Time-dependent density-functional studies on strength functions in neutron-rich nuclei

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The electric dipole (E1) strength functions have been systematically calculated based on the time-dependent density functional theory (TDDFT), using the finite amplitude method and the real-time approach to the TDDFT with pairing correlations. The low-energy E1 strengths in neutron-rich isotopes show peculiar behaviors, such as sudden enhancement and reduction, as functions of the neutron numbers. They seem to be due to the interplay between the neutron shell effect and the deformation effect.

Keywords: Time-dependent density-functional theory; E1 strength function; Neutron-rich nuclei

1. Introduction

The electric dipole (E1) response is a fundamental mode of excitation in nuclei and a useful tool to probe the isovector property of nuclei. The giant dipole resonance may provide information on the symmetry energy near the saturation density $\rho_0$. In contrast, the low-energy E1 modes, which are often referred to as pygmy dipole resonances, is sensitive to the nuclear structure and may carry information on the symmetry energy $E_{\text{sym}}(\rho)$ at densities away from $\rho_0$. Thus, the low-energy dipole modes in neutron-rich nuclei are of significant interest at present.

The low-energy dipole strengths have been experimentally observed in several neutron-rich isotopes; O isotopes,$^{1,2}$ $^{26}$Ne,$^3$ and Sn isotopes.$^4$–$^8$ The low-energy E1 strength observed in stable isotopes carries only less than $\leq 1 \%$ of the Thomas-Reiche-Kuhn (TRK) sum-rule value. In contrast, it may amount up to about 5 % in neutron-rich nuclei. Therefore, we may
expect a qualitative difference in properties of the low-energy dipole modes of excitation between in stable and in neutron-rich nuclei.

The time-dependent density-functional theory (TDDFT) provides us with a practical and reasonable description of nuclear strength functions. Its rigorous theoretical foundation is given by the one-to-one correspondence between the time-dependent external potential $v(t)$ and the time-dependent one-body density $\rho(t)$. In the Kohn-Sham scheme, it gives the time-dependent Kohn-Sham (TDKS) equations that are practically identical to the one known as the time-dependent Hartree-Fock (TDHF) equations in nuclear physics. An extension for the study of superconducting systems has been also carried out by including the time-dependent pair potential $\Delta(t)$ and the time-dependent pair density $\kappa(t)$. This eventually leads to the “time-dependent Bogoliubov-de-Gennes-Kohn-Sham (TDBdGKS) scheme”, which is, in nuclear physics, much more familiar with the name of “time-dependent Hartree-Fock-Bogoliubov (TDHFB) equation”. The TDBdGKS equations determine the time evolution of quasiparticle orbitals whose number is $2M$ where $M$ indicates the dimension of the single-particle model space. Since $M$ is significantly larger than the particle number $N$, it requires a huge computational task and becomes a challenging subject in computational nuclear physics.

In this paper, alternative approaches based on the TDDFT, which are computationally more feasible than the full solution of the TDBdGKS equations, are utilized to study the properties of the low-energy $E1$ strength. These methods will be briefly explained in Sec. 2. The numerical applications are given in Sec. 3.

2. Theoretical tools

We use the canonical-basis formulation of the TDBdGKS method and the finite amplitude method (FAM) to obtain low-energy $E1$ strength functions in neutron-rich nuclei. We briefly recapitulate these methods in the followings. Details of the method can be found in references given below.

2.1. Canonical-basis TDBdGKS equations

The real-time calculations of the TDKS equations have been carried out in real space. However, the computational cost is significantly increased by inclusion of the pairing correlation (TDKS $\rightarrow$ TDBdGKS), which makes practical applications very difficult. This numerical cost can be reduced, by several orders of magnitude, introducing an approximation for
the time-dependent pair potential, similar to the BCS approximation in static cases.\textsuperscript{16} This may lead to the following set of equations:

\[ i \frac{\partial}{\partial t} |φ_k(t)\rangle = (h(t) - η_k(t)) |φ_k(t)\rangle, \]
\[ i \frac{\partial}{\partial t} |φ_{¯k}(t)\rangle = (h(t) - η_{¯k}(t)) |φ_{¯k}(t)\rangle, \]

(1)

\[ i \frac{\partial}{\partial t} \rho_k(t) = κ_k(t) Δ_k^*(t) - κ_k^*(t) Δ_k(t), \]

(2)

\[ i \frac{\partial}{\partial t} κ_k(t) = (η_k(t) + η_{¯k}(t)) κ_k(t) + Δ_k(t) (2\rho_k(t) - 1). \]

(3)

Here, Eqs. (1) and (2) describes the time evolution of a pair of canonical states, \(|φ_k(t)\rangle\) and \(|φ_{¯k}(t)\rangle\). Their occupation and pair probabilities are given by Eqs. (3) and (4). The Hamiltonian \(h(t)\) is a functional of density \(h[ρ(t)]\), and \(η_k(t)\) and \(η_{¯k}(t)\) are arbitrary real parameters. In numerical calculations in Sec. 3, we adopt \(η_k(t) = \langle φ_k(t)|h(t)|φ_k(t)\rangle \) and \(η_{¯k}(t) = \langle φ_{¯k}(t)|h(t)|φ_{¯k}(t)\rangle\). The computational task for solution of these equations is roughly similar to that of TDKS equation.

### 2.2. Finite amplitude method for linear response

The finite amplitude method (FAM)\textsuperscript{17} is another feasible approach to the linear response calculation. The formulation has been extended to superfluid systems as well.\textsuperscript{18} The method allows us to easily construct a computer code for the linear response calculation based on the TDDFT. The FAM has been applied to the coordinate-space representation,\textsuperscript{17–21} and to the harmonic-oscillator-basis representation.\textsuperscript{22} The essential idea is that the complicated residual induced part of the Hamiltonian \(δh\) can be calculated in terms of the finite difference associated with the non-Hermitian density \(ρ_η\). Provided that \(|φ_k\rangle\) are the canonical single-particle states at the ground state \((h_0|φ_k⟩ = ε_k|φ_k⟩\) and \(ρ_0 = \sum_{i:hole} |φ_i⟩⟨φ_i|\),

\[ δh = \frac{1}{η} (h[ρ_η] - h_0), \]

(5)

\[ ρ_η = ρ_0 + ηδρ = \sum_{i:hole} |ψ_i⟩⟨ψ_i|, \]

(6)

where

\[ |ψ_i⟩ = |φ_i⟩ + η \sum_{m:particle} X_{mi}|φ_m⟩, \]

(7)

\[ ⟨ψ_{i}⟩ = ⟨φ_i⟩ + η \sum_{m:particle} Y_{mi}⟨φ_m⟩. \]

(8)
In the FAM, the induced field $\delta h$ for a given $(X,Y)$ can be estimated using Eq. (5). This only requires us to calculate the single-particle (Kohn-Sham) Hamiltonian $h[\rho]$ with different bra’s and ket’s in Eq. (6). Then, we resort either to iterative algorithms\textsuperscript{17,19,22} or to the matrix diagonalization,\textsuperscript{21} in order to obtain solutions of the linear-response equation $(X,Y)$.

3. Low-energy $E1$ strength

The $E1$ strength functions in even-even isotopes are systematically calculated. For relatively light nuclei, the FAM was used neglecting the pairing correlations.\textsuperscript{20} For heavier nuclei, in which the pairing is expected to play an important role, we use the real-time method based on the canonical-basis TDBdGKS method with a time-dependent perturbation of the external $E1$ field.\textsuperscript{15,16}

3.1. Shell effects

The photoabsorption cross sections for Ca isotopes ($N = 20 - 40$), estimated in the dipole approximation, are shown in Fig. 1. For Ca isotopes with $N = 20 - 28$, we see only negligible $E1$ strengths below $E = 10$ MeV. In contrast, those with $N = 30 - 40$ shows sizable $E1$ strengths below 10 MeV. This indicates that a sudden appearance of the low-energy $E1$ modes takes place beyond the magic number $N = 28$ in Ca isotopes. We have confirmed the same behavior in neighboring isotopes.\textsuperscript{20} Similar jumps of the low-energy $E1$ strengths can be observed at $N = 14 \rightarrow 16$ and $N = 50 \rightarrow 52$.\textsuperscript{20} These indicate a strong shell effect on the appearance of the low-energy $E1$ strength. These numbers are related to the occupation of single-particle orbitals with low orbital angular momenta, such as $s_{1/2}$ ($N = 14 \rightarrow 16$), $p_{3/2}$ ($N = 28 \rightarrow 30$), and $d_{5/2}$ ($N = 50 \rightarrow 52$). When these low-$\ell$ orbitals are weakly bound having spatially extended characters, we may expect the threshold effect which may enhance the $E1$ strengths near the neutron emission threshold energy. Thus, we suppose that the low-energy $E1$ strengths predominantly possess a single-particle nature.

3.2. Effects of deformation and separation energy

Let us move toward heavier isotopes. We use the canonical-basis TDBdGKS method to calculate the $E1$ strength distribution.\textsuperscript{9,16} We have found that the effect of pairing correlation is not so significant, in general. However,
for selected nuclei, the pairing correlation affects the shape of the ground state, which modifies the $E1$ properties accordingly.

We calculate the integrated energy-weighted $E1$ strength up to $E = E_c$, defined as

$$m_1(E_c) \equiv \int_0^{E_c} E \frac{dB(E1)}{dE} dE = \sum_{\mu=x,y,z} \int_0^{E_c} E \frac{dB(E1;\mu)}{dE} dE.$$  
(9)

In Fig. 2, the ratio of $m_1(10\text{ MeV})$ to $m_1(\infty)$ is shown for Sr isotopes. The ratio is less than 1% for isotopes with $N \leq 50$. Then, the ratio jumps up beyond $N = 50$, which is consistent with the argument given above. However, there are sudden drops of the low-energy $E1$ ratio at $N = 58 \rightarrow 60$ and $N = 72 \rightarrow 74$. This seems to be due to changes of the ground-state deformation.
The calculated ground states in even-even Sr isotopes with \( N = 40 - 50 \) are all spherical \((\beta = 0)\). The two-neutron separation energies, which are equal to twice of the chemical potential, gradually decrease as the neutron number increases. Then, the calculation predicts that the onset of the ground-state deformation takes place at \( N = 58 \rightarrow 60 \), from spherical to prolate shapes \((\beta = 0 \rightarrow 0.37)\). This shape transition result in the increase of the two-neutron separation energy and the decrease of the low-energy \( E1 \) strengths. The deformation stays rather constant for \( N = 60 - 72 \), with prolate shapes of \( \beta = 0.34 - 0.38 \) and with decreasing separation energies as increasing the neutron number. At \( N = 72 \rightarrow 74 \), again, the shape transition takes place, from prolate to oblate shapes, \((\beta, \gamma) = (0.34, 0) \rightarrow (0.14, 60^\circ)\). This shape change accompanies the increase of the separation energy and decrease of the low-energy \( E1 \) strength.

The low-energy strength can be decomposed into those associated with \( x, y, \) and \( z \) directions, as in the last equation in Eq. (9). This decomposition is also shown in Fig. 2. The \( z \) axis is chosen as the symmetry axis for axially deformed nuclei. For prolate Sr isotopes with \( N = 60 - 72 \), the strength associated with the \( z \) \((K = 0)\) component is dominant. The \( K = 0 \) dominance was also reported for neutron-rich Sn isotopes using the relativistic quasiparticle random phase approximation.\textsuperscript{23} This was interpreted by the conjecture that the neutron skin is thicker in the \( z \) direction than the \( x \) and \( y \) directions. We calculate the neutron-skin thickness in the \( x \) direction as

Fig. 2. \( m_1(E)/m_1(\infty) \) with \( E = 10 \) MeV for even-even Sr isotopes. The calculation was performed with the SkM* functional using the canonical-basis TDBdGKS equations. See text for details.
\[ \Delta x_{np} = \sqrt{\langle x^2 \rangle_n} - \sqrt{\langle x^2 \rangle_p}, \] and those for y and z directions in exactly the same way. It turns out that \( \Delta r_{np} \) is even larger with respect to the x (y) direction than the z direction, for prolate nuclei. Therefore, the observed \( K = 0 \) dominance in the low-energy \( E1 \) strength cannot be attributed to the different neutron skin thickness. This suggests that these low-energy strengths are not associated with the skin modes.

4. Summary

The \( E1 \) strength functions have been systematically calculated with the finite amplitude method and the real-time method, based on the time-dependent density functional theory. The low-energy \( E1 \) strength distributions in stable and neutron-rich isotopes were estimated from these calculations. We have found a strong neutron shell effect and have identified magic numbers for the appearance of low-energy \( E1 \) modes. The deformation and separation energies also play an important role in the low-energy \( E1 \) strength distribution.

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