Double Giant Quadrupole Resonance in Time-Dependent Density-Matrix Theory

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A time-dependent method for studying the double-phonon states of giant resonances is proposed based on an extended version of the time-dependent Hartree-Fock theory known as the time-dependent density-matrix theory. The method is applied to the double phonon state of the isoscalar giant quadrupole resonance in $^{16}$O. It is found that the peak energy of the double phonon state is nearly twice the energy of the single phonon state calculated in the random phase approximation and that its width is slightly larger than that of the single-phonon state.

The double phonon states of giant resonances have been the subject of a number of recent experimental and theoretical investigations, and some microscopic calculations have been performed based on various time-dependent theories. In this note we propose a new time-dependent approach based on the time-dependent density-matrix theory (TDDM). TDDM is an extended version of the time-dependent Hartree-Fock theory (TDHF), and its equations of motion determine the time evolution of both one-body and two-body density matrices. We demonstrate that, using appropriate initial conditions for the two-body density matrix, we can calculate the strength functions of the double-phonon states in a manner similar to that used to calculate the strength functions of single phonon states in TDHF and TDDM. The new method is applied to the double phonon state of the isoscalar quadrupole resonance in $^{16}$O.

We first briefly discuss the equations of motion in TDDM and then present the method for calculating the strength function of the double giant quadrupole resonance (DGQR). The formulation of TDDM is based on a truncation of the BBGKY hierarchy of reduced density matrices, in which genuine correlated parts of a three-body density matrix and higher reduced density matrices are neglected. TDDM thus determines the time evolution of a one-body density matrix $\rho$ and a two-body density matrix $\rho_2$. The equations of motion in TDDM consist of the following three coupled equations for the single-particle wavefunctions $\psi_\alpha$, the occupation matrix $n_{\alpha\alpha'}$ (the expansion coefficients of $\rho$) and the correlation matrix $C_{\alpha\beta\alpha'\beta'}$ (the expansion coefficients of $C_2$, where $C_2$ is a correlated part of $\rho_2$):}

$$i\hbar \frac{\partial}{\partial t} \psi_\alpha(1, t) = h(1, t)\psi_\alpha(1, t), \quad (1)$$
\[ i\hbar \dot{\alpha} = \sum_{\beta\gamma \delta} \{ (\alpha|\beta|\gamma\delta) C_{\gamma\delta} \alpha' \beta - C_{\alpha\beta\gamma\delta} \langle \gamma\delta | \alpha' \beta \rangle \}, \tag{2} \]

\[ i\hbar \dot{\beta} = B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'}, \tag{3} \]

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. (3) 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. (3) contain \( C_{\alpha\beta\alpha'\beta'} \) and represent higher-order particle-particle (hole-hole) and particle-hole type correlations, respectively. Thus full two-body correlations including those induced by the Pauli principle are taken into account in the equation of motion for \( C_{\alpha\beta\alpha'\beta'} \). The explicit expressions of \( B_{\alpha\beta\alpha'\beta'} \), \( P_{\alpha\beta\alpha'\beta'} \), and \( H_{\alpha\beta\alpha'\beta'} \) are given in Ref. 11. It has also been discussed \(^{(14)} \) that the second RPA (random phase approximation) \(^{(15)} \) can be obtained from the small amplitude limit of TDDM.

The strength function of DGQR is calculated as follows. We assume that the motion of DGQR is generated by a two-body operator \( \hat{Q}_2 \):

\[ |\Psi(t = 0)\rangle = e^{ik\hat{Q}_2}|\Phi_0\rangle, \tag{4} \]

where \( |\Phi_0\rangle \) is the ground-state wavefunction and \( \hat{Q}_2 \) is a two-body part of \( \hat{Q}^2 \). Here \( \hat{Q} \) is a one-body operator generated by the quadrupole velocity field \( Q = z^2 - (x^2 + y^2)/2 \):

\[ \hat{Q} = \sum_{\alpha\alpha'} \langle \alpha|Q|\alpha'\rangle a^\dagger_\alpha a_{\alpha'}. \tag{5} \]

We use \( \hat{Q}_2 \) instead of \( \hat{Q}^2 \) to reduce the excitation of single phonon states. Assuming that \( |\Phi_0\rangle \) is the Hartree-Fock (HF) ground-state wavefunction and that \( k \) is sufficiently small, we evaluate the initial \( C_{\alpha\beta\alpha'\beta'} \) as

\[ C_{\alpha\beta\alpha'\beta'}(t = 0) = \langle \Psi(t = 0)|a^\dagger_\alpha a^\dagger_\beta a_\beta a_{\alpha'}|\Psi(t = 0)\rangle. \tag{6} \]

At first order in \( k \), the initial correlation matrix becomes

\[ C_{\rho\mu,\nu\sigma} = \langle \Psi|a^\dagger_\rho a^\dagger_\sigma a_\mu a_\nu|\Psi\rangle = 2ik\langle \mu|Q|\rho\rangle \langle \nu|Q|\sigma \rangle - \langle \mu|Q|\sigma \rangle \langle \nu|Q|\rho \rangle, \tag{7} \]

\[ C_{\mu\nu,\rho\sigma} = \langle \Psi|a^\dagger_\mu a^\dagger_\nu a_\sigma a_\rho|\Psi\rangle = -2ik\langle \rho|Q|\sigma \rangle \langle \nu|Q|\mu \rangle - \langle \rho|Q|\mu \rangle \langle \sigma|Q|\nu \rangle, \tag{8} \]

where \( \rho \) and \( \sigma \) refer to unoccupied single-particle states, and \( \mu \) and \( \nu \) refer to occupied ones. Other elements of the initial correlation matrix vanish at first order in \( k \). For the initial values of \( \psi_\alpha \) and \( n_{\alpha\alpha'} \) we use the HF values. The strength function of DGQR defined by

\[ S(E) = \sum_n |\langle \Phi_n|\hat{Q}_2|\Phi_0\rangle|^2 \delta(E - E_n) \tag{9} \]

is given by the Fourier transformation of the expectation value of \( \hat{Q}_2 \) as in the case of single phonon states: \(^{(11)} \)

\[ S(E) = \frac{1}{\pi k \hbar} \int_0^\infty Q_2(t) \sin \frac{Et}{\hbar} dt, \tag{10} \]
where $Q_2$ is calculated as

$$
Q_2(t) = \langle \Psi(t)|\hat{Q}_2|\Psi(t)\rangle
= \sum_{a\beta,a'\beta'} \langle \alpha|Q|\alpha'\rangle \langle \beta|Q|\beta'\rangle \{ A[n_{a'\alpha}n_{\beta'\beta}] + C_{a'\beta'\alpha\beta}\}'.
$$

(11)

Here $A[\ ]$ denotes that the quantity in the brackets is antisymmetrized. The dependence of $S(E)$ on $k$ is negligible as long as $k$ is sufficiently small. The energy weighted sum rule (EWSR) for DGQR is given as

$$
\int ES(E)dE = \frac{1}{2}\langle \Phi_0|[\hat{Q}_2,[H,\hat{Q}_2]]|\Phi_0\rangle
= \frac{2\hbar^2}{m}\langle \Phi_0|\hat{Q}^2 \hat{R} - 2\hat{Q}(\hat{Q}\hat{R})_1 + (\hat{Q}^2\hat{R})_1|\Phi_0\rangle,
$$

(12)

where $H$ is the total hamiltonian, $m$ is the nucleon mass, $\hat{R}$ is a one-body operator generated by the function $4x^2 + x^2 + y^2$, and $(\ )_1$ denotes that the quantity in the parentheses is a one-body operator. The last two terms on the right-hand side of the above equation appear because we use the operator $\hat{Q}_2$ instead of $\hat{Q}^2$ in Eq. (4). The EWSR value is evaluated using the HF wavefunction for $|\Phi_0\rangle$.

To treat DGQR consistently with the giant quadrupole resonance (GQR), we should employ as the residual force the same effective interaction as that used for the calculation of the mean-field potential. We use the Skyrme III force\(^{16}\) as such an effective interaction and assume that $^{16}$O is a completely spin-isospin symmetric system. The part of the mean-field potential that contains the parameter $x_0$\(^{17}\) 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 form\(^{17}\)

$$
v(r-r') = t_0\delta^3(r-r') + \frac{1}{2}t_1\{k'^2\delta^3(r-r') + \delta^3(r-r')k^2\}
+ t_2k' \cdot \delta^3(r-r')k + \frac{1}{2}t_3\rho \left(\frac{r + r'}{2}\right) \delta^3(r-r'),
$$

(13)

where $k = (\nabla_{\rho} - \nabla_{\rho'})/2i$ acts to the right and $k' = (\nabla_{\rho'} - \nabla_{\rho})/2i$ acts to the left. The factor 1/2 on the density dependent term contains the contribution of a rearrangement effect.\(^{17}\) The spin-orbit force is neglected, as in most TDHF calculations.\(^{18}\) The coupled equations (1) - (3) 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 to a cylinder of length 16 fm and radius 8 fm, as was done in Ref. 19. Since the integration in Eq. (10) is performed for a finite time interval of $1 \times 10^{-21}$ s, $S(E)$ has small fluctuations. To reduce the fluctuations in $S(E)$, we multipy $Q_2(t)$ by the damping factor $e^{-\Gamma t/2}$ before performing the integration in Eq. (10). This corresponds to smoothing the strength function with a width $\Gamma$. We use $\Gamma = 1$ MeV. Other calculational details are explained in our previous publications.\(^{11,19}\)

The strength distribution of DGQR calculated in TDDM is shown in Fig. 1 (solid line), together with the unperturbed one (dotted line). The peak at $E = 49.8$ MeV
corresponds to DGQR. The fraction of the EWSR value for the double phonon state exhausted in the energy interval 10 - 80 MeV is 73%. The small bump around $E = 20$ MeV seen in Fig. 1 corresponds to GQR. This is due to a coupling of DGQR to GQR. We also calculate the frequency distribution of a quadrupole oscillation of the mean field induced by the coupling of DGQR to GQR. The result is shown in Fig. 2. In this distribution the GQR component is dominant and DGQR is seen as a small bump around 50 MeV. The spectral distribution of GQR in Fig. 2 is quite similar to the strength function of GQR calculated in TDDM\textsuperscript{19} with an initial condition for the one-body density matrix; in Ref. 19), GQR was excited by boosting the single-particle wavefunctions with a quadrupole velocity field. The results in Figs. 1 and 2 show that the energy of DGQR is more than twice the mean energy of GQR. Before a comparison between the energies of DGQR and GQR is made, it should be noted that Eqs. (1) (describing GQR) and (3) are solved using different truncation schemes of the single-particle space: Eq. (1) is solved in coordinate space and Eq. (3) with the truncated single-particle space, as described above. To clarify this point, we made a TDHF calculation for GQR in coordinate space which corresponds to the continuum RPA calculation in the small amplitude limit and found that the centroid energy of the GQR distributions in Figs. 1 and 2 is nearly equal to the result of the TDHF calculation: such a TDHF calculation for GQR gives a single peak at 21.6 MeV with 97% of the EWSR value exhausted in the energy interval 0 - 40 MeV. On the other hand, an RPA calculation in the truncated single-particle space as described above gives a peak energy of 24.8 MeV and 86% of the EWSR value exhausted in the same energy interval. The strength function of GQR obtained from such an RPA calculation is shown in Fig. 3. Thus the peak energy of DGQR shown in Fig. 1 is nearly twice the GQR energy obtained from the RPA calculation done with the same truncated single-particle space. The width of DGQR is only 1 MeV larger than that of GQR in RPA: The full width at half maximum $\Gamma_{FWHM}$ of GQR in Fig. 3 is 3.2 MeV and $\Gamma_{FWHM}$ of DGQR is 4.2 MeV. (Only the difference between these widths may be meaningful because of the limited time interval to calculate $S(E)$ in Eq. (10).) These results show that DGQR calculated in TDDM has properties similar to those of the double phonon state of GQR in RPA. This is consistent with the results
of other theoretical calculations for DGQR. Our results indicate that RPA-type correlations in each single-phonon state dominate various two-body correlations considered in Eq. (3). The shape of the strength distribution of DGQR shown in Fig. 1 is quite different from that of GQR: Although the strength of GQR is strongly fragmented, that of DGQR is not. Since the coupling of DGQR to more complicated states like 3 particle-3 hole and 4 particle-4 hole states is neglected, a comparison of the width of DGQR with that of GQR is beyond the scope of our approach, as is the case for most microscopic calculations.

In summary, we have proposed a new time-dependent approach for studying the double phonon states of giant resonances based on TDDM, in which the strength function of the double phonon states is calculated in a manner similar to that used for giant resonances. We have applied this approach to DGQR in $^{16}$O. To treat DGQR consistently with GQR, we have used the same effective interaction in the calculation of both the mean field and two-body correlations. It was found that DGQR in TDDM has properties similar to those of the double phonon state of GQR calculated in RPA.

17) D. Da Providência, Nucl. Phys. 61 (1965), 87.