New truncation scheme for a time-dependent density-matrix approach applied to the ground state of ^{16}O

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The ground state of ^{16}O is calculated by using a time-dependent density-matrix approach derived from a new truncation scheme of the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy for reduced density matrices, where a three-body density matrix is approximated by an antisymmetrized product of two-body density matrices. The new scheme is compared with a simpler truncation scheme previously used for the calculation of the ground state of ^{16}O where the three-body density matrix is neglected and only two-particle–two-hole elements of the two-body density matrix are considered. It is shown that the results obtained from the two truncation schemes agree well with the exact solution.

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The equations of motion for reduced density matrices have a coupling scheme known as the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy where an n-body density matrix couples to n-body and $(n+1)$-body density matrices. The time-dependent Hartree–Fock theory is obtained from the truncation scheme of the BBGKY hierarchy where the two-body density matrix in the equation of motion for the one-body density matrix is approximated by an antisymmetrized product of the one-body density matrices. If we replace the three-body density matrix in the equation of motion for the two-body density matrix with antisymmetrized products of the one-body and two-body density matrices, we can truncate the BBGKY hierarchy and obtain a closed set of the equations of motion for the one-body and two-body density matrices. This is the truncation scheme used in the time-dependent density-matrix theory (TDDM) [1,2]. TDDM has been applied to model Hamiltonians [3,4] and realistic cases [4–8] to investigate two-body correlation effects. On the other hand it has been pointed out [9,10] that TDDM can give unphysical results because an identity that the one-body and two-body density matrices should satisfy is not conserved in TDDM. Obviously, the problems of TDDM originate in the truncation scheme of the BBGKY hierarchy where genuine three-body and higher-level correlations are completely neglected. One way of overcoming the problems may be to include the three-body correlation explicitly, as has been done in Ref. [11] for a model Hamiltonian. However, such an extension of TDDM is impractical for realistic cases. We recently proposed a new truncation scheme [12] where the three-body density matrix is approximated by the antisymmetrized products of the two-body density matrices. The truncation scheme was applied to model Hamiltonians and good agreement with the exact solutions was obtained [12]. In the previous TDDM applications to the ground state of ^{16}O [4,13] were included only two-particle–two-hole (2p-2h) and 2p-2h elements of the two-body density matrix to facilitate numerical calculations. The aim of this paper is to further investigate the new truncation scheme in a realistic case of ^{16}O and also to test the validity of the simplified treatment of TDDM by comparing with the results of exact diagonalization.

I consider the Hamiltonian H consisting of a one-body part and a two-body interaction:

$$H = \sum_{\alpha} \langle \alpha | t | \alpha' \rangle a^{\dagger}_{\alpha} a_{\alpha'} + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle \alpha\beta | v | \alpha'\beta' \rangle a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\beta'} a_{\alpha'}, \quad (1)$$

where $a^{\dagger}_{\alpha}$ and a_{α} are the creation and annihilation operators of a particle at a time-independent single-particle state α. TDDM gives the coupled equations of motion for the one-body density matrix (the occupation matrix) $n_{\alpha\alpha'}$ and the correlated part of the two-body density matrix $C_{\alpha\beta\alpha'\beta'}$. These matrices are defined as

$$n_{\alpha\alpha'}(t) = \langle \Phi(t) | a^{\dagger}_{\alpha'} a_{\alpha} | \Phi(t) \rangle, \quad (2)$$

$$C_{\alpha\beta\alpha'\beta'}(t) = \langle \Phi(t) | a^{\dagger}_{\alpha'} a^{\dagger}_{\beta'} a_{\beta} a_{\alpha} | \Phi(t) \rangle - [n_{\alpha\alpha'}(t) n_{\beta\beta'}(t) - n_{\alpha\beta'}(t) n_{\beta\alpha'}(t)], \quad (3)$$

where $|\Phi(t)\rangle$ is the time-dependent total wave function $|\Phi(t)\rangle = \exp[-iHt/\hbar]|\Phi(t=0)\rangle$. The equations of motion for $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$ are written as

$$\begin{aligned} i\hbar \dot{n}_{\alpha\alpha'} = & \sum_{\lambda} (\epsilon_{\alpha\lambda} n_{\lambda\alpha'} - n_{\alpha\lambda} \epsilon_{\lambda\alpha'}) \\ & + \sum_{\lambda_1\lambda_2\lambda_3} \big[\langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle C_{\lambda_2\lambda_3\alpha'\lambda_1} \\ & - C_{\alpha\lambda_1\lambda_2\lambda_3} \langle \lambda_2\lambda_3 | v | \alpha'\lambda_1 \rangle \big], \end{aligned} \quad (4)$$

$$\begin{aligned} i\hbar \dot{C}_{\alpha\beta\alpha'\beta'} = & \sum_{\lambda} (\epsilon_{\alpha\lambda} C_{\lambda\beta\alpha'\beta'} + \epsilon_{\beta\lambda} C_{\alpha\lambda\alpha'\beta'} \\ & - \epsilon_{\lambda\alpha'} C_{\alpha\beta\lambda\beta'} - \epsilon_{\lambda\beta'} C_{\alpha\beta\alpha'\lambda}) \\ & + B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'} \\ & + \sum_{\lambda_1\lambda_2\lambda_3} \big[\langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle C_{\lambda_2\lambda_3\beta\alpha'\lambda_1\beta'} \\ & + \langle \lambda_1\beta | v | \lambda_2\lambda_3 \rangle C_{\lambda_2\lambda_3\alpha\alpha'\lambda_1\beta'} \\ & - \langle \lambda_1\lambda_2 | v | \alpha'\lambda_3 \rangle C_{\alpha\lambda_3\beta\lambda_1\lambda_2\beta'} \\ & - \langle \lambda_1\lambda_2 | v | \lambda_3\beta' \rangle C_{\alpha\lambda_3\beta\lambda_1\lambda_2\alpha'} \big], \end{aligned} \quad (5)$$

where $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ is the correlated part of a three-body density-matrix which is neglected in the original version of TDDM.

The energy matrix $\epsilon_{\alpha\alpha'}$ is given by

$$\epsilon_{\alpha\alpha'} = \langle\alpha|t|\alpha'\rangle + \sum_{\lambda_1\lambda_2}\langle\alpha\lambda_1|v|\alpha'\lambda_2\rangle_A n_{\lambda_2\lambda_1}, \tag{6}$$

where the subscript A means that the corresponding matrix is antisymmetrized. The matrix $B_{\alpha\beta\alpha'\beta'}$ in Eq. (5) does not contain $C_{\alpha\beta\alpha'\beta'}$ and describes 2p-2h and 2h-2p excitations, while $P_{\alpha\beta\alpha'\beta'}$ and $H_{\alpha\beta\alpha'\beta'}$ contain $C_{\alpha\beta\alpha'\beta'}$ and describe p-p (and h-h) and p-h correlations to infinite order, respectively [2]. These matrices are explicitly given in Ref. [2]. Equations (4) and (5) satisfy the conservation laws of the total energy and the total number of particles [1,2].

The new truncation scheme for Eq. (5) is the following [12]: Instead of neglecting $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ we use

$$C_{\mathrm{p_1p_2h_1p_3p_4h_2}} = \sum_{\mathrm{h}} C_{\mathrm{hh_1p_3p_4}} C_{\mathrm{p_1p_2h_2h}}, \tag{7}$$

$$C_{\mathrm{p_1h_1h_2p_2h_3h_4}} = \sum_{\mathrm{p}} C_{\mathrm{h_1h_2p_2p}} C_{\mathrm{p_1ph_3h_4}}, \tag{8}$$

where p and h refer to particle and hole states, respectively. These expressions were derived from a perturbative consideration [12] by using the following ground state $|Z\rangle$:

$$|Z\rangle = e^Z|\mathrm{HF}\rangle \approx (1+Z)|\mathrm{HF}\rangle, \tag{9}$$

with

$$Z = \frac{1}{4}\sum_{\mathrm{pp'hh'}} z_{\mathrm{pp'hh'}} a^\dagger_{\mathrm{p}} a^\dagger_{\mathrm{p'}} a_{\mathrm{h'}} a_{\mathrm{h}}, \tag{10}$$

where $|\mathrm{HF}\rangle$ is the Hartree–Fock (HF) ground state and $z_{\mathrm{pp'hh'}}$ is antisymmetric under the exchanges of $\mathrm{p} \leftrightarrow \mathrm{p'}$ and $\mathrm{h} \leftrightarrow \mathrm{h'}$. In the lowest order of $z_{\mathrm{pp'hh'}}$ the two-body correlation matrices are given by

$$C_{\mathrm{pp'hh'}} \approx z_{\mathrm{pp'hh'}}, \tag{11}$$

$$C_{\mathrm{hh'pp'}} \approx z^*_{\mathrm{pp'hh'}}, \tag{12}$$

and the three-body correlation matrices are given by

$$C_{\mathrm{p_1p_2h_1p_3p_4h_2}} \approx \sum_{\mathrm{h}} z^*_{\mathrm{p_3p_4hh_1}} z_{\mathrm{p_1p_2h_2h}}, \tag{13}$$

$$C_{\mathrm{p_1h_1h_2p_2h_3h_4}} \approx \sum_{\mathrm{p}} z^*_{\mathrm{p_2ph_1h_2}} z_{\mathrm{p_1ph_3h_4}}. \tag{14}$$

These relations suggest the expressions for $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ in terms of $C_{\mathrm{pp'hh'}}$ given by Eqs. (7) and (8).

There are identities which are satisfied by exact reduced density matrices. The identity for the one-body and two-body density matrices is

$$n_{\alpha\alpha'} = \frac{1}{N-1}\sum_{\lambda}\rho_{\alpha\lambda\alpha'\lambda}. \tag{15}$$

This is also expressed by using $C_{\alpha\beta\alpha'\beta'}$ as

$$n_{\alpha\alpha'} - \sum_{\lambda}(n_{\alpha\lambda}n_{\lambda\alpha'} - C_{\alpha\lambda\alpha'\lambda}) = 0. \tag{16}$$

When the three-body correlation matrix is neglected in Eq. (5), this identity is not conserved [9]. It has been shown [12] that the inclusion of the three-body correlation matrix using Eqs. (7) and (8) improves the conservation of Eq. (16). This is also the case in ^{16}O as shown below.

The ground state in TDDM is given as a stationary solution of the time-dependent equations [Eqs. (4) and (5)]. I use the following adiabatic method to obtain a nearly stationary solution [14]: Starting from the HF configuration, I solve Eqs. (4) and (5), gradually increasing the strength of the residual interaction such as $v(\boldsymbol{r}-\boldsymbol{r}')\times t/T$. To suppress oscillating components which come from the mixing of excited states, we must take large T: I use $T = 2400$ fm/c. To compare with the results from the exact diagonalization of the Hamiltonian, I use a small single-particle space: The occupation probability $n_{\alpha\alpha}$ and the correlation matrix $C_{\alpha\beta\alpha'\beta'}$ are calculated by using the $1p_{3/2}$, $1p_{1/2}$, and $1d_{5/2}$ states for both protons and neutrons. For the calculations of the single-particle states I use the Skyrme III force. A simplified interaction which contains only the t_0 and t_3 terms of the Skyrme III force is used as the residual interaction. The spin-orbit force and Coulomb interaction are also omitted from the residual interaction. Since it is difficult to satisfy antisymmetry properties of $C_{\alpha\beta\alpha'\beta'}$ by using a density-dependent force as the residual interaction [15], I adopt the three-body version of the Skyrme interaction, $v_3 = t_3\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_3)$, which gives the following density-dependent two-body residual interaction: $t_3\rho_n\delta^3(\boldsymbol{r}-\boldsymbol{r}')$, $t_3\rho\delta^3(\boldsymbol{r}-\boldsymbol{r}')/2$, and $t_3\rho_p\delta^3(\boldsymbol{r}-\boldsymbol{r}')$ for the proton-proton, proton-neutron, and neutron-neutron interactions, respectively, where ρ_p, ρ_n, and ρ are the proton, neutron, and total densities, respectively. For simplicity I use the time-independent HF single-particle states and neglect the effects of ground-state correlations on the mean field. This means that all density matrices are defined by using the HF single-particle states and that $\epsilon_{\alpha\alpha'}$ in Eqs. (4) and (5) is replaced by the HF single-particle energy accordingly. To be consistent with this treatment of the single-particle states, I subtract from the Hamiltonian (1) the mean-field potential $\sum_\lambda\langle\alpha\lambda|v|\alpha\lambda\rangle_A n^0_\lambda a^\dagger_\alpha a_\alpha$, where n^0_λ is the HF occupation probability ($n^0_\lambda = 1$ or 0).

The occupation probabilities of the proton $1p_{3/2}$, $1p_{1/2}$, and $1d_{5/2}$ states are shown in Figs. 1–3 as a function of the strength of the residual interaction t/T. The solid line depicts the result in TDDM with $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ given by Eqs. (7) and (8). The dotted line shows the result in TDDM without the three-body correlation matrix and the dot-dashed line the TDDM result where the three-body density matrix and the two-body correlation matrix other than 2p-2h and 2h-2p types are neglected. The results for the neutron single-particle states are similar and not shown here. The results obtained from the exact diagonalization in the same single-particle space are shown with the squares at $t/T = 1$. The deviation from the HF values ($n_{\alpha\alpha} = 1$ or 0) is more than 10%, which means that the ground state of ^{16}O is a strongly correlated state. A recent shell-model calculation by Utsuno and Chiba [16] also gives a similar result for the ground state of ^{16}O. It is clear from Figs. 1–3 that the original truncation scheme of TDDM where the three-body correlation matrix is neglected but all elements of $C_{\alpha\beta\alpha'\beta'}$ are included overestimates the ground-state correlations. It has been pointed out in Ref. [12] that the three-body correlation matrix plays a role in suppressing

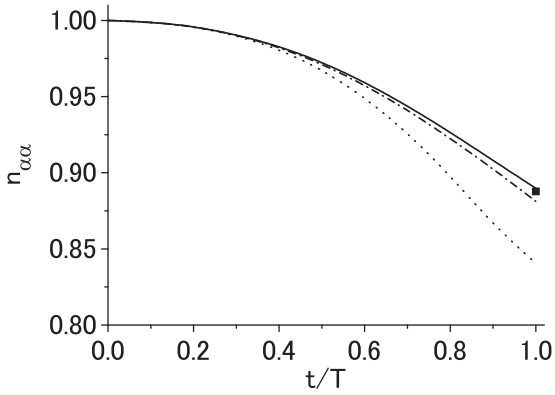

FIG. 1. Occupation probability of the proton $1p_{3/2}$ state as a function of t/T calculated in TDDM with $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ given by Eqs. (7) and (8) (solid line). The dotted line depicts the results in the original truncation scheme of TDDM where the three-body correlation matrix is neglected but all components of $C_{\alpha\beta\alpha'\beta'}$ are included. The dot-dashed line shows the results of the simplified version of TDDM where only the 2p-2h and 2h-2p elements of the two-body correlation matrix are included. The exact solution is shown with the square at $t/T = 1$.

the particle-hole correlations. In fact the neglect of $C_{\mathrm{php'h'}}$ is the main reason why the results of the simplified truncation scheme where only $C_{\mathrm{pp'hh'}}$ and $C_{\mathrm{hh'pp'}}$ are included are in good agreement with the results of the new truncation scheme.

To investigate how the two-body correlation matrix depends on the truncation schemes, I consider the correlation energy E_{cor} defined by $E_{\mathrm{cor}} = \sum_{\alpha\beta\alpha'\beta'}\langle\alpha\beta|v|\alpha'\beta'\rangle C_{\alpha'\beta'\alpha\beta}/2$. The obtained results are shown in Fig. 4 as a function of t/T. Figure 4 shows that the neglect of the three-body correlation matrix overestimates the correlation energy, as is the case for the occupation probabilities. Figure 4 also indicates that the inclusion of only $C_{\mathrm{pp'hh'}}$ and $C_{\mathrm{hh'pp'}}$ underestimates E_{cor}, although the occupation probabilities are reasonable. This underestimation is due to the omission of other elements of the two-body correlation matrix. Therefore, I calculate $C_{\mathrm{p_1h_1p_2h_2}}$, $C_{\mathrm{p_1p_2p_3p_4}}$, and $C_{\mathrm{h_1h_2h_3h_4}}$ by using $C_{\mathrm{p_1h_1p_2h_2}} = \sum_{\mathrm{ph}} C_{\mathrm{p_1ph_1h}} C_{\mathrm{hh_2p_2p}}$, $C_{\mathrm{p_1p_2p_3p_4}} = \sum_{\mathrm{hh'}} C_{\mathrm{p_1p_2hh'}} C_{\mathrm{hh'p_3p_4}}/2$, and

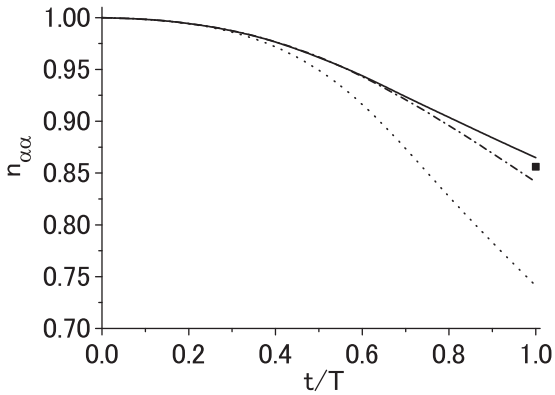

FIG. 2. Same as Fig. 1 but for the proton $1p_{1/2}$ state.

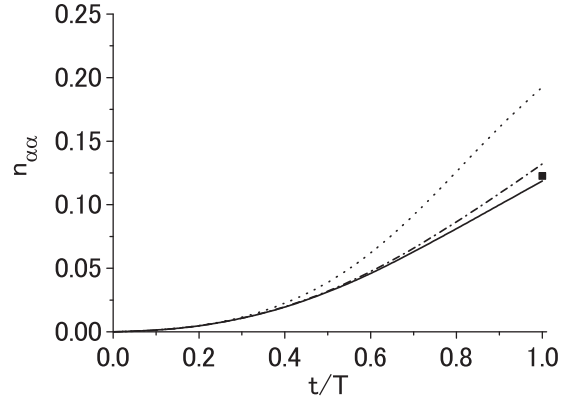

FIG. 3. Same as Fig. 1 but for the proton $1d_{5/2}$ state.

$C_{\mathrm{h_1h_2h_3h_4}} = \sum_{\mathrm{pp'}} C_{\mathrm{h_1h_2pp'}} C_{\mathrm{pp'h_3h_4}}/2$. These relations have also been derived from a perturbative consideration [12]. The obtained E_{cor} is shown in Fig. 4 with the green (gray) solid line. Now good agreement is obtained with the result given by Eqs. (7) and (8) and with the exact solution.

I now show that the inclusion of the three-body correlation matrix also stabilizes the long-time behavior of the ground state. To show the stability of the ground-state solution in TDDM, I present the sum S of the absolute value of Eq. (16) $S = \sum_\alpha |n_{\alpha\alpha} - n^2_{\alpha\alpha} + \sum_\lambda C_{\alpha\lambda\alpha\lambda}|$ in Fig. 5: In the model single-particle space considered here, $n_{\alpha\alpha'}$ has no off-diagonal elements. The time step 4000 corresponds to T and, for $t > T$, the interaction strength is fixed at the original value. The solid line shows the result in TDDM with the three-body correlation matrix given by Eqs. (7) and (8), while the result in the original truncation scheme of TDDM where the three-body correlation matrix is neglected is given by the dotted line. The latter becomes unstable after the 6000th time step. The dot-dashed line depicts the result with only $C_{\mathrm{pp'hh'}}$ and $C_{\mathrm{hh'pp'}}$. The green (gray) line shows the result where $C_{\mathrm{php'h'}}$, $C_{\mathrm{pp'p''p'''}}$, and $C_{\mathrm{hh'h''h'''}}$ are calculated with $C_{\mathrm{pp'hh'}}$ and $C_{\mathrm{hh'pp'}}$. Comparison of the dot-dashed line with the green (gray) solid line shows that the

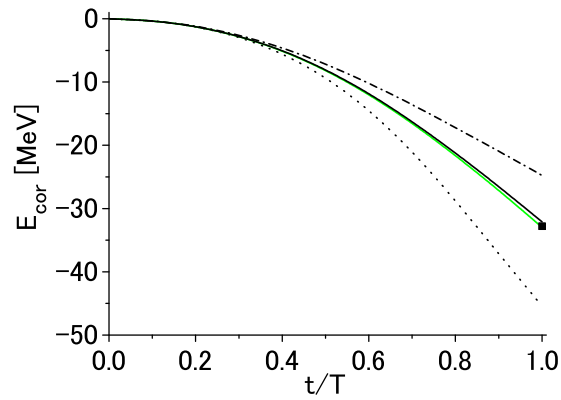

FIG. 4. (Color online) Correlation energy in TDDM as a function of t/T. The meaning of the three lines is the same as in Fig. 1. The green (gray) solid line depicts the result where $C_{\mathrm{php'h'}}$, $C_{\mathrm{pp'p''p'''}}$, and $C_{\mathrm{hh'h''h'''}}$ are calculated by using $C_{\mathrm{pp'hh'}}$ and $C_{\mathrm{hh'pp'}}$ (see text). The exact solution is shown with the square.

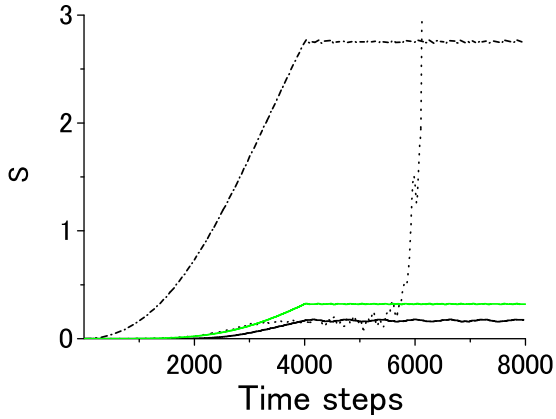

FIG. 5. (Color online) Sum of the absolute value of Eq. (16) as a function of time steps. The meaning of the four lines is the same as in Fig. 4. Time step 4000 corresponds to T.

inclusion of $C_{\mathrm{php'h'}}$, $C_{\mathrm{pp'p''p'''}}$, and $C_{\mathrm{hh'h''h'''}}$ drastically improves the identity Eq. (16). The difference between the solid and dotted lines demonstrates that the three-body correlation matrix given by Eqs. (7) and (8) plays a role in stabilizing the time evolution of the ground state.

In summary, I applied a new truncation scheme for the time-dependent density-matrix approach to the ground state of ^{16}O. The scheme consists of approximating the three-body correlation matrix with the antisymmetrized product of the two-body correlation matrices. The validity of a simpler truncation scheme where only the two-particle–two-hole elements of the two-body correlation matrix are included was also tested. It was found that the results obtained from the two truncation schemes agree well with the exact solution when other neglected elements of the two-body correlation matrix in the latter approach are evaluated by using the two-particle–two-hole elements. It was pointed out that the three-body correlation matrix plays a role in suppressing the particle-hole correlations and stabilizing the long-time behavior of the ground state. This study shows that the previous truncation scheme of TDDM applied to ^{16}O, where only the two-particle–two-hole elements of the two-body correlation matrix are included, are justifiable.

[1] S. J. Wang and W. Cassing, Ann. Phys. (NY) **159**, 328 (1985).
[2] M. Gong and M. Tohyama, Z. Phys. A - Hadrons and Nuclei **335**, 153 (1990).
[3] S. Takahara, M. Tohyama, and P. Schuck, Phys. Rev. C **70**, 057307 (2004).
[4] M. Tohyama, Phys. Rev. C **75**, 044310 (2007).
[5] F. V. De Blasio, W. Cassing, M. Tohyama, P. F. Bortignon, and R. A. Broglia, Phys. Rev. Lett. **68**, 1663 (1992).
[6] A. Pfitzner, W. Cassing, and A. Peter, Nucl. Phys. A **577**, 753 (1994).
[7] M. Assié and D. Lacroix, Phys. Rev. Lett. **102**, 202501 (2009).
[8] M. Tohyama, J. Phys. Soc. Jpn. **81**, 054707 (2012).
[9] K.-J. Schmitt, P.-G. Reinhard, and C. Toepffer, Z. Phys. A - Hadrons and Nuclei **336**, 123 (1990).
[10] T. Gherega, R. Krieg, P.-G. Reinhard, and C. Toepffer, Nucl. Phys. A **560**, 166 (1993).
[11] M. Tohyama and P. Schuck, Eur. Phys. J. A **45**, 257 (2010).
[12] M. Tohyama and P. Schuck, Eur. Phys. J. A **50**, 77 (2014).
[13] M. Tohyama, Phys. Rev. C **87**, 054330 (2013).
[14] M. Tohyama, Phys. Rev. A **71**, 043613 (2005).
[15] D. Gambacurta, M. Grasso, and F. Catara, J. Phys. G **38**, 035103 (2011).
[16] Y. Utsuno and S. Chiba, Phys. Rev. C **83**, 021301(R) (2011).