Non-empirical description of nuclear collective motion with optimized basis for multi-reference density functional theory

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Abstract. The generator coordinate method (GCM) has been a well-known method to describe nuclear collective motions. In this method, one *a priori* specifies collective degrees of freedom as inputs of the method based on empirical and/or phenomenological assumptions. We here present an extension of the GCM, in which both the basis Slater determinants and weight factors are optimized in a non-empirical manner. The result for ^{16}O nucleus with the Skyrme functional suggests that a collective coordinate should be determined in a more complex way than what has been assumed so far.

1 Introduction

Collective motions are characteristics of many-body systems. Typical examples in atomic nuclei include giant resonances and low-lying surface vibrations with several multipolarities. Furthermore, in collective phenomena such as fission and shape coexistence, large amplitude motions play an essential role. It is one of the major goals of the quantum many-body problems to describe such collective motions microscopically.

A widely used theoretical method for describing large-amplitude collective motion is the generator coordinate method (GCM) [1, 2]. In GCM, one *a priori* specifies collective degrees of freedom (that is, collective coordinates), such as nuclear deformations and distances between clusters, and superposes many Slater determinants (SDs) within the selected collective subspace. The weight coefficients of SDs are then determined according to the variational principle. Many numerical calculations have been performed using this method, which is often referred to as the beyond-mean-field method [3–7].

However, GCM has a serious problem that there always exists arbitrariness in the choice of collective coordinates, which one has to select in empirical and phenomenological manners. With such choice, it is not trivial whether the collective motion of interest can be optimally described. Therefore, a description of collective motions which avoids pre-set collective coordinates is always desirable in order not to miss important degrees of freedom.

To discuss collective motion in a non-empirical way, several methods have been developed. For example, a stochastic selection of the basis is carried out with anti-symmetrized molecular dynamics (AMD) [8–10] and multi-reference density functional theory (DFT) [11, 12]. Even though the basis is constructed in an unbiased way with these methods, it is not obvious whether such basis is optimal for the ground or low-lying excited states of a system. Similar attempts have been taken in the Monte Carlo shell model (MCSM), in which the optimization of the basis is performed not only stochastically, but also variationally [13].

In this contribution, we introduce the optimized-basis GCM (OptGCM) for multi-reference DFT that we recently proposed in Ref. [14]. In our new method, a trial many-body state is given by a superposition of SDs as in GCM, but both the weights and the basis SDs are determined by variation as in the MCSM [13]. The method thus avoids pre-fixed collective coordinates. With this formulation, the collective space covered by the basis states is automatically optimized to the ground state of a system of interest. Note that a similar technique was recently developed in the context of AMD as well [15].

2 Ground state of ^{16}O

Let us assume that the ground state wave function is given by

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

where $|\Phi_a\rangle$ are the basis SDs with the antisymmetrized product of N orthonormal single-particle orbitals $\varphi_i^{(a)}(i = 1, \ldots, N)$. We minimize the total energy for a given Hamiltonian H,

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

where $N_{ab} = \langle\Phi_a|\Phi_b\rangle$ and $H_{ab} = \langle\Phi_a|H|\Phi_b\rangle$ are the norm and Hamiltonian kernels, respectively. We take variation

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Table 1. The ground state energies, the quadrupole moments, Q_2, and the hexadecupole moments, Q_4, obtained with the HF, GCM and OptGCM methods. Taken from Ref. [14].

Method	Energy (MeV)	Q_2 (fm^2)	Q_4 (fm^4)
HF	−142.024	0.000	0.000
GCM	−142.407	0.179	4.662
OptGCM	−143.109	0.165	0.563

of E with respect to both $\varphi_i^{(a)}$ and f_a [14] and search for the minimum of the total energy by the conjugate gradient method [16].

In this work, the initial set of SDs are prepared with Woods-Saxon potentials with different deformations, and the initial values of the weight factors are set to be $f_a = 1$ for all a. The SIII parameter set [17] of the Skyrme functional is adopted for the energy density functional, while the pairing correlation is not included. For simplicity, the time-odd terms of the functional and the Coulomb interaction are neglected. The single-particle states are expanded on the axial harmonic-oscillator (HO) basis [18]. For simplicity, the weight factors f_a are restricted to be real numbers.

Let us apply the OptGCM to ^{16}O and compare our results with those of the conventional GCM, in which the basis SDs are prefixed and only the weight factors f_a are optimized. For this purpose, the results for the 8 SDs with 14 HO major shells are used as basis sets. Since quadrupole collectivity is important for many nuclei, the quadrupole moments are used in the GCM calculations as the collective coordinates. That is, in the GCM calculations, the basis SDs are the local ground state obtained with constrained Hartree-Fock (CHF) method with $\langle\Phi_a(Q_2^{(a)})|\hat{Q}_2|\Phi_a(Q_2^{(a)})\rangle = Q_2^{(a)}$. Here,

$$\hat{Q}_\lambda = \int d^3r\, r^\lambda Y_{\lambda 0}(\hat{\boldsymbol{r}})\hat{\rho}(\boldsymbol{r}) \tag{3}$$

is the multipole moment operator with $\hat{\rho}$ and $Y_{\lambda 0}$ being the density operator and the spherical harmonics, respectively. For $Q_2^{(a)}$, we take the eight values equally spaced between -7.73 fm^2 and 8.36 fm^2, which are the smallest and largest values of the quadrupole moment of the optimized basis SDs.

In Table 1, the ground state energies obtained with HF, GCM and OptGCM are listed. In the case of GCM, the total energy is about 0.4 MeV lower than that of HF. On the other hand, in OptGCM, the ground state energy is further lowered from the GCM energy by about 0.7 MeV. This implies that the optimized basis states gain more correlations than the Q_2-CHF basis states.

In order to understand the difference between OptGCM and conventional GCM, the basis obtained with OptGCM and Q_2-CHF calculations are analyzed in Fig. 1. Firstly, Fig. 1 (a) shows the eigenvalues of the norm kernel. In the CHF case, the eigenvalues range from ~ 1 to 10^{-10}. The small eigenvalues of the norm kernel mean that the basis SDs are not completely linearly independent. On the other hand, in the case of OptGCM, all eigenvalues are larger than $\approx 10^{-1}$, which indicates that the optimized basis set spans a larger subspace than the basis obtained in the CHF calculation.

Figure 1 (b) shows the energies of each SD, $E^{(a)} = E[\rho^{(a)}] = \langle\Phi_a|H|\Phi_a\rangle$, as a function of the quadrupole moment for each SD, $Q_2^{(a)} = \langle\Phi_a|\hat{Q}_2|\Phi_a\rangle$. It is worth mentioning that the optimized bases have higher energies than those obtained using the CHFs. In other words, the optimized bases correspond to excited states above the potential energy curve obtained with CHF. In particular, there are some bases that reach energies more than 20 MeV above the potential energy curve. This result indicates that the excitations of nuclei should be taken into account in determining collective coordinates. Even if the expectation values, that is, the diagonal components, of the Hamiltonian H with the OptGCM are larger than those with the GCM, the off-diagonal components with different SDs are larger either in the Hamiltonian or in the norm kernels, which result in the lower value of the ground state energy. This point will be discussed in the next section.

Figure 1 (c) shows the quadrupole moments $Q_2^{(a)}$ and the hexadecupole moment $Q_4^{(a)} = \langle\Phi_a|\hat{Q}_4|\Phi_a\rangle$ for each of the SDs on the two-dimensional (Q_2, Q_4) plane. The filled and the open circles are for the SDs with the OptGCM and the Q_2-CHF, respectively. In the OptGCM, Q_4 fluctuates significantly around the valley and takes both positive and negative values compared to the Q_2-CHF case. As a result, the total Q_4 becomes smaller than the Q_4 in the Q_2-CHF. This suggests that Q_2 alone does not make a good collective coordinate and at least one needs to take into account both Q_2 and Q_4. A recent GCM calculation includes not only Q_2 but also Q_4 as collective coordinates [19]. See Table 1 also for the quadrupole and hexadecupole moments of the total densities. The Q_2 values for GCM and OptGCM are almost the same, while the Q_4 value is smaller in OptGCM.

Figures 1 (d) and 1 (e) show the neutron density distributions of each SD obtained with the Q_2-CHF and the OptGCM, respectively. With the OptGCM, a variety of shapes are obtained for the bases, that cannot be genearated with the Q_2-CHF.

3 Discussion

One of the major conclusions presented in the previous section is that the optimized bases correspond to excited states along a collective path, unlike the conventional GCM which superposes only the local ground states. Here we demonstrate the role of off-diagonal components in lowering the ground state energy. To this end, we use the case of two SDs. The Hamiltonian (in units of MeV) and the norm kernels with the OptGCM read,

$$H_{\rm OPT} = \begin{pmatrix} -138.61 & -110.18 \\ -110.18 & -139.28 \end{pmatrix}, \tag{4}$$

$$N_{\rm OPT} = \begin{pmatrix} 1.00 & 0.74 \\ 0.74 & 1.00 \end{pmatrix}, \tag{5}$$

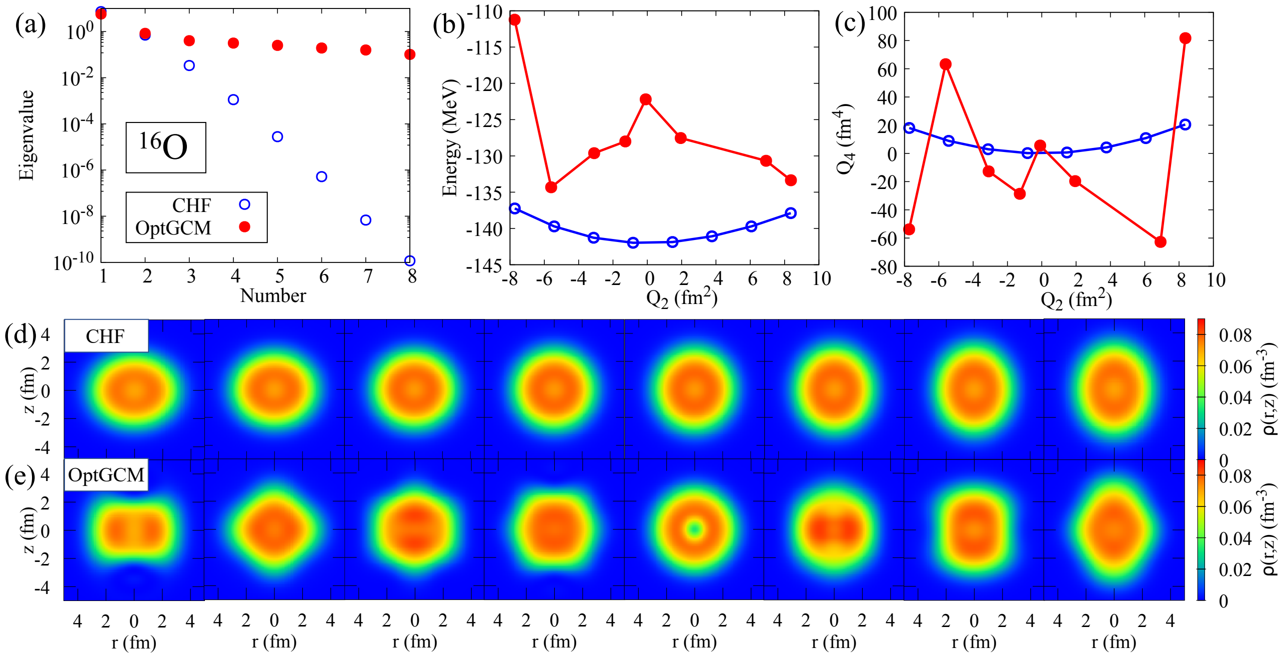

Figure 1. The properties of the basis SDs obtained with the constrained-HF (CHF) and the OptGCM. (a) The eigenvalues of the norm kernels plotted in the descending order. The CHF and the OptGCM results are shown by the blue open circles and the red filled circles, respectively. (b) The expectation value of the Hamiltonian as a function of the expectation value of Q_2 for each SD. The meaning of each symbol is the same as in the panel (a). (c) The quadrupole (Q_2) and the hexadecupole (Q_4) moments of each SD in the two-dimensional Q_2-Q_4 plane. The meaning of each symbol is the same as in the panel (a). (d) The neutron density distributions of each SD obtained with the CHF. (e) The same as the panel (d), but with the OptGCM. Taken from Ref. [14].

respectively, while those for the conventional GCM read

$$H_{\rm GCM} = \begin{pmatrix} -139.64 & -115.18 \\ -115.18 & -140.07 \end{pmatrix}, \tag{6}$$

$$N_{\rm GCM} = \begin{pmatrix} 1.00 & 0.79 \\ 0.79 & 1.00 \end{pmatrix}. \tag{7}$$

Here, the two configurations for the conventional GCM were obtained with CHF, with the same values of Q_2 as those obtained with OptGCM. One can see that both of the diagonal components of $H_{\rm OPT}$ are significantly larger than those of $H_{\rm CHF}$. The ground state energy within the collective space corresponds to the lowest eigenvalue of $H' \equiv N^{-1/2}HN^{-1/2}$. This matrix reads,

$$H'_{\rm OPT} = \begin{pmatrix} -127.69 & -14.39 \\ -14.39 & -128.69 \end{pmatrix}, \tag{8}$$

$$H'_{\rm GCM} = \begin{pmatrix} -129.89 & -12.14 \\ -12.14 & -130.60 \end{pmatrix}, \tag{9}$$

from which the lower eigenvalue is obtained to be -142.59 and -142.40 MeV for the OptGCM and the conventional GCM, respectively. Notice that the diagonal components of $H'_{\rm OPT}$ are larger than those of $H'_{\rm GCM}$. However, the absolute values of the off-diagonal components are also larger in $H'_{\rm OPT}$ than in $H'_{\rm GCM}$. This results in the lower ground state energy with the OptGCM.

To further clarify the role of off-diagonal components of the Hamiltonian matrix, we consider a simple model, in which the Hamiltonian matrix is given by

$$H' = \begin{pmatrix} \left[H'_{\rm GCM}\right]_{11} + \Delta E & f \cdot \left[H'_{\rm GCM}\right]_{12} \\ f \cdot \left[H'_{\rm GCM}\right]_{21} & \left[H'_{\rm GCM}\right]_{22} + \Delta E \end{pmatrix}. \tag{10}$$

Figure 2 (a) plots the difference between the lower eigenvalue of H', E', and that for $H'_{\rm GCM}$, $E'_{\rm GCM}$, that is, $E' - E'_{\rm GCM}$ as a function of ΔE and f. One can see that the energy E' is lowered than $E'_{\rm GCM}$ as long as f is large enough even if ΔE is positive. This clearly indicates that the diagonal components of the Hamiltonian alone do not determine the ground state energy, and one also needs to consider the off-diagonal components as well. Figure 2(b) schematically shows this situation.

4 Conclusion

We have developed a method to optimize both the weights and the basis SDs in GCM. We have performed numerical calculations for the ground state of ^{16}O with this method using a Skyrme interaction. We have pointed out that a multidimensional GCM calculation including not only Q_2 but also higher moments is necessary to describe the ground state of ^{16}O. Furthermore, from the analysis of the optimal basis obtained, we have suggested that it may not be a good approximation to superpose the local ground states along the collective coordinate as in the conventional GCM calculation. Furthermore, we have demonstrated that the off-diagonal components of the Hamiltonian as well as those of the norm kernels play an important role in the ground state.

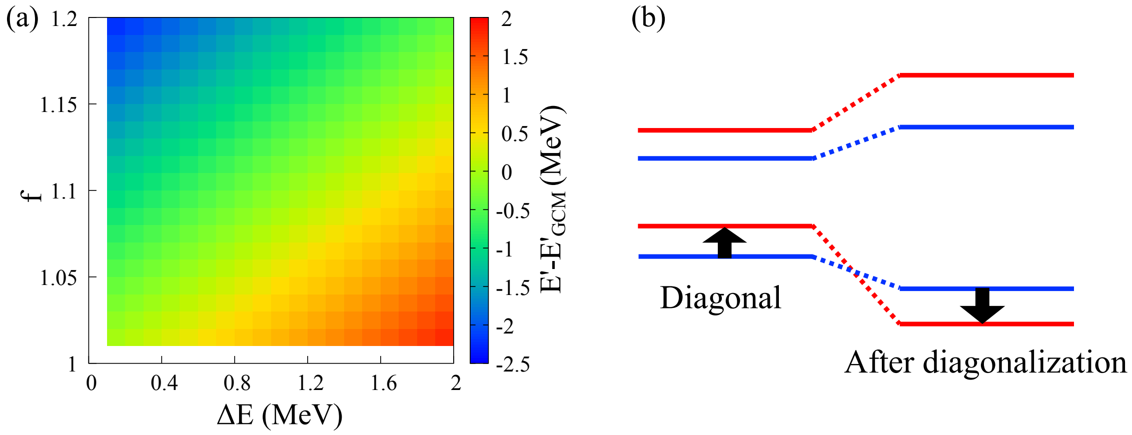

Figure 2. (a) The difference between the lowest eigenvalue of Eq. (10) and that for H'_{GCM} as a function of ΔE and f defined in Eq. (10). (b) A schematic picture of energies. Even if the diagonal components are not optimized, the lowest energy may be lowered after diagonalization due to the off-diagonal components.

It would be interesting to compare the collective space obtained with this method to that obtained with existing other theories for collective motion, such as the self-consistent collective coordinate method [20–23]. Since the basis obtained in this work are local excited states with respect to the collective coordinates, it would be also interesting to discuss the relation between this method and the dynamical GCM with collective momenta [24, 25].

It would also be of interest to extend the method of optimizing the basis to time-dependent calculations and to provide a microscopic description for fusion and fission. A preliminary calculation with the AMD basis has suggested that such calculations would have a capability of describing many-body quantum tunneling [26]. Therefore, it would be an interesting future work to clarify whether it is possible to describe sub-barrier fusion and spontaneous fission with such methods. In this regards, we mention that several research groups have recently been working on extensions of time-dependent GCM [27, 28], and further prospects in these directions would be highly expected.

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References

[1] P. Ring, P. Schuck, *The Nuclear Many-Body Problem* (Springer, 1980)

[2] P.G. Reinhard, K. Goeke, Rep. Prog. Phys. **50**, 1 (1987)

[3] M. Bender, P.H. Heenen, P.G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003)

[4] T. Nikšić, D. Vretenar, P. Ring, Prog. Part. Nucl. Phys. **66**, 519 (2011)

[5] L.M. Robledo, T.R. Rodríguez, R.R. Rodríguez-Guzmán, J. Phys. G **46**, 013001 (2018)

[6] J.M. Yao, J. Meng, P. Ring, D. Vretenar, Phys. Rev. C **81**, 044311 (2010)

[7] J.M. Yao, K. Hagino, Z.P. Li, J. Meng, P. Ring, Phys. Rev. C **89**, 054306 (2014)

[8] N. Itagaki, A. Kobayakawa, S. Aoyama, Phys. Rev. C **68**, 054302 (2003)

[9] P. Descouvemont, N. Itagaki, Phys. Rev. C **97**, 014612 (2018)

[10] P. Descouvemont, N. Itagaki, Prog. Theor. Exp. Phys. **2020**, 023D02 (2020)

[11] S. Shinohara, H. Ohta, T. Nakatsukasa, K. Yabana, Phys. Rev. C **74**, 054315 (2006)

[12] Y. Fukuoka, S. Shinohara, Y. Funaki, T. Nakatsukasa, K. Yabana, Phys. Rev. C **88**, 014321 (2013)

[13] N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Prog. Theor. Exp. Phys. **2012** (2012)

[14] M. Matsumoto, Y. Tanimura, K. Hagino, Phys. Rev. C **108**, L051302 (2023)

[15] T. Myo, M. Lyu, Q. Zhao, M. Isaka, N. Wan, H. Takemoto, H. Horiuchi, Phys. Rev. C **108**, 064314 (2023)

[16] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical Recipes in Fortran 77*, Vol. 1 Fortran Numerical Recipes (Cambridge University Press, 1986)

[17] M. Beiner, H. Flocard, N. Van Giai, P. Quentin, Nucl. Phys. A **238**, 29 (1975)

[18] D. Vautherin, Phys. Rev. C **7**, 296 (1973)

[19] C.V.N. Kumar, L.M. Robledo, Phys. Rev. C **108**, 034312 (2023)

[20] T. Marumori, T. Maskawa, F. Sakata, A. Kuriyama, Prog. Theor. Phys. **64**, 1294 (1980)

[21] M. Matsuo, Prog. Theor. Phys. **76**, 372 (1986)

[22] M. Matsuo, T. Nakatsukasa, K. Matsuyanagi, Prog. Theor. Phys. **103**, 959 (2000)

[23] N. Hinohara, T. Nakatsukasa, M. Matsuo, K. Matsuyanagi, Prog. Theor. Phys. **119**, 59 (2008)

[24] N. Hizawa, K. Hagino, K. Yoshida, Phys. Rev. C **103**, 034313 (2021)

[25] N. Hizawa, K. Hagino, K. Yoshida, Phys. Rev. C **105**, 064302 (2022)

[26] N. Hasegawa, K. Hagino, Y. Tanimura, Phys. Lett. B **808**, 135693 (2020)

[27] B. Li, D. Vretenar, T. Nikšić, P.W. Zhao, J. Meng, Phys. Rev. C **108**, 014321 (2023)

[28] P. Marević, D. Regnier, D. Lacroix, Eur. Phys. J. A **60** (2024)