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Uncertainty evaluation of peak energy of giant dipole resonance propagated from uncertainty of parameters of effective interaction

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Abstract. We evaluate uncertainty of giant dipole resonance (GDR) peak energy propagated from the uncertainty of effective interaction parameter. The Monte Carlo calculation of microscopic random phase approximation using randomized parameter sets is performed. Under the condition that correlations between the parameters are considered, the calculated GDR peak energy has an uncertainty of ~1 MeV irrespective of nuclear mass and is strongly correlated with the parameters, in the present calculations. Our result serves as a guide for a new parametrization of effective interaction.

1 Introduction

Random phase approximation (RPA) calculation with effective interaction is one of the standard theoretical tools to calculate photoabsorption cross section in MeV region from the degree of freedom of nucleons, and has been applied to systematic calculations of nuclei covering wide range of the nuclear chart [1,2]. However, it is known that the RPA calculation with Skyrme effective interaction underestimates peak energies of giant dipole resonances (GDRs) in light nuclei by a few MeV.

The parameters of effective interactions are determined to reproduce limited sets of experimental data of ground states and nuclear matter properties. This limitation raises the question of its predictive power especially for excited states. Therefore, uncertainty estimation of the calculated values and feedback to the parameters are strongly desired. In the last decade, many theoretical studies have estimated uncertainty of calculated values and correlations of calculated values and the parameters [3-10]. However, these results are not used to improve the parameters of the effective interactions. This is because the relations between the parameters and the calculated values are not known clearly.

In this study, we performed Monte Carlo calculation of RPA using randomized parameters in Skyrme interaction. We evaluated the uncertainty of the GDR peak energy, propagated from the uncertainties of Skyrme parameters. By explicit taking the correlations of the parameters in randomization, we found that there are strong correlations between the Skyrme parameters and the calculated GDR peak energy.

2 Method

We employ Skyrme SLy5-min parameter set as the effective interaction. The SLy5-min parameters and their uncertainties Δp_i [8] are listed in Table **1**. Note that parameters x_2, W_0, and α are fixed when the SLy5-min parameters were determined and thus they do not have uncertainties. Table **2** shows a part of correlation matrix of the SLy5-min parameters. Other matrix elements of correlation $\boldsymbol{C}$ are listed in Ref. [11].

Table 1. Parameter name $\boldsymbol{p}$, their optical value $\boldsymbol{p_0}$, uncertainty $\boldsymbol{\Delta p}$ for SLy5-min parameters [8].

$\boldsymbol{p}$	$\boldsymbol{p_0} \pm \boldsymbol{\Delta p}$	Unit
t_0	-2475.408±149.455	MeV fm^3
t_1	482.842±55.537	MeV fm^5
t_2	-559.374±144.534	MeV fm^5
t_3	13697.07±1672.93	MeVfm$^{3+\alpha}$
x_0	0.741185±0.189191	
x_1	-0.146374±0.468173	
x_2	-1: fixed	
x_3	1.162688±0.340537	
W_0	126: fixed	MeV fm^5
α	1/6: fixed	

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Table 2. Part of correlation matrix elements of SLy5-min parameters, $\boldsymbol{C}$.

	t_0	t_1	t_2	t_3
t_0	1.0000	0.9837	0.9854	-0.9997
t_1	0.9837	1.0000	0.9575	-0.9870
t_2	0.9854	0.9575	1.0000	-0.9863
t_3	-0.9997	-0.9870	-0.9863	1.0000

For the Monte Carlo calculation using randomized SLy5-min parameter sets, we generate $n = 1000$ random samples, $\boldsymbol{X}^{(j)}$ $(j = 1,2, \ldots, n)$, which satisfy the correlation $\boldsymbol{C}$. Before generating the random samples, we introduce a one-dimensional normal distribution $N(\mu, \sigma)$, where μ and σ are mean value and standard deviation of the distribution, respectively. And in preparation, the correlation matrix $\boldsymbol{C}$, which is positive semidefinite matrix, is factorized as $\boldsymbol{C} = \boldsymbol{Q}^T\boldsymbol{Q}$ by the singular value decomposition.

First, we generate n sets of random independent samples $\overline{\boldsymbol{X}}^{(j)} = \left(\overline{x}_1^{(j)}, \overline{x}_2^{(j)}, \ldots\, \overline{x}_m^{(j)}\right)^T$ from a normal distribution $N(0,1)$. Namely, each variable is $N(0,1)$ and is uncorrelated with each others. Secondly, we act the factorized matrix $\boldsymbol{Q}$ on each $\overline{\boldsymbol{X}}^{(j)}$, i.e., creating correlated samples $\left(\boldsymbol{Q}\overline{\boldsymbol{X}}\right)^{(j)}$ satisfying the correlation $\boldsymbol{C}$. Thirdly, we shift the mean value and standard deviation, $X_i^{(j)} = p_{0i} + \left(Q\overline{X}\right)_i^{(j)} \Delta p_i$, employing $\boldsymbol{p_0}$ and $\boldsymbol{\Delta p}$ in Table 1. These are the correlated random parameter sets of SLy5-min.

Using these randomized parameter sets $\boldsymbol{X}^{(j)}$, we perform the RPA calculations n times. The RPA solver is Skyrme-rpa [12]. The Skyrme-rpa solves the RPA equation for spherical nuclei in the coordinate representation. The calculation space is a sphere with radius 25 fm and mesh span 0.1 fm. The photoabsorption cross section is computed from the resulting dipole strength functions and smeared with a width $\Gamma = 2$ MeV. From this photoabsorption cross section, we extract the position of the GDR peak top of jth random parameter set, $E_{GDR}^{(j)}$. This calculated $E_{GDR}^{(j)}$ is different form one that the original SL5-min parameter set $\boldsymbol{p_0}$ produces because different parameter set $\boldsymbol{X}^{(j)}$ is used. These are repeated $n = 1000$ times. The mean value and the standard deviation of the calculated GDR peak energies are obtained by statistical process from these 1000 results. This is the uncertainty evaluation of E_{GDR} propagated from the uncertainties of the parameters.

3 Results and discussion

The photoabsorption cross sections in ^{40}Ca calculated with the random parameter sets are plotted in **Figs. 1**. In **Fig. 1(b)**, the red line shows the photoabsorption cross section calculated with the original SLy5-min parameter set, and black lines are those with the randomized parameter sets. **Figure 1(a)** shows histogram of the randomized GDR peak energies. Arrow denotes mean value of the peak energies and its standard deviation, 17.9 ± 1.5 MeV. Remarkably, the randomized GDR peak energies have two regions separated in their energy. In upper energy region, the randomized peak energies scatter around $E_{GDR} = 18.3$ MeV that the original SLy5-min results. In the lower energy region at ≤ 17 MeV, the bunch is clearly separated from the upper one, while the number of the low-energy randomized peaks is ~ 200. These peaks originate from a shoulder at 17 MeV of the original cross section denoted by led line in **Fig. 1(b)**.

Figure 1(c) shows averaged cross section and its standard deviations. If the parameter uncertainties are small, $\frac{|p_i - \Delta p_i|}{|p_i|} \ll 1$, the averaged cross section is expected to be close to the original cross section. However, the averaged cross section is different from the original one. The GDR peak height is lowered, its width is broadened

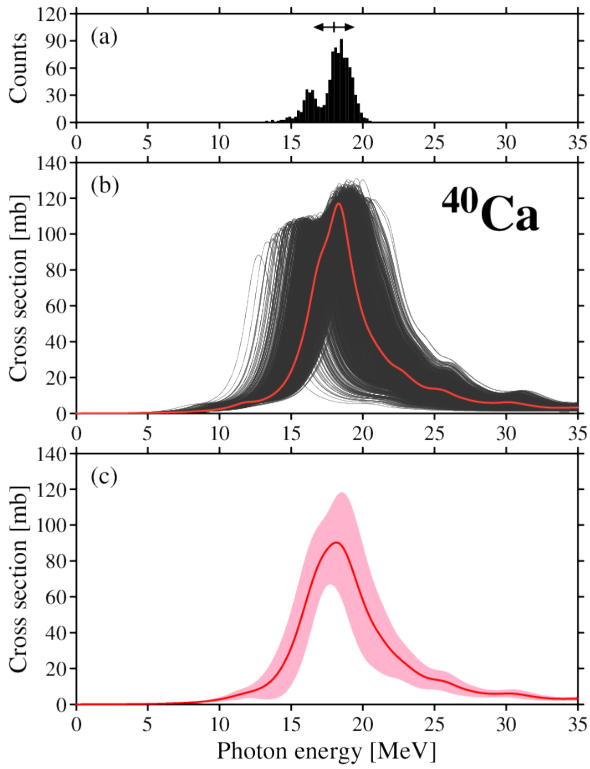

Fig. 1 ^{40}Ca photoabsorption cross sections with randomized parameter sets of SLy5-min interaction. (a) histogram of peak energies. Arrow denotes the mean value of randomized peak energies and standard deviation. (b) photoabsorption cross section calcauated with the original SLy5-min interatrction (red) and those with randomized parameters (black). (c) Averaged cross section (red) with standard deviation (shaded red area).

To see which parameter affects the GDR peak energy, we calculate the Pearson correlation coefficient of the GDR peak energies and the parameters p_i. **Figures 2** show relations of the randomized parameters

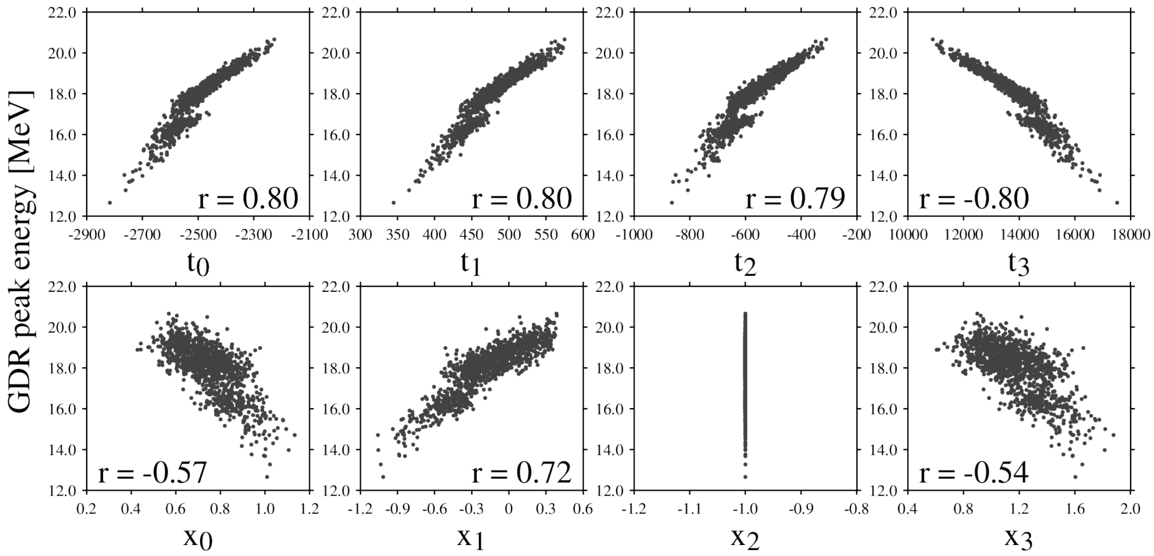

Fig. 2 Relations between the radomized GDR peak energies and paramers, $\boldsymbol{t_0}, \boldsymbol{t_1}, \boldsymbol{t_2}, \boldsymbol{t_3}, \boldsymbol{x_0}, \boldsymbol{x_1}, \boldsymbol{x_2}$, and $\boldsymbol{t_3}$, and Pearson correlation coefficients.

and the corresponding randomized GDR peak energies. Note that the parameters x_2, W_0, and α are fixed in the SLy5-min parameter set, and therefore the relations of W_0 and α are not plotted and always $x_2 = -1$. The randomized GDR peak energies have strong correlations with t_0, t_1, t_2, and t_3, and their Pearson correlation coefficients calculated from all randomized GDR peak energies are 0.8 or -0.8. Since the randomized GDR peak energies has two separated bunches [See **Fig. 1(a)**], the plotted relations are also separated into upper- and lower-energy regions. If we pick up the upper-energy region only, the correlations become stronger.

Similar values of these Pearson correlation coefficients are related to the strong correlations between t_0, t_1, t_2, and t_3, shown in **Table 2**. The moduli of the correlations between t_0, t_1, t_2, and t_3 are larger than 0.95. This means that uncertainties of t_1, t_2, and t_3 are almost redundant and can be approximated by the uncertainty of t_0. Similar is seen in the relations of the randomized GDR peak energies and the parameters x_0, x_1, and x_3. The moduli of the correlations between x_0, x_1, and x_3 are larger than 0.93. The strong correlations between the randomized GDR peak energies and the parameter enable us to improve the calculated GDR peak energy by tuning the parameters.

Same Monte Carlo calculations are performed for spherical nuclei, ^{16}O, ^{90}Zr, and ^{208}Pb. **Figures 3** show the averaged cross sections and the standard deviations in ^{16}O, ^{90}Zr, and ^{208}Pb. The averaged GDR peak energies and their standard deviations are listed in **Table 3**. The standard deviations of the GDR peak energies are 1.0-1.5 MeV, irrespective of nuclear mass. The Pearson correlation coefficients between the randomized GDR peak energies and the randomized parameters $t_{0,1,2,3}$ in ^{16}O, ^{90}Zr, and ^{208}Pb are strong, similar to those in ^{40}Ca. These moduli are approximately 0.83, 0.86, 0.65, respectively. Also, the correlation coefficients of $x_{0,1,3}$ are almost same as those in ^{40}Ca. The uncertainty propagation from the parameters to the GDR peak energies are not sensitive to nuclear mass.

Table 3. Averaged GDR peak energies and standard deviations for ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb, obtained by Monte Carlo calculation using randomized SLy5-min parameter sets.

	Averaged E_{GDR} and deviations
^{16}O	19.10 $\pm$ 1.21 MeV
^{40}Ca	17.89 $\pm$ 1.46 MeV
^{90}Zr	15.70 $\pm$ 1.08 MeV
^{208}Pb	12.93 $\pm$ 1.19 MeV

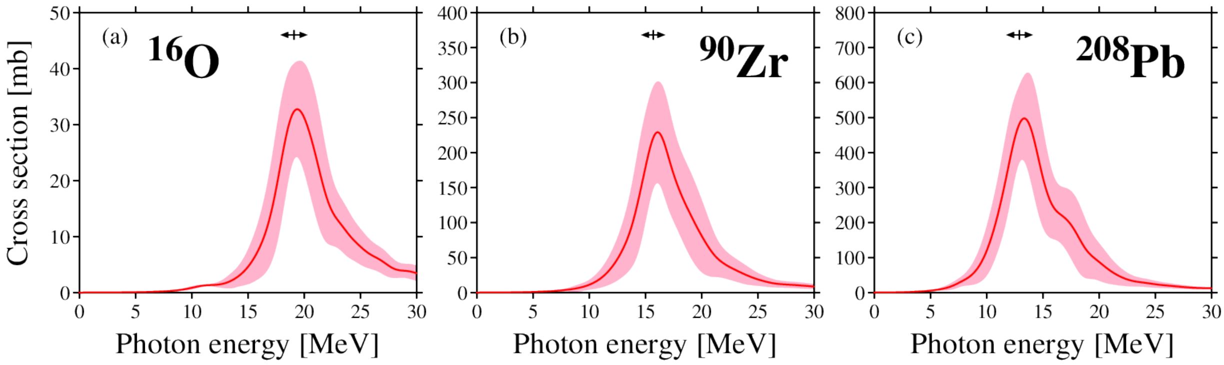

Fig. 3 Same as Fig. 1(c) but for (a) ^{16}O, (b) ^{90}Zr, and (c) ^{208}Pb.

4 Conclusion

We performed the Monte Carlo calculation to evaluate the uncertainty of the GDR peak energy, propagated from the uncertainties of effective interaction parameters. The RPA calculation with randomized parameters is applied to spherical nuclei, ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb. In the case that SLy5-min parameters is employed with the correlations between the parameters, the standard deviations of the GDR peak energies E_{GDR} are ~ 1 MeV, irrespective of nuclear mass. The GDR peak energy has strong correlations with the parameters. These correlations enable us to handle the calculated GDR peak energy by tuning the parameters.

One of the promising ways to tune the parameters is by shifting some parameters in directions that calculated E_{GDR} becomes higher, such as $t_0 \rightarrow t_0 + \frac{f\Delta t_0}{A}$, with satisfying the correlation matrix (**Table 2**). Here f is a free parameter. We introduce mass dependence to push up E_{GDR} larger (smaller) for lighter (heavier) nuclei. We have the plan to propose a new parameter set that reproduces E_{GDR} properly.

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