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# Towards Microscopic Descriptions of Thermal Fission Rates

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**Abstract:** The studies of thermal fission rates are relevant to novel reactors, astrophysical environments, and survival probabilities of compound superheavy nuclei. This has been conventionally studied by the Bohr-Wheeler statistical model that depends on phenomenological level densities and fission barriers. In this context, we propose to study the thermal fission rates based on microscopic temperature dependent nuclear energy density functional theory. The microscopic temperature dependent fission barrier heights and curvatures, and collective mass parameters can be self-consistently obtained. The fission lifetimes from low to high temperatures can be given by the imaginary free energy method in a consistent framework. Microscopic temperature dependent fission barriers play an essential role in fission studies.

**Key words:** fission rate; induced fission; imaginary free energy method

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## 1 Introduction

The fission studies and related experimental evaluations are of practical application interests. In particular, the cross sections, lifetimes, fragment distributions, energy release modes, *etc.*, of actinide nuclei have been extensively studied. A number of models with parameterized inputs of level densities, potential energy surfaces and scission shapes, were developed at the application level. However, the microscopic fission mechanism as a large amplitude collective motion of nuclear many body systems has not yet been fully understood[1]. The microscopic fission studies are also desirable to make predictions because experimental fission studies of exotic nuclei are difficult.

The goal of microscopic studies of fission process is to accurately describe various fission observations based on effective nuclear forces and the nuclear energy density functional theory, without free parameters. The renaissance of microscopic studies is only possible with the recent development of computing capability. Indeed, the fission description involves large scale calculations of multi-dimensional potential energy surfaces[2] and collective mass inertia[3]. The non-adiabatic description that involves time dependent evolutions of a 3-dimensional nuclear system in coordinate spaces[4] are even more costly.

The thermal fission can evolve from quantum tunneling to statistical decays with increasing excitation energies[5]. To describe the thermal fission, or induced fission, the method should be consistent at all temperatures. Obviously, the conventional statistical models can't be applied to low temperatures for which quantum effects are important. To this end, we employed the imaginary free energy method (ImF)[6, 7] which is a general thermal dynamic approach at all temperatures. The ImF method has been widely applied in studies of chemical reactions. In the ImF method, the fission barrier is given in terms of free energy which is naturally temperature dependent.

In our approach, the thermal excited nuclei are described by the finite-temperature Skyrme-Hartree-Fock+BCS framework[8]. Previously we have studied the temperature dependent fission barriers based on the finite-temperature Hartree-Fock-Bogoliubov[9] which is computationally more costly. In our calculations, it is crucial to include the quadrupole deformation $\beta_2$ and the reflection-asymmetric deformation $\beta_3$. The calculations are performed in deformed coordinate spaces that can naturally describe elongated shapes to scission points. The temperature dependent fission barriers are given in terms of free energies $F=E-TS$. The collective mass parameters are calculated by the temperature dependent cranking approximation[10].

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## 2 Theoretical framework

The thermal fission lifetimes are calculated by the imaginary free energy method[6, 7]. In the ImF method, it is crucial to calculate the partition function $Z$ of the metastable system.

$$Z=\sum_n \mathrm{e}^{-\beta z_n}=\sum_n \mathrm{e}^{-\beta(E_n-i\hbar\gamma_n/2)} \ . \tag{1}$$

The widths $\gamma_n$ of each quasi-stationary states have been taken into account. Therefore the obtained free energy $F$ can have an imaginary part that is related to the fission width $\Gamma_\mathrm{f}$,

$$F=-\ln Z/\beta, \quad \Gamma_\mathrm{f}=-\frac{2}{\hbar}\mathrm{Im}F \ , \tag{2}$$

where $\beta=1/kT$. The partition function can be calculated by the functional integral over the counter.

$$Z=\oint D\left[\boldsymbol{x}(\tau)\right]\mathrm{e}^{-S[\boldsymbol{x}(\tau)]/\hbar} \ , \tag{3}$$

$$S[\boldsymbol{x}(\tau)]=\int_0^{\hbar\beta}\left[\frac{1}{2}\left(\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}\tau}\right)^2+V(\boldsymbol{x}(\tau))\right]\mathrm{d}\tau \ . \tag{4}$$

The real part of $Z$ is determined by the potential well and the imaginary part is determined by the potential barrier. The real part of the partition function, $Z_0$, can be calculated as:

$$Z_0=N\left[\mathrm{Det}\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\omega_0^2\right)\right]^{-1/2}=\left[2\sinh\left(\frac{1}{2}\hbar\omega_0\beta\right)\right]^{-1} . \tag{5}$$

The imaginary part of the partition function, $Z_b$, can be calculated as:

$$\mathrm{Im}Z_b=\sqrt{\frac{W}{2\pi\hbar}}N\left|\mathrm{Det}'\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+V''(X_b)\right]\right|^{-\frac{1}{2}}\mathrm{e}^{-S/\hbar} \ , \tag{6}$$

$$W(E)=\int\sqrt{2M(V(s)-E)}\mathrm{d}s \ , \tag{7}$$

where $W(E)$ is the tunneling action through the barrier. Finally, the thermal fission rates at low temperatures can be given as:

$$\Gamma_\mathrm{f}=Z_0^{-1}\frac{1}{2\pi\hbar}\int\mathrm{d}E\mathrm{e}^{-W(E)/\hbar}\mathrm{e}^{-\beta E} \ . \tag{8}$$

The thermal fission rates at high temperatures can be given as:

$$\Gamma_\mathrm{f}=Z_0^{-1}\omega_\mathrm{b}\left[4\pi\sin\left(\frac{1}{2}\beta\omega_\mathrm{b}\hbar\right)\right]^{-1}\mathrm{e}^{-\beta V_\mathrm{b}} \ . \tag{9}$$

From low to high temperatures, the calculated fission rates has a crossover. The transition temperature $T_\mathrm{c}$ is given as

$$T_\mathrm{c}=\frac{\omega_\mathrm{b}}{2\pi k} \ . \tag{10}$$

In the above equations, the curvatures around the potential well and the barrier are $\omega_0$ and $\omega_\mathrm{b}$, respectively. The Bohr-Wheeler fission model[11] and the Kramers model[12] are based on classical statistical theory, which should be not applicable at low temperatures. The ImF method is applicable for thermal fission rates at all temperatures based on a consistent framework. In this respect, the ImF method has been extended to include the dissipation[13] and the deformation dependent mass inertia[14]. The ImF method can also been extended to study reaction rates of multi-dimensional systems[15]. At high temperatures, the results of the ImF method is close to the Kramers results.

To calculate the thermal fission rates based on the ImF method, we need to calculate the microscopic temperature-dependent potential energy surfaces, the collective mass parameters, the barrier heights and curvatures, based on the Skyrme-Hartree-Fock+BCS calculations in axially-deformed coordinate-spaces. The coordinate-space solver can naturally describe very elongated shapes. The thermal excited nuclei with reduced quantum effects can be self-consistently described by the finite-temperature Skyrme-Hartree-Fock+BCS theory. The temperature dependent fission barriers are given in terms of the free energy. The microscopic mass parameters are given by the finite-temperature cranking approximation. The fission at low temperatures can be described mainly as a barrier-tunneling process. While the fission at high temperatures has to incorporate the reflection above barriers. The details of these calculations have been given in Ref. [16].

## 3 Results and discussion

Firstly we studied the spontaneous fission rates of some interested nuclei. The formula is based on the one dimensional WKB tunneling method, with microscopically calculated fission barriers and cranking mass inertia parameters. The results are given in Table 1, using the SkM*[19] force. The decay energy $E_0$ is given by the quantized condition. The fission lifetime of $^{240}$Pu is much larger than the experimental value. This is mainly due to the absence of triaxial deforma-

Table 1 The calculated spontaneous fission lifetimes (in seconds) of selected nuclei, in which $E_0$ is obtained by the quantization condition. The experimental data are also given for comparison.

| Nuclei | Expt/s[17] | $T_\mathrm{SF}$/s | $E_0$/MeV |
|---|---|---|---|
| $^{240}$Pu | $3.6\times10^{18}$ | $2.73\times10^{22}$ | 0.92 |
| $^{260}$Fm | $5.8\times10^{-3}$ | $4.25\times10^{-3}$ | 0.65 |
| $^{278}$Cn | | $6.39\times10^{-5}$ | 0.90 |
| $^{292}$Fl | | $8.56\times10^{4}$ | 0.46 |

tions in our calculations. In addition, the results could be dependent on the Skyrme parameters and pairing interactions. Indeed, multi-dimensional calculations are expected to be more realistic although which are computationally much more costly.

Next, we discuss the calculated thermal fission rates of $^{240}$Pu, which has been studied extensively as a benchmark for microscopic fission descriptions[18]. The calculations adopt the SkM*[19] Skyrme nuclear interaction and the mixed delta pairing interaction[20].

Fig. 1 displays the calculated fission barriers of $^{240}$Pu at temperature $T$=0, 1.0, 1.5 MeV, respectively. The symmetric and asymmetric fission barriers have been given for comparison. The octuple deformation is important to reduce the second barrier. As temperatures increase, the difference between the symmetric and asymmetric fission barriers are reduced. The triaxial deformation has not been considered in this work which is also important to reduce the first barrier height. We demonstrated the increasing symmetric fission mode at high excitation energies self-consistently.

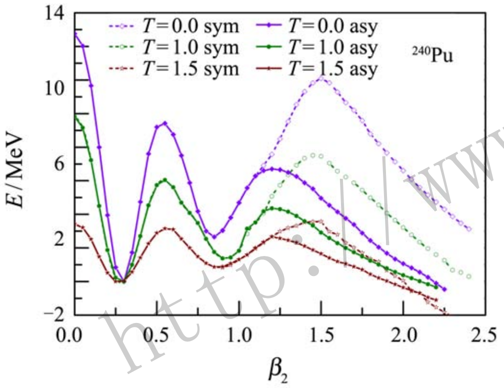

Fig. 1　(color online) The temperature-dependent fission barriers of $^{240}$Pu as a function of quadrupole deformations $\beta_2$. The symmetric and asymmetric fission barriers are given for comparison.

Fig. 2 displays the calculated mass inertia parameters with the cranking approximations. Compared to fission barriers, the mass parameters at high temperatures are rather nonsmooth. At zero temperature, the mass parameters is smooth due to the existence of pairing correlations. At the temperature of $T = 0.75$ MeV, it is around the critical temperature for the pairing phase transition and the mass parameters are increased and become very much irregular. It is known that the collective inertia mass is inversely proportional to the square of the pairing gap[21]. As the temperature increases from $T = 0$ to $T = 0.75$ MeV the pairing gap decreases and therefore the mass parameters must increase. At the high temperature of $T = 1.5$ MeV, the mass parameters are much reduced and large peaks fade away due to statistical effects.

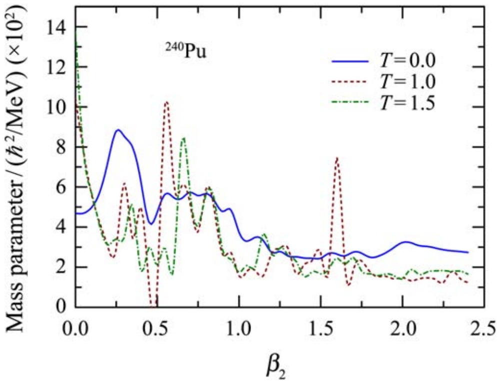

Fig. 2　(color online) The temperature-dependent mass parameters of $^{240}$Pu as a function of quadrupole deformations $\beta_2$.

Fig. 3 displays the calculated fission barrier curvatures $\omega_0$ and $\omega_\mathrm{b}$ as a function of temperatures. We see that $\omega_0$ is very large due to a narrow potential well. $^{240}$Pu has a double-humped barrier and $\omega_\mathrm{b}$ is obtained with an approximate parabolic potential. Thus the obtained $\omega_\mathrm{b}$ is small due to a very broad barrier. Consequently, the resulted crossover temperature $T_\mathrm{c}$ is very low. We say the low temperature ImF formula maybe not suitable. In the future, we should consider the double-humped structure of the barrier which can lead to resonances in cross sections.

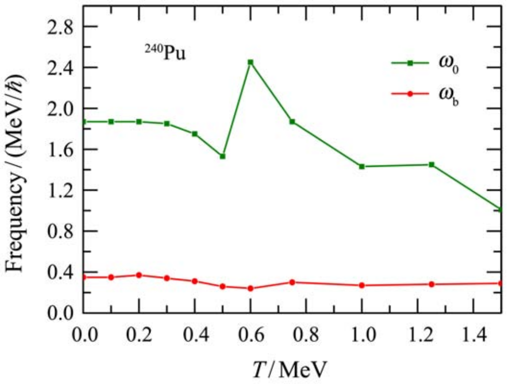

Fig. 3　(color online) The temperature-dependent curvatures around the potential well ($\omega_0$) and the fission barrier ($\omega_\mathrm{b}$) of $^{240}$Pu.

Fig. 4 displays the calculated fission lifetimes by the low and high temperature ImF formulas. We see the lifetime decreases very rapidly at low temperatures. There is a smooth crossover between the low and high temperature formulas around the excitation energy of 1 MeV. At low temperatures, the high-temperature ImF formula give large lifetimes than the low-temperature ImF formula. Generally, the Kramers formula overestimate fission lifetime than the high temperature ImF formula at low temperatures.

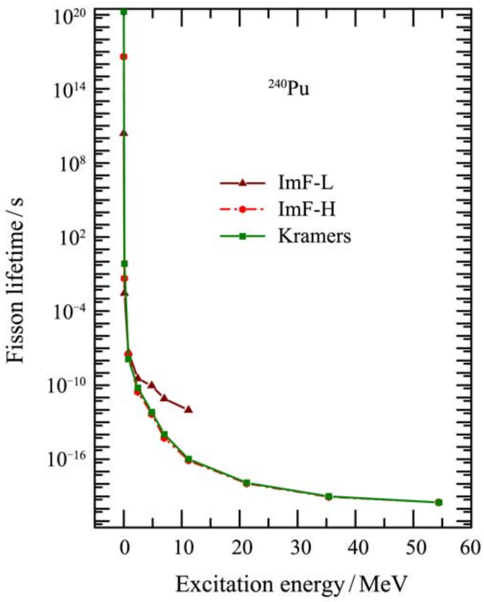

Fig. 4 (color online) The excitation energy dependent fission lifetimes of $^{240}$Pu. The lifetimes are calculated by the imaginary free energy formulas at low temperatures (ImF-L) and high temperatures (ImF-H), respectively. The results of the Kramers[12] formula is also given.

## 4 Conclusions

In summary, we studied the thermal fission rates from low to high excitation energies based on the imaginary free energy method and microscopic inputs. The temperature dependent fission barriers and mass parameters from microscopic nuclear energy functional calculations are employed. We demonstrated the temperature dependencies of fission barrier heights, curvatures and fission pathways. Conventionally, the statistical fission models rely on phenomenological inputs of level densities and potential energy surfaces, in which quantum effects are not properly considered. At high temperatures, the imaginary free energy method is close to the Kramers method. Our studies provide a consistent framework to calculate the induced fission rates. In the future, the multi-dimensional descriptions of thermal fission rates and fragment distributions are in progress.

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# 微观描述热核裂变寿命

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**摘要:** 有关热核裂变的研究与反应堆中的诱发裂变，天体环境中的裂变，以及超重元素的合成等密切相关。热核裂变的研究通常是基于Bohr-Wheeler的统计裂变理论。而统计模型的研究十分依赖唯像的能级密度和位能面。因此，提出基于微观的有限温度的能量密度泛函理论计算热核的裂变寿命。可以微观自洽地计算出温度相关的裂变位垒高度，曲率，集体质量参数。基于虚自由能法，从低温到高温的裂变寿命可以由一个统一的框架给出。展示了在裂变研究中温度相关裂变位垒的重要性，并讨论了微观描述热核裂变的前景。

**关键词:** 裂变寿命；诱发裂变；虚自由能法

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