Asymmetric fission of $^{180}\mathrm{Hg}$ and the role of hexadecapole moment*

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Abstract

In current work, the fission property of ^{180}Hg is investigated based on the Skyrme density functional theory (DFT). The impact of the high-order hexadecapole moment (q_{40}) is found at large deformations. With the q_{40} constraint, a smooth and continuous potential energy surfaces (PES) could be obtained. Especially, the hexadecapole moment constraint is essential to get proper scission configurations. The static fission path based on the PES supports the asymmetric fission of ^{180}Hg. The asymmetric distribution of the fission yields of ^{180}Hg is further reproduced by the time-dependent generator coordinate method (TDGCM), and agrees well with the experimental data.

Full Text

Asymmetric fission of ^{180}Hg and the role of hexadecapole moment*

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In this work, the fission properties of ^{180}Hg are investigated based on Skyrme density functional theory (DFT). The impact of the higher-order hexadecapole moment (q_{40}) is found at large deformations. With the q_{40} constraint, smooth and continuous potential energy surfaces (PESs) can be obtained. In particular, the hexadecapole-moment constraint is essential for obtaining proper scission configurations. The static fission path based on the PES supports the asymmetric fission of ^{180}Hg. The asymmetric distribution of the fission yields of ^{180}Hg is further reproduced by the time-dependent generator coordinate method (TDGCM), and agrees well with the experimental data.

Keywords: Nuclear fission, density functional theory, hexadecapole moment, potential energy surface, mass distribution

I. INTRODUCTION

The asymmetric fission mode in neutron-deficient ^{180}Hg was discovered in 2010 via the β decay of ^{180}Tl [1]. For the fission of ^{180}Hg, its splitting into two ^{90}Zr fragments with magic $N = 50$ and semimagic $Z = 40$ was believed to dominate the fission process. However, unlike the initial theoretical prediction, ^{180}Hg has been observed to fission asymmetrically, with the heavy- and light-fragment mass distributions centered around $A = 100$ and 80 nucleons, respectively [1, 2].

A great deal of theoretical attention has been drawn to the puzzling fission behavior of ^{180}Hg. For example, macroscopic-microscopic models [1, 3-5] and self-consistent microscopic approaches [6–8] were used to analyze multidimensional potential energy surfaces (PESs), and the presence of an asymmetric saddle point with a rather high ridge between the symmetric and asymmetric fission valleys was explained as the main factor determining the mass split in fission.

Calculations of fission-fragment yields have also been performed for ^{180}Hg by means of the Brownian Metropolis shape-motion treatment [3, 5, 9], the Langevin equation [10], the scission-point model [4, 11, 12], and the random-neck-rupture mechanism [13], based on the PESs or scission configurations. The results are in approximate agreement with the experimental data, with a deviation of ~ 4 nucleons for the peak positions. There have also been several attempts to describe the fragment mass distribution in a fully microscopic way, i.e., using the time-dependent generator coordinate method (TDGCM) based on covariant density functional theory (CDFT) [8]. The asymmetric peaks are reproduced very well, while a more asymmetric fission mode with $A_{\mathrm{H}} \sim 116$ is predicted, which was not observed in the experimental measurement.

In theoretical studies of nuclear fission, the PES is an important framework that describes the evolution of nuclear energies with shape variations on the way from the initial configuration toward scission. In nuclear physics, there are generally two approaches to generating PESs. One ranges from the historical liquid-drop model [14, 15] to the well-known macroscopic-microscopic model, using parametrization of the nuclear mean-field deformation [16–19]. The other is based on microscopic self-consistent methods [20–26], or on the constrained relativistic mean-field method [8, 27–30].

In the macroscopic-microscopic method, a predefined class of nuclear shapes is uniquely defined by selecting appropriate collective coordinates, and a relatively smooth potential energy surface can be obtained. However, because of limitations in computing resources, microscopic calculations of PESs can be performed only within a limited number of deformation degrees of freedom. In the microscopic self-consistent method, the higher-order collective degrees of freedom are incorporated self-consistently based on the variational principle. In fission studies, quadrupole and octupole deformation (moment) constraints are the natural and most frequently used constraints for calculating microscopic PESs.

However, several studies have shown that, as a consequence of the absence of hexadecapole deformation (q_{40} or β_4), PESs may exhibit discontinuities in the large-deformation scission regions [31–35]. Ref. [36] investigated the role of hexadecapole deformation in the PES calculation of ^{240}Pu by applying a disturbance on β_4. The results show that one can obtain a smooth two-dimensional PES in (β_2, β_3) by parallel calculations with a suitable disturbance of the hexadecapole deformation.

But for the asymmetric fission of ^{180}Hg, there have been no reports on the effect of q_{40} or β_4 on the PES of ^{180}Hg. The self-consistent calculation in quadrupole and octupole deformation spaces indicated that the PES of ^{180}Hg exhibits behavior different from that of ^{240}Pu or ^{236}U with increasing quadrupole moment [6, 8]. Thus, it is interesting to examine the influence of the hexadecapole moment on the PES of ^{180}Hg at large deformation, and also to analyze some properties of the scission configuration. In this paper, we will extend two-dimensional (q_{20}, q_{30}) constraint calculations in the large-deformation region by adding the q_{40} constraint to the microscopic PES calculation of ^{180}Hg. The importance of q_{40} in the self-consistent calculation of the PES for ^{180}Hg at large deformation will be investigated. Moreover, the fission dynamic of

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^{180}Hg, the total kinetic energies and the fragment mass-yield distributions based on the TDGCM [37] will be described and discussed.

II. THEORETICAL FRAMEWORK

To study the static fission properties, the PES was determined using Skyrme density functional theory (DFT). The dynamic process is further investigated within the framework of TDGCM. Thus, in this section, we briefly explain these two methods. A detailed description of Skyrme DFT can be found in Ref. [38], and the formulations of TDGCM can be found in Refs. [37, 39–41].

A. Density functional theory

In the local-density approximation of DFT, the total energy of finite nuclei can be calculated from the spatial integration of the Hamiltonian density $\mathcal{H}(\mathbf{r})$,

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau(\mathbf{r}) + \sum_{t=0,1} \chi_t(\mathbf{r}) + \sum_{t=0,1} \breve{\chi}_t(\mathbf{r}). \tag{1}$$

In the above equation, $\tau(\mathbf{r})$, $\chi_t(\mathbf{r})$, and $\breve{\chi}_t(\mathbf{r})$ stand for the kinetic-energy density, the potential energy, and the pairing energy, respectively. The symbol $t = 0, 1$ denotes the isoscalar or isovector channel, respectively [42].

The mean-field potential energy $\chi_t(\mathbf{r})$ in Skyrme DFT generally has the form

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

Here the particle density ρ_t, kinetic density τ_t, and spin-current vector densities $\mathbf{J}_t$ $(t = 0, 1)$ can be calculated from the density matrix $\rho_t(\mathbf{r}\sigma, \mathbf{r}'\sigma')$, with dependence on the spatial $(\mathbf{r})$ and spin (σ) coordinates. The quantities $C_t^{\rho\rho}$, $C_t^{\rho\tau}$, etc., are coupling constants for different types of densities in the Hamiltonian density $\mathcal{H}(\mathbf{r})$, which are usually real numbers. As an exception, $C_t^{\rho\rho} = C_{t0}^{\rho\rho} + C_{tD}^{\rho\rho}\rho_0^{\gamma}$ is the density-dependent term. The formulae relating the coupling constants to traditional Skyrme parameters can be found in Ref. [43]. For example, the spin-orbit force of the Skyrme interaction corresponds to the term $C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t$.

Pairing correlations are often taken into account through the Hartree–Fock–Bogoliubov (HFB) approximation in DFT [38]. In the case of the Skyrme energy density functional, a commonly adopted pairing force is the density-dependent surface-volume, zero-range potential, as given in Refs. [26, 44]:

$$\hat{V}_{\mathrm{pair}}(\mathbf{r}, \mathbf{r}') = V_0^{(\mathrm{n,p})}\left[1 - \frac{1}{2}\frac{\rho(\mathbf{r})}{\rho_0}\right]\delta(\mathbf{r} - \mathbf{r}'), \tag{3}$$

where $V_0^{(\mathrm{n,p})}$ is the pairing strength for the neutron (n) and the proton (p), ρ_0 is the saturation density of nuclear matter fixed at 0.16 fm^{-3}, and $\rho(\mathbf{r})$ indicates the total density. As studied in Ref. [26], this type of pairing force is a suitable choice for nuclear fission studies.

The DFT solver HFBTHO (V3.00) [45] is used to generate the PESs, in which axial symmetry is assumed. Twenty-six major shells of the axial harmonic-oscillator single-particle basis are used, and the number of basis states is further truncated to 1140. In this work, the Skyrme DFT with SkM* parameters [46] is adopted, which is commonly used for fission studies. For the pairing strengths, $v_0^{(\mathrm{n})} = -268.9$ MeV fm^3 and $v_0^{(\mathrm{p})} = -332.5$ MeV fm^3 are used for neutrons and protons, respectively, with a pairing window of $E_{\mathrm{cut}} = 60$ MeV. This pairing strength, together with the choice of the SkM* force and model space, has been adopted in Refs. [6, 47], in which the two-dimensional PES related to the fission of ^{180}Hg has been studied.

B. Time-dependent generator coordinate method

Nuclear fission is a large-amplitude collective motion, which can be approximated as a slow adiabatic process driven by several collective degrees of freedom. In TDGCM, the many-body wave function of the fissioning system takes the generic form

$$|\Psi(t)\rangle = \int_{\mathbf{q}} f(\mathbf{q}, t)|\Phi(\mathbf{q})\rangle\, d\mathbf{q}. \tag{4}$$

Here $|\Phi(\mathbf{q})\rangle$ is composed of known many-body wave functions with the vector of continuous variables $\mathbf{q}$. The $\mathbf{q}$ are collections of variables chosen according to the physics problem.

For the fission study, two collective variables, the quadrupole moment $\hat{q}_{20}$ and the octupole moment $\hat{q}_{30}$, are usually adopted. In the above equation, $f(\mathbf{q}, t)$ is a weighted function. It is determined by the time-dependent Schrödinger-like equation,

$$i\hbar \frac{\partial g(\mathbf{q}, t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q}) g(\mathbf{q}, t), \tag{5}$$

in which the Gaussian overlap approximation (GOA) is used. $\hat{H}_{\text{coll}}(\mathbf{q})$ is the collective Hamiltonian, as

$$\hat{H}_{\text{coll}}(\mathbf{q}) = -\frac{\hbar^2}{2} \sum_{ij} \frac{\partial}{\partial q_i} B_{ij}(\mathbf{q}) \frac{\partial}{\partial q_j} + V(\mathbf{q}), \tag{6}$$

in which $V(\mathbf{q})$ is the collective potential, and $B_{ij}(\mathbf{q}) = \mathcal{M}^{-1}(\mathbf{q})$ is the inertia tensor, the inverse of the mass tensor $\mathcal{M}$. The potential and mass tensor are solved by Skyrme DFT in this work. $g(\mathbf{q}, t)$ contains information about the dynamics of the fissioning nuclei and is the complex collective wave function with collective variables $\mathbf{q}$.

To describe nuclear fission, the collective space is divided into an inner region and an external region, corresponding respectively to the nucleus remaining as a whole and the nucleus separated into two fragments. The scission contour, which is a hypersurface, is used to separate these two regions. The flux of the probability current passing through the scission contour can be

used to evaluate the probability of observing the two fission fragments at time t. For the surface element ξ on the scission contour, the integrated flux $F(\xi, t)$ is calculated by

$$F(\xi, t) = \int_{t=0}^{t} dt \int_{\mathbf{q}\in\xi} \mathbf{J}(\mathbf{q}, t) \cdot d\mathbf{S}, \tag{7}$$

as in Ref. [37], in which $\mathbf{J}(\mathbf{q}, t)$ is the current

$$\mathbf{J}(\mathbf{q}, t) = \frac{\hbar}{2i} B(\mathbf{q}) \left[g^*(\mathbf{q}, t) \nabla g(\mathbf{q}, t) - g(\mathbf{q}, t) \nabla g^*(\mathbf{q}, t) \right]. \tag{8}$$

The yield of the fission product with the mass number A can be obtained by

$$Y(A) = C \sum_{\xi\in A} \lim_{t\to+\infty} F(\xi, t) \tag{9}$$

where A denotes an ensemble of all the surface elements ξ on the scission contour containing the fragment with mass number A, and C is the normalization factor to ensure that the total yield is normalized to be 200. In the same way, the yield of fission fragment with charge number Z can also be obtained. In this work, the computer code FELIX(version 2.0) [41] is used for describing the time evolution of the nuclear fission in TDGCM-GOA framework.

III. RESULTS AND DISCUSSION

In the adiabatic approximation approach for fission dynamic, the precise multidimensional PES is the first and the essential step toward the dynamical description of fission. Fig. 1 displayed the PES contour of ^{180}Hg obtained by the HFB calculation in the collective space of (q_{20}, q_{30}), in which q_{20} is from -20 b to 300 b and q_{30} is from 0 b$^{3/2}$ to 40 b$^{3/2}$ with the step of $\Delta q_{20} = 2$ b and $\Delta q_{30} = 2$ b$^{3/2}$. Overall, the pattern of PES obtained in this work based on the DFT solvers HFBTHO with Skyrme SkM* functional is similar to that obtained using the symmetry unrestricted DFT solver HFODD [6] with the same functional and that obtained using covariant density functional theory with the relativistic PC-PK1 functional [8]. The static fission path starts from a nearly spherical ground state ($q_{20} = 20$ b$, q_{30} = 0$ b$^{3/2}$), the reflection symmetric fission path can be found for small quadruple deformations, and the reflection-asymmetric path branches away from the symmetric path about $q_{20} = 100$ b. One can see that unlike the PES of actinide nuclei, there is no valley towards to scission for ^{180}Hg, it undergoes a continuous uphill process till the mass asymmetric scission point with high q_{30} asymmetry.

In the (q_{20}, q_{30})-constrained PES calculations by DFT, the other degree of deformations are obtained based on the variational principle. In Refs. [35, 36], it has been learned that at given q_{20} and q_{30}, there are two minimum with different value of q_{40}, and the minimum with larger q_{40} disappears when the q_{20} is large enough, which indicates the transition toward the scission. The hexadecapole deformation is an important degree of freedom for the description of PES at large deformation, and especially, a disturbation of hexadecapole deformation is required for a smooth and reasonable PES, as shown in Ref. [36]. Thus, in our work, at large quadrupole moments, i.e., larger than $q_{20} \simeq 200$ b ($\beta_2 \simeq 3.2$), a further constraint of hexadecapole moment q_{40} is introduced. It is done in a "perturbative" way. A smaller hexadecapole moment than the one obtained variationally is used as a further constraint in the first ten steps of DFT iterations, and it is then released to vary freely. Thus a lower energy minimum with smaller q_{40} might be obtained. This treatment is used for the calculation of PES in Fig. 1, and labeled "(B)" in Figs. 2-3. The calculation with the constraints of q_{20} and q_{30} only is labeled "(A)" in Figs. 2-3.

Fig. 1. (color online) Potential energy surface of ^{180}Hg in the collective space of (q_{20}, q_{30}). The pink solid line and purple circle dots denote the static fission path and scission line respectively.

Fig. 2. (color online) HFB energies along the symmetric-fission and asymmetric-fission pathways of ^{180}Hg as a function of q_{20}. The least-energy

fission pathway (static fission path) is given as a blue curve. The symmetric-fission pathways are shown as the black or green curves, labeled as (A) or (B) respectively. These two curves are obtained with different treatment of q_{40} (see text for details). The red line shows the transitional valley that bridges the asymmetric and symmetric paths.

In Fig. 2, the energies of the static fission path as a function of quadruple moment q_{20} are shown. The symmetric ($q_{30} = 0$ b$^{3/2}$) and the asymmetric fission path in ^{180}Hg are given respectively. One can see clearly that these energies increase with q_{20} steadily. At around $q_{20} \sim 100$ b, the asymmetric fission path starts to be favoured in energy compared to the

Fig. 3. (color online) The hexadecapole moment (q_{40}), the neck particle number (q_N), and the HFB energies as functions of q_{20} are shown in panels (a), (b), and (c), respectively, for $q_{30} = 0$ b$^{3/2}$ and 10 b$^{3/2}$.

symmetric fission path. The transitional valley that bridges the asymmetric and symmetric paths is also drawn in red in Fig. 2. Notably, this connection occurs at the deformation where the symmetric and asymmetric paths are nearly equivalent in energy. This characteristic of ^{180}Hg has also been verified in Ref. [48] using the HFB-Gogny D1S interaction. From Fig. 2, for case (A), one can see that the energy of ^{180}Hg increases continuously with q_{20}, and it is difficult for the nucleus to rupture even at very large elongation, e.g., $q_{20} \geq 300$ b ($\beta_{20} \geq 4.8$). As seen in case (B), with the inclusion of the q_{40} constraint, a gentle decreasing trend in the energy occurs at $q_{20} \sim 240$ b, and a sudden drop in energy occurs at $q_{20} \sim 280$ b, indicating nuclear scission.

In Fig. 3, the hexadecapole moment (q_{40}), the average particle number around the neck (q_N), and the HFB energies are given as functions of q_{20}, respectively, at given q_{30}. To investigate the role of q_{40}, only the region with large q_{20} is shown. From Fig. 3(a), one can see that q_{40} increases nearly linearly up to very large q_{20} values, especially for case (A), in which q_{40} can become very large during the elongation. After a "perturbative" constraint on q_{40}, as in case (B) in the figure, the q_{40} value drops suddenly and then grows linearly. In the study of nuclear fission, q_N is often adopted as the indicator of nuclear scission. For example, $q_N = 4$ has been used for the determination of the scission line of ^{240}Pu in Refs. [26, 34, 49]. In Fig. 3(b), q_N decreases gradually with q_{20}. However, for case (A), the reduction of q_N becomes rather slow with increasing q_{20}. Especially at $q_{20} \sim 340$ b ($\beta_2 \sim 5.4$), $q_N > 4$ for $q_{30} = 0$ and 10 b$^{3/2}$, and the total energies increase continuously at large q_{20}, as seen in Fig. 3(c). After the q_{40} constraint is considered, as shown for case (B) in Fig. 3(b) and (c), both q_N and the total energy have a sudden drop at around $q_{20} \sim 280$ b ($\beta_2 \sim 4.5$), indicating nuclear rupture. It is seen that when $q_N \leq 4$, q_N becomes close to zero with increasing q_{20}.

Fig. 4. (color online) HFB energies [panel (a)] and q_N [panel (b)] of ^{180}Hg obtained by constrained q_{20}, q_{30}, and q_{40} calculations. These values are shown as functions of q_{40}, and different curves correspond to different q_{20} values. $q_{30} =$

0 b$^{3/2}$.

To investigate the role of q_{40} in the PES, the HFB energies and q_N as functions of q_{40} at given q_{20} and q_{30} are plotted in Fig. 4, obtained through exact constrained calculations of q_{20}, q_{30}, and q_{40}. In the figure, q_{30} is constrained to be 0 b$^{3/2}$. Other q_{30} values were also tested, and the results are similar to those in Fig. 4. In Fig. 4(a), one can see that there are two local minima along the q_{40} degree of freedom, corresponding to distinct valleys on the multidimensional potential energy surface. In Ref. [36], a similar trend in ^{240}Pu was found, and the minimum related to the larger q_{40} disappears with increasing quadrupole deformation (at roughly $\beta_2 \sim 3.8$), leading to a natural transition to the minimum with the smaller q_{40}. This transition is the cause of the discontinuity and the sudden drop of energy in the two-dimensional PES of (q_{20}, q_{30}). However, for ^{180}Hg, there remains an extremely soft and relatively flat minimum with larger q_{40} values even at very large q_{20} values, e.g., at $q_{20} = 340$ b ($\beta_2 \sim 5.4$). In PES calculations with only

Fig. 5. (color online) Density distributions of ^{180}Hg obtained from (q_{20}, q_{30}, q_{40})-constrained calculations. Results are obtained with different constrained q_{40} values for the symmetric fission channel $(q_{20}, q_{30}) = (240\ \text{b}, 0\ \text{b}^{3/2})$ (upper panels) and for the asymmetric fission channel $(q_{20}, q_{30}) = (240\ \text{b}, 10\ \text{b}^{3/2})$ (lower panels).

the (q_{20}, q_{30}) constraint, the q_{40} degree of freedom is obtained through variations of the total energies. As seen for case (A) in Fig. 3, q_{40} after the variation calculation grows steadily even at very large q_{20}, and no transition to the minimum with smaller q_{40} occurs. With only the (q_{20}, q_{30}) constraint, it is difficult to find the proper scission configuration, at least for ^{180}Hg. After the "perturbative" inclusion of the q_{40} constraint, as in case (B) in Fig. 3, such a transition can occur at large q_{20}. In Fig. 4(b), it is seen that q_{N} generally increases with q_{40}. q_{N} around the minimum with larger q_{40} is roughly larger than 4, and when $q_{20} > 200$ b, its value around the minimum with smaller q_{40} is close to zero (numerically 10^{-3}–10^{-4}, effectively near zero). For $q_{\mathrm{N}} \sim 0$, the nucleus becomes well separated into two fragments. From this calculation, one can learn that introducing the q_{40} constraint into the self-consistent calculation of the PES can ensure the continuity of the potential-energy surface. q_{40} is essential in DFT calculations for fission studies, especially for the transition to scission.

Several results of (q_{20}, q_{30}, q_{40})-constrained calculations are shown in Fig. 5 for the density-distribution profiles of ^{180}Hg. q_{20} is constrained to be 240 b, and q_{40} changes from 140 b^2 to 60 b^2 for $q_{30} = 0$ b$^{3/2}$ and $q_{30} = 10$ b$^{3/2}$ in the upper and lower panels, respectively. The q_{40} degree of freedom influences the formation of the neck and the scission configurations. From the figure, one can see that with large q_{40}, there is no neck in the nucleus and the nucleus is simply stretched to a very large extent. For the calculation with only the (q_{20}, q_{30}) constraint, as in case (A) in Figs. 2–3, q_{40} has a very large value with increasing q_{20}, and thus the nucleus cannot undergo scission. With decreasing q_{40}, the neck structure of the nucleus appears and becomes well separated when q_{40} has small values.

Fig. 6. (Color online) The calculated Coulomb repulsive energy of the nascent fission fragments for ^{180}Hg as functions of fragment mass, in comparison with the experimental data of the total kinetic energy [2].

One of the most important quantities in induced fission is the total kinetic energy (TKE) carried by the fission fragments. In this work, the total kinetic energy of the two separated fragments at the scission point can be approximately estimated as the Coulomb repulsive interaction using the simple formula $e^2 Z_{\mathrm{H}} Z_{\mathrm{L}}/d_{\mathrm{ch}}$, where e stands for the proton charge, Z_{H} and Z_{L} denote the charge numbers of the heavy and light fragments, respectively, and d_{ch} is the distance between the centers of charge of the two fragments at the scission point. Fig. 6 displays the distribution of the calculated Coulomb repulsive energy based on the scission line shown by the purple circle in Fig. 1 and compares it with the measured TKE [2]. It can be seen that the calculated results reproduce the trend of the measured TKE quite well, especially the dip at $A_{\mathrm{H}} = 90$ and the peak at $A_{\mathrm{H}} = 94$, although the calculated results are generally overestimated by several MeV compared with the data, which may be caused by neglecting the dissipation effect.

Plot labels: GCM; ATDHFB; EXP.
y-axis: Yields (normalized to 200). x-axis: Mass.

Fig. 7. (color online) Mass distribution of the fission fragments of ^{180}Hg calculated by the TDGCM method (open symbols), in comparison with the experimental data (black squares) [1, 2]. The open upper triangle and lower triangle stand for the calculated results with the ATDHFB mass tensor and GCM mass tensor, respectively.

Finally, we performed the TDGCM+GOA calculation to model the time evolution of the fission dynamics of ^{180}Hg. Fig. 7 shows the calculated mass distributions of the fission fragments of ^{180}Hg and compares them with the experimental data [1, 2]. As one of the most important microscopic inputs for fission-dynamics calculations, the mass tensor is calculated by the GCM or ATDHFB methods in the present work. The calculated mass distribution is generally similar when using the mass tensor from these two methods, and better agreement is obtained by using the GCM method for the height of the asymmetric peaks and the symmetric valley. Overall, the calculation reproduces the experimental data well. The calculated peak position deviates by one unit from the experimental peak position. Moreover, a more asymmetric fission mode with $A_{\mathrm{H}} \sim 117$ is predicted in our calculation, which was also predicted by the covariant density functional theory with the PC-PK1 functional [8].

IV. SUMMARY

In this work, the static fission properties and the fission dynamics of ^{180}Hg were investigated by the Skyrme DFT and TDGCM, respectively. During the calculation of multidimensional PES, it is found that the hexadecapole moment is crucial to obtain a smooth PES and proper scission configurations, and thus it is essential for fission-dynamic studies. For the calculation of PES with only the q_{20} and q_{30} constraints, the nuclear rupture does not happen even at very large q_{20}. Through the calculations with q_{20}, q_{30} and q_{40} constraints, it is found that a rather soft and flat minimum with large hexadecapole moment still exists in the PES of ^{180}Hg even with a very elongated shape, which hinders the transition to the lower-energy minimum with smaller q_{40}. With the strategy of "perturbative" constraint of the collective freedom q_{40}, the transition to the minimum corresponding to the nuclear rupture could happen naturally, and thus reasonable scission configurations can be obtained. From these scission configurations, the estimated distribution of TKE reproduces the trend of experimental data.

Based on the static PES calculation, it is learned that the asymmetric fission channel is favoured in ^{180}Hg. Finally, the fission-fragment yields were calculated with the TDGCM. The calculated mass distributions also support the asymmetric fission for ^{180}Hg. The calculation agrees well with the experimental data. Moreover, a more asymmetric peak with $A_{\mathrm{H}} \sim 117$ is predicted, which is also predicted by the covariant DFT with the PC-PK1 parameter set [8].

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Note: Figure translations are in progress. See original paper for figures.