Ab initio Monte Carlo shell model calculations for ^{7}Li and ^{9}Li low-lying spectra*

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Abstract: The low-lying spectra of ^{7}Li and ^{9}Li are investigated within an *ab initio* Monte Carlo Shell Model (MCSM) employing a realistic potential obtained via the Unitary Correlation Operator Method (UCOM). The MCSM calculations in a 4-major-shells model space for the binding energy and mass quadrupole moment of ^{7,9}Li show good convergence when the MCSM dimension reaches 20. The excitation energy of the $J^{\pi}=1/2^{-}$ state for ^{7}Li and the magnetic moments for ^{7,9}Li ground states in the MCSM with a treatment of spurious center-of-mass motion are close to the experimental data. Correct level ordering of $J^{\pi}=3/2^{-}$ and $1/2^{-}$ states for ^{7,9}Li can be reproduced due to the inclusion of three-body correlations in the MCSM+UCOM. However, the excitation energy of $J^{\pi}=1/2^{-}$ state for ^{9}Li is not reproduced in the MCSM mainly due to the lack of larger model space.

Key words: Monte Carlo shell model, unitary correlation operator method, *ab initio*, ^{7,9}Li

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1 Introduction

One of the central challenges for nuclear physics is to understand nuclear structure from first principle calculations. Much progress on these *ab initio* investigations have been made based on the development of studies of the reputed bare nucleon-nucleon (NN) potentials and nuclear many-body theory in the last decade. For example, a two-body potential can be constructed phenomenologically by fitting experimental data on NN scattering, such as the Argonne V18 potential [1], the CD-Bonn potential [2] and the Nijmegen potential [3]. Alternatively, a consistent two- and many-body interactions can also be constructed in the framework of chiral effective field theory using the symmetries and the effective degrees of freedom of low-energy QCD as a guiding principle, such as the chiral N^{3}LO potential [4–6]. By using these realistic nuclear interactions, *ab initio* nuclear many-body calculations have been performed. In Green's Function Monte Carlo (GFMC) calculations the exact ground-state wave function is calculated by treating the many-body Green's functions in a Monte Carlo approach [7–9]. Another *ab initio* approach for nuclei up to A=14 is the No-Core Shell Model (NCSM) [10–12].

However, the straightforward application of those realistic interactions in nuclear many-body calculations is still difficult due to the strong short-range repulsion and the tensor correlations. The Unitary Correlation Operator Method (UCOM) is one of the methods to tackle this problem by introducing a unitary transformation such that the transformed many-body states contain the information on the dominant correlations in nuclear many-body system [13–15]. In the UCOM approach two unitary transformation operators are defined: a central correlation operator and a tensor correlation operator, which correspond to the two most important correlations: the central correlations induced by the strong short-range repulsion and the tensor correlations, respectively. Through a unitary transformation of the Hamiltonian, a soft phase-shift equivalent two-nucleon interaction can be obtained.

In the shell model calculations, the direct diagonalization of the Hamiltonian matrix in the full valence-nucleon Hilbert space is difficult, as the dimension of such a space becomes larger and larger when one moves from light nuclei to heavier nuclei. As one way to overcome this difficulty, the stochastic approaches have been introduced. Among them, the Shell Model Monte Carlo (SMMC) method has been successfully proposed [16]. Nevertheless, the SMMC is basically suitable for the ground state and thermal properties, and suffers from the so-called "sign problem". As a completely different approach, the Quantum Monte Carlo Diagonalization (QMCD) method has been proposed for solving quan-

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tum many-body systems with a two-body interaction [17–19]. The QMCD can describe not only the ground state but also the excited states, including their energies, wave functions and hence transition matrix elements. Thus, on the basis of the QMCD method, the Monte Carlo Shell Model (MCSM) has been introduced [20]. An extrapolation method in the Monte Carlo Shell Model has been proposed recently [21]. In parallel, a revised MCSM method is also outlined for future directions [22–24].

For the first time, *ab initio* Monte Carlo shell model (MCSM) has been successfully applied to study the low-lying spectra of light nuclei by employing a realistic potential obtained via UCOM [25]. The magnetic moment of $J^\pi=2_1^+$ state for ^{10}Be has also been studied in terms of the single-particle orbits under the same framework [26].

^{7,9}Li are also good candidates for testing *ab initio* calculations, as there are adequate experimental data both in the ground state and in the excited states, for instance, excitation energies of two $J^\pi=3/2^-,1/2^-$ states, as well as the magnetic moments for the ground states. In this work, the low-lying spectra of ^{7,9}Li are investigated with the MCSM plus UCOM. In Section 2, the theoretical framework for the MCSM is briefly outlined. The numerical details, results, and discussion of many-body calculation results are presented in Section 3. Finally, a brief summary is given in Section 4.

2 Theoretical framework

The main idea of the MCSM is to diagonalize the Hamiltonian in a subspace spanned by the MCSM basis, which is generated in a stochastic way. We begin with the imaginary-time evolution operator

$$\mathrm{e}^{-\beta H}, \tag{1}$$

where H is a given general (time-independent) Hamiltonian and $\beta\propto T^{-1}$ is a real number with T being analogous to a temperature. If this operator in Eq. (1) acts on a state $|\Psi^{(0)}\rangle$, one obtains

$$\mathrm{e}^{-\beta H}|\Psi^{(0)}\rangle=\sum_i \mathrm{e}^{-\beta E_i}c_i|\psi_i\rangle, \tag{2}$$

where E_i is the i-th eigenvalue of H, $|\psi_i\rangle$ is the corresponding eigenstate and c_i its amplitude in the initial state:

$$|\Psi^{(0)}\rangle=\sum_i c_i|\psi_i\rangle. \tag{3}$$

For β large enough, only the ground and low-lying states survive. But the actual handling is very complicated for H containing a two-body (or many-body) interaction.

The Hubbard-Stratonovich (HS) transformation [27, 28] can be used to ease the difficulty mentioned above. We then move to the formula

$$|\Phi(\sigma)\rangle\propto \mathrm{e}^{-\beta h(\sigma)}|\Psi^{(0)}\rangle, \tag{4}$$

where $h(\sigma)$ is a one-body Hamiltonian obtained through the HS-transformation and σ is a set of random numbers (auxiliary fields). The right-hand-side of this relation can be interpreted as a mean to generate all basis vectors needed for describing the ground state and the low-lying states. For different values of the random variable, σ, one obtains different state vectors, $|\Phi(\sigma)\rangle$, by Eq. (4). These vectors are labeled as candidate states and selected as MCSM basis by a procedure of energy comparison [20].

During the MCSM generation of the basis vectors, symmetries, e.g. rotational and parity symmetry, are restored before the diagonalization as more basis vectors are included. All MCSM basis states are projected onto good parity and angular momentum quantum numbers by acting with the corresponding projection operators. We diagonalize the Hamiltonian in a subspace spanned by those projected basis vectors. The number of the MCSM basis states is referred to as the MCSM dimension. The basis generation process for general cases is outlined in Ref. [20].

As more than one major shell is included in the MCSM calculation, the spurious center-of-mass motion must be accounted for. The Lawson's prescription is adopted to suppress the spurious center-of-mass motion in good approximation for major shell truncation [29]. The total Hamiltonian can be separated into an intrinsic part and a center-of-mass part

$$H'=H_{\mathrm{int.}}+\beta_{\mathrm{c.m.}}H_{\mathrm{c.m.}}, \tag{5}$$

where $H_{\mathrm{int.}}$ is the intrinsic Hamiltonian. The $H_{\mathrm{c.m.}}$ is defined by

$$H_{\mathrm{c.m.}}=\frac{\boldsymbol{P}^2}{2AM}+\frac{1}{2}MA\omega^2\boldsymbol{R}^2-\frac{3}{2}\hbar\omega, \tag{6}$$

where $\boldsymbol{R}$ and $\boldsymbol{P}$ are the coordinate and momentum of the center of mass, respectively. In general, by taking sufficiently large values of $\beta_{\mathrm{c.m.}}$, the spurious components become smaller and smaller for the low-lying eigenstates of H'.

With these wave functions without spurious center-of-mass motion, any physical quantities can be evaluated in the MCSM. For example, the nuclear magnetic moments are calculated with

$$\begin{aligned}\mu &= \sqrt{\frac{4\pi}{3}}\langle J,M=J|O(\mathrm{M1})|J,M=J\rangle \\ &= \sqrt{\frac{4\pi}{3}}\begin{pmatrix} J & 1 & J \\ -J & 0 & J\end{pmatrix}\langle J||O(\mathrm{M1})||J\rangle,\end{aligned} \tag{7}$$

where J and M is the quantum numbers of total angular momentum and corresponding third component of

the nucleus. The total M1 transition operator is defined as:

$$O(\mathrm{M1})=\sqrt{\frac{3}{4\pi}}\left[\boldsymbol{l}g_{\mathrm{q}}^{\mathrm{l}}+\boldsymbol{s}g_{\mathrm{q}}^{\mathrm{s}}\right]\mu_{\mathrm{N}}, \tag{8}$$

where μ_{N} is the nuclear magneton. The g-factors $g_{\mathrm{q}}^{\mathrm{l}}$ and $g_{\mathrm{q}}^{\mathrm{s}}$ are the orbital and spin g-factor, respectively. The free-nucleon values for the g-factors are adopted with $g_{\mathrm{p}}^{\mathrm{l}}=1$, $g_{\mathrm{n}}^{\mathrm{l}}=0$, $g_{\mathrm{p}}^{\mathrm{s}}=5.586$, and $g_{\mathrm{n}}^{\mathrm{s}}=-3.826$.

Under the same theoretical framework, the electric quadrupole moments can be evaluated with:

$$\begin{aligned} Q &= \sqrt{\frac{16\pi}{5}}\langle J,M=J|O(\mathrm{E2})|J,M=J\rangle \\ &= \sqrt{\frac{16\pi}{5}}\begin{pmatrix} J & 2 & J \\ -J & 0 & J \end{pmatrix}\langle J||O(\mathrm{E2})||J\rangle, \end{aligned} \tag{9}$$

where the E2 transition operator is defined as:

$$O(\mathrm{E2})=r^2Y_{\mu}^2(\hat{r})e_{\mathrm{q}}e, \tag{10}$$

where Y_{μ}^2 are the spherical harmonics and q stands for proton q=p or neutron q=n. The e_{q} are the electic charges for the proton and neutron in units of e. In our calculations, we take $e_{\mathrm{p}}=1$ and $e_{\mathrm{n}}=0$, for the proton and neutron, respectively.

3 Results and discussion

The model space of the MCSM is spanned by a harmonic oscillator basis truncated with respect to the unperturbed single-particle energies with $e_{\max}=2n+l$. Our calculations are performed in the model space $e_{\max}=3$, namely 4 major shells. We use UCOM-transformed realistic two-nucleon interactions (hereinafter referred to as V_{UCOM}) as the input potential in the MCSM. The transformed potentials are derived from the N^{3}LO interaction. The Coulomb interaction in all of our calculations is neglected throughout this work for simplicity. The parameter $\beta_{\mathrm{c.m.}}$ of Lawson's prescription for treatment of spurious center-of-mass motion is adopted as 10.

The convergence of the MCSM calculations in the $e_{\max}=3$ model space should be examined at first. Fig. 1 shows the binding energies of the $3/2^-$ (full circles) and $1/2^-$ states (open circles) of ^{7}Li as a function of the MCSM dimension for the $e_{\max}=3$ model space, as well as the $3/2^-$ (red full triangles) and $1/2^-$ states (black open triangles) of ^{9}Li. If we evaluate the energy difference ε between results corresponding to the last two consecutive MCSM dimensions, we obtain $\varepsilon=39$ keV for the $3/2^-$ and 14 keV for the $1/2^-$ states of ^{7}Li, 29 keV for the $3/2^-$ and 124 keV for the $1/2^-$ states in the case of ^{9}Li. The relative accuracy of these excitation energies is 0.2%, 0.07%, 0.2%, and 0.9%, respectively. All of them are less than 1%, and indicates a reasonably converged MCSM calculations. Usually, the diagonalization of the MCSM is performed in a subspace comprised of 10^{1-2} optimally generated basis states. The size (dimension) of this subspace is quite small compared to that of the entire Hilbert space taken in the direct diagonalization in the conventional shell model. This advantage will be even more obvious for heavier nuclei by the fact that the full diagonalization in the $e_{\max}=3$ is hardly feasible with other calculational techniques available presently. Meanwhile, it can be found that the MCSM results for the total energy in the $e_{\max}=3$ model space present some difference compared with the experimental data [30]. For example, the binding energy of ^{7}Li ground state of the MCSM is -18.624 MeV, which is about 20 MeV deviation in comparison with the experimental one (-39.242 MeV). In order to investigate this difference, we also perform the MCSM calculations in the $e_{\max}=2$ model space for the ^{7}Li ground state. This energy is about 10 MeV higher than that in the $e_{\max}=3$ model space. We believe that the larger model spaces will improve dramatically the total energy in the MCSM calculations. However, it is difficult to perform these kind of calculations in larger model spaces due to the numerical technique limitations at present.

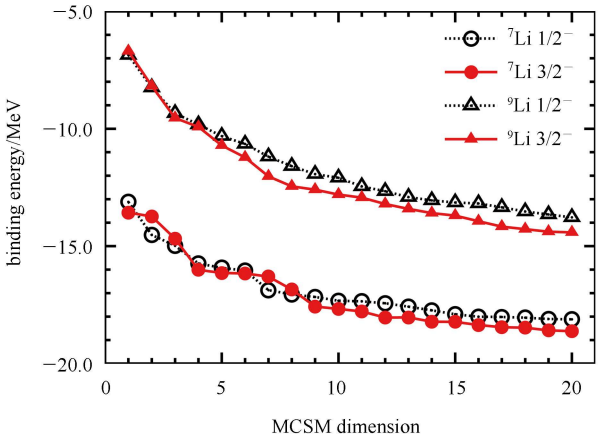

Fig. 1. (color online). Binding energy of the $J^{\pi}=3/2^-$ (full symbols) and $1/2^-$ (open symbols) states for ^{7}Li (circles) and ^{9}Li (triangles) as a function of the MCSM dimension in the $e_{\max}=3$ model space.

Besides binding energy, the convergence of other physical observables, for example, mass quadrupole moments in the MCSM calculations should also be checked in the $e_{\max}=3$ model space. In Fig. 2, the expectation values of mass quadrupole moments of neutrons (full symbols) and protons (open symbols) for ^{7}Li (circles) and ^{9}Li (triangles) respectively as a function of the MCSM dimension in the $e_{\max}=3$ model space. The mass quadrupole moments can be evaluated with Eq. (9) by replacing the E2 transition operator $r^2Y_{\mu}^2(\hat{r})e_{\mathrm{q}}e$ as

$r^2Y^2_\mu(\hat{r})$. One finds that beyond MCSM dimension 10, those mass quadrupole moments reach stable values. Both nuclei ^{7}Li and ^{9}Li have negative mass quadrupole moments for neutrons and protons in the ground state.

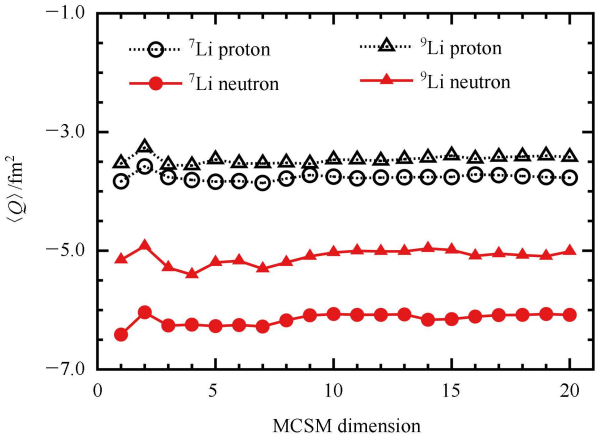

Fig. 2. (color online). The expectation values of mass quadrupole moment of neutrons (full symbols) and protons (open symbols) states for ^{7}Li (circles) and ^{9}Li (triangles) as a function of the MCSM dimension in the $e_{\max}=3$ model space, where $e_{\rm q}$=1 for protons and $e_{\rm q}$=0 for neutrons.

Figure 3 shows energy levels of the $1/2^-$ excited states of ^{7,9}Li calculated by the MCSM in comparison with the experiment data [30]. It is found that the excitation energy (506 keV) of $1/2^-$ state for ^{7}Li in MCSM with proper treatment of spurious center-of-mass motion shows good agreement with the experimental value (477.6 keV). However, our calculation underestimates the excited energy for ^{9}Li $1/2^-$ state to a large extent. The large excitation energy of ^{9}Li $1/2^-$ state suggests a possible neutron sub-shell closure at N=6. However, our MCSM calculation in the $e_{\max}$=3 model space do not reproduce this property due to the deficiency of large $e_{\max}$ orbits contribution, which might imply the high $e_{\max}$ intruder states are crucial for the neutron sub-shell closure. In addition, the *ab initio* calculation, for instance, GFMC can not present correct level ordering of $3/2^-$ and $1/2^-$ states for ^{7}Li with only two-body interaction. The right level sequence can be reproduced with the including of three-body forces in their calculations. Although the three-body forces are not included in our MCSM calculation with UCOM-transformed interaction, the correct level ordering can be presented since the three-body correlations are taken into account in the unitary transformation.

The electromagnetic moments are also investigated in the MCSM. Table 1 shows the nuclear magnetic moments and electric quadrupole moments of the ground state for ^{7}Li and ^{9}Li calculated with Eqs. (7) and (9) under the MCSM in comparison with the experiment values as well as NCSM with CDB2k interaction results. Our results reproduce the nuclear magnetic moments of ^{7}Li and ^{9}Li quite well. By choosing the bare effective charge ($e_{\rm p}$=1 and $e_{\rm n}=0$), the MCSM presents a better description of electric quadrupole moment than that of NCSM with only a two-body interaction. It is possible that the high $e_{\max}$ intruder states, which are important to reproduce the total energy, are not crucial for ^{7,9}Li electromagnetic moments.

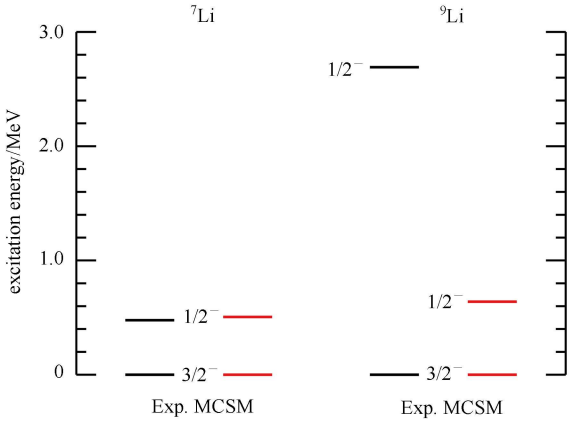

Fig. 3. (color online) Excitation energy of the $1/2^-$ states for ^{7}Li (left) and ^{9}Li (right) calculated by the MCSM (red lines) in the $e_{\max}$=3 model space in comparison with the experimental data [30] (black lines).

Table 1. Nuclear magnetic moments and electric quadrupole moments of the ground state for ^{7}Li and ^{9}Li in the MCSM calculation as well as the NCSM calculation results with CDB2k interaction [31] and the experimental data [31, 32]. The bare effective charge ($e_{\rm p}$=1 and $e_{\rm n}$=0) is adopted in our calculation.

isotope	Exp.	MCSM	NCSM
		$\mu/\mu_{\rm N}$	
^{7}Li	3.256427(2)	3.116	3.01(2)
^{9}Li	3.434(5)	3.183	2.89(2)
		Q/efm^2	
^{7}Li	−4.00(3)	−3.770	−3.20(22)
^{9}Li	−3.06(2)	−3.452	−2.66(22)

4 Summary

In summary, the low-lying excited states of ^{7}Li and ^{9}Li are investigated within an *ab initio* MCSM employing a realistic potential obtained via the UCOM. The MCSM calculations $e_{\max}$=3 model space for the binding energies and mass quadrupole moments of ^{7,9}Li show good convergence when the MCSM dimension reaches 20. The excited states are studied in terms of excitation energy, level ordering and electromagnetic moments. The excitation energies of the $J^\pi=1/2^-$ state for ^{7}Li

and the magnetic moments for ^{7,9}Li ground states in the MCSM with a treatment of spurious center-of-mass motion are close to the experimental data. Correct level ordering of $J^{\pi}=3/2^{-}$, $1/2^{-}$ states for ^{7,9}Li is presented due to the partial inclusion of three-body correlations in the MCSM+UCOM. The high $e_{\max}$ orbits might be important to investigations of possible neutron sub-shell closure of ^{9}Li.

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