Self-consistent calculation of nuclear photoabsorption cross sections: Finite amplitude method with Skyrme functionals in the three-dimensional real space

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The finite amplitude method (FAM), which we have recently proposed [T. Nakatsukasa, T. Inakura, and K. Yabana, Phys. Rev. C **76**, 024318 (2007)], significantly simplifies the fully self-consistent calculation of the random-phase approximation (RPA). This article presents a computational scheme of FAM suitable for systematic investigation and shows its performance for realistic Skyrme energy functionals. We adopt the mixed representation in which the forward and backward RPA amplitudes are represented by index of hole orbitals and of the spatial grid points for the three-dimensional real space. We solve a linear algebraic problem with a sparse non-Hermitian matrix, using an iterative method. We show results of the dipole response for selected spherical and deformed nuclei. The calculated peak energies of the giant dipole resonance well agree with experiments for heavy nuclei. However, they are systematically underestimated for light nuclei. We also discuss the width of the giant dipole resonance in the fully self-consistent RPA calculation.

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I. INTRODUCTION

Nuclear density-functional theory has been successful for a systematic description of ground-state properties such as binding energies, density distributions, deformations, and so on. In the past decade, systematic calculations for the whole nuclear chart become feasible and a variety of energy functionals are tested $[1,2]$. One of the major goals of such systematic investigations is an assessment and an improvement of the energy functional. A rapid progress of experimental research on unstable nuclei also necessitates a development of an accurate and universal energy functional that describes nuclei far from the stability line. These efforts are aiming at an ultimate theory with high predictive power and high accuracy.

The nuclear density-functional theory is also capable of describing excited state properties. The random-phase approximation (RPA), which is derived by linearizing the time-dependent mean-field equation [\[3\]](#page-10-0), describes the nuclear excitation as a small-amplitude oscillations around the ground state. It has been successful for describing both giant resonances and low-lying modes of excitations. In practical calculations, the RPA equation has been solved mostly in the matrix diagonalization scheme. In these calculations, it was common to ignore a part of the residual interaction, sacrificing the full self-consistency. This is because the inclusion of the full residual interaction for a realistic interaction involves a cumbersome and complicated task. Recently, several groups have reported fully self-consistent RPA calculations [\[4–8\]](#page-10-0). However, they are mostly restricted to spherical nuclei. There are a few recent attempts for deformed nuclei [\[9–14\]](#page-10-0).

Recently, we have proposed a new method to solve the RPA equation, the finite amplitude method (FAM) [\[15\]](#page-10-0). The FAM allows us to evaluate the fully self-consistent residual fields as a finite difference, employing a computational code for the *static* mean-field Hamiltonian alone with a minor modification. In Ref. [\[15\]](#page-10-0), the FAM was successful in solving

the linear-response equation for a deformed nucleus 20 Ne with a simplified interaction.

In most cases, the RPA forward and backward amplitudes are expressed in the *particle-hole* representation [\[3\]](#page-10-0). In the present work, we employ the mixed representation in which the *particle* index is replaced by the three-dimensional (3D) real space. In this representation, the RPA equation becomes a linear algebraic equation with a sparse, non-Hermitian matrix. The typical matrix dimension is order of $10⁶$. We will show that such a large-scale linear algebraic problem can be solved using an iterative method and then demonstrate that the FAM excellently works for realistic calculations with complicated energy functionals.

At present, we ignore the pairing terms. The pairing effects will not be important for high-lying negative-parity excitations such as the dipole excitation we investigate in this article. However, the pairing may have significant effects on the low-lying modes such as quadrupole excitations. An extension to inclusion of the pairing is now under study. To treat the particle escape properly, we need to impose the continuum boundary condition [\[16\]](#page-10-0). Although it can be managed in the present scheme [\[14\]](#page-10-0), the accurate description requires a heavy computational task. For our systematic investigation, we must make a compromise with the computational feasibility at the sacrifice of the exact treatment of the continuum. We will approximately take into account the continuum effects by solving the RPA equation inside the large 3D space.

We are undertaking the systematic investigation of nuclear response for a wide mass region ($A \le 100$). The purpose of this article is to explain the implementation of the FAM with the realistic Skyrme functional and to show that the FAM is suitable for the systematic investigation. The results of the systematic calculations will be reported in a forthcoming article.

We summarize here main features of our calculations:

(i) Fully self-consistent RPA calculation. The identical Skyrme energy functional is used for both ground-state and linear response calculations, including spin-orbit, Coulomb, and time-odd-density terms.

- (ii) 3D mixed representation applicable to nuclei with any kind of deformation. No truncation of the *particle* space is introduced.
- (iii) Use of the iterative method for the large-scale linear response equation with the fixed frequency.

This article is organized as follows. In Sec. \mathbf{II} , we review formalism of the FAM. The numerical details and the related techniques are discussed in Sec. ΠC . To show the accuracy of the method, the FAM results are compared with the fully self-consistent RPA results in the conventional diagonalization scheme. Calculated results are shown in Sec. [III](#page-4-0) for selected nuclei in light and heavy mass regions. Convergence with respect to the model space and to the smoothing factor (imaginary part of the frequency), dependence on the functionals will be discussed. Finally, our fully self-consistent RPA results are compared with experimental data. Conclusions are presented in Sec. [IV.](#page-9-0)

II. LINEAR-RESPONSE CALCULATION WITH A SKYRME FUNCTIONAL

A. Linear response equation in the mixed representation

Under a weak, time-dependent external field $V_{ext}(t)$, the transition density $\delta \rho(t)$ follows the equation ($\hbar = 1$)

$$
i\frac{d}{dt}\delta\rho(t) = [h_0, \delta\rho(t)] + [V_{\text{ext}}(t) + \delta h(t), \rho_0], \qquad (1)
$$

where ρ_0 and $h_0 = h[\rho_0]$ are the ground-state density and the single-particle Hamiltonian, respectively. The residual field *δh*(*t*) is induced by density fluctuation, $h[\rho(t)] = h_0 + δh(t)$. Assuming that $\delta \rho(t)$, $V_{ext}(t)$, and $\delta h(t)$ oscillate with a frequency *ω* like *δρ*(*t*) = *δρ*(*ω*)*e*−*iωt* + *δρ*† (*ω*)*eiωt* , Eq. (1) is recast to

$$
\omega \delta \rho(\omega) = [h_0, \delta \rho(\omega)] + [V_{ext}(\omega) + \delta h(\omega), \rho_0]. \tag{2}
$$

Because $\delta \rho(\omega)$ is not necessarily Hermitian, we need forward and backward amplitudes, $|X_i(\omega)\rangle$ and $|Y_i(\omega)\rangle$, to express the transition density *δρ*(*ω*).

$$
\delta \rho(\omega) = \sum_{i=1}^{A} \left\{ |X_i(\omega)\rangle \langle \phi_i| + |\phi_i\rangle \langle Y_i(\omega)| \right\},\tag{3}
$$

where $A = N + Z$ is the mass number of the nucleus and the orbitals $|\phi_i\rangle$ are occupied orbitals in the ground state, $h_0|\phi_i\rangle =$ $\epsilon_i|\phi_i\rangle$ (*i* = 1, ..., *A*). Substituting this expression into Eq. (2), we obtain the RPA linear-response equation:

$$
\omega|X_i(\omega)\rangle = (h_0 - \epsilon_i) |X_i(\omega)\rangle + \hat{P} \{V_{ext}(\omega) + \delta h(\omega)\} |\phi_i\rangle,
$$

(4)

$$
-\omega\langle Y_i(\omega)| = \langle Y_i(\omega) | (h_0 - \epsilon_i) + \langle \phi_i | \{V_{ext}(\omega) + \delta h(\omega)\} \hat{P},
$$

(5)

where \hat{P} denotes the projector onto the particles space, $\hat{P} = 1 - \sum_{i=1}^{A} |\phi_i\rangle\langle\phi_i|$. In Eqs. (4) and (5), if we expand *δh*(*ω*) with respect to the forward and backward amplitudes in the linear order, we obtain the well-known $A - B$ matrix form of the RPA equations $[3,15]$. When the single-particle Hamiltonian and the external field are both local in coordinate space, Eqs. (4) and (5) may be conveniently expressed in the coordinate representation,

$$
\omega X_i(\xi, \omega) = [h_0(\xi) - \epsilon_i] X_i(\xi, \omega)
$$

+ $\hat{P} \{V_{ext}(\xi, \omega) + \delta h(\xi, \omega)\} \phi_i(\xi),$ (6)
- $\omega Y_i^*(\xi, \omega) = [(h_0(\xi) - \epsilon_i)Y_i(\xi, \omega)$
+ $\hat{P} \{V_{ext}^{\dagger}(\vec{\xi}, \omega) + \delta h^{\dagger}(\xi, \omega)\} \phi_i(\xi)]^*$, (7)

where the coordinate ξ may contain the spin index σ as well as the spatial coordinate \vec{r} , $\xi = (\vec{r}, \sigma)$. This is often referred to the mixed representation [\[12,13,17\]](#page-10-0). It should be noted that because $\delta h(\omega)$ has a linear dependence on $X_i(\omega)$ and $Y_i^*(\omega)$, this is an inhomogeneous linear algebraic equation of the form $\mathbf{A}\vec{x} = \vec{b}$, where $\vec{x} \equiv [X_i(\xi, \omega), Y_i^*(\xi, \omega)]$ [\[15\]](#page-10-0). In our implementation, we employ the grid representation of the 3D Cartesian-coordinate space. Denoting the number of the spatial grid points as $N_{\vec{r}}$, the dimension of the vector \vec{x} is $N_{\vec{r}} \times A \times$ 2×2 (a factor of two for the forward and backward amplitudes and another factor of two for the spin degrees of freedom). $N_{\vec{r}}$ is order of 10,000 (see Sec. [II C1\)](#page-2-0). For systems described by local potentials, we need not introduce any further truncations in the particle space. In the 3D grid representation, the particle escape is better treated than in other representations, for example, the harmonic-oscillator-basis representation.

B. Finite amplitude method

If we expand the residual field *δh*(*ξ,ω*) explicitly with respect to the forward $X_i(\xi, \omega)$ and backward $Y_i(\xi, \omega)$ amplitudes, it requires us to calculate the residual two-body kernel, $v(\xi, \xi') = \delta h(\xi, \omega) / \delta \rho(\xi')$. However, if one employs a realistic energy functional, the explicit construction of the residual two-body kernel involves a complicated coding and a large numerical task. For this reason, it has been a common procedure to approximate or ignore a part of the residual interaction in most RPA calculations. For example, the velocity-dependent terms are sometimes replaced with the Landau-Migdal interaction. The spin-spin, the spin-orbit, and the Coulomb residual interactions are often neglected.

To achieve a fully self-consistent RPA calculation, we believe that the FAM [\[15\]](#page-10-0) is one of the simplest methods, at least, with respect to programming. In the FAM, we evaluate *δh*(*ξ,ω*) directly from the single-particle Hamiltonian *h*[*ρ*] by means of the finite difference method, thus avoiding an explicit construction of the residual two-body kernel. In this section, we recapitulate the essence of the FAM. Readers are referred to Ref. [\[15\]](#page-10-0) for details.

The residual field *δh*(*ξ,ω*) depends linearly on *δρ*(*ω*): *δh*(*ω*) = $∂h/∂ρ|_{ρ=ρ_0}$ · $δρ(ω)$. In the first order with respect to a small parameter *η*, we have

$$
h_0 + \eta \delta h(\omega) = h[\rho_0 + \eta \delta \rho(\omega)] \equiv h[\tilde{\rho}_{\eta}(\omega)].
$$
 (8)

Here, the one-body *pseudodensity* operator $\tilde{\rho}_\eta(\omega) \equiv \rho_0 + \rho_0 \rho_0$ $\eta \delta \rho(\omega)$ is a non-Hermitian operator expressed with bra and ket vectors as follows:

$$
\tilde{\rho}_{\eta}(\omega) = \sum_{i} (|\phi_{i}\rangle + \eta |X_{i}(\omega)\rangle) (\langle \phi_{i}| + \eta \langle Y_{i}(\omega)|). \quad (9)
$$

In the linear order in η , Eq. [\(8\)](#page-1-0) is expressed as

$$
\delta h(\omega) = \frac{1}{\eta} (h[\tilde{\rho}_{\eta}(\omega)] - h_0).
$$
 (10)

This is the basic result of the FAM. In Eq. (10), $h[\tilde{\rho}_n(\omega)]$ can be evaluated in the same manner as in $h_0 = h[\rho_0]$, with a replacement of the ordinary densities with the *pseudodensities*. For instance, the *pseudolocal density*, *pseudokinetic density*, and *pseudocurrent density* are given by

$$
\tilde{\rho}_{\eta}(\vec{r}) = \sum_{i} \sum_{\sigma} \psi_{i}^{*}(\xi) \varphi_{i}(\xi),
$$
\n
$$
\tilde{\tau}_{\eta}(\vec{r}) = \sum_{i} \sum_{\sigma} \nabla \psi_{i}^{*}(\xi) \cdot \nabla \varphi_{i}(\xi),
$$
\n
$$
\vec{j}_{\eta}(\vec{r}) = \frac{1}{2i} \sum_{i} \sum_{\sigma} \{ \psi_{i}^{*}(\xi) \nabla \varphi_{i}(\xi) - (\nabla \psi_{i}^{*}(\xi)) \varphi_{i}(\xi) \},
$$
\n(11)

respectively, where $\varphi_i = \phi_i + \eta X_i(\omega)$ and $\psi_i = \phi_i + \eta Y_i(\omega)$. The spin-dependent pseudodensities are also defined in the same manner. Once $X_i(\omega)$, $Y_i(\omega)$, and η are given, the pseudodensities are calculated as in Eq. (11).

Equations [\(6\)](#page-1-0) and [\(7\)](#page-1-0) are the linear algebraic equation of the form, $A\vec{x} = \vec{b}$. Here,

$$
\vec{x} = \begin{bmatrix} X_i(\xi, \omega) \\ Y_i^*(\xi, \omega) \end{bmatrix}, \qquad \vec{b} = \begin{bmatrix} -V_{\text{ext}}(\xi, \omega)\phi_i(\xi) \\ -\{V_{\text{ext}}(\xi, \omega)\phi_i(\xi)\}^* \end{bmatrix}. \tag{12}
$$

To solve Eqs. (6) and (7) , we utilize the iterative scheme, as described below. In the iterative scheme, we need not construct the matrix elements of **A** explicitly but only to evaluate $A\vec{x}$ for a given vector \vec{x} :

$$
\mathbf{A}\vec{x} = \begin{bmatrix} (h_0(\xi) - \epsilon_i - \omega)X_i(\xi, \omega) + \delta h(\xi, \omega)\phi_i(\xi) \\ \{ (h_0(\xi) - \epsilon_i + \omega^*)Y_i(\xi, \omega) + \delta h^\dagger(\xi, \omega)\phi_i(\xi) \}^* \end{bmatrix},
$$
\n(13)

where $\delta h(\xi, \omega)\phi_i(\xi)$ is calculated using Eq. (10) and *δh*[†](ξ, ω) ϕ_i (ξ) using the same equation but $\tilde{\rho}_{\eta}$ replaced by $\tilde{\rho}_{\eta}^{\dagger}$. To find a solution of Eqs. (6) and (7) , we employ extensions of the conjugate gradient method for linear algebraic equations involving a non-Hermitian matrix. In the literature, quite a few solvers for this purpose have been developed. However, we find only a few methods work for the present problem. We will discuss it in Sec. II C.

To calculate the strength function for a given one-body operator *F*, we adopt an external field of $V_{ext}(t) = \eta F e^{-i\omega t} +$ *η[∗]F*[†]*e*^{*iωt*}. Then, the transition strength is expressed with the forward and backward amplitudes,

$$
\frac{dB(E;F)}{dE} \equiv \sum_{n} |\langle n|F|0\rangle|^{2} \delta(E - E_{n})
$$

$$
= -\frac{1}{\pi} \text{Im} \sum_{i} \{ \langle \phi_{i} | F^{\dagger} | X_{i}(\omega) \rangle + \langle Y_{i}(\omega) | F^{\dagger} | \phi_{i} \rangle \}
$$
(14)

for a real frequency $\omega = E$. Here, $|n\rangle$ are energy eigenstates of the total system. In the following calculations, we use complex frequencies with a finite imaginary part, $\omega = E + i\gamma/2$. Then,

the transition strength becomes

$$
\frac{dB(E;F)}{dE} = \frac{\gamma}{2\pi} \sum_{n} \left\{ \frac{|\langle n|F|0\rangle|^2}{(E - E_n)^2 + (\gamma/2)^2} - \frac{|\langle n|F^{\dagger}|0\rangle|^2}{(E + E_n)^2 + (\gamma/2)^2} \right\}.
$$
(15)

The second term in the right-hand side is not important, if $\gamma \ll E + E_n$. For a Hermitian operator *F* this leads to

$$
\frac{dB(E;F)}{dE} = \frac{2E\gamma}{\pi} \sum_{n} \frac{\tilde{E}_n |\langle n|F|0\rangle|^2}{\left(E^2 - \tilde{E}_n^2\right)^2 + E^2 \gamma^2},\tag{16}
$$

where $\tilde{E}_n^2 = E_n^2 + \gamma^2/4$.

In this article, we consider an electric dipole operator for *F*:

$$
D_z^{E1} = \frac{N}{A}e\sum_{p=1}^{Z}z_p - \frac{Z}{A}e\sum_{n=1}^{N}z_n, \qquad (17)
$$

and similar operators for D_x^{E1} and D_y^{E1} . The photoabsorption cross section in the dipole approximation is given as follows [\[18\]](#page-10-0),

$$
\sigma_{\text{abs}}(E) = \frac{4\pi^2 E}{3c} \sum_{\mu = x, y, z} \frac{dB(E; D_{\mu}^{E1})}{dE}.
$$
 (18)

C. Numerical details

1. Adaptive 3D grid representation

We employ a model space of 3D grid points inside a sphere of a radius R_{box} . All the single-particle wave functions and potentials except for the Coulomb potential are assumed to vanish outside the sphere. For the calculation of the Coulomb potential, we follow the prescription in Ref. [\[19\]](#page-10-0). The differentiation is approximated by a finite difference with the nine-point formula.

To obtain nuclear response with a reasonable accuracy, we need a large model space, typically $R_{\text{box}} \gtrsim 15$ fm (see Sec. III B₁). This is much larger than the typical nuclear size R_0 . Outside the nuclear radius R_0 , we do not need to use a fine mesh. Thus we adopt an adaptive coordinate system to reduce the number of grid points in the outer region, $R_0 < r < R_{\text{box}}$. We use the following coordinate transformation, $(u, v, w) \rightarrow$ (x, y, z) , which was also adopted in Ref. [\[14\]](#page-10-0),

$$
x(u) = ku \left[1 + (k-1) \left\{ \frac{u}{x_0 \sinh(u/x_0)} \right\}^n \right]^{-1}, \quad (19)
$$

and the same form for $y(v)$ and $z(w)$. In this transformation, we have $x(u) \approx u$ for spatial region of $u \ll x_0$, and $x(u) \approx ku$ for $u \gg x_0$. We adopt a uniform mesh spacing of $\Delta h = 0.8$ fm in the (u, v, w) space. The parameters $k = 5.0$, $x_0 = 8$ fm, and $n = 2$ are used in the following calculations. The number of grid points in the sphere of $r \le R_{\text{box}}$ is significantly reduced; $27,609 \rightarrow 11,777$ for $R_{\text{box}} = 15$ fm and $221,119 \rightarrow 39,321$ for $R_{\text{box}} = 30$ fm.

2. Choice of iterative algorithms

In this section, we discuss performance of different iterative solvers to solve the linear response equations. We first discuss the calculation for the ground state. To obtain ground-state solutions, the imaginary-time iterative method is used [\[20\]](#page-10-0). We impose constraints in the iteration process so that the center of mass always coincides with the origin of the coordinate system and the principal axes of the density distribution coincide with three Cartesian axes of *x*, *y*, and *z*. It is important to obtain a well-converged ground-state solution because the convergence properties of the linear-response calculation crucially depend on this. To assure the strict convergence in the ground-state calculation, we impose the convergence condition not only for the total energy but also for the deformation parameters (β, γ) , single-particle energies ϵ_i , single-particle angular momenta, and so on.

For the Skyrme energy functional, the RPA matrix **A** that appears in Eqs. (6) and (7) is sparse in the \vec{r} -space grid representation. Therefore, the iterative methods, such as the conjugate gradient (CG) method [\[21\]](#page-10-0), should work efficiently. The CG method is very powerful for the Hermitian matrix. However, because we calculate for the complex frequency *ω*, the matrix **A** is no longer Hermitian. Therefore, a simple CG method is not applicable. There are a lot of variants of the CG method extended for non-Hermitian problems. We test some of them: biconjugate gradient (Bi-CG) method [\[21\]](#page-10-0), generalized conjugate residual (GCR) method [\[22\]](#page-10-0), generalized product-type biconjugate gradient (GPBi-CG) method [\[23\]](#page-10-0), Bi-CGSTAB method [\[24\]](#page-10-0), and Bi-CGSTAB2 method [\[25\]](#page-10-0). In the original GCR method, it is necessary to store all the vectors $\vec{x}_0, \ldots, \vec{x}_{n-1}$ to calculate the vector at the *n*-th iteration. Because this is rather impractical, we restart the GCR procedure every 20 iterations. In Fig. 1, we show the convergence behavior of the different iterative solvers. The magnitude of the relative residue,

$$
r_n = |\vec{b} - \mathbf{A}\vec{x}_n|/|\vec{b}|,\tag{20}
$$

is plotted against the number of iterations.

At very low energies ($\omega = 0 + 0.5i$ MeV), all the solvers except for the Bi-CG method quickly reach the convergence. However, at higher energies ($\omega = 10 + 0.5i$ MeV), only the GCR and the GPBi-CG methods lead to the convergence. In most cases, the convergence of the GPBi-CG method is faster than that of the GCR. However, after the convergence, the residue by the GPBi-CG method start to increase again. Therefore, only the result of the GCR method shows a stable convergence property in Fig. 1. We thus employ the GCR in the following calculations, although it has a disadvantage that it requires larger computer memory size than other methods based on the Bi-CG.

In the iteration procedure, we need to set up the initial vector \vec{x}_0 . It turns out that the convergence property depends very little on the selection of the initial vector. We simply take the initial vector of $\vec{x}_0 = 0$. We stop the GCR iteration procedure if the relative residue becomes smaller than a threshold, $r_n < 10^{-6}$. We find the typical number of the iteration necessary to reach the convergence is about $10³$ around the excitation energy region of giant dipole resonance (GDR), while the convergence is much faster for smaller energy, $E = \text{Re}\omega$. The necessary iteration number also depends on the imaginary part of the frequency, $\gamma = 2\text{Im}\omega$, and is roughly proportional to $1/\gamma$.

In Sec. [III,](#page-4-0) the calculation is performed with the following settings, unless otherwise specified: The energy range of $0 \le E \le 38.1$ MeV, discretized in spacing of $\Delta E = 0.3$ MeV (128 points). The imaginary part of the frequency is fixed at 0.5 MeV, corresponding to $\gamma = 1.0$ MeV. The calculated strength is interpolated using the cubic spline function. We find that the computational time scales linearly both with the number of grid points and with the particle number *A*. Utilizing PC cluster systems with either 64 or 128 processors in parallel, we can obtain the photoabsorption cross section for $A \approx 20$ nuclei within a few hours.

3. Choice of the FAM parameter η

The FAM parameter η in Eq. [\(10\)](#page-2-0) should be as small as possible to validate the linearity. In practice, there is a

FIG. 1. Convergence properties of different iterative methods to solve the linear response Eqs. [\(6\)](#page-1-0) and [\(7\)](#page-1-0) for electric dipole response in ¹⁶O calculated at complex frequencies of $\omega = 0 + 0.5i$ MeV (a) and 10 + 0.5*i* MeV (b). Relative residue, r_n , is shown as a function of iteration number *n*.

lower limit to avoid the round-off error. In the numerical computation, we use real variables with double precision (8 bytes) and complex variables with 8×2 bytes. We use the following value for η that differs for every iteration to ensure the linearity [\[15\]](#page-10-0):

$$
\eta = \frac{\eta_{\text{Lin}}}{\max\{N(X), N(Y)\}}, \quad N(\psi) = \frac{1}{A} \sqrt{\sum_{i=1}^{A} \langle \psi_i | \psi_i \rangle} \quad (21)
$$

with $\eta_{\text{Lin}} = 10^{-4}$. The convergence property of the GCR iteration is not sensitive to the value of η_{Lin} , as far as the value is in the range of $\eta_{\text{Lin}} = 10^{-2} - 10^{-6}$. However, if we use too small a value, r_n oscillates in the iteration and never reaches the convergence.

III. CALCULATED RESULTS

A. Numerical accuracy

In this section, we demonstrate that the FAM, described in Sec. [II,](#page-1-0) really works as a simple and accurate method for the fully self-consistent linear-response calculation with realistic Skyrme functionals. In Ref. [\[15\]](#page-10-0), we have already done it for a simple Bonche-Koonin-Negele interaction [\[26\]](#page-10-0).

In the following calculations, we adopt the same functional form as that of Ref. [\[27\]](#page-10-0) (Appendix A). In Ref. [\[27\]](#page-10-0), every single-particle orbital is assumed to have a definite parity and *z*-signature symmetries. However, we assume none of these in this article. The functional depends on densities $\rho_{\tau}(\vec{r})$, kinetic densities $\tau_{\tau}(\vec{r})$, spin-orbit densities $\vec{J}_{\tau}(\vec{r})$, current densities $\vec{j}_\tau(\vec{r})$, and spin densities $\vec{\rho}_\tau(\vec{r})$, where $\tau = n$ and *p*. The exchange part of the Coulomb energy is evaluated by the Slater approximation. The center-of-mass correction is achieved by using the recoil nucleon mass, $M \to AM/(A-1)$.

In Fig. 2, we show photoabsorption cross section for ${}^{16}O$ calculated with two different methods: The dots are obtained by solving the linear response Eqs. (6) and (7) in which the FAM is employed to evaluate the residual fields. The vertical lines are obtained by the matrix diagonalization method [\[12,13\]](#page-10-0) in which the residual interactions, second derivatives of the Skyrme energy functional, are constructed explicitly. The positions of the vertical lines indicate the energy eigenvalues, while the heights show the calculated cross section. The solid curve is obtained by smoothing the vertical lines with the energy-weighted Lorentzian. In both calculations of the linear response and the matrix diagonalization, the same Skyrme functional and the same grid representation of the \vec{r} space are used. The width parameter is set common, $\gamma = 2$ MeV. In the matrix diagonalization method, the spurious solutions corresponding to the center-of-mass motion appear around a few tens keV. They do not carry *E*1 strength.

This figure clearly demonstrates that the linear response calculation with the FAM completely agrees with the fully selfconsistent RPA calculation with an explicit construction of the residual interaction. We should note that the computer program of the diagonalization method requires heavy and complicated coding for the residual interaction, while that of the FAM can be achieved with the static mean-field calculation alone, with

FIG. 2. Comparison of the results for electric dipole response of 16O calculated by the present linear response formalism with FAM (dots) and by the eigenvalue formalism with an explicit construction of the residual interaction (curve). Both calculations use the cubic box of $(21 \text{ fm})^3$ and the SIII functional. See text for details. The vertical lines indicate eigenenergies and strengths of the RPA normal modes calculated by the matrix diagonalization method, whose vertical magnitude is in units of mb MeV.

a minor modification. The accuracy and the simplicity of the FAM is clearly demonstrated.

Let us next consider the merit of the linear response calculation for a fixed frequency in comparison with the matrix diagonalization method, apart from the FAM. In the matrix diagonalization method, the number of normal modes increases rapidly as the excitation energy becomes higher. Even when we assume the parity and the *z*-signature symmetries, the number of excited states is an order of 1000 in the energy range below 50 MeV. If we achieve matrix diagonalization in the mixed representation, we must calculate eigenvalues and eigenvectors of the RPA solution one by one. Then the calculations of a thousand of eigenstates require huge computational time. Therefore, to calculate responses for a wide energy region, the computation time with the linear response method is much smaller than that of the diagonalization method. Furthermore, we can easily parallelize the calculation in the linear response calculation, assigning different processors to solve the equation at different frequencies *ω*.

Combining these features, we consider the linear response calculation with the FAM is the best choice for the systematic, fully self-consistent calculations over a periodic table.

B. Light nuclei

1. Dependence on box size and smoothing parameter

In this section, we show how the results depend on the box size R_{box} and the smoothing parameter *γ*. In the present mixed representation, the model space is specified with R_{box} and the 3D mesh size Δh . The dependence on the mesh size is discussed in details in Ref. [\[12\]](#page-10-0) for spurious and low-energy excitations in ¹⁶O and ²⁰⁸Pb. According to this study, $\Delta h \approx$ 0*.*8 fm produces a converged result. In addition, we have also

FIG. 3. (Color online) Photoabsorption cross sections in (a) ¹⁶O and (b) ⁴⁰Ca calculated with the FAM in a spherical box of different sizes: $R_{\text{box}} = 10, 15, 20, \text{ and } 30 \text{ fm. } \text{``ABC''}$ indicates a result with the absorbing boundary condition that properly treats the continuum effect [\[14\]](#page-10-0). The SkM[∗] interaction and the smoothing parameter $\gamma = 1$ MeV are used. Convergence properties as a function of the CPU time for (c) ¹⁶O and (d) ⁴⁰Ca, at $E = 19.2$ MeV and $E = 18.0$ MeV, respectively.

carefully examined the convergence with respect to the grid spacing in the adaptive-coordinate, Eq. [\(19\)](#page-2-0).

In Fig. 3, results of the calculations with $R_{\text{box}} = 10, 15$, 20, 25, and 30 fm are shown. Small peaks in higher energies $(E > 20$ MeV) are disappearing with increasing R_{box} . These small peaks at high energies are all spurious, due to the discretization of the continuum. In fact, the calculation with the proper continuum boundary condition [\[14\]](#page-10-0), which is denoted as "ABC," shows only a smooth tail in this energy region above the main GDR peak. With the energy resolution of $\gamma = 1$ MeV, the effect of the discretized continuum is still visible at $E > 20$ MeV, even for the case of $R_{\text{box}} \simeq 30$ fm. To remove the spurious effect, we need to increase either R_{box} or *γ*. In Fig. 4, we show results for ⁴⁰Ca calculated with different box sizes and with different magnitudes of the smoothing parameter *γ*. Using $\gamma > 2$ MeV, the calculation roughly converges with $R_{\text{box}} > 15$ fm. Thus, in the calculation with the vanishing (box) boundary condition, it is difficult to

distinguish small physical peaks from unphysical ones in the high-energy continuum region, *E >* 20 MeV. In this article, we concentrate our discussion on gross structure of the main GDR peaks.

Next, in Fig. [5,](#page-6-0) we show results for ^{24}Mg . Because the ground state of ²⁴Mg is deformed with a prolate shape (β_2 = 0.39), the GDR splits into two major peaks, $K = 0$ mode (dashed line) and $K = 1$ mode (long dashed line). The $K = 0$ mode corresponds to the oscillation parallel to the symmetry axis (*z* direction) and $K = 1$ mode to that perpendicular to the symmetry axis $(x \text{ and } y \text{ directions})$. In the calculations with $R_{\text{box}} = 10$ and 15 fm, we observe a peak at $E = 25 \text{ MeV}$ for the $K = 1$ mode. However, this peak becomes smaller for larger R_{box} . This suggests that the peak at 25 MeV comes from the effect of the box discretization and is spurious.

Although the calculated profile functions of cross section in the high-energy continuum region are affected by the box discretization, the gross property of the GDR is less

FIG. 4. (Color online) Photoabsorption cross sections in spherical nucleus 40Ca calculated with different R_{box} and with different *γ* values. The functional parameter set of SkM[∗] is used.

FIG. 5. Photoabsorption cross sections in deformed nucleus 24Mg calculated with a spherical box of (a) $R_{\text{box}} = 10$ fm, (b) 15 fm, (c) 20 fm, and (d) 30 fm. Dashed, long dashed, and solid lines correspond to cross sections of $K = 0$ mode, $K = 1$ mode, and the total one, respectively. The functional parameter set of SkM^{*} and the smoothing parameter $\gamma = 1$ MeV are used.

sensitive to the value of R_{box} . We estimate the GDR peak energy and the width according to the electric dipole (*E*1) strength distribution and the photoabsorption cross section (oscillator strength distribution). For spherical nuclei, the nuclear response does not depend on the direction of the external dipole field. Thus, we can arbitrary choose it, for instance, $F = D_z^{E1}$. Then, *E*1 strength is fitted by a single Lorentzian function,

$$
\frac{dB(E; D_z^{E1})}{dE} \approx B_{\text{tot}} \times L(E),
$$

$$
L(E) = \frac{1}{\pi} \frac{\Gamma/2}{(E - E_{\text{peak}})^2 + (\Gamma/2)^2},
$$
(22)

where E_{peak} and Γ are fitting parameters and $B_{\text{tot}} =$ $\int dEdB(E)/dE$. The fitting is also performed for the photoabsorption cross section $\sigma_{\text{abs}}(E)$, using the energy-weighted Lorentzian, $f_{\text{tot}} \times EL(E)$. The results are shown in Table I.

TABLE I. R_{box} dependence of the GDR peak positions and widths in units of MeV, for ¹⁶O and ⁴⁰Ca. The smoothing parameter of $\gamma = 1$ MeV is used. See text for details.

	dB(E)/dE		$\sigma_{\text{abs}}(E)$		
	$E_{\rm peak}$	Г	$E_{\rm peak}$	Г	
	16 _O				
$R_{\text{box}} = 10$ fm	18.993	3.869	18.798	3.876	
$R_{\text{box}} = 15$ fm	19.063	3.475	19.103	3.944	
$R_{\rm{box}} = 20$ fm	19.141	3.096	19.151	3.435	
$R_{\text{box}} = 30$ fm	19.162	3.035	19.165	3.330	
	40Ca				
$R_{\text{box}} = 10$ fm	17.794	1.545	17.766	1.550	
$R_{\text{box}} = 15$ fm	17.797	2.334	17.796	2.492	
$R_{\text{box}} = 20$ fm	17.904	2.789	17.901	2.886	
$R_{\text{box}} = 30$ fm	17.963	2.956	17.959	3.014	

These two definitions of the peak energy and the width lead to nearly identical results.

The dependence of E_{peak} on the box size R_{box} is very small. However, the GDR width Γ shows a substantial dependence on the box size. For $\gamma = 1$ MeV, to estimate the width with a reasonable accuracy requires $R_{\text{box}} > 20$ fm. However, the width also depends on the smoothing parameter γ , which is shown in Fig. 6. The value of Γ is converged at $R_{\text{box}} \geq 20$ fm for $\gamma = 1$ MeV. When we use a larger γ value, the model space of $R_{\text{box}} = 15$ fm is good enough to calculate the width. From the approximate linear dependence of Γ on the parameter *γ*, we can estimate the width at $\gamma = 0$ as $\Gamma^{RPA} \approx 2$ MeV. This value can be regarded as the damping width in the RPA, namely due to the Landau damping and escaping: $\Gamma^{RPA} = \Gamma^{Landau} + \Gamma^{\uparrow}$. Because the smoothing parameter *γ* can be regarded as the spreading width, $\gamma = \Gamma^{\downarrow}$, we may extract Γ^{\downarrow} from experimental data. This will be discussed in the followings.

FIG. 6. Estimated GDR width for 40 Ca as a function of the parameter *γ* .

2. Comparison with experiments and Skyrme-functional dependence

In Fig. 7 calculated photoabsorption cross sections for spherical nuclei (${}^{16}O$, ${}^{40}Ca$) and deformed nucleus ${}^{24}Mg$ are compared with experimental data. The calculated energies of the GDR peaks are underestimated by a few MeV, but the overall structures are reproduced. For spherical nuclei, the GDR widths calculated with $\gamma = 1$ MeV are narrower than the corresponding experimental data. This seems to suggest that the spreading width Γ^{\downarrow} , which takes account of effects decaying into compound states, such as two-particletwo-hole excitations, is slightly larger than $\gamma = 1$ MeV. The cross section at higher energies (*E >* 25 MeV) is larger in experiment. This may be due to effect of the ground-state correlation produced by the tensor and short-range parts in the two-body nuclear interaction $[18]$. For ¹⁶O, all the calculations fail to reproduce a double-peak structure of the GDR, present in experimental data. If we neglect the time-odd spin densities, the double peaks can be reproduced [\[14\]](#page-10-0). The GDR peak energy in ⁴⁰Ca is better reproduced compared to the case for 16O. The calculated cross sections in the high-energy region also becomes closer to the experimental data. It seems that the discrepancy is more prominent for lighter nuclei.

For the deformed nucleus $24Mg$, the GDR peak splitting caused by the ground-state deformation well agree with the experiments, although the magnitude of the deformation splitting is slightly too large in the calculation. We may interpret that the experimental GDR peak around $E = 20$ MeV is associated with the $K = 0$ mode, and those at $E = 22 \sim 25$ MeV correspond to the $K = 1$ mode. The double-peak structure of the $K = 1$ GDR peak is well reproduced. Approximately, the calculated cross section is shifted to lower energy from the experimental ones by about 3 MeV.

We next show results obtained with different Skyrme-parameter sets in Fig. [8;](#page-8-0) SkM[∗] [\[30\]](#page-10-0), SIII [\[31\]](#page-10-0), SGII [\[32\]](#page-10-0), and SLy4 [\[33\]](#page-10-0). Two parameter sets, SkM[∗] and SLy4, produce similar results. In $16O$, the GDR peak position is calculated around $E = 19$ MeV. In contrast, the SIII functional produces the GDR peak near $E = 21$ MeV. The result with the SGII functional is intermediate, around $E = 20$ MeV. However, all the calculations underestimate the experimental GDR

peak energy, $E \approx 22$ MeV. These difference in the GDR peak energy cannot be simply explained only by the symmetry energy, because the symmetry energy is the largest for SLy4 and the smallest for SGII. The cross section at higher energies $E > 25$ MeV is also systematically underestimated in the calculations. For deformed $24Mg$, all the calculations again underestimate the peak energies. The peak energy obtained with the SIII functional are located highest among these four functionals.

3. Transition density

We obtain the forward and backward amplitudes, $X_i(\xi, \omega)$ and $Y_i(\xi, \omega)$, using the FAM. Then, the local part of the transition density in the intrinsic frame, Eq. (3) , can be calculated as

$$
\delta \rho_{\tau}(\vec{r}, \omega) = \sum_{i \in \tau} \sum_{\sigma} {\{\phi_i^*(\xi)X_i(\xi, \omega) + Y_i^*(\xi, \omega)\phi_i(\xi)\}}, \quad (23)
$$

where $\tau = n$ or p. In this section, we adopt the external field of $D_z^{E1}(K = 0)$. Using $\delta \rho(\omega)$ with $\omega = E + i\gamma/2$, the strength function can be written as

$$
\frac{dB(E; D_z^{E1})}{dE} = -\frac{1}{\pi} \text{Im} \int d\vec{r}
$$

$$
\left[\frac{Ne}{A} z \delta \rho_p(\vec{r}, \omega) - \frac{Ze}{A} z \delta \rho_n(\vec{r}, \omega) \right]
$$

$$
= \frac{2E\gamma}{\pi} \sum_n \frac{\tilde{E}_n |\langle n| D_z^{E1} |0 \rangle|^2}{\left(E^2 - \tilde{E}_n^2\right)^2 + E^2 \gamma^2}.
$$
(24)

Substituting $\langle n | D_z^{E_1} | 0 \rangle$ by the following expression

$$
\langle n|D_z^{E1}|0\rangle = \int d\vec{r} \frac{Ne}{A} z \langle n|\hat{\rho}_p(\vec{r})|0\rangle - \frac{Ze}{A} z \langle n|\hat{\rho}_n(\vec{r})|0\rangle, \tag{25}
$$

we find

Im
$$
\delta \rho_{n(p)}(\vec{r}, \omega) \propto \sum_{n} \frac{\tilde{E}_n \langle 0 | D_z^{E_1} | n \rangle \langle n | \hat{\rho}_{n(p)}(\vec{r}) | 0 \rangle}{\left(E^2 - \tilde{E}_n^2\right)^2 + E^2 \gamma^2},
$$
 (26)

FIG. 7. Calculated (a)–(c) and experimental (d)–(f) [\[28,29\]](#page-10-0) photoabsorption cross sections in spherical nuclei 16O, 40 Ca and deformed nucleus 24 Mg. We use the box size $R_{\text{box}} = 30$ fm and the SkM^{*} parameter set with $\gamma = 1$ MeV.

FIG. 8. Comparison of the calculated photoabsorption cross sections with different Skyrme parameter sets in ¹⁶O (a)–(d) and ²⁴Mg (g)–(j). The calculation is performed with the box size $R_{\text{box}} = 25$ fm. The experimental data are shown in panels (e) ¹⁶O and (f) ²⁴Mg.

where $\hat{\rho}_\tau(\vec{r}) = \sum_{i \in \tau} \delta(\vec{r} - \vec{r}_i)$. If there is a single state $|n\rangle$ that gives a dominant contribution in the vicinity of $E = \tilde{E}_n$ (within the width of γ), we have Im $\delta \rho(\omega) \propto \langle n|\hat{\rho}|0\rangle$.

In Fig. [9,](#page-9-0) we show the calculated transition densities of neutrons and protons, at $E = 19.4$ MeV for ¹⁶O [panel (a)] and at $E = 16.1$ MeV for the $K = 0$ mode of ²⁴Mg [panel (b)]. These energies correspond to the peak energies of the GDR. In the transition density of $16O$, one can clearly see the isovector character. In Fig. 9(c), we show $\partial \rho_0 / \partial r$ for ¹⁶O, where the $\rho_0(r)$ is the ground-state density profile. This corresponds to the transition density predicted by the Tassie model for an irrotational and incompressible fluid. As is discussed in the literatures [\[3\]](#page-10-0), the GDR of light nuclei is approximately represented by this classical fluid model. However, the transition density of $24Mg$ shows more complicated features. We show, in Fig. $9(d)$, a contour plot of the transition density in the Tassie model, $\delta \rho \propto \nabla \rho_0 \cdot \nabla r Y_{10}(\hat{r}) \sim \partial \rho_0 / \partial z$. Compared to the RPA transition density, there is a deviation, especially in the nodal structure in the interior region. This may suggest the importance of coupling of the dipole mode to the octupole and higher-multipole modes.

C. Heavy nuclei

For heavier nuclei, the calculation better agrees with experiments. As is well known, in heavy spherical nuclei, a single energy-weighted Lorentzian curve can fit the experimental data of the photoabsorption cross section very well [\[34\]](#page-10-0). We calculate photoabsorption cross sections in spherical nuclei ^{90}Zr , ¹²⁰Sn, and ²⁰⁸Pb within a box of radius $R_{\text{box}} = 15$ fm

and compare them with experimental data in Fig. [10.](#page-9-0) The calculated GDR peak shows a splitting, however, this may be due to the spurious effect coming from the box discretization. Except for this splitting, the results agree well with the experimental data. Table II shows the calculated and the experimental values of the GDR peak positions and the widths. Both values are extracted from the Lorentzian fit to the photoabsorption cross section. According to Ref. [\[34\]](#page-10-0), the Lorentzian function of the form of Eq. [\(16\)](#page-2-0),

$$
\sigma_{\rm abs}(E) = \frac{\sigma_0}{1 + \left(E^2 - E_{\rm peak}^2\right)^2 / (E^2 \Gamma^2)},\tag{27}
$$

is used. The GDR peak positions are well reproduced within an error of 400 keV. The systematic deviation of the peak energies, seen in calculations for light nuclei, are not observed for these heavy systems. Therefore, we may conclude that the SkM[∗] functional reproduces peak energies of the *E*1 resonances in heavy nuclei.

TABLE II. Calculated and experimental [\[34\]](#page-10-0) GDR peak energies and widths for $90Zr$, $120Sn$, and $208Pb$. The FAM calculation was performed with the same parameter set as Fig. [10.](#page-9-0)

Nucleus	Calculation		Experiment	
	E_{peak} (MeV) Γ (MeV)		$E_{\rm peak}$ (MeV)	Γ (MeV)
90Zr	16.37	3.85	16.74	4.16
^{120}Sn	15.22	4.52	15.40	4.89
208Ph	13.26	3.47	13.63	3.94

FIG. 9. (a) Contour maps of the calculated transition densities of $K = 0$ mode, Im $\delta \rho(\omega)$, in the *y*-*z* ($x = 0$) plane at $\omega = 19.4 + 0.5i$ MeV in 16O. Contour lines with positive, negative, and zero values are denoted by solid, dashed, and longdashed lines, respectively. Thick solid lines correspond to nuclear surface, defined by $y^2/(y^2)$ + $z^2/(z^2) = 1$. (b) The same as in (a) but for ²⁴Mg at $16.1 + 0.5i$ MeV. (c) Transition densities for the GDR in 16 O predicted by the Tassie model. The magnitude is fitted to the RPA result at the maximum value. (d) The transition densities of the Tassie model ($K = 0$ mode) for ²⁴Mg. See text for details.

The calculated widths are slightly smaller than the experiments, by 300 \sim 700 keV. Because we use $\gamma = 1$ MeV in these calculations, this indicates the spreading width of $\Gamma^{\downarrow} = 1.3 \sim 1.7$ MeV. The total damping width is about 4 MeV for these nuclei. Thus, the spreading width is less than half of the total width. This is rather surprising because, for heavy nuclei, the spreading width was supposed to be a major part of the total damping width [\[35,36\]](#page-10-0). However, the fragmentation of the strength into noncollective 1p-1h states (Landau damping), which can be described by the RPA theory, is significant for these heavy systems. Thus, the spreading width of $\Gamma^{\downarrow} \sim 1.5$ MeV is able to reproduce a broadening of the experimental strength distribution. This observation seems consistent with recent self-consistent RPA calculations for spherical nuclei [\[5,7\]](#page-10-0).

IV. CONCLUSIONS

We have presented an implementation of the FAM to make a fully self-consistent RPA calculation employing realistic Skyrme energy functionals. Although the RPA is a wellestablished theory and have been widely applied, a fully self-consistent calculation with a realistic functional is rather limited. This is mostly because of the complexity to construct the residual two-body kernels for realistic functionals. The FAM, which was proposed recently by the present authors, makes it possible to achieve a fully self-consistent RPA calculation without an explicit construction of the residual two-body kernels. Instead, the residual fields are evaluated by the finite difference, employing a computational code for the static mean-field Hamiltonian alone with a minor modification.

We implemented the FAM in the mixed representation where the *particle* index is replaced by the three-dimensional Cartesian grid points. In this representation, the linear response equation is a linear algebraic problem with a large, sparse, and non-Hermitian matrix. We have tested several solvers for the problem and have found that the generalized conjugate residual method works stably to obtain the solution. We also examined the accuracy of the FAM employing different values of the parameters η and have found that the method works robust; namely accurate results can be obtained for a certain wide range of the parameter *η*.

FIG. 10. Calculated photoabsorption cross sections for (a) $90Zr$, (b) $120Sn$, and (c) 208Pb. The calculation has been performed with $R_{\text{box}} = 15$ fm, the SkM^{*} parameter set, and $\gamma = 1$ MeV. The experimental data (symbols) are taken from Refs. [\[37–39\]](#page-10-0).

We show results for the electric dipole responses of several nuclei of spherical and deformed shapes. For light nuclei, we have found systematic underestimation of the average excitation energy, irrespective of the energy functional employed.We further notice the underestimation of the strength at energies higher than the GDR peak. The discrepancy is significant only for light nuclei. The average excitation energies of heavy nuclei are reasonably described. For a deformed nucleus ^{24}Mg , the calculation shows a deformation splitting of the giant dipole resonance, which well agrees with measurements. For spherical heavy nuclei, we have found a substantial part of the width can be explained within the RPA, leaving less than half of the total width for the spreading width, in contrast to the previous studies that reported that most of the width is attributed to the spreading mechanism for heavy nuclei [36].

We are currently performing a systematic calculation of the electric dipole responses for light to medium mass nuclei using the present method and Skyrme energy functionals. In a forthcoming article, we will report a systematic analysis of the

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properties of the giant dipole resonance, including the average excitation energy, width, and the low-lying dipole mode around the threshold.

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