Microscopic calculations of $^6$He and $^6$Li with real-time evolution method

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Abstract The low-lying cluster states of $^6$He ($\alpha+n+n$) and $^6$Li ($\alpha+n+p$) are calculated by the real-time evolution method (REM) which generates basis wave functions for the generator coordinate method (GCM) from the equation of motion of Gaussian wave packets. The $0^+$ state of $^6$He as well as the $1^+$, $0^+$, and $3^+$ states of $^6$Li are calculated as a benchmark. We also calculate the root-mean-square (r.m.s.) radii of the point matter, the point proton, and the point neutron of these states, particularly for the study of the halo characters of these two nuclei. It is shown that REM can be one constructive way for generating effective basis wave functions in GCM calculations.

Keywords $\alpha$ cluster · Halo nuclei · r.m.s. radius

1 Introduction

The light nuclei have been studied within the view of the cluster feature for more than five decades [1–3], and various nuclear theories have been developed for the study of nuclear clustering [4–6]. By assuming the cluster structure, various cluster states of light nuclei have been investigated explicitly [7–9]. However, as the number of the constituent clusters and nucleons increases or nuclear system becomes dilute, the number of required basis wave functions increases very quickly. Therefore, a method which can efficiently shift out the basis is highly desired. For this purpose, many efforts have been made, such as the stochastic sampling [10–12] and the imaginary-time development method [13].

Recently, a new time-dependent many-body theory has been developed in Refs. [14–16] for the calculations of Be and C isotopes. This real-time evolution method (REM) generates the basis wave function using the equation of motion (EOM) which has been applied in the study of heavy-ion collisions [17–19], but now is found to be very effective in searching for the basis wave functions for the microscopic calculations because of its ergodic nature.

$^6$He is well known as a Borromean nucleus consisting of loosely bound and spatially extended three-body systems, typically composed of a compact core plus two weakly bound neutrons (n+n+core) [20–22]. These properties lead to huge computational difficulties and many methods have been taken to investigate this nucleus, like the three-body resonance group method (RGM) performed in Refs. [23–25]. Despite its simple physical structure, the description of the motion of the dineutron is highly desired by theoretical studies. For example, the contraction of the size of nucleon pairs on the surface of nuclei is investigated under the view of the nucleon correlation [26,27], and the deuteron-alpha scattering data is successfully explained by this kind of behavior [28].

We intend to apply the REM on the $0^+$ ground state of $^6$He nucleus ($\alpha+n+n$). Meanwhile, the low lying states of $^6$Li ($\alpha+n+p$) also can be a good comparison, where the more compact states ($1^+$ and $3^+$ states with $T = 0$) and the dilute state ($0^+$ state with $T = 1$) are present simultaneously. In this study, aiming to explore the applicability of REM, we will calculate the $0^+$ ground state of $^6$He as well as the low lying states of $^6$Li to reproduce the halo and anti-halo properties of these states.

This paper is organized as follows: Sect. 2 explains the framework of the wave function and the real-time evolution method (REM). The numerical results including the energy and the root-mean-square (r.m.s.) radius are presented and discussed in Sect. 3. The conclusion is summarized in Sect. 4.

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2 Framework

2.1 Hamiltonian

We begin with the Hamiltonian given below

\[
\hat{H} = \sum_{i=1}^{A} \hat{t}_i + \hat{T}_{c.m.} + \sum_{i<j}^{A} \hat{v}_N + \sum_{i<j}^{A} \hat{v}_C + \hat{v}_{LS}
\]

(1)

where \(\hat{t}_i\) and \(\hat{T}_{c.m.}\) denote the kinetic energies of each nucleon and the center of mass, respectively. \(\hat{v}_N\) denotes the effective nucleon-nucleon interaction and \(\hat{v}_C\) denotes the Coulomb interaction. \(\hat{v}_{LS}\) denotes the spin-orbit interaction.

For the nucleon-nucleon interaction, we take the Volkov No.2 interaction \([29]\) as

\[
\hat{v}_N = (W - M \hat{P}_0 \hat{P}^* \hat{P} - B \hat{P}^* \hat{P} - H \hat{P}^* \hat{P})
\]

\[
\times \left[ V_1 \exp(-r^2/c_1^2) + V_2 \exp(-r^2/c_2^2) \right].
\]

(2)

The corresponding exchange parameters are, \(W = 0.4, M = 0.6\) and \(B = H = 0.125\). The parameters in the Gaussian terms are, \(V_1 = -60.65\) MeV, \(V_2 = 61.14\) MeV, \(c_1 = 1.80\) fm and \(c_2 = 1.01\) fm.

We take the G3RS potential \([30,31]\) as the spin-orbit interaction,

\[
\hat{v}_{LS} = V_0(e^{d_1 r^2} - e^{d_2 r^2}) \hat{P}_{31} \hat{L} \cdot \hat{S}.
\]

(3)

The strength parameter \(V_0\) is set to be 2000 MeV. The Gaussian parameters \(d_1\) and \(d_2\) are set to be 5.0 fm\(^{-2}\) and 2.778 fm\(^{-2}\), respectively.

2.2 Generator coordinate method

In the current work, the single-particle wave function \(\phi(r, Z)\) are expressed in a Gaussian form multiplied by the spin-isospin part \(\chi_{\tau, \sigma}\) as

\[
\phi(r, Z) = \left( \frac{2^v}{\pi} \right)^{3/4} \exp \left[ -v \left( \frac{r - z}{\sqrt{v}} \right)^2 + \frac{1}{2} z^2 \right] \chi_{\tau, \sigma}.
\]

(4)

Here the coordinate \(Z\) represents the generator coordinates, which includes the three-dimensional coordinate \(z\) for the spatial part of the wave function as well as the spinor \(a\) and \(b\) for the spin part \(\chi_{\sigma} = a |\uparrow\rangle + b |\downarrow\rangle\). In this work, the spinor \(a\) and \(b\) are also regarded as time-dependent variables which will be generated similarly to the spatial coordinates as introduced later. The harmonic oscillator parameter \(b = \sqrt{1/(2v)} = 1.46\) fm, which is same with that used in Refs. \([11,32]\).

We describe the \(^6\text{He}\) and \(^6\text{Li}\) as the \(\alpha\)-cluster plus two valence nucleon systems in the wave function. Thus the corresponding wave function can be written as

\[
\Phi(Z_1, Z_2, z_a) = A[\phi(r_1, Z_1) \phi(r_2, Z_2) \Phi_{a}(r_{3-6}, z_a)].
\]

(5)

Here \(\Phi_{a}\) is the wave function of the \(\alpha\)-cluster with (0s\(^4\)) configuration. \(\phi\) are the single-particle wave functions as introduced above, which are used to describe the valence nucleons in \(^6\text{He}\) and \(^6\text{Li}\). Thus, the coordinates \(r_1\) and \(r_2\) represent the real spatial position of valence nucleons while \(r_{3-6}\) are for the nucleons in the \(\alpha\)-cluster.

Within the framework of generator coordinate method (GCM), the final wave function is the superposition of the basis wave functions with different sets of generator coordinates \((Z_1, Z_2, z_a)\):

\[
\Psi = \sum_{i} f_i \hat{P}_{MK} \Phi_i(Z_{1,i}, Z_{2,i}, z_{a,i})
\]

(6)

where \(\hat{P}_{MK}\) is the parity and the angular momentum projector. The corresponding coefficients \(f_i\) will be determined by the diagonalization of the Hamiltonian.

There are several technical methods to prepare the basis wave functions for GCM calculation. For example, in Refs. \([11,32]\), a stochastic multi-configuration mixing (SMCM) method is employed with the cluster structure to obtain the wave functions of the \(^6\text{He}\) and \(^6\text{Li}\) nuclei. In this method, the basis wave functions with different generator coordinates are generated stochastically and selected by the energy optimal variation. However, such a method can be only proper for the calculation of the ground state of the nuclei. In the current work, the generator coordinates \(Z\) can be obtained by solving the equation of motion in REM without any selections. The detail of this method will be explained in the next subsection.

2.3 Real-time evolution method

In the quantum system, the wave function should satisfy the Schrodinger equation at all times. Thus, the time-dependent variational principle holds for the intrinsic wave function mathematically:

\[
\delta \int dt \frac{\langle \Phi(Z_1, Z_2, z_a) | i \hbar \frac{d}{dt} - \hat{H} | \Phi(Z_1, Z_2, z_a) \rangle}{\langle \Phi(Z_1, Z_2, z_a) | \Phi(Z_1, Z_2, z_a) \rangle} = 0
\]

(7)

Regarding the coordinate \(Z\) as the function of the time \(t\), we obtain the equation of the motion (EOM) as

\[
i\hbar \sum_{i=1,2, a} \sum_{\sigma = x,y,z} C_{ij\sigma} \frac{dZ_{j\sigma}}{dt} = \frac{\partial \mathcal{H}_{\text{int}}}{\partial Z_{i\rho}}
\]

(8)

\[
\mathcal{H}_{\text{int}} = \frac{\langle \Phi(Z_1, Z_2, z_a) | \hat{H} | \Phi(Z_1, Z_2, z_a) \rangle}{\langle \Phi(Z_1, Z_2, z_a) | \Phi(Z_1, Z_2, z_a) \rangle}
\]

(9)

\[
C_{ij\sigma} = \frac{\partial^2 \ln\langle \Phi(Z_1, Z_2, z_a) | \Phi(Z_1, Z_2, z_a) \rangle}{\partial Z_{i\rho} \partial Z_{j\sigma}}
\]

(10)
By following the EOM, from an initial wave function at \( t = 0 \), the sets of the generator coordinates \((Z_1, Z_2, z_α)\) for GCM can be yielded as a function of time \( t \). The ensemble of the basis wave functions \( \Phi_i(Z_{1,i}, Z_{2,i}, z_{α,i}) \) denoted by these sets of the generated coordinates will hold the information of the quantum system. Thus, effective basis can be generated.

In practical calculations, we choose the proper initial excitation energy (the definition can be found in Refs. [14,15]) for obtaining various cluster configurations in the evolution. To avoid the clusters or valence nucleons move to unphysical regions, the rebound condition is imposed in our REM calculations. By following the work in Ref. [18], we add a potential barrier to the Hamiltonian during the REM procedure with the form:

\[
V_{reb} = \frac{k}{2} \sum_i f(\|\mathbf{R}_i - \mathbf{R}_{c.m.}\|) \\
\quad f(x) = (x - d)^2 \theta(x - d) \\
\mathbf{R}_i = \frac{\text{Re}(z_i)}{\sqrt{\nu}} \quad \mathbf{R}_{c.m.} = \frac{1}{6} \sum_j \mathbf{R}_j 
\]

Here \( \mathbf{R}_i \) and \( \mathbf{R}_{c.m.} \) represent the spatial position of the \( i \)th valence nucleon and the center of mass, respectively, so that \( \|\mathbf{R}_i - \mathbf{R}_{c.m.}\| \) is the distance between them. Because of the step function \( \theta(x - d) \), the evolving valence nucleon will face potential barrier when it is \( d \) fm far from the center of mass, and be smoothly pushed back in later evolution. We set the strength of the potential barrier \( k = 6 \text{ MeV/fm}^2 \), which determines how rapidly the height of the barrier increases. This value is not physically important as long as it is not too large or too small. The rebound radius parameter \( d \) is set to be \( 8 \) fm in our calculations, which is large enough for the current work.

We perform the above REM process for the intrinsic wave function of \(^6\text{He}\) and obtain an ensemble of basis. This ensemble of basis is used for both the calculations of \(^6\text{He}\) and \(^6\text{Li}\).

### 3 Results

We firstly show the energy spectra for the low-lying states of \(^6\text{He}\) and \(^6\text{Li}\) nuclei in Fig. 1.

The experimental data and the corresponding results in the referenced works [11,32] are also included for comparison. In Fig. 1, it clearly shows that our REM method provides the almost consistent results for the 0\(^+\) states of \(^6\text{He}\) and \(^6\text{Li}\) nuclei as the references. Besides, for the 1\(^+\) ground state and the 3\(^+\) excited state of \(^6\text{Li}\), the wave functions from our REM procedure provide better results than the reference work, which means that we have found more sufficient wave function through the evolution with the EOM. These results support the validity of the REM. Furthermore, it should be noted that we are using one ensemble of the basis for both of the \(^6\text{He}\) and \(^6\text{Li}\) calculations. It is interesting that one EOM can reproduce both the \( T = 0 \) states and \( T = 1 \) states, and it indicates that the REM may have the potential for the investigation of the isospin mixing states in the future study.

Next we shall check the accuracy of our calculations. We show the energy convergences with the increasing number of basis in Fig. 2. It shows that the huge number of the basis have been included and the binding energies of all these states are well converged. These results prove that the number of basis in our calculations is sufficient to converge the energy results. Furthermore, we can see that the converged results of 1\(^+\) and 3\(^+\) states in our calculation give much lower energy than the results from the reference works. It denotes that the REM procedure has found more effective basis, which should be included to the total wave function.

It is also an essential topic to investigate the halo property of the \(^6\text{He}\) nucleus as well as the \(^6\text{Li}\) nucleus. The 0\(^+\) ground state of \(^6\text{He}\) is the well known two-neutron halo. Likewise, the 0\(^+\) excited states of \(^6\text{Li}\) also has the controversial halo property [34]. To investigate the halo property in these two nuclei, we calculate the root-mean-square (r.m.s.) radii of \(^6\text{He}\) and \(^6\text{Li}\) with the wave function from REM. The corresponding results are shown in Fig. 3.

In the left panel of this figure, the calculated r.m.s. radii of point matter, point proton and point neutron of the 0\(^+\) state of \(^6\text{He}\) are 2.71 fm, 2.03 fm, and 2.99 fm, respectively. These
Fig. 2 The energy convergence of $^6\text{He}$ and $^6\text{Li}$ from the REM calculations concerning the successive addition of bases. The dash lines are the corresponding results from the reference works [11,32].

![Graph showing energy convergence of $^6\text{He}$ and $^6\text{Li}$](image)

Fig. 3 The r.m.s. radii of $^6\text{He}$ and $^6\text{Li}$ from the REM calculations concerning the successive addition of bases. The dotted lines denote the results in the reference works [11,32].

![Graph showing r.m.s. radii of $^6\text{He}$ and $^6\text{Li}$](image)

Table 1 The numerical results of the 0$^+$ ground state of $^6\text{He}$, as well as the 1$^+$, 3$^+$ and 0$^+$ states of $^6\text{Li}$ from the calculations of REM.

|           | Energy (MeV) | Point matter (fm) | Point proton (fm) | Point neutron (fm) |
|-----------|--------------|-------------------|------------------|-------------------|
| $^6\text{He}$ (0$^+$) | $-28.37$    | $2.71$            | $2.03$           | $2.99$            |
| $^6\text{Li}$ (1$^+$) | $-30.92$    | $2.65$            | $2.66$           | $2.65$            |
| $^6\text{Li}$ (3$^+$) | $-29.87$    | $2.42$            | $2.43$           | $2.41$            |
| $^6\text{Li}$ (0$^+$) | $-27.58$    | $2.79$            | $2.81$           | $2.77$            |

results are showing the explicit halo property of the ground state of $^6\text{He}$. From the right panel of Fig. 3, one can also find that the r.m.s. radius of point matter of the 0$^+$ state of $^6\text{Li}$ (2.79 fm) is larger than the radii of its 1$^+$ (2.65 fm) and 3$^+$ (2.42 fm). It implies that the 0$^+$ state of $^6\text{Li}$ can be treated as a halo state, which is consistent with the experimental conclusion [34]. These results show that the halo property of these states can be naturally included in the ensemble of the basis from the REM. Comparing with the reference works, we notice that our results on the r.m.s. radii are larger than the results in the reference works, which are denoted by the dotted lines in Fig. 3. It indicates that our ensemble of basis from REM includes the basis, where valence nucleons spread far from the core, so that we provide more dilute structure for the halo states of $^6\text{He}$ and $^6\text{Li}$ nuclei than theirs.

In the end, the detailed numerical results are summarized in Table 1. We notice that the binding energies of the 0$^+$ states obtained in our calculations are slightly different from the reference works. Besides, we may overestimate the r.m.s. radii of these nuclei compare with the experimental data.
These deviations indicate that we still missing something in the total wave functions or the Hamiltonian, which will be further studied in our future work with the REM method.

4 Conclusion

We perform the calculations for $^6$He and $^6$Li nuclei with a recently developed model named REM, which can generate the ergodic ensemble of the basis wave functions. During this work, we generate the basis wave functions from the procedure of REM and superpose them to construct the total wave functions. The converged results for the energy and the r.m.s. radius of the $0^+$ state of $^6$He as well as the $1^+$, $0^+$ and $3^+$ states of $^6$Li nuclei have been obtained in this work. The halo properties of $^6$He and $^6$Li are well described in the current work, which indicates that the REM can search for the basis more efficiently. However, there is still something missing in the total wave functions or the Hamiltonian in the current work, since the calculated binding energies of $0^+$ states still have slight deviation with the previous reference works, and we also overestimate the r.m.s. radii of these nuclei. We will continue developing this new method in future work. The benchmark calculations performed in this work can be instructive for further calculation with REM. This method has shown its potential in the description of the motion of the nucleons and we will take its advantage in future research to study the neutron Cooper pairs or other physical problems.

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