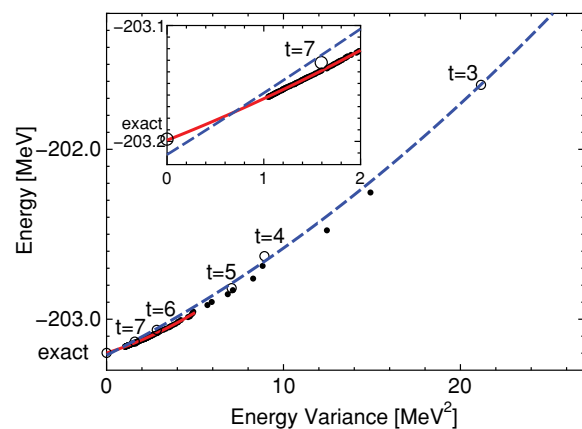


FIG. 2. (Color online) Second-order extrapolations of the ground-state energy into a zero energy variance of the $J^\pi = 0^+$ ground state of ^{56}Ni in the pf -shell. The solid symbols, open symbols, solid red line, and dotted blue line denote the E_N of MCSM, the results of the diagonalization method with PHT, and their second-order fits, respectively. The exact energy is also shown by open symbols on the y axis. The inset shows a magnified view around $\langle \Delta H^2 \rangle \simeq 0$.

close to the true eigenstate. Moreover, the MCSM points of $N < 10$ show comparably large fluctuation due to the stochastic procedure and should have strong dependence on the initial states of the stochastic sampling.

For comparison, we also show another extrapolation result for the conventional SM calculation with the particle-hole truncation (PHT) in Fig. 2. The configuration of the PHT is $(0f_{7/2})^{16-t}(0f_{5/2}, 1p_{3/2}, 1p_{1/2})^t$, with $t = 3, 4, 5, 6, 7$, and the practical calculation was performed by the MSHELL code [17]. These energies and their variances are also fitted by a quadratic curve in the same manner as Ref. [12]. While both the MCSM and the PHT calculation succeed in reproducing the exact energy well, minor deviation can be seen in the inset of Fig. 2. The extrapolated energy with PHT is -203.217 MeV, and its discrepancy with the MCSM and the exact energy is 19 keV. Note that we discuss precision in the unit of a few keVs, while previous works using the energy-variance extrapolation provided the precision of a few tens or hundreds of keVs [12,13].

An advantage of the MCSM for the extrapolation method is that the MCSM provides us with the sequence of many (more than 50) successive approximate wave functions simultaneously. It provides us with good statistics for the extrapolation. However, the conventional PHT scheme yields only 6 points in the case of ^{56}Ni , for example.

To test the applicability to larger systems, we assume that the MCSM result with $N \leq 50$ is available in the ground state of the ^{56}Ni case. In practical calculations, the N is often limited so small that the E_N cannot reach good convergence. The MCSM result with $N = 50$ is $E_{N=50} = -203.115$ MeV, which is worse than $t = 7$ energy and -203.132 MeV. Nevertheless, the extrapolated energy of the MCSM is -203.202 MeV, which is still much closer to the exact result than that of PHT. This good agreement provides us with a promising perspective for its application to larger systems.

Figure 3 shows the results of 0_1^+ , 2_1^+ , 0_2^+ , and 0_3^+ states in order to discuss the behavior of the MCSM extrapolation concerning excited states and some observables. In Fig. 3(a), all of the MCSM-extrapolation results of these energies agree excellently with the exact ones in a unit of keV, too. Figures 3(b) and 3(c) show the occupation numbers of the $0f_{7/2}$ orbit and the quadrupole moment of the 2_1^+ state by the MCSM and their first-order extrapolations. In the case of these observables, a first-order polynomial is appropriate for the extrapolation because the positive and negative contributions of the contamination of excited states cancel each other. Obviously, such cancelation does not occur in the case of the energy eigenvalue. The first-order extrapolation for these observables provides us with excellent improvement of the agreement with the exact value, while some other extrapolation methods do not [13].

Finally, we discuss the case of ^{64}Ge with $pf + g_{9/2}$ model space to demonstrate the applicability of the present method to large-scale SM calculations. Its m -scheme dimension is 1.7×10^{14} , which is roughly 10^3 times larger than the current limitation of the conventional diagonalization method, $\sim 10^{11}$. We adopt the PFG9B3 effective interaction [18], which was used also in Ref. [19]. In Fig. 4, the result of the MCSM-extrapolation method shows stable behavior while the

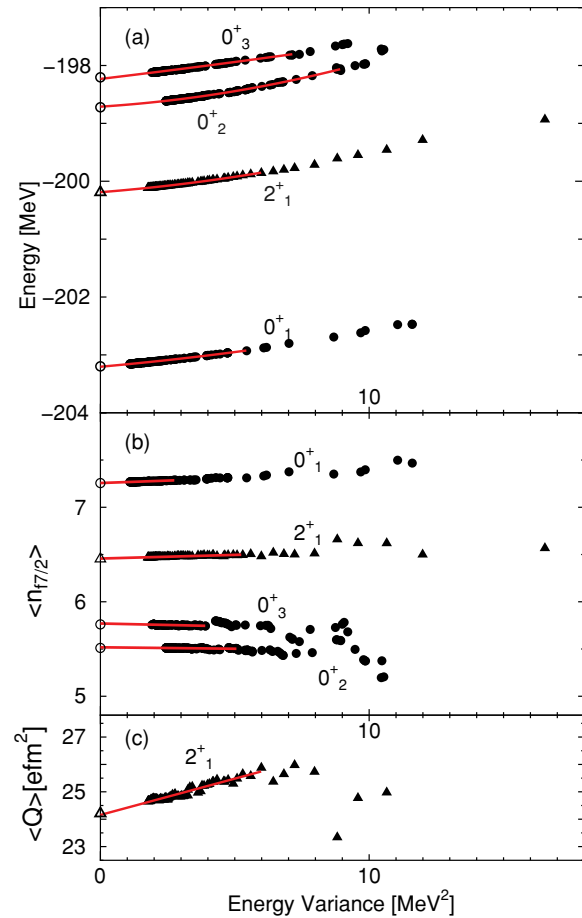


FIG. 3. (Color online) (a) Second-order extrapolations of the energies of $J^\pi = 0_1^+, 2_1^+, 0_2^+$, and 0_3^+ states of ^{56}Ni in the pf -shell. The notation is the same as that of Fig. 2. (b) First-order extrapolation of the occupation number of the $0f_{7/2}$ orbit by the MCSM. (c) First-order extrapolation of the quadrupole moment of the 2_1^+ state. The results obtained by exact diagonalization are also shown by the corresponding open symbols.

exact value is not available. The 82 points for the ground state are obtained by the MCSM and fitted by a quadratic curve. The excitation energy of 2^+ state is 0.95 MeV, which is close to the experimental value, 0.90 MeV [20]. We also see the reasonable agreement between the ground-state energy of MCSM extrapolation and that of the first-order extrapolation with the PHT calculation. We point out that the PHT extrapolation is based on the 4 points ($1 \leq t \leq 4$), and the fitted line shows certain deviations from these points already, suggesting possible ambiguities. Note that the guess by the statistics of the nuclear level density is rather low, -306.7 MeV [19].

In summary, we have proposed the MCSM-extrapolation method, which provides us with accurate correction to the MCSM. Equation (5) considerably reduces the computation time by orders of magnitudes to calculate the energy variance with deformed Slater determinants. The energy as a function of its variance is well fitted by a quadratic curve, and the result of the MCSM is improved down to a unit of keV especially in ^{56}Ni case. We demonstrate that this method works

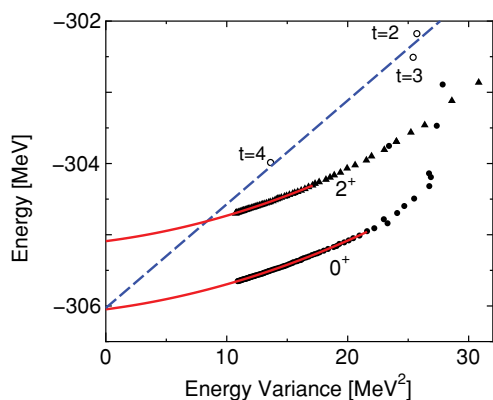


FIG. 4. (Color online) Second-order extrapolations of the ground-state and 2^+ energies of ^{64}Ge in the $pf+g_{9/2}$ -shell. The blue dashed line shows the first-order extrapolation of the ground-state energy of the PHT calculation. The notation is the same as that of Fig. 2.

quite well not only for energy eigenvalues, but also for other physical quantities of some low-lying states. By adopting the

extrapolation method with the energy variance, we obtain a self-contained framework that removes the ambiguity of the energy convergence in the MCSM. We applied this framework also to large-scale shell-model problems, like the case of ^{64}Ge , that cannot be solved by existing conventional solvers. These results look quite promising and encourage us to apply the present method to larger-scale problems. In such cases, the error estimation of the extrapolation method itself becomes important and will be discussed in a future publication.

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