A deeper understanding of fission from a droplet of condensed nuclear matter splitting into fragments is still strongly motivated, even though its discovery occurred more than 80 years ago [1]. Firstly, fission data is crucial for increasingly wide applications [2] such as for nuclear energy, production of medical isotopes, radiation shielding, as well as for basic sciences such as synthesis of superheavy elements [3, 4] and constraints on r-process in neutron-star mergers [5, 6]. Due to experimental difficulties, however, fission yields are only available at neutron energies of thermal energy, 0.5 MeV and 14 MeV in major nuclear data libraries [8]. Energy dependent fission data is very needed. Secondly, the fission process is extremely complex from the microscopic view as a probe of non-equilibrium quantum many-body dynamics [9–11].

It is known that the pioneer Bohr-Wheeler statistical theory is very successful but not applicable for highly excited fission with experimental observations of exceeding precission neutron multiplicities [12]. Strong viscosity and dissipation in hot nuclear matter has to be invoked [13]. The realistic fission of compound nuclei is not only determined by the barrier but also the later phase of fission evolutions towards scission becomes important [14]. In addition, the quantum effects such as shell effects and pairing would gradually fade away as excitation energies increase [4, 15]. There were studies of the role of static temperature-dependent fission barriers [4, 15, 16], however, the microscopic fission dynamics in terms of excitation energy dependence is still absent.

For experiments, the well-known semi-empirical model by Brosa et al. [17] is the primary tool for evaluations of fission data with high accuracy. This model has great physics intuition on the multi-channel fission and the random neck-rupture assumptions, which is well established by detailed fission observations, in particular correlations between distributions of mass yields, total kinetic energies (TKE) and neutron multiplicities. However, as a major obstacle for extrapolations when experiments are absent, the origin and pathways of two asymmetric standard channels (denoted S1, S2) in Brosa model are still ambiguous, although shell effects are present in nascent fragments [10, 18]. This also hinders shape dynamics models [14, 19, 22] based on potential energy surfaces (PES) to take into account these intuitive assumptions. Therefore, the validation of physics assumptions of the Brosa model from microscopic dynamical models would be significant.

The microscopic time-dependent density functional theory (TD-DFT) is promising to describe the later phase of fission from saddle to scission [23–27]. TD-DFT has provided valuable clues about the overdamped assumption [28], non-adiabatic effects [29], the excitations of fragments [24], the role of shell effects [18] and pairing effects [27], but the lack of fluctuations undermines TD-DFT to reproduce distributions of fission yields [28, 30]. It is an evident defect that strongly dissipated fission has no dissipation-fluctuation correspondence. At low excitations, the probability of orbital exchanges is connected to the Landau-Zener effect and is dependent on the pairing gap [23]. At high excitations, as the pairing is diminished, it is expected that thermal fluctuations are the main source of orbital changes. There are efforts such as the stochastic TD-DFT with initial fluctuations [30, 31] or by including dynamical density fluctuations [32], aiming to bridge the Langevin descriptions [20]. The time-dependent random-phase approximation [33] can describe particle-number fluctuations but not actual distributions of fission observables [29, 34]. In addition to quantal fluctuations, it is essential to include thermal fluctuations based on TD-DFT which would become significant in fission of highly excited compound nuclei. Thermal fluctuations in the mean-field picture can be naturally linked to random transitions between single-particle levels around Fermi surfaces. Actually the fluctuations in single-particle and collective motions are interweaved in the TD-DFT approach.

In this Letter, we study the energy dependence of fission observables of the compound nucleus 240Pu with microscopic TD-DFT, including dynamical pairing and thermal fluctuations. This is an attempt to develop....
a consistent understanding of fission mechanism connecting microscopic dynamical models and statistical Langevin models. As a reward, it turns out that our results can explain the origin of the two asymmetric fission channels of the Brosa model.

We describe the fission of compound nuclei with the time-dependent Hartree-Fock+BCS (TD-BCS) approach [32–36]. The initial configuration of compound nuclei $^{240}$Pu is obtained by finite-temperature Hartree-Fock+BCS calculations [13, 37]. The evolutions of compound nuclei is similar to that of the zero-temperature time-dependent Hartree-Fock-Bogoliubov (TD-HFB) formulism [35],

$$i\hbar \frac{d\mathcal{R}}{dt} = [H, \mathcal{R}],$$

where $H$ is the HFB hamiltonian, $\mathcal{R}$ is the general density matrix. The initial $H$ and $\mathcal{R}$ are associated with a finite temperature [27]. The time-dependent Hartree-Fock+BCS equations can be obtained by using BCS basis or canonical basis [32–36]. Note that TD-BCS can describe dynamical pairing approximately compared to the fully dynamical pairing in TD-HFB.

In TD-BCS, the evolution of densities is actually related to the evolution of occupation numbers of single-particle levels. In the mean-field picture, the single-particle levels around Fermi surfaces are active for orbital exchanges due to dynamical pairing fluctuations [27]. To mimic thermal fluctuations, we implement random transitions between single-particle levels without explicit external forces, in which the occupation number $n_k$ is modified with a random additive $\delta n_k$. The random $\delta n_k$ is designed as a transition so that the total particle number is strictly conserved. The transition occurs as a random Gaussian noise around Fermi surfaces and the transition amplitude $\delta n_k$ is proportional to $e^{-|E_k-E_j|/T}$ as a symmetric Boltzmann distribution, where $T$ is an effective temperature and $E_{k,j}$ are single-particle energies. The random transitions are connected to statistical collisions approximately, while the exact treatment of two-body collision terms beyond TDHF is very sophisticated [38]. The transition amplitudes are also constrained by the Pauli exclusion principle. The thermal transitions are naturally prohibited at low temperatures. At high temperatures, the orbital exchanges are mainly induced by thermal fluctuations, even when two levels are not close.

The calculations are performed with the time-dependent Hartree-Fock solver Sky3D [33, 40] with the addition of our modifications of TD-BCS plus thermal fluctuations. The initial configurations at finite temperatures are obtained using the SkyAx solver [15, 41], to interface with Sky3D [42]. The time evolution operator is based on the Taylor expansion at the fourth order and time step is taken as 0.1 fm/c. The box size $(x, y, z)$ is taken as $48 \times 48 \times 64$ fm and the grid space is 0.8 fm. The nuclear interaction we adopted is the widely used SkM* parameterization [43] and the paring interaction is the mixed pairing [44].

We firstly studied the fission of compound nuclei $^{240}$Pu with different initial temperatures with TD-BCS. The initial deformation in this work adopts the dimensionless quadrupole-octupole deformations as $\beta_2=2.3$ and $\beta_3=1.0$ (see the definition [45]). The timescale is an important quantity characterizing nuclear dynamics with dissipations and fluctuations [46]. Fig. (a) displays the evolutions of the number of particles in the neck. The zero-temperature TD-BCS calculations is slower than TDHF calculations, due to dynamical pairing effects [27]. With increasing temperatures $T$, the evolution times become considerably lengthened. Note that fission would not oc-
In this case, thermal fluctuations have to be invoked. The damping time from the beginning stage of evolutions. Furthermore, the hot nuclei, we see that pairing energies dissipate rapidly compared to zero-temperature results in Fig. 2(a). In BCS calculations at high temperatures but with an initial temperature increases. This also indicates that the initial pairing can reduce viscosity to some extent. With a considerable initial pairing, the fission now happens at $T=1.0$ and $1.25$ MeV, but still not happen at $T=1.5$. In this case, thermal fluctuations have to be invoked.

Fig. 3 displays the evolutions of octupole deformations and pairing energies at $T=0.9$ and $1.5$ MeV with thermal fluctuations. The resulting evolution times of different pathways are distributed widely. At $T=1.5$ MeV, the fission now occurs with thermal fluctuations as an indispensable driving source. The resulted scission deformations are widely distributed compared to that of $T=0.9$ MeV, as a result of larger effects of thermal fluctuations at higher temperatures. Pairing energies decrease at the beginning due to dissipations and then induced dynamical pairings increase towards the scission due to thermal fluctuations, exhibiting interesting competing roles of dissipation and fluctuation. The induced pairing becomes prominent after long time evolutions.

One of the key issues is the distributions of outcomes of TD-BCS calculations with thermal fluctuations. Fig 4 shows the fission pathways in the quadrupole-octupole deformation space. At $T=0.9$ MeV ($E^*=16.1$), the fission yields are mainly distributed around two asymmetric channels. The average masses of heavy fragments are around $A_H=134.8$ and $139.3$ for S1 and S2 channels, respectively. The associated average TKE are around $187.3$ and $172.3$ MeV respectively. This is exactly the two standard asymmetric fission channels of $^{240}$Pu in the Brosa model [4]. The two channels of pathways are close in the deformation space while S2 corresponds to a larger deformation or a longer neck. The onset of two asymmetric channels is mainly due to dynamical effects while it would be difficult to distinguish them by models based on static PES. It is understandable that the longer neck structure leads to smaller TKE and wider distributions. The longer

![Graph](image_url)

**TABLE I:** Calculated fission observables of $^{240}$Pu at different initial temperatures $T$ (MeV) and associated excitation energies $E^*$, including mass of heavy fragment $A_H$, excitation energies of heavy fragments $E^*_H$ and light fragments $E^*_L$, and TKE. All energies are in MeV. TDHF results are also listed. TD-BCS results with an initial pairing of zero temperature are listed for comparisons. With thermal fluctuations, averaged values and standard deviations in brackets are shown.

| $T$ (MeV) | $A_H$ | $E^*_H$ | $E^*_L$ | TKE |
|----------|-------|--------|--------|-----|
| TDHF     | 134.9 | 9.9    | 12.0   | 186.9 |
| TD-BCS with temperature | | | | |
| 0.5 (4.7) | 135.3 | 9.1 | 19.3 | 186.9 |
| 0.75 (10.6) | 135.8 | 13.8 | 21.3 | 185.3 |
| 0.9 (16.1) | 135.6 | 17.8 | 24.8 | 185.6 |
| with initial pairing | | | | |
| 0.0 | 138.6 | 10.6 | 22.6 | 172.1 |
| 0.75 (10.6) | 137.7 | 13.5 | 25.1 | 175.6 |
| 1.0 (20.5) | 138.4 | 19.8 | 28.8 | 174.2 |
| 1.25 (34.6) | 137.0 | 28.9 | 32.9 | 176.9 |
| with thermal fluctuations | | | | |
| 0.9 (16.1) | 137.5(2.7) | 20.7(4.1) | 26.4(2.8) | 178.3(7.9) |
| 1.5 (53.2) | 138.5(4.9) | 41.4(5.7) | 42.3(4.9) | 172.6(3.9) |
Figure 4: The fission pathways of $^{240}$Pu within TD-BCS plus thermal fluctuations in the space of quadrupole-octupole deformations ($Q_{20}$, $Q_{30}$), at temperatures of 0.9 MeV (upper panel) and 1.5 MeV (lower panel). At $T=0.9$ MeV, the fission pathway without fluctuations (yellow color) is also shown. Specific results of S1 and S2 channels are also shown inside the upper panel.

S2 pathways also lead to more dissipations and higher excitations of fragments, leading to the sawtooth structure of neutron multiplicities. At $T=1.5$ MeV ($E^* = 53.2$ MeV), the splitting of S1 and S2 is not clear any more. The distributions of scission deformations and masses are much wider than that of 0.9 MeV. This demonstrated that the splitting of S1 and S2 disappears at high excitations as quantal effects fade away. Systematic analysis has also found that S2 is dominated and the percentage of S1 channel decreases with increased energies.

Finally, Table I displays the calculated fission observables. The complete results of all fluctuated pathways are given in the supplement. In experiments, the averaged TKE of $^{239}$Pu($n$, f) is about 175 MeV and slightly decreases with increasing energies. It is related to generally larger scission deformations at higher excitations as shown in Fig. 4. The experimental averaged mass of heavy fragments $A_H$ is about 140 rather than the magic number 132. It is shown that TKE and $A_H$ from TD-BCS with temperatures and TDHF are about 186 MeV and 135.5, which are around S1 channel. On the other hand, TKE and $A_H$ from TD-BCS with initial pairings are about 175 MeV and 138. We see that a considerable initial pairing is favorable for S2 channel. With thermal fluctuations, averaged TKE and $A_H$ come back to experiments with spreading widths. We have demonstrated the essential role of thermal fluctuations in fission of compound nuclei when initial pairings are diminished, to correspond to increased dissipations. The obtained excitation energies of fragments are also useful for understanding energy dependence of neutron emission. The heavy fragments have less excitation energies at low excitations but become close to that of light fragments at high excitations. It is promising to calculate distributions of fission observables with more pathways and also varying initial deformations. Our work sheds a new light on the intuitive Brosa model for extrapolations and provides valuable clues towards a predictive microscopic fission theory.

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Supplement Material for “Fission Dynamics of Compound Nuclei: Pairing versus Fluctuations”

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TABLE I: Calculated detailed fission observables of compound $^{240}$Pu with TD-BCS plus thermal fluctuations. Results include 10 individual cases at temperature of 0.9 and 1.5 MeV, respectively. The table lists the fission evolution time ($T_f$) (in fm/c), mass of heavy fragment $A_H$, the proton number $Z_H$ and neutron number $N_H$ of heavy fragments, the proton number $Z_L$ and neutron number $N_L$ of light fragments, excitation energies of heavy fragments $E^*_H$ and light fragments $E^*_L$, the total excitation energies of fragments $TXE$, total kinetic energies $TKE$, the quadrupole deformation $Q_{20}$ and octupole deformation $Q_{30}$ before scission. All energies are in MeV.

| Case | $T_f$ | $A_H$ | $N_H$ | $Z_H$ | $N_L$ | $Z_L$ | $E^*_H$ | $E^*_L$ | TXE | TKE | TKE+TXE | $Q_{20}$ (b) | $Q_{30}$ (b^{3/2}) |
|------|-------|-------|-------|-------|-------|-------|---------|---------|-----|-----|---------|-------------|------------------|
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |
|      |       |       |       |       |       |       |         |         |     |     |         |             |                  |

(T=0.9)
- S1 channels-
1  974.0 134.2 82.4 51.8 63.5 42.2 15.3 25.1 40.4 188.6 229.0 389.1 43.7
2  1567.0 134.9 82.3 52.6 63.6 41.4 18.8 21.6 40.4 189.2 226.6 376.4 39.7
3  1176.0 134.9 82.7 52.2 63.3 41.8 15.9 25.9 41.8 186.2 228.0 397.6 46.8
4  873.0 135.1 82.9 52.2 63.0 41.8 18.0 26.0 44.0 185.1 229.1 402.0 45.1

- S2 channels-
5  2992.0 136.2 83.3 53.0 62.7 41.0 27.7 28.8 56.5 173.5 230.0 452.7 54.7
6  950.0 139.2 85.0 54.2 60.9 39.8 21.9 27.1 49.0 173.0 222.0 443.6 57.4
7  1380.0 139.5 85.0 54.5 60.9 39.5 22.0 24.5 46.4 173.2 219.7 434.2 53.6
8  5007.0 139.5 85.6 53.9 60.3 40.5 26.5 30.0 56.5 173.3 229.8 435.8 51.4
9  2385.0 140.1 86.2 53.9 59.8 40.1 21.1 30.4 51.5 170.2 221.7 444.4 53.8
10  3061.0 141.7 86.5 55.1 59.4 38.8 19.6 24.2 43.8 170.6 214.4 432.0 57.4

(T=1.5)
1  1915 127.6 77.7 49.8 67.6 44.1 35.1 49.7 84.8 173.5 258.3 483.5 43.3
2  3012 135.4 82.0 53.4 63.3 40.6 39.7 39.9 79.6 180.5 260.1 429.2 49.2
3  2972 136.0 83.2 52.8 62.1 41.2 40.1 44.2 84.4 175.9 260.2 431.4 47.4
4  3754 137.8 84.6 53.2 60.6 40.7 50.9 36.9 87.8 170.5 258.4 456.1 47.6
5  3871 138.1 84.8 53.4 60.4 40.6 30.8 47.9 78.7 173.1 252.5 451.1 61.0
6  3774 138.6 84.5 54.1 60.7 39.9 40.4 40.7 81.1 175.5 256.6 426.4 56.7
7  881 141.8 86.9 54.8 58.5 39.1 46.9 40.9 87.8 168.8 256.5 488.4 71.2
8  2027 142.3 86.4 55.9 58.9 38.1 42.0 40.8 82.7 169.5 252.2 438.7 61.8
9  2382 143.8 87.7 56.2 57.6 37.8 44.3 47.2 91.5 168.7 260.2 446.8 71.5
10  1337 143.9 87.9 56.0 57.4 38.0 43.8 34.7 78.5 169.8 248.3 433.5 62.5