GENERATOR COORDINATE METHOD WITH BASIS OPTIMIZATION*

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The generator coordinate method (GCM) is a well-known method to describe nuclear collective motions. In this method, one needs to specify *a priori* the relevant collective degrees of freedom as input of the method, based on empirical and/or phenomenological assumptions. Recently, we extended the GCM to include simultaneous optimization of both the basis Slater determinants and the weight factors based on the variational principle. This extension allows for the automatic optimization of the collective subspace. In this study, we apply the extended GCM to analyze ^{20}Ne using the Skyrme interaction. We demonstrate that the optimized basis states correspond to excited states along a collective path, in contrast to the conventional GCM, which typically superposes only local ground states. We further calculate the low-lying excited states with the angular momentum projection and discuss the capabilities of the extended method.

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1. Introduction

Developing a theory for the microscopic description of collective motion is one of the major goals of nuclear many-body problems. In particular, there are several phenomena in nuclear systems, such as shape coexistence phenomena and nuclear fission, in which large-amplitude collective motion is crucial. The generator coordinate method (GCM) has been widely used to describe collective motions including large-amplitude motions.

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A trial wave function of GCM is given by a superposition of basis Slater determinants (SDs). The basis states are parametrized by appropriate collective coordinates to describe the dynamics of the system. In practice, the local ground states along selected collective coordinates are generated by the constrained Hartree–Fock (CHF) method. Then, a set of weights is determined based on the variational principle.

However, there is a serious problem of GCM that collective coordinates must be selected based on empirical or phenomenological assumptions. There is no guarantee that the commonly used collective coordinates are sufficient to describe the ground state of a given nucleus. Therefore, it is necessary to develop a theory that does not rely on the empirical determination of collective coordinates and that describes the collective motion non-empirically.

Recently, we have proposed a method based on GCM with basis optimization [1, 2]. Such an extension allows us to obtain an optimal collective space. Similar attempts have been made with the Monte Carlo shell model [3] and more recently with anti-symmetrized molecular dynamics [4]. We have studied the intrinsic ground states of the *sd*-shell region using Skyrme interactions in our previous work [1]. In this work, as the next step, we analyze the low-lying excited states of ^{20}Ne.

2. Method

We optimize the basis for the intrinsic ground states using the method proposed in [1]. We call this method the optimized-basis GCM (OptGCM). The trial function is given by

$$|\Psi\rangle = \sum_{a=1}^{M} f_a |\Phi_a\rangle \,, \tag{1}$$

where $|\Phi_a\rangle$ are the basis Slater determinants, which are given by anti-symmetrized product of N orthonormal single-particle orbitals $\varphi_i^{(a)} (i = 1, \ldots, N)$.

The total energy to be minimized is given by

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_{ab} f_a^* f_b H_{ab}}{\sum_{ab} f_a^* f_b N_{ab}} \,, \tag{2}$$

where N_{ab} and H_{ab} are the norm and the Hamiltonian kernels, respectively,

$$N_{ab} = \langle\Phi_a|\Phi_b\rangle \,, \tag{3}$$

$$H_{ab} = \langle\Phi_a|H|\Phi_b\rangle \,. \tag{4}$$

The total energy E should be stationary under an arbitrary variation of the variational parameters f_a and $\varphi_i^{(a)}$. We take the variation of E with respect to $\varphi_i^{(a)}$ and weight function f_a using the conjugate gradient method [5].

In this work, the initial set of SDs for the conjugate gradient iterations is prepared by Woods–Saxon potentials with different deformations, and the initial values of the weight factors are set as $f_a = 1$ for all a. For the energy density functional, we adopt the SIII parameter set of the Skyrme functional [6]. We assume axial and reflection symmetries and omit the time-odd terms of the functional for simplicity. The pairing correlation is also neglected. The single-particle states are expanded on the axial harmonic-oscillator basis [7]. We take 14 major shells of harmonic-oscillators and 10 basis SDs.

After the optimum set of the basis and the weight factors are obtained, we perform the angular momentum projection to restore the rotational symmetry and obtain low-lying excited states. The weights are re-determined by GCM after projection for each angular momentum. For comparison, we also perform GCM calculations with quadrupole moments Q_2 as the collective coordinates. That is, the basis obtained by the CHF method with constraints on Q_2 is superposed, and the weights are determined by GCM after the angular momentum projection.

3. Results and discussions

Figure 1 (a) shows the bases obtained by basis optimization for the intrinsic ground states. It also includes the potential energy curve calculated by CHF. Note that for the CHF, a level crossing takes place near $Q_2 = 0$ in ^{20}Ne, and the CHF does not converge near that point. Therefore, the calculation is performed up to the smallest Q_2 possible to be calculated. As we show for the cases of ^{16}O and ^{28}Si in [1], the optimized bases correspond to excited states along a collective path. This result implies that one needs to take into account excitations of nuclei in determining a collective coordinate.

Figures 1 (d) and (e) show neutron-density distributions obtained by CHF and OptGCM, respectively. With the OptGCM, a variety of shapes are obtained for the bases that cannot be obtained with the Q_2-CHF. This indicates that a wider collective subspace and nontrivial fluctuation in higher moments can be obtained by optimizing the basis. Using the basis shown here, the calculation of physical quantities, such as the energy by the angular momentum projection, is carried out.

Figure 1 (b) shows the calculated and observed rotational bands of ^{20}Ne obtained with the HF, GCM, and OptGCM. The experimental results are taken from [8]. The energies of the 0^+, 2^+, 4^+, and 6^+ states are lowered, as compared to those in HF, by the configuration mixing in GCM and further by

the mixing of the optimized bases in OptGCM. According to the variational principle, the OptGCM results are better than those of GCM and HF for the given Hamiltonian. For the 8^+ state, GCM gives the lowest energy, reversing the results for GCM and OptGCM. It is reasonable that OptGCM cannot reproduce well the structure of the spectrum for the higher states, since the basis in OptGCM is optimized for the intrinsic ground state in this calculation. Optimization of the basis states after the angular momentum projection would improve the results for the excited states as well as the ground state.

Figure 1 (c) shows the B(E2) values obtained with HF, GCM, and OptGCM. The experimental values are also presented [8]. The results for GCM and OptGCM are in better agreement with the experimental values than those of HF. In particular, the decrease in $B(\mathrm{E2}; 6^+ \to 4^+)$ and $B(\mathrm{E2}; 8^+ \to 6^+)$ is better reproduced by GCM and OptGCM.

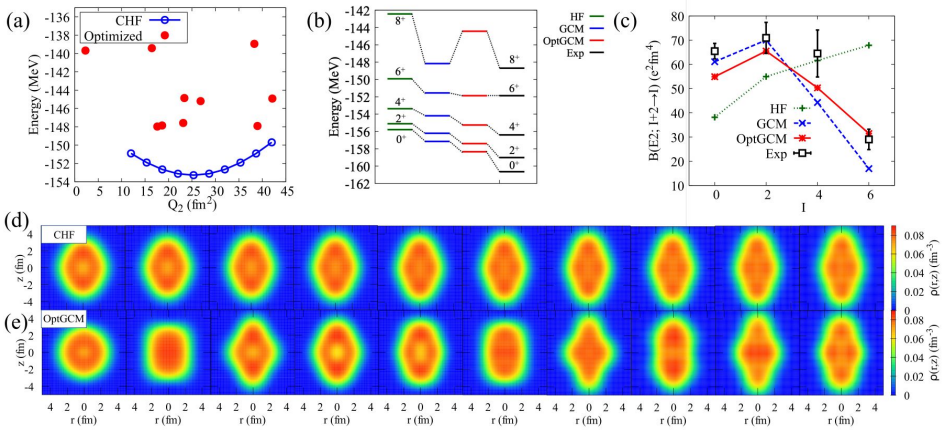

Fig. 1. (a) Expectation value of the Hamiltonian H_{aa} as a function of the expectation value of Q_2 for each SD. (b) Energy spectra of ^{20}Ne calculated with AMP. The experimental data is taken from [8]. (c) Observed and calculated B(E2) strengths of ^{20}Ne. The experimental data is taken from [8]. (d) Neutron density distribution of each SD obtained with CHF. (e) The same as (d), but with OptGCM.

4. Conclusion

We obtained the optimal collective subspace for the intrinsic ground state of ^{20}Ne using OptGCM, which we recently proposed. From information of the obtained basis, it is expected that one needs to take into account excitations of nuclei in determining collective coordinates. It was shown that the fluctuations of higher multipole moments could also contribute to the ground-state correlations.

In addition, we calculated the low-lying excited states from the obtained basis with the angular momentum projection. The energies of the ground-state rotational band and $B(\mathrm{E2})$ value were discussed. For the 0^+, 2^+, 4^+, and 6^+ states, whose excitation energies are approximately 10 MeV or less, the OptGCM calculations show lower energies than the GCM calculations with the Q_2 taken as the generator coordinate. The $B(\mathrm{E2})$ calculated by OptGCM and GCM was in good agreement with the experimental values.

To extend the applicability of OptGCM to a broader range of collective excitations, it is crucial to perform basis optimization after angular momentum projection [3]. It would enlarge the applicability of OptGCM to the analysis of large-amplitude collective motions, such as shape coexistence. Another interesting future work is to employ OptGCM to determine collective paths in various nuclei and compare the results with those obtained from other existing approaches to collective motion, such as the dynamical GCM [9, 10].

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