Correlated ground state of ^{16}O and $E2$ giant resonance built on it

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A correlated ground state of ^{16}O and an $E2$ giant resonance built on it are calculated using an extended version of the time-dependent Hartree-Fock theory called the time-dependent density-matrix (TDDM) theory. The Skyrme III force is used as an effective interaction for the calculation of both a mean field and two-body correlations. It is found that a TDDM calculation with the Skyrme force gives reasonable ground-state correlations and a large spreading width of the $E2$ giant resonance. [S0556-2813(98)07710-3]

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The time-dependent density-matrix (TDDM) theory [1,2] is an extended version of the time-dependent Hartree-Fock (TDHF) theory to include the effects of two-body correlations. TDDM theory has recently been extended to calculate a correlated ground state using an adiabatic method in which, starting with the Hartree-Fock (HF) ground state, a residual interaction is gradually turned on in time [3]. It has been shown that correlated ground states of ^{16}O [4] and ^{40}Ca [5] can be obtained in this way and that spurious components in an $E2$ giant resonance can be eliminated using such a correlated ground state. In order to make the calculation of matrix elements of the residual interaction feasible, however, we have used in our previous calculations a simple force of the single δ-function form $v_0\delta(\mathbf{r}-\mathbf{r}')$ as the residual interaction. Such an interaction is not consistent with the effective interaction (the Skyrme force [6]) used for the calculation of a mean-field potential. In this Brief Report we calculate a correlated ground state and an $E2$ giant resonance of ^{16}O using a residual interaction which is the same as that used for the mean-field potential and investigate the effect of a consistent treatment of the effective interaction in TDDM theory.

We first present the equations of motion in TDDM theory and explain the method to obtain a correlated ground state. The equations of motion in TDDM theory have been derived from the truncation of the well-known Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [7], neglecting a genuine correlated part in a three-body density matrix [8], and therefore consist of a closed set of equations of motion for a one-body density matrix ρ and a two-body correlation function C_2 defined by $C_2=\rho_2-A(\rho\rho)$. Here $A(\rho\rho)$ is an antisymmetrized product of the one-body density matrices and ρ_2 is a two-body density matrix. In TDDM theory ρ and C_2 are expanded with a finite number of single-particle states $\{\psi_\alpha\}$,

$$\rho(11',t)=\sum_{\alpha\alpha'} n_{\alpha\alpha'}(t)\psi_\alpha(1,t)\psi^*_{\alpha'}(1',t), \tag{1}$$

$$C_2(121'2',t)=\sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'}(t)\psi_\alpha(1,t)\psi_\beta(2,t) \times\psi^*_{\alpha'}(1',t)\psi^*_{\beta'}(2',t), \tag{2}$$

where the numbers denote space, spin, and isospin coordinates. The time evolution of ρ and C_2 is determined by the following three coupled equations [1]:

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(1,t)=h(1,t)\psi_\alpha(1,t), \tag{3}$$

$$i\hbar\dot{n}_{\alpha\alpha'}=\sum_{\beta\gamma\delta}[\langle\alpha\beta|v|\gamma\delta\rangle C_{\gamma\delta\alpha'\beta}-C_{\alpha\beta\gamma\delta}\langle\gamma\delta|v|\alpha'\beta\rangle], \tag{4}$$

$$i\hbar\dot{C}_{\alpha\beta\alpha'\beta'}=B_{\alpha\beta\alpha'\beta'}+P_{\alpha\beta\alpha'\beta'}+H_{\alpha\beta\alpha'\beta'}, \tag{5}$$

where $h(1,t)$ is the mean-field Hamiltonian and v the residual interaction. The term $B_{\alpha\beta\alpha'\beta'}$ on the right-hand side of Eq. (5) represents the Born terms (the first-order terms of v). The terms $P_{\alpha\beta\alpha'\beta'}$ and $H_{\alpha\beta\alpha'\beta'}$ in Eq. (5) contain $C_{\alpha\beta\alpha'\beta'}$ and represent higher-order particle-particle- and particle-hole-type correlations, respectively. The explicit expressions for $B_{\alpha\beta\alpha'\beta'}$, $P_{\alpha\beta\alpha'\beta'}$, and $H_{\alpha\beta\alpha'\beta'}$ have been presented in Ref. [1]. The small amplitude limit of TDDM theory was investigated in Ref. [9] and it was shown that in such a limit TDDM theory can be reduced to the second random phase approximation (RPA) [10], which has often been used to study decay properties of giant resonances [11].

To obtain a correlated ground state as a stationary solution of the coupled TDDM equations, we use an adiabatic method: Starting with the HF ground state, we gradually turn on the residual interaction. This is done by making the residual interaction time dependent as

$$v\rightarrow(1-e^{-t/\tau})v, \tag{6}$$

where time constant τ is chosen to be larger than the period corresponding to the energies of two-particle–two-hole excitations. To solve the coupled equations, we assume that ^{16}O is a completely spin-isospin symmetric system. The part of the mean-field potential which contains the parameter x_0 [6] associated with the spin exchange operator disappears for such a system. Therefore, terms depending on x_0 are neglected also in the residual interaction. The residual interaction used is of the following form [6]:

$$v(\mathbf{r}-\mathbf{r}')=t_0\delta^3(\mathbf{r}-\mathbf{r}')+\frac{1}{2}t_1\{k'^2\delta^3(\mathbf{r}-\mathbf{r}')+\delta^3(\mathbf{r}-\mathbf{r}')k^2\}$$
$$+t_2\mathbf{k}'\cdot\delta^3(\mathbf{r}-\mathbf{r}')\mathbf{k}+\frac{1}{2}t_3\rho\left(\frac{\mathbf{r}+\mathbf{r}'}{2}\right)\delta^3(\mathbf{r}-\mathbf{r}'), \tag{7}$$

where $\mathbf{k}=(\nabla_{\mathbf{r}}-\nabla_{\mathbf{r}'})/2i$ acts to the right and $\mathbf{k}'=(\nabla_{\mathbf{r}'}-\nabla_{\mathbf{r}})/2i$ acts to the left. The factor 1/2 of the density-dependent term contains the contribution of a rearrangement effect [6]. The spin-orbit force is neglected as in most TDHF calculations [12]. We use the parameter set of the Skyrme III force (SKIII) [13]. The coupled equations (3)–(5) are solved using the $1s$, $1p$, $2s$, $1d$, $2p$, and $1f$ single-particle orbits. The $2s$, $2p$, and $1f$ states are in the continuum. The wave functions of these states are obtained by confining them in a cylinder with a length of 16 fm and a radius of 8 fm. (Axial symmetry is used to calculate the single-particle wave functions [12].) We have checked that a smaller cylinder disturbs the wave functions of the bound sates ($1s$, $1p$, and $1d$) and that the use of a larger cylinder gives weak transitions to the continuum states. The energy-weighted sum rule (EWSR) value [14] for $E2$ states calculated in the RPA may give a criterion of the size of the cylinder. The fraction of the EWSR value exhausted in the energy interval 0–40 MeV with the above size of the cylinder is 86%, which is large enough and comparable with a shell-model calculation [15] done with harmonic oscillator wave functions in the same single-particle space.

The property of the Skyrme interaction as the residual interaction is also studied for the damping of an $E2$ giant resonance. The $E2$ giant resonance built on the correlated ground state is excited by boosting the single-particle wave functions $\phi_\alpha(1)$ with a phase factor corresponding to the $E2$ mode,

$$\psi_\alpha(1,t=t_0)=e^{ikV(\mathbf{r})}\phi_\alpha(1), \tag{8}$$

where k is a parameter determining the amplitude of the motion and $V(\mathbf{r})$ is

$$V(\mathbf{r})=z^2-\frac{1}{2}(x^2+y^2). \tag{9}$$

The boost is done at $t_0=5\tau$. The strength function, defined by

$$S(E)=\sum_n |\langle n|\hat{V}|0\rangle|^2\delta(E-E_n), \tag{10}$$

is related to the Fourier transformation of the expectation value $V(t)$ of the transition operator $\hat{V}$ [1]:

$$S(E)=\frac{1}{\pi k\hbar}\int_0^\infty V(t)\sin\frac{Et}{\hbar}\,dt, \tag{11}$$

where $V(t)$ is calculated with the one-body density $\rho(\mathbf{r},t)$ as

$$V(t)=\langle\hat{V}\rangle=\int V(\mathbf{r})\rho(\mathbf{r},t)d^3\mathbf{r}. \tag{12}$$

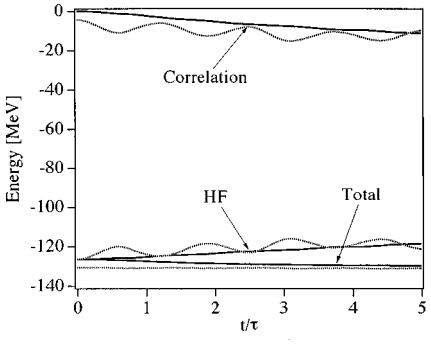

FIG. 1. Time evolution of the HF, correlation, and total energies of ^{16}O calculated in TDDM theory with $\tau=20\times10^{-23}$ s (solid line) and that with $\tau=0$ (dotted line).

Since the integration in Eq. (11) is performed for a finite time interval of 150×10^{-23} s, $S(E)$ has small fluctuations. To reduce the fluctuations in $S(E)$, we multiply $V(t)$ by a damping factor $e^{-\Gamma t/2}$ before performing the integration in Eq. (11). This corresponds to smoothing the strength function with a width Γ. We use $\Gamma=1$ MeV. Other calculational details are given in Refs. [1,16].

The correlation, HF, and total energies calculated in TDDM theory are shown in Fig. 1 as functions of time for $\tau=20\times10^{-23}$ s (solid lines). The correlation energy $E_{\rm cor}$ is given by [1]

$$E_{\rm cor}=\frac{1}{2}\sum_{\alpha\beta\gamma\delta}C_{\alpha\beta\gamma\delta}\langle\gamma\delta|v|\alpha\beta\rangle. \tag{13}$$

Note that the periods corresponding to the lowest energies ($2\hbar\omega$) of two-particle–two-hole excitations in ^{16}O are about 14×10^{-23} s. The results with $\tau=0$ (dotted lines) are also shown in Fig. 1. In this calculation $C_{\alpha\beta\alpha'\beta'}$ in the Born approximation is used as its initial condition to avoid a rapid change in the initial stage of the time evolution. As shown in Fig. 1, the oscillations in the HF and correlation energies are drastically reduced by using a time constant which is slightly larger than the the periods corresponding to two-particle–two-hole excitation energies. The results in Fig. 1 demonstrate that the adiabatic method for obtaining a stationary solution in TDDM theory works well even for SKIII, which is more complicated than the simple force used in our previous calculations. The value of the correlation energy reached at $t=5\tau$ is -11.1 MeV. The decrease in the correlation energy is largely canceled by the increase in the HF energy. As a result, the total energy is decreased only by 3.2 MeV from the HF value. The occupation probabilities of single-particle states averaged over the $2s$ and $1d$ orbits are 0.025 in TDDM theory, while the observed value for these orbits is 0.021 [17]; SKIII seems to induce ground-state correlations to a reasonable extent.

In the following we discuss the difference between SKIII and the simple force of the single δ-function form $v=v_0\delta^3(\mathbf{r}-\mathbf{r}')$. First, we determined the strength v_0 of the simple force so as to reproduce approximately the correlation energy calculated with SKIII. The value of v_0 so obtained is -220 MeV fm^3, which is about 70% of the strength used in our previous studies [4,5]. (As has been discussed in Ref. [1] and will be shown below, the simple force with this strength

does not give any spreading width of the $E2$ giant resonance.) Although the correlation energies given by SKIII and the simple force are the same, there is a difference in the two-particle–two-hole matrix elements. The transitions to the high-lying $1f$ and $2p$ states play a more important role in SKIII than in the simple force. In the case of SKIII the correlation energy calculated without the $1f$ and $2p$ states is 52% of that with the $1f$ and $2p$ states, while the value is 78% in the case of the simple force. In other words, SKIII induces weaker transitions to the $2s$ and $1d$ states than the simple force. This property of SKIII seems common to any Skyrme force. Using the Skyrme II force [6] and the Bonche-Koonin-Negele (BKN) force [18], the density and momentum dependence of which significantly differ from SKIII, we performed a similar calculation and found again weak transitions to the $2s$ and $1d$ states. Since each term in Eq. (7) is quite large, this is a consequence of a cancellation among various terms in the Skyrme force. For example, a strong repulsive contribution of the density-dependent part reduces an attractive contribution of the first term in Eq. (7). Such a property of the Skyrme interaction was discussed by Arima *et al.* [19]. This cancellation mechanism may be associated with the fact that only a small portion of the EWSR value for negative-parity states is given in the truncated single-particle space. (The negative-parity states consist of one-particle–one-hole excitations involving the $2s$ and $1d$ orbits.) For example, a RPA calculation done in the truncated space gives only 14% of the EWSR value of 3^- states in the energy interval 0–40 MeV. In this RPA calculation the strength distribution of 3^- states is almost equivalent to the unperturbed one. On the other hand, a TDHF calculation for 3^- states which is equivalent to a continuum RPA calculation (no truncation made) [14] in a small amplitude limit gives 70% of the EWSR value in the same energy interval and a coherent state appears in a much lower-energy region than the unperturbed states. Thus the weak transitions to the $2s$ and $1d$ states observed in the calculation of the correlation energy are related to the properties of negative-parity states in the truncated single-particle space. In contrast to SKIII the simple force with $V_0=-220$ MeV fm^3, which is not consistent with the effective interaction used for the mean-field potential, gives a collective 3^- state in a RPA calculation in the truncated single-particle space, which is shifted downward by 3.7 MeV from the unperturbed states.

The damping of the $E2$ giant resonance was also studied using SKIII. The $E2$ strength distributions obtained are shown in Fig. 2. The solid line denotes the $E2$ resonance built on the correlated ground state, and the dotted line represents the result of a TDHF calculation (corresponding to a continuum RPA calculation). The fraction of the energy-weighted sum rule [14] exhausted in the energy interval 5–35 MeV is 97% in TDDM theory, while it is 96% in TDHF theory. The average energy and the full width at half maximum of the peaks distributed from 10 to 25 MeV are 19.5 and 8.4 MeV, respectively. The fraction of the EWSR exhausted in the energy interval from 10 to 25 MeV is 87%. The energy and width of the $E2$ giant resonance obtained in TDDM theory are comparable with experiment. In experiment the $E2$ giant resonance in ^{16}O was observed at $E=20.7$ MeV with a width of 7.5 ± 1 MeV and 58 ± 25 % of the EWSR value [20]. The splitting of the $E2$ strength shown in Fig. 2 is also consistent with a recent experimental observation [21]. When the simple force $v=v_0\delta^3(\mathbf{r}-\mathbf{r}')$ with $v_0=-220$ MeV fm^3 is used (dot-dashed line), the main peak is shifted downward by 1.2 MeV, but there is little broadening of the main peak as shown in Fig. 2. We also made a calculation of the $E2$ spectrum with SKIII without the high-lying $1f$ and $2p$ states. The obtained result is quit similar to the TDHF result. The contribution of the $2s$ and $1d$ states to the damping of the $E2$ giant resonance is also small in the case of SKIII.

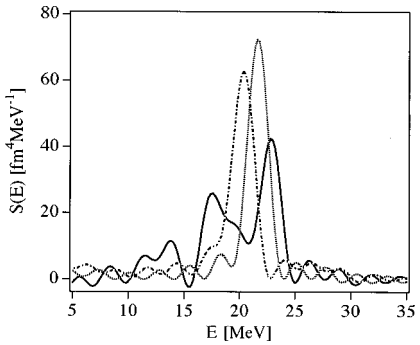

FIG. 2. $E2$ strength distribution of ^{16}O calculated in TDDM theory (solid line) and TDHF theory (dotted line). The dot-dashed line depicts that in TDDM theory with the simple force of the single δ-function form.

In summary, using a single effective interaction SKIII for the calculation of the mean-field potential and the two-body correlation function, we calculated a correlated ground state of ^{16}O in TDDM theory. It was found that SKIII induces reasonable ground-state correlations when the single-particle states are taken up to the $1f$ and $2p$ orbits. It was also found that the transitions to the $2s$ and $1d$ states are small as compared with the simple force of the single δ-function form. This is a consequence of a cancellation among various components of the Skyrme force and may be associated with the fact that the portion of the EWSR value for negative-parity states is quite small in such truncated single-particle space. The energy distribution of the $E2$ giant resonance built on the correlated ground state was also calculated in TDDM theory. It was found that the obtained spreading width is comparable with experiment. It was also found that the matrix elements involving the $2s$ and $1d$ states are quite small as in the ground-state calculation. The present study suggests that the Skyrme force may be used as a residual interaction in TDDM theory to study ground-state correlations and giant resonances without major modifications, and encourages us to do further studies for other excitation modes with larger single-particle space and also for heavier nuclei.

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