Random-phase-approximation calculations of nuclear response in the continuum

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A method is presented for random-phase-approximation calculations of nuclear response in the continuum. It utilizes the Lanczos method for solving the basic inhomogeneous coupled-channel integral equation. The method can provide information on both the direct and statistical decay components. We illustrate the usefulness of the method by applying it to calculate the 2^+ strength functions for 16 O, 40 Ca, and 208 Pb in the giant quadupole resonance region. It is shown that the calculations reproduce the observed peak positions and widths very well.

Giant resonances (GR) are collective states described as a coherent superposition of many one-particle-onehole (*ph*) configurations. Since these states appear in the continuum where the level density is high, the states decay either by emitting particles or by spreading (damping) into more complicated compound nuclear states. From a number of studies made in the past,^{1,2} the collective nature of GR has been well established. The decay properties, however, have not been well understood to date, and currently the subject is under intensive study from both experimental³⁻⁶ and theoretical⁷⁻¹⁴ points of view.

In this theoretical study, we are concerned with the strength function. One, and perhaps the best, possible approach is the continuum random-phase-approximation (\mathbf{RPA}) approach.^{1,7-16} The central problem there is to solve an inhomogeneous coupled-channel (CC)differential or integral equations for particles excited by an external force. The dimension of the CC equation, however, becomes very large for heavy nuclei. Take, e.g., the 2^+ strength function for ²⁰⁸Pb. In this case, the dimension becomes 298. To solve such a large set of CC equations in the usual way is extremely time consuming and practically impossible. Because of this reason, no calculation has ever been made so far for nuclei heavier than ⁴⁰Ca.

The aim of this paper is to demonstrate that it is possible to perform the continuum RPA calculation, even for 208 Pb, with a reasonable computer time, if one modifies the basic equation slightly, and applies the Lanczos method¹⁷ for solving it. Because of the use of continuum RPA, the calculation can naturally take into account continuum effects. Damping effect may also be taken into account by utilizing a complex optical potential for excited particles, which we do in this approach. We thus present here the formalism of such RPA calculations and then apply it to the 2⁺ strength functions in the giant quadrupole resonance (GQR) region.

The strength function S that we need here may generally be given as

$$S = \frac{1}{\pi} \operatorname{Im} \left[-\int d\mathbf{r} \, d\mathbf{r}' \rho^*(\mathbf{r}) R\left(\mathbf{r}, \mathbf{r}'; E\right) \rho(\mathbf{r}') \right], \qquad (1)$$

where ρ is the external field and $R(\mathbf{r}, \mathbf{r}'; E)$ is the response function defined as¹⁸

$$R(\mathbf{r},\mathbf{r}';E) \equiv \langle \Phi_0 | \psi^+(\mathbf{r})\psi(\mathbf{r})G\psi^+(\mathbf{r}')\psi(\mathbf{r}') | \Phi_0 \rangle .$$
(2)

In (2), $|\Phi_0\rangle$ is the target ground-state wave function, and $\psi^+(\mathbf{r})$ and $\psi(\mathbf{r})$ are the nucleon field creation and annihilation operators, respectively. Further, G is the (particle-hole) Green's function of the target system,

$$G = \frac{1}{E - H_{\rm h} - H_{\rm p} - V + i\varepsilon} , \qquad (3)$$

where E is the excitation energy of the system, H_h is the hole-nucleus Hamiltonian, and $H_p = T_p + U_p$ is the Hamiltonian for the excited particle p, consisting of the kinetic energy T_p and the complex optical potential U_p . V is the effective ph interaction. We assume that V already includes exchange effects, which means in practice that the calculation of the direct matrix element of V automatically generates the antisymmetrized matrix element of the original interaction Hamiltonian.^{7,8}

Further, we assume that the interaction V is a local two-body operator. This requires that we use the well-known pseudo-potential (δ function) approximation¹⁹ for dealing with the exchange term in V, which has, however, been known to be a good approximation. Under this assumption, R satisfies the following RPA equation:¹⁸

$$R(\mathbf{r},\mathbf{r}'E) = R_0(\mathbf{r},\mathbf{r}';E) + \int d\mathbf{r}_1 d\mathbf{r}_1' R_0(\mathbf{r},\mathbf{r}_1;E) \times V(\mathbf{r}_1,\mathbf{r}_1') R(\mathbf{r}_1',\mathbf{r}';E) , \qquad (4)$$

where $R_0(\mathbf{r}, \mathbf{r}'; E)$ is the free response function given as

$$R_0(\mathbf{r},\mathbf{r}';E) \equiv \langle \Phi_0 | \psi^+(\mathbf{r})\psi(\mathbf{r})G_0\psi^+(\mathbf{r}')\psi(\mathbf{r}') | \Phi_0 \rangle , \qquad (5)$$

$$G_0 = \frac{1}{E - H_h - H_p + i\varepsilon}$$
 (6)

In RPA, R_0 can more explicitly be given as¹⁸

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$$R_{0}(\mathbf{r},\mathbf{r}';E) = \Sigma_{h} \left[\phi_{h}^{*}(\mathbf{r}) \langle \mathbf{r} | \frac{1}{E + \varepsilon_{h} - H_{p} + i\varepsilon} | \mathbf{r}' \rangle \phi_{h}(\mathbf{r}') + \phi_{h}^{*}(\mathbf{r}') \langle \mathbf{r}' | \frac{1}{-E + \varepsilon_{h} - H_{p} + i\varepsilon} | \mathbf{r} \rangle \phi_{h}(\mathbf{r}) \right], \tag{7}$$

where $\phi_h(\mathbf{r})$ is the single-particle wave function for the single hole state *h*. R_0 is given in terms of $\phi_h(\mathbf{r})$ and the optical-model Green's function for *p*, and we may calculate it without any problem.

We now introduce $\lambda(\mathbf{r})$ through the following equation:

$$\Psi(\mathbf{r}) \equiv \int R(\mathbf{r}, \mathbf{r}'; E) \rho(\mathbf{r}') d\mathbf{r}'$$

$$\equiv \int R_0(\mathbf{r}, \mathbf{r}'; E) \lambda(\mathbf{r}') d\mathbf{r}' , \qquad (8)$$

and consider the equation that $\lambda(\mathbf{r})$ must satisfy. Using Eqs. (4) and (8), it is easy to show that $\lambda(\mathbf{r})$ satisfies

$$\lambda(\mathbf{r}) = \rho(\mathbf{r}) + \int d\mathbf{r}_1 d\mathbf{r}_1' V(\mathbf{r}, \mathbf{r}_1) R_0(\mathbf{r}_1, \mathbf{r}_1'; E) \lambda(\mathbf{r}_1') . \quad (9)$$

Equation (9) is our basic equation. In contrast to this, in previous studies,¹⁶ the equation for $\Psi(\mathbf{r})$ has been considered. The merit of dealing with $\lambda(\mathbf{r})$, instead of $\Psi(\mathbf{r})$, is in the fact that the former is a function localized only in the nuclear region. This is not the case for the latter function. This makes it much easier to solve the equation.

In solving (9), we further reduce the equation to that for the radial functions $\lambda_{ph}^{J}(r)$ and $\overline{\lambda}_{hp}^{J}(r)$, defined, respectively, as

$$(y_p|\lambda|\phi_{\tilde{h}}) = \sum_{JM} \langle j_p m_p j_h m_h | JM \rangle \frac{1}{r} \lambda_{ph}^J(r) , \qquad (10)$$

$$\langle \phi_h | \lambda | y_{\bar{p}} \rangle = \Sigma_{JM} \langle j_h m_h j_p m_p | JM \rangle \frac{1}{r} \overline{\lambda}_{hp}^J(r) , \qquad (11)$$

where y_p is the spin-angle wave function for p, \tilde{p} being the time reversal state corresponding to p. Further, the symbols ($||\rangle$ and $\langle ||$) were used to indicate that the integrals are carried over only the spin-angle variables, thus leaving the resultant integrals as functions of the radial distance r. Similarly, we may define the radial functions, $\rho_{ph}^J(r)$ and $\bar{\rho}_{hp}^J(r)$ for $\rho(\mathbf{r})$. Note that $\lambda_{ph}^J(r)$ and $\bar{\lambda}_{hp}^J(r)$ correspond to the forward and backward RPA particlehole amplitudes.¹⁸ In the present case, these amplitudes are functions of r, and satisfy the following CC integral equations,

$$\lambda_{ph}(r) = \rho_{ph}(r) + \sum_{p'h'} \int dr' dr'' V_{ph,p'h'}^{J}(r,r') g_{p'h'}^{(+)}(r',r'') \lambda_{p'h'}(r'') + \sum_{h'p'} \int dr' dr'' V_{ph,h'p'}^{J}(r,r') g_{h'p'}^{(+)}(r',r'') \overline{\lambda}_{h'p'}(r'') , \qquad (12)$$

$$\bar{\lambda}_{hp}(r) = \bar{\rho}_{hp}(r) + \sum_{p'h'} \int dr' dr'' V^{J}_{hp,p'h'}(r,r') g^{(+)}_{p'h'}(r',r'') \lambda_{p'h'}(r'') + \sum_{h'p'} \int dr' dr'' V^{J}_{hp,h'p'}(r,r') g^{(+)}_{h'p'}(r',r'') \bar{\lambda}_{h'p'}(r'')$$
(13)

In Eqs. (12)–(13), we omitted, for brevity, the superscript J in $\lambda_{ph}^{J}(r)$ and $\rho_{ph}^{J}(r)$, etc. Also, $V_{ph,p'h'}^{J}(r,r')$ is the ph matrix elements defined as

$$V_{ph,p'h'}^{J}(\mathbf{r},\mathbf{r}') = \Sigma_{m_{p}m_{h}m_{p}'m_{h}'} \langle j_{p}m_{p}j_{h}m_{h}|JM\rangle \langle j_{p}m_{p}'j_{h}m_{h}'|JM\rangle rr'(y_{p}\phi_{\tilde{h}'}|V|\phi_{\tilde{h}}y_{p'}) .$$

$$(14)$$

Expressions for $V_{ph,h'p'}^{J}(\mathbf{r},\mathbf{r})$, $V_{hp,p'h'}^{J}(\mathbf{r},\mathbf{r}')$, and $V_{hp,h'p'}^{J}(\mathbf{r},\mathbf{r}')$ may simply be obtained by interchanging p' and h', and/or p and h in (14). Further, $g_{ph}^{(+)}(\mathbf{r},\mathbf{r}')$ is the radial Green's function for the particle p with the orbital and total angular momenta l_p and j_p , respectively, and the energy $\varepsilon_p = E + \varepsilon_h$, while $g_{hp}^{(+)}$ is the similar Green's function with $\varepsilon_p = -E + \varepsilon_h$. We use here $g_i^{(+)}(i = ph$ or hp) given by Ichimura *et al*,²⁰ in which care is taken into account for eliminating contributions from the occupied hole states. The explicit form of $g_i^{(+)}$ may be given in terms of the well-known radial Green's function

$$g_{i0}^{(+)} = \frac{2m}{\hbar^2} f_{l_p j_p}(r_<) h_{l_p j_p}(r_>) / W$$
(15)

as

$$g_i^{(+)}(r,r') = g_{i0}^{(+)}(r,r') - \Sigma_{mn'} g_n(r) (O^{-1})_{nn'} g_{n'}(r') .$$
(16)

In (15), $f_{l_p j_p}(r)$ and $h_{l_p j_p}(r)$ are the regular and irregular

solutions of H_p , respectively, while W is the Wronskian. Also $O_{nn'}$ and $g_n(r)$ in (16) are defined as

$$O_{mn'} = \int dr \, dr' u_n(r) g_{io}^{(+)}(r,r') u_{n'}(r) , \qquad (17)$$

$$g_n(r) = \int dr' g_{i0}^{(+)}(r,r') u_{n'}(r') , \qquad (18)$$

where $u_n(r)$ is the radial wave function for the occupied orbit with the node *n*. The sum over *n* and *n'* in Eq. (16) is taken over all the occupied orbits (with definite l_p and j_p). The second term in (16) serves to forbid *p* to propagate in the occupied orbits. [The error caused by allowing *p* to propagate in the occupied orbits, i.e., by neglecting the second term in (16) is, however, rather small; the errors were found to be less than 5% for those cases considered in this study.] $g_i^{(+)}$ satisfies the outgoing or decaying boundary condition, depending on whether $\varepsilon_p > 0$ or $\varepsilon_p < 0$.

Let us now define column vectors $(1 \times N_c \text{ matrices})$

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$$|\lambda\rangle = \begin{pmatrix} \lambda_{ph} \\ \cdots \\ \overline{\lambda}_{hp} \\ \cdots \end{pmatrix}, \qquad (19)$$
$$|\rho\rangle = \begin{pmatrix} \rho_{ph} \\ \cdots \\ \overline{\rho}_{hp} \\ \cdots \end{pmatrix}. \qquad (20)$$

We may rewrite our basic equations (12)-(13) in a matrix form as

$$|\lambda\rangle = |\rho\rangle + \mathcal{V}\mathcal{G}_0|\lambda\rangle , \qquad (21)$$

where \mathcal{V} and \mathcal{G}_0 are the $N_c \times N_c$ matrices, whose elements are $V_{ph,p'h'}^J$, and $g_{ph}^{(+)}\delta_{ph,p'h'}$ and $g_{hp}^{(+)}\delta_{hp,h'p'}$, respectively.

Using (8), (10), (11), and (21), one can rewrite Eq. (1) as

$$S = \frac{1}{\pi} \operatorname{Im}(-\langle \rho | \mathcal{G}_0 | \lambda \rangle) .$$
 (22)

S may be decomposed into two components, S^{\downarrow} and S^{\uparrow} ; S^{\downarrow} describes the contribution from the damping or spreading process, i.e., the absorption due to W_p in U_p $(=V_p+iW_p)$, while S^{\uparrow} is due to direct particle emission. Following the technique used to derive the knockoutfusion cross-section formula,²¹ one can show that the contribution S^{\downarrow} can be given explicitly as

$$S^{\downarrow} = (-\langle \mathcal{G}_0 \lambda | \mathcal{W}_p | \mathcal{G}_0 \lambda \rangle), \qquad (23)$$

where \mathcal{W}_p is a diagonal matrix whose diagonal element is \mathcal{W}_p . The contribution S^{\uparrow} from the particle emission may then simply be obtained as (we may derive for S^{\downarrow} a more explicit DWBA-type expression, which however, will be given elsewhere)

$$S^{\uparrow} = S - S^{\downarrow} . \tag{24}$$

We now discuss the method for solving our basic equation (21). As already stated, we adopt the Lanczos method,¹⁷ which has been extensively used in the past for large shell-model calculations. In this method, we expand $|\lambda\rangle$ with a set of N+1 biorthogonal basic wave functions $|D_i\rangle(i=0,1,\ldots,N)$, which we generate iteratively as

$$|D_0\rangle = \frac{1}{N_0} |\rho\rangle , \qquad (25)$$

$$|D_{i+1}\rangle = \frac{1}{N_i} \left[\mathcal{V}\mathcal{G}_0 | D_i \rangle - \sum_{j=0}^i | D_j > \alpha_{ji} \right], \qquad (26)$$

with

$$\alpha_{ji} = \begin{cases} \langle \tilde{D}_j | \mathcal{VG}_0 | D_i \rangle & \text{if } j \le i+1 \\ 0.0 & \text{if } j > i+1 \end{cases}$$
(27)

 N_i in (26) is the normalization constant determined from the condition $\langle \tilde{D}_i | D_i \rangle = 1$, $|\tilde{D}_i \rangle$ being the conjugate state to $|D_i \rangle$. The coefficients α_{ji} given by (27) are nothing but those determined from the Schmidt orthonormalization procedure.

In terms of $|D_i\rangle$, $|\lambda\rangle$ is expanded as

$$|\lambda\rangle = \sum_{i=0}^{N} C_i |D_i\rangle .$$
⁽²⁸⁾

Inserting (28) into (21), one can easily derive an inhomogeneous linear equation for the expansion coefficient C_i , i.e.,

$$\sum_{j} (\delta_{ij} - \alpha_{ij}) C_j = N_0 \delta_{0i} \quad . \tag{29}$$

The values of C_i are then determined by solving (29). Note that Eq. (29) can be solved rather easily, because $\alpha_{ji} = 0$ for j > i + 1 [See Eq. (27)]. In addition, the value of N, i.e., the number of the basic wave functions $|D_i\rangle$, can be chosen as a small number, much smaller than the number of dimension N_c of the CC equation. This helps greatly in making the actual numerical calculations possible and practical. Typical values of N and N_c will be given below.

We have developed a computer code CRPA (continuum RPA) for carrying out the numerical calculations. As a test of the method and also the computer code, we have first repeated the calculation of Shlomo and Bertsch (SB) (Ref. 7) for the 2^+ strength function S for 16 O, 40 Ca, and ²⁰⁸Pb. As already noted, for the case of ²⁰⁸Pb, $N_c = 298$. For the ph interaction used in Ref. 7, however, it is possible to reduce the dimension of the CC equation to half. This could be done since the matrix elements between the forward and backward amplitudes are the same as those between the forward and forward, and the backward and backward amplitudes, except for a phase factor. $\overline{\lambda}_{hp}$ then becomes equal to λ_{ph} [except a factor of $(-1)^{j_p - j_h + J}$]. The CC equations we actually solved could thus be reduced to that of $N_c = 149$. Note that the dimension is still quite large. Nevertheless, with the use of the Lanczos method, we were able to solve the equation in 10 seconds with an X-MP Cray computer (for a given excitation energy E). The total time used for reproducing the 2^+ strength function of SB turned out to be about 5 min. For the cases of ¹⁶O and ⁴⁰Ca, the computer times needed were even much less than the time required for ²⁰⁸Pb. The required value of N for obtaining enough accuracy was about 8, which is far smaller than $N_c = 149$. It is thus seen that the method is indeed very efficient.

It is worth remarking here that the *ph* interaction used by SB is a δ interaction. This reduces the double dimensional integral involved in our basic Eqs. (12)-(13) to a single integral, making it much easier than otherwise to carry out the computation. This is, however, not a required condition. In fact, in a recent study of Δ excitations by charge-exchange reactions,²² we have carried out the finite-range calculation, though the calculation was done in the Tamm-Dancoff-Approximation.

We have then carried out calculations using the mass quadrupole field as an external field [i.e., assuming $\rho(r) = \sum_i r_i^2 Y 2_{\mu}(\Omega_i)$] for the same nuclei as considered above. Use is made of the same parameters as used in SB, excepting that the imaginary potential W_p is now added



FIG. 1. Comparison of calculated distributions of the energy-weighted quadrupole transition strength in units of the sum-rule limit with experiment. Histograms with an 1 MeV bin are experimental data deduced from hadronic inelastic scattering experiments of Refs. 26–28.

to the real U_p in order to account for the damping effect. In this calculation, it is important to take into account the energy dependence of W_p , not only in the particleunbound region, but also in the bound region, since the calculated width Γ is expected to depend mainly on W_p . Fortunately, such information on the energy variation of W_p has recently become available^{23,24} for $n + {}^{40}\text{Ca}$ and $n + {}^{208}\text{Pb}$. In these calculations, we thus use the W_p determined in Refs. 23 and 24 for both neutrons and protons. For ${}^{16}\text{O}$, use is made of the same W_p as that determined for ${}^{40}\text{Ca}$. Note that in this calculation, we ignore for simplicity damping effects due to those of hole singleparticle states and also those arising from the interference between particle and hole states.²⁵

In Fig. 1, we present the calculated distribution F(E)

of the energy-weighted quadrupole transition strength in units of the total sum rule, i.e.,

$$F(E) = [ES(E) / \int_0^\infty E'S(E')dE'] \times 100 .$$
 (30)

The corresponding experimental data are also presented by a histogram with an 1 MeV bin. These experimental data are those deduced from hadronic inelastic scattering experiments.²⁶⁻²⁸ As seen, the calculations reproduce the observed distributions fairly well. The calculated peak energies (E_R) and widths (Γ) of GQR are $E_R = 21.2$, 16.8, and 11.1 MeV and $\Gamma = 6.4$, 4.4, and 1.8 MeV for ¹⁶O, ⁴⁰Ca, and ²⁰⁸Pb, respectively. These are compared with the experimental values of $E_{R, exp} = 21$, 18, and 11 MeV, and $\Gamma_{exp} = 7.5$, 4.0, and 2.0 MeV, respectively.

As already noted, these calculations ignore the damping effects of the hole states as well as the interference between the particle and hole states. In spite of this, the calculation could reproduce fairly well the observed width Γ_{exp} . This suggests that the neglected effects are small as expected from the fact that the dominant contribution to S comes from ph components, whose hole states are in the last occupied shell, and that the contribution to the spreading from such hole states may be small. It might also be possible that this is achieved because the two contributions neglected are canceling for each other.^{25,29}

Finally we note that the calculations predicted S^{\dagger}/S at the peak energy to be 12%, 8%, and 5%, respectively, for ¹⁶O, ⁴⁰Ca, and ²⁰⁸Pb. This result shows that the decay should be dominated by the damping, which agrees with the data taken so far, although there are no data which would permit a quantitative comparison with the calculated results.

In summary, we have presented an approach for the continuum RPA response calculations, including the damping effect as well as the continuum effect. The damping effects have been treated by means of the imaginary potential for the particle excited by an external force. The essence of this approach is to use the Lanczos method for solving the basic coupled-channel RPA equation. The method was then applied to calculate 2^+ strength functions in the GQR region for a few example nuclei, demonstrating that the calculations are indeed very fast. It has also been shown that the calculated distributions of the quadrupole strength GQR agreed well with the data. The method may thus be used to make realistic analyses of experimental data.

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