Sensitivity of Fission Properties to Variations in Zero-Range Pairing Forces within Density Functional Theory

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Date: 2024-02-21T13:08:44+00:00

Abstract

By the Skyrme density functional theory (DFT), potential energy surfaces (PES) of ^{240}Pu with constraints on the axial quadrupole and octupole deformations(q_{20} and q_{30}) are calculated.The volume-like, and the surface-like pairing forces, and the mixing between these two forces are used, within the Hartree-Fock-Bogoliubov (HFB) approximation. The variations of the least-energy fission path, fission barrier, paring energy, total kinetic energy, scission line, and mass distribution of fission fragments by the different forms of paring force are analyzed and discussed. The fission dynamics is studied based on the time-dependent generator coordinate method (TDGCM) plus Gaussian overlap approximation (GOA). The results show a sensitivity of the mass and charge distributions of fission fragments to the form of the pairing force. Based on the investigation of the neutron-induced fission of ^{239}Pu, among the volume, mixed, and surface pairing forces, the mixed-type of pairing force can give a good reproduction of experimental data.

Full Text

Preamble

Using the Skyrme density functional theory (DFT), we calculated potential energy surfaces (PES) of ^{240}Pu with constraints on the axial quadrupole and octupole deformations (q_{20} and q_{30}). The Hartree-Fock-Bogoliubov (HFB) approximation was employed with volume-like and surface-like pairing forces, as well as a combination of these two forces. We analyzed and discussed variations in the least-energy fission path, fission barrier, pairing energy, total kinetic energy, scission line, and mass distribution of fission fragments based on the different forms of the pairing forces. Fission dynamics were studied using

the time-dependent generator coordinate method (TDGCM) plus the Gaussian overlap approximation (GOA). The results demonstrated sensitivity of the mass and charge distributions of the fission fragments to the form of the pairing force. Based on our investigation of neutron-induced fission of ^{239}Pu, the mixed pairing force provided the best reproduction of experimental data among the volume, mixed, and surface pairing forces.

Keywords: Nuclear fission, density functional theory, pairing force, potential energy surfaces, fission fragment distribution

Introduction

Nuclear fission—the phenomenon in which a (usually heavy) atomic nucleus separates into two or more fragments—was discovered more than eighty years ago [?, ?]. It is accompanied by the release of abundant energy [?] and has a wide range of applications. In addition to its important applications in energy production and rare isotope generation, fission also plays a crucial role in fundamental physics, such as synthesizing superheavy elements [?, ?, ?] and constraining the r-process in neutron-star mergers [?]. Consequently, several theoretical approaches have been utilized to describe the fission process and observations [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. As shown in Ref. [?], microscopic models applied to fission thus far utilize density functional theory (DFT), which is based on effective nucleon-nucleon interactions.

As one of the dominant residual correlations in atomic nuclei, the pairing interaction is critical for understanding the fission process. Extensive studies regarding the influence of pairing interactions on fission properties have been performed, examining effects on fission barrier heights, fission isomer excitation energies, and collective inertia [?, ?, ?, ?, ?, ?]. In Ref. [?], a fission dynamic calculation based on covariant DFT was performed for the fission of ^{226}Th, in which both symmetric and asymmetric fission modes co-exist. The asymmetric fission mode dominated as the pairing force decreased, whereas the symmetric fission mode dominated as the pairing force increased. The time-dependent superfluid local density approximation (TDSLDA) method has demonstrated that fission significantly accelerates as the pairing force increases [?]. The effect of dynamic pairing correlations on the fission process was studied in Refs. [?, ?].

In our previous work, we studied the role of the pairing force on static fission properties and the fission dynamic process [?, ?, ?, ?], which demonstrated that variation in the strength of the pairing correlation can significantly influence the fission process. However, whether the form of the pairing force can also impact fission properties is noteworthy. A schematic pairing force was originally introduced in [?], and parameters of the density-dependent pairing correlation were studied in Refs. [?, ?, ?]. Specifically, considering Skyrme-DFT, different types of pairing forces have been used for studying nuclear structure, such as volume-like, surface-like, and mixed-type pairing forces. In Refs. [?, ?, ?], various types of pairing interactions (volume-, surface-, and mixed-type pairing forces) were used to study pairing gaps in even-even nuclei across the entire nuclear chart, the odd-even staggering behavior of binding energies around tin isotopes, and to predict two-neutron separation energies and neutron pairing gaps [?]. In this study, we investigated whether the form of the pairing force can influence both the static aspects of fission properties and dynamics. We studied the fission process of ^{240}Pu in the Skyrme DFT and time-dependent generator coordinate method (TDGCM) + Gaussian overlap approximation (GOA) framework.

In Section II, we briefly describe the main features of our theoretical approach. Section III presents and discusses detailed results for the least-energy fission path, fission barrier, pairing energy, total kinetic energy, scission line, and mass distribution of fission fragments using various types of pairing forces. Finally, Section IV summarizes our principal results.

II. Theoretical Framework

We applied Skyrme DFT as the microscopic method to study static fission properties and prepare input files for dynamic calculations. The dynamic process was further investigated within the TDGCM framework. In this section, we briefly explain these two methods. Detailed formulations of Skyrme DFT can be found in Ref. [?], and those of TDGCM can be found in Refs. [?, ?, ?].

A. Density Functional Theory Approach for Static Fission Properties

For the local density approximation of DFT, the total energy of finite nuclei can be calculated using the space integral of the Hamiltonian density $\mathcal{H}(\mathbf{r})$, which consists of the kinetic energy τ, potential energy χ_t, and pairing energy $\tilde{\chi}_t$ densities:

$$\mathcal{H}(\mathbf{r}) = \tau(\mathbf{r}) + \sum_{t=0,1} \chi_t(\mathbf{r}) + \sum_{t=0,1} \tilde{\chi}_t(\mathbf{r}).$$

Here, $\tau(\mathbf{r})$ is the kinetic energy density, and the symbol $t = 0, 1$ indicates isoscalar or isovector, respectively [?].

The mean-field potential energy in the Skyrme DFT usually has the following form:

$$\chi_t(\mathbf{r}) = C_t^{\rho\rho}\rho_t^2 + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\tau}\rho_t\tau_t + C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t + C_t^{J^2}\mathbf{J}_t^2 + C_t^{\nabla\rho}\nabla\rho_t\cdot\nabla\rho_t + C_t^{\nabla J}\nabla\cdot\mathbf{J}_t.$$

Here, the particle density ρ_t, kinetic density τ_t, and spin-current vector densities $\mathbf{J}_t$ $(t = 0, 1)$ can be obtained from the density matrix $\rho_t(\mathbf{r}\sigma, \mathbf{r}'\sigma')$, depending on the spatial $(\mathbf{r})$ and spin (σ) coordinates. In the aforementioned formula, $C_t^{\rho\rho}$, $C_t^{\rho\Delta\rho}$, and etc. are the coupling constants in the Hamiltonian density $\mathcal{H}(\mathbf{r})$, corresponding to different types of densities, most of which are real numbers;

$C_t^{\rho\rho}$ is an exception, which is the traditional density-dependence term. Expressions relating the coupling constants to the standard Skyrme parameters can be found in Ref. [?]. Specifically, the spin-orbit interaction in the Skyrme force corresponds to the term $C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t$.

In DFT, the pairing correlation is usually incorporated by the Hartree-Fock-Bogoliubov (HFB) method [?]. For the Skyrme energy density functional, a commonly used pairing force is the density-dependent, zero-range potential, which can be expressed as follows [?, ?]:

$$\hat{V}_{\text{pair}}(\mathbf{r},\mathbf{r}') = V_0^{(n,p)}\left[1-\eta\left(\frac{\rho(\mathbf{r})}{\rho_0}\right)^{\gamma}\right]\delta(\mathbf{r}-\mathbf{r}').$$

Here, $V_0^{(n,p)}$ is the pairing strength for neutrons (n) and protons (p), the exponent γ of the density-dependence affects the appearance of neutron skins and halos [?], for which $\gamma = 1$ is widely used [?, ?]. ρ_0 is the average density inside the nucleus (often considered as the saturation density of nuclear matter, and set as 0.16 fm^{-3}), and $\rho(\mathbf{r})$ is the total density. Different types of pairing forces can be obtained by choosing different values of η. The pairing force is "volume-like" when $\eta = 0$, indicating no explicit density dependence. The pairing force acts equivalently inside the nuclear volume. In contrast, the pairing force will be "surface-like" for $\eta = 1$, which has a significant effect around the nuclear surface and a small impact in the central area of the nucleus. The choice of $\eta = \frac{1}{2}$ is often called a mixed-pairing force, which is the average of these two types of pairing forces. To test sensitivities of fission-related properties based on the form of the pairing force, we considered $\eta = 0, 0.25, 0.5, 0.75$, and 1. Values $\eta = 0.25$ and 0.75 were used for test purposes, while the other choices of η values have been frequently used for structural studies.

B. Time-Dependent Generator Coordinate Method for Fission Dynamics

Fission is a large-amplitude collective motion that can be described as a slow adiabatic process driven by a few collective degrees of freedom within the framework of TDGCM. In this approach, the many-body state wave function of the fissioning system can be expressed by the following generic form:

$$|\Psi(t)\rangle = \int f(\mathbf{q},t)|\Phi(\mathbf{q})\rangle d\mathbf{q}.$$

Here, $|\Phi(\mathbf{q})\rangle$ consists of a set of known many-body wave functions parameterized by a vector of continuous variables $\mathbf{q}$. Each of these $\mathbf{q}$ is a collective variable chosen based on the specific physics problem. The quadrupole moment $\hat{Q}_{20}$ and octupole moment $\hat{Q}_{30}$ are usually chosen as collective variables for fission studies. $f(\mathbf{q},t)$ is the weight function, which is solved using the time-dependent

Schrödinger-like equation in the space of the coordinates $\mathbf{q}$. Under the GOA, this equation can be expressed as follows:

$$i\hbar \frac{\partial g(\mathbf{q},t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q}) g(\mathbf{q},t).$$

The collective Hamiltonian $\hat{H}_{\text{coll}}(\mathbf{q})$ is:

$$\hat{H}_{\text{coll}}(\mathbf{q}) = -\sum_{ij} \frac{\partial}{\partial q_i} B_{ij}(\mathbf{q}) \frac{\partial}{\partial q_j} + V(\mathbf{q}),$$

where $V(\mathbf{q})$ is the collective potential, and the inertia tensor $B_{ij}(\mathbf{q}) = \mathcal{M}^{-1}(\mathbf{q})$ is the inverse of the mass tensor $\mathcal{M}$. The potential and mass tensor are determined by the Skyrme DFT in this study. $g(\mathbf{q},t)$ is the complex collective wave function of the collective variables $\mathbf{q}$ and contains all information regarding the dynamics of the fission system.

For the description of fission, the collective space is divided into an inner region with a single nuclear density distribution and an external region that contains the two fission fragments. The scission contour defines the hyper-surface that separates these two regions. The flux of the probability current through this hyper-surface provides a measure of the probability of observing a given pair of fragments at time t. The integrated flux $F(\xi,t)$ for the surface element ξ on the scission hyper-surface is calculated as follows:

$$F(\xi,t) = \int_0^t \int_\xi \mathbf{J}(\mathbf{q},t) \cdot d\mathbf{S},$$

as in Ref. [**?**], where $\mathbf{J}(\mathbf{q},t)$ is the current:

$$\mathbf{J}(\mathbf{q},t) = \mathbf{B}(\mathbf{q})[g^*(\mathbf{q},t)\nabla g(\mathbf{q},t) - g(\mathbf{q},t)\nabla g^*(\mathbf{q},t)].$$

The yield of the fission fragment with mass number A can be calculated as follows:

$$Y(A) = C \sum_{\xi \in A} F(\xi,t),$$

where A indicates a set of all the surface elements ξ on the scission hyper-surface with a fragment mass of A, and C is the normalization constant to ensure that the total yield is normalized to 200 as usual. The yield of the fission fragment with charge number Z can also be obtained from the integrated flux $F(\xi,t)$. The mass number A can be replaced with the charge number Z in Eq. (9); the summation is then over the set of all ξ values on the scission frontier with the fragment charge number Z. In this study, the FELIX (version 2.0) [?] computer code was used to model the time evolution of the fissioning nucleus in the TDGCM+GOA framework.

III. Results and Discussion

We studied the influence of different types of pairing forces on fission properties based on Skyrme DFT with SkM* parameters [?]. The DFT solvers HFBTHO (V3.00) [?] were used to calculate the potential energy surfaces (PESs). Axial symmetry was assumed. Thirty-one major shells of the axial harmonic-oscillator single-particle basis were used, and the number of basis states was further truncated to 1100. In this study, we considered five values of η (0, 0.25, 0.5, 0.75, and 1) in Eq. (3) as different types of pairing forces. For each value of η, the pairing strength for neutrons and protons was adjusted to reproduce the pairing gap of ^{240}Pu extracted from the three-point formula of the odd-even mass staggering. A cutoff of 60 MeV was used as the pairing window in all calculations.

Figure 1 presents the pairing strengths of neutrons and protons for pairing forces with different values of η. For η near 0, pairing tends to occur equivalently throughout the nuclear volume. When η is near 1, pairing tends to peak at the nuclear surface. For η between 0.0 and 0.5, the absolute value of the pairing strength increased nearly linearly. However, for $\eta = 1.00$, there was a sudden increase in pairing strength. The surface-like pairing force requires a significantly larger strength to produce the same pairing gap compared to volume-like or mixed-type pairing forces. These results are consistent with previous studies. As demonstrated in Refs. [?, ?], the surface pairing force is also significantly stronger than the volume and mixed pairing forces.

A. Potential Energy Surface

The calculation of multidimensional PESs is the first step toward the dynamical description of fission. In this study, we chose the quadrupole moment (q_{20}) and octupole moment (q_{30}) as collective parameters, which are the most important collective degrees of freedom for nuclear fission studies; they describe the elongation of the nucleus and mass asymmetry, respectively. Figure 2 presents the PESs of ^{240}Pu calculated using the HFB method with five different types of pairing forces ($\eta = 0, 0.25, 0.5, 0.75$, and 1.0) in the collective space of (q_{20}, q_{30}). The collective variables ranged from 0 to 600 b for q_{20} and from 0 to 60 b$^{3/2}$ for q_{30} with steps of $\Delta q_{20} = 2$ b and $\Delta q_{30} = 2$ b$^{3/2}$.

As shown in Figure 2, there is no notable difference in the topological properties of PESs with different types of pairing forces. Double-humped fission barriers were predicted for all cases. An inner symmetric fission barrier followed by an outer asymmetric barrier was clearly distinguished. At $q_{20} > 200$ b, symmetric valleys with large elongations were found. The symmetric and asymmetric fission valleys were well-separated by a ridge from $(q_{20}, q_{30}) \approx (150\text{ b}, 0\text{ b}^{3/2})$ to $(350\text{ b}, 20\text{ b}^{3/2})$, and the height of the ridge gradually decreased as the η value increased. Therefore, the density-dependent surface pairing force led to a reduction in ridge height. In addition, the asymmetric fission channel was favored for all least-energy fission pathways, as indicated by the red lines in Figure 2.

Energies along the symmetric and asymmetric fission paths as functions of the quadrupole moment (q_{20}) are provided in Figures 3(a) and 3(b), respectively. The value of η varied from 0 to 1, indicating a transition from "volume-like" to surface pairing force. Figure 3 demonstrates that fission barrier heights and isomeric-state energies decrease as η increases. Specifically, when $\eta > 0.5$, the fission barriers explicitly decrease. For the least-energy fission pathway shown in Figure 3(b), a smaller quadrupole moment is needed for scission to occur for larger η.

As indicated in Sec. II.B, obtaining the precise collective mass tensor is essential for the adiabatic approximation approach to fission dynamics. Table 1 lists the energies of the ground state, isomeric states, and fission barrier heights for different types of pairing forces, along with the corresponding quadrupole and octupole moments for each state. The energies of the isomeric state and heights of the fission barrier decrease as the η value increases. Owing to the lack of triaxial deformation in our collective space, the heights of the fission barriers would be higher than those experimentally obtained, especially for the inner fission barrier [**?**, **?**]. As indicated in the table, for $\eta = 1$, the inner fission barrier height was near that demonstrated by the data, and the outer fission barrier was lower than that in the data, leaving no room for the triaxial degree of freedom. Thus, $\eta = 1$ (surface pairing force) may not be a good choice for fission studies. Based on Table 1, the deformations of these states, including the ground state, isomeric state, and inner and outer barriers, are generally not influenced by the type of pairing force. These deformations are mainly determined by the shell structure given by the mean-field potential. In our previous study [**?**], we also found that these deformations were relatively stable against variations of the pairing strength.

B. Pairing Energies

Figure 4 presents the pairing energies at different deformations for various types of pairing forces. The pairing energies at the ground and isomeric states are smaller than those at the fission barriers. At the same state, the pairing energy increases as the value of η increases, especially for $\eta = 1$, which corresponds to the surface-type pairing force. The pairing gaps at different deformations are provided in Figure 5. Once again, the pairing gap has a minimum at the ground state and a second minimum at the isomeric states. The pairing gaps are large around the fission barriers. For the adjustment of the strength of the different pairing forces used in this study, the same values of the pairing gaps in ^{240}Pu were used. The figure demonstrates that in the smaller deformation region, the pairing gaps from the different types of pairing forces were relatively similar. However, when the deformation was large, explicit discrepancies appeared ($q_{20} > 150$ b). For the pairing force with a smaller η value, the neutron and proton pairing gaps were generally smaller.

C. Mass Tensor

The mass tensor $\mathcal{M}$ reflects the response of the fissioning system to changes in collective coordinates. In this study, mass tensors were obtained from static calculations using the Skyrme DFT with the perturbative cranking approximation. As shown in Figure 6, the elements of the mass tensor M_{22}, M_{33}, and M_{23} are plotted as functions of q_{20} along the lowest-energy fission path for different choices of η. The mass tensor given by ATDHFB was larger than that by GCM for all types of pairing forces. As indicated in Ref. [**?**], this was caused by missing correlations in the GCM method. Generally, as the quadrupole moments increase, M_{22} and M_{33} gradually decrease. M_{23} is negative, and its absolute value increases with explicit fluctuations when the deformation is large. For different types of pairing forces tuned by η, the mass tensor apparently decreases and demonstrates reduced fluctuation against deformations when η is large. As indicated in Ref. [**?**], considering the mixed pairing force with $\eta = 0.5$, the mass tensor decreases and fluctuates less when the pairing strength is decreased. The systematic behavior of the $\eta > 0.5$ pairing force resembles that of increasing the strength of the pairing force.

D. Scission Lines

Determining the scission frontier is critical for describing fission dynamics. In DFT, the operator $q_N = \langle \hat{Q}_N \rangle = \langle e^{-(z-z_N)^2/a_N^2} \rangle$ is often used to evaluate the neck size of the fissioning nuclei, with $a_N = 1$ fm typically chosen. z_N is the neck position, which has the lowest density between the two fragments. Generally, the neck size smoothly decreases as the fissioning nucleus elongates, and decreases to nearly zero after scission, where the two fragments are sufficiently separated. In this study, we chose $q_N = 4$ as the critical value for determining the scission line in ^{240}Pu, which has been used in Refs. [**?**, **?**]. This value was chosen at the edge of the sudden decrease in neck size, maintaining most of the pre-fission configurations for further fission dynamic calculations. The scission lines in the PES of the (q_{20}, q_{30}) collective spaces obtained by DFT using different types of pairing forces are shown in Figure 7. Generally, the scission contours for different η values display similar patterns. For different η values, in or around the region of symmetric fission, the increase of η leads to a smaller quadrupole moment at the scission point. For $\eta = 1.0$, symmetric fission occurred at $q_{20} \sim$ 480 b, whereas it occurred at approximately 550 b for other η values. The shortest elongation occurred at $q_{20} \sim 300$ b when the asymmetry increased to the octupole moment $q_{30} \sim 30$ b$^{3/2}$. Subsequently, the scission lines turned toward the upper-right direction until significant asymmetry appeared. The pre-fission region for $\eta = 1$ is explicitly smaller than in other cases.

E. Total Kinetic Energy

An important quantity in induced fission is the total kinetic energy (TKE) obtained by the fission fragments. In this study, the total kinetic energy of the two separated fragments at the scission point can be estimated as the Coulomb repulsive interaction:

$$E_{\mathrm{TKE}} = \frac{e^2 Z_H Z_L}{d_{\mathrm{ch}}},$$

where e indicates the proton charge, Z_H and Z_L denote the charge numbers of the heavy and light fragments, respectively, and d_{ch} is the relative distance between the centers of charge of the two fragments at the scission point. This approximation for TKE has been frequently used for simplification, as demonstrated in Refs. [?, ?, ?, ?, ?, ?]. However, it neglects dissipation and shell effects, among others, which can lead to overestimated TKE compared to experimental data [?, ?, ?, ?, ?, ?]. The dissipation effect has been recently considered [?], allowing calculated TKE to better agree with data. The TKE values of ^{240}Pu fission fragments with different types of pairing forces are plotted as functions of the heavy fragment mass in Figure 8. Open circles represent calculated results for different η values, whereas solid circles indicate experimental data from thermal neutron-induced ^{239}Pu fission experiments [?, ?, ?]. Considering the general trend, a qualitative dip is reproduced for all types of pairing forces at $A_H = 120$, as well as a peak at $A_H = 134$. Near the dip or peak, the TKE is larger for larger η values. For $A_H > 144$, the discrepancies are fairly small for different pairing forces.

F. Fission Yields

Figure 9 presents the mass and charge yields obtained with the code FELIX (version 2) [?] based on the TDGCM-GOA framework using different types of pairing forces, compared with experimental data. As a critical microscopic input for fission dynamic calculations, the mass tensor is calculated by the GCM or ATDHFB methods. In this calculation, $q_N = 4$ was used to determine the scission line. Generally, the discrepancies between the calculated pre-neutron mass distributions and charge distributions obtained using mass tensors from the GCM and ATDHFB methods are small. Furthermore, the mass and charge yields calculated using the mixed-pairing force with $\eta = 0.5$ combined with the ATDHFB mass tensor demonstrated the best agreement with experimental data.

The impact of different types of pairing forces on mass and charge distributions is apparent. For calculated results obtained with the ATDHFB mass tensor, the position of the peak was nearly constant for $\eta = 0.0, 0.25$, and 0.5, and moved toward heavier fragments for $\eta = 0.75$ and 1.0. For results with the GCM mass tensor, the mass and charge distributions of fission fragments shifted toward heavier fragments as η increased (panels (a) and (c)). Furthermore, theoretical calculations obtained with TDGCM using ATDHFB mass tensors (panels (b) and (d)) demonstrated that yields from the symmetric fission channel increased as η increased, which was related to the decrease in ridge height as η increased, as shown in Figure 2.

IV. Summary

In this study, we focused on analyzing the influence of different types of pairing forces on fission properties within the framework of SkM*-DFT and TDGCM, considering the ^{239}Pu(n, f) reaction as an example. Different types of pairing interactions were considered in the HFB approximation. The η parameter was tuned to obtain different types of pairing forces and test the sensitivity of calculations. Values $\eta = 0, 0.5$, and 1.0 correspond to volume-, surface-, and mixed-type pairing forces, respectively; we also used $\eta = 0.25$ and 0.75 for test purposes.

We calculated the PES, mass tensor, scission line, and TKE. The results demonstrated significant sensitivity of the fission process to the choice of η. An increase in the η value led to lower ground-state and isomeric-state energies, as well as lower fission barriers. For surface pairing ($\eta = 1$), the calculated outer barrier was lower than the empirical value, suggesting it may not be a good choice for fission studies. The strength of these pairing forces was fixed by reproducing empirical pairing gaps at ground states. However, for large deformations, pairing forces with larger η values tended to produce larger pairing gaps. The collective mass tensor decreased and fluctuated less against deformation with larger η values. For scission lines, the pre-fission region decreased with larger η values, especially around the symmetric fission channel. The TKE tended to be larger for larger η around the symmetric fission channel and around the peak of the TKE distribution. In the asymmetric fission region, TKEs obtained using different pairing forces were fairly similar. For fission yield calculations, results using the mixed-pairing force ($\eta = 0.5$) best aligned with data. The peaks of mass and charge distributions shifted toward heavier fragments as η increased. When the ATDHFB mass tensor was used, a small peak in the symmetric fission channel appeared for $\eta = 0.75$ and 1.0, contradicting experimental data.

This work has been supported by the National Key R&D Program of China (No. 2022YFA1602000), National Natural Science Foundation of China under Grant Nos. 12275081, 11790325, U2067205, and U1732138, and the Continuous-support Basic Scientific Research Project.

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