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A new generator coordinate method to describe gas-like states

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Abstract. A new theoretical model which employs the real time as the generator coordinate is developed to describe gas-like cluster states. The model exploits the quantum ergodic nature of the time-evolution of the wave packets. The result of the benchmark calculation shows that the new method describes the dynamics of the 3α system reasonably comparable with or even better than the Tohsaki-Horiuchi-Schuck-Röpke wave function.

1. Introduction

In this decade, the α particle condensates in finite nuclei attract a lot of interest. In the very begging [1, 2], the Hoyle state of ^{12}C was the icon of the α particle condensate. Later, a lot of theoretical and experimental efforts revealed that there are many families of the 3α condensates in ^{12}C and established that the α particle condensate also exists in the 4α system, ^{16}O [3, 4].

Different from the cold atomic systems, the α particle condensates are self-bound systems without the confinement potential, hence the question "how many α particles can form the condensate?" is very interesting and essential. The experiments [5] imply the possible formation of 10 and 15 α particle condensates in the compound states of ^{40}Ca and ^{60}Zn. Theoretically, Yamada and Schuck [6] showed that up to approximately 10α particles can form self-bound condensate. However, their prediction is based on the macroscopic model which approximates α particles as structureless bosons. Therefore, the microscopic model studies which take the Fermi statistics of nucleons into account are highly desirable for more detailed and reliable discussions.

Unfortunately, we immediately find serious difficulty in describing the dynamics of many α particles with the full microscopic models. Imagine that one tries to describe $N\alpha$ particle system by the generator coordinate method (GCM) which superposes basis wave functions Φ_i,

$$\Psi = \sum_i c_i \Phi_i. \tag{1}$$

It is easy to understand that the number of basis wave function Φ_i very quickly increases as the number of α particle increases, which makes the practical numerical calculation impossible. Therefore, the effective method to generate the basis wave function Φ_i is indispensable. Several methods have been suggested, which are based on the random generation of the basis wave function [7] and the imaginary-time development [8]. In this contribution, we suggest an alternative but surprisingly effective method which relies on the ergotic nature of the real-time evolution of the α particle wave packets. We here discuss the result of the benchmark calculation for 3α system.

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2. Methodology

The Hamiltonian of the 3α system used in the benchmark calculation is given as,

$$H = \sum_{i=1}^{12} t_i + \sum_{i<j}^{12} v_N(r_{ij}) + \sum_{i<j}^{6} v_C(r_{ij}) - t_{cm}, \tag{2}$$

where t_i and t_{cm} respectively denote the kinetic energies of the nucleons and the center-of-mass. As an effective nucleon-nucleon interaction, we used Volkov No. 2 with a slight modification. In short, the Hamiltonian is common to the other studies using resonating group method (RGM) [9] and Tohsaki-Horiuchi-Schuck-Röpke (THSR) wave function [10].

Our basis wave function for 3α system is the Brink-Bloch wave function,

$$\Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3) = \mathcal{A}\left\{ \Phi_\alpha(\boldsymbol{Z}_1)\Phi_\alpha(\boldsymbol{Z}_2)\Phi_\alpha(\boldsymbol{Z}_3) \right\}, \tag{3}$$

$$\Phi_\alpha(\boldsymbol{Z}) = \mathcal{A}\left\{ \phi(\boldsymbol{r}_1, \boldsymbol{Z})\chi_{p\uparrow}\phi(\boldsymbol{r}_2, \boldsymbol{Z})\chi_{p\downarrow}\phi(\boldsymbol{r}_3, \boldsymbol{Z})\chi_{n\uparrow}\phi(\boldsymbol{r}_4, \boldsymbol{Z})\chi_{n\downarrow} \right\}, \tag{4}$$

$$\phi(\boldsymbol{r}, \boldsymbol{Z}) = \left(\frac{2\nu}{\pi}\right)^{3/4} \exp\left\{ -\nu\left(\boldsymbol{r} - \frac{\boldsymbol{Z}}{\sqrt{\nu}}\right)^2 + \frac{1}{2}Z^2 \right\}, \tag{5}$$

where $\Phi_\alpha(\boldsymbol{Z})$ denotes the wave function of α particle located at $\boldsymbol{Z}$. Here, the three-dimensional vector $\boldsymbol{Z}$ is complex numbered differently from the ordinary Brink-Bloch wave function, and hence, they are regarded as the dynamical variable. By applying the time-dependent variational principle, one obtains the equation of motion (EoM) for the α particle centroids $\boldsymbol{Z}_1, \boldsymbol{Z}_2$ and $\boldsymbol{Z}_3$,

$$\sum_{j,\sigma} C_{i\rho j\sigma} \frac{dZ_{j\sigma}}{dt} = \frac{\partial \mathcal{H}}{\partial Z^*_{i\rho}}, \quad i = 1, 2, 3, \quad \rho, \sigma = x, y, z, \tag{6}$$

$$\mathcal{H} \equiv \frac{\langle \Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)|H|\Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)\rangle}{\langle \Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)|\Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)\rangle}, \quad C_{i\sigma j\rho} \equiv \frac{\partial^2 \ln \langle \Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)|\Phi(\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3)\rangle}{\partial Z^*_{i\sigma}\partial Z_{j\sigma}}. \tag{7}$$

We evolve the system by solving the EoM (Eq. (6)). As a result, we obtain the wave function of the 3α system at each time t; $\Phi(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t))$. Despite of its classical-like look, this EoM possesses the following excellent properties [11, 12],

(i) The wave function $\Phi(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t))$ has ergodic nature.

(ii) The ensemble of $\Phi(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t))$ follows *quantum* statistics.

This means that, if time is evolved long enough, the set of wave functions $\Phi(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t))$ spans a good model space for 3α system. Therefore, the superposition of the basis wave function,

$$\Psi = \int_0^T dt\ c(t)\left\{ \Phi(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t)) + \Phi^*(\boldsymbol{Z}_1(t), \boldsymbol{Z}_2(t), \boldsymbol{Z}_3(t)) \right\}, \tag{8}$$

should give a good description for 3α system. Here, the basis wave functions are conjugated to guarantee that Ψ is time even. The coefficients $c(t)$ should be determined by the diagonalization of the Hamiltonian. In other words, by using the EoM, we perform the generator coordinate method by employing the real time t as the generator coordinate.

3. Numerical benchmark

The practical numerical calculation was done as follows. First, we randomly generate the excited 3α wave function by the imaginary-time evolution. The excitation energy is set $E^* \simeq 15$ MeV. Then we solve the EoM and perform the GCM calculation by discretizing the time t in Eq. (8).

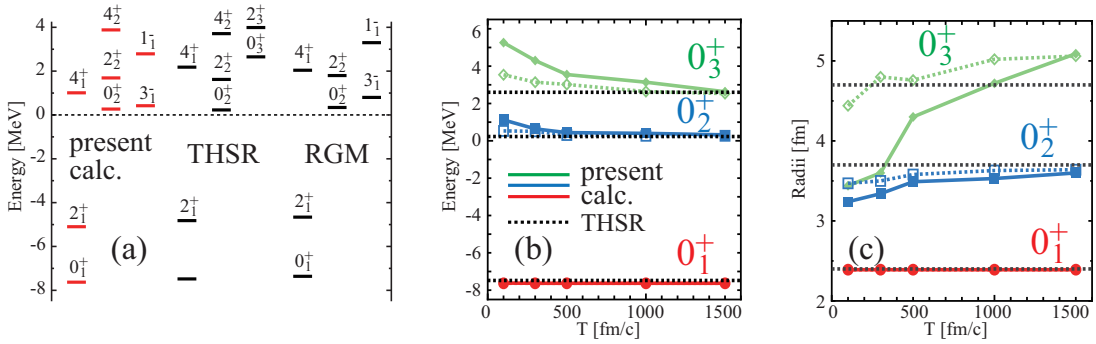

Figure 1. (a) Energy spectra of 3α system calculated by the present method, THSR [10] and RGM [9]. (b) and (c) The convergence of the energies and radii of the eigenstates as functions of the time evolution duration T.

Figure 1 (a) compares the present result with other theoretical calculations which employ the same Hamiltonian. It is clear that our model gives very reasonable result and consistent with the previous methods including the THSR wave function. It is also noted that the radii are also properly described. For example, the radius of the Hoyle state is calculated as 3.66 fm and 3.7 fm by the present model and THSR respectively, while the ordinary RGM yields much smaller radius, 3.47 fm. Thus, the our method can reasonably describe the cluster gas-like states and has the advantage over the ordinary cluster model. Figure 1 (b) and (c) show how the binding energies and radii are converged as the duration T increases. Solid and dashed lines show the results obtained by starting from different initial condition. We see that, except for the 0_3^+ state which has broad width, the calculation converges as T becomes large and the result is independent of the initial condition of the time evolution. Since the extension of this model is rather straightforward, the application to 4α,5α, ... systems looks fascinating and promising.

4. Summary

In summary, we have developed a new theoretical model which employs the real time as the generator coordinate. The model relies on the quantum ergodic nature of the EoM of the wave packets. The result of the benchmark calculation shows that our model can describe the 3α system reasonably.

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