Modified fusion probability by reflection boundary *

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Abstract: We investigate the time-dependent probability for a Brownian particle passing over the barrier to stay at a metastable potential pocket against escaping over the barrier. This is related to the whole fusion-fission dynamical process and can be called the reverse Kramers problem. By the passing probability over the saddle point of an inverse harmonic potential multiplying the exponential decay factor of a particle in the metastable potential, we present an approximate expression for the modified passing probability over the barrier, in which the effect of the reflection boundary of the potential is taken into account. Our analytical result and Langevin Monte-Carlo simulation show that the probability of passing and against escaping over the barrier is a non-monotonous function of time and its maximal value is less than the stationary result of the passing probability over the saddle point of an inverse harmonic potential.

Key words: barrier passage, modified passing probability, Langevin Monte-Carlo simulation

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1 Introduction

Metastable system decay can be applied widely to describe various science problems such as chemical reaction kinetics, phase transition, nuclear fission, and so on. The well-known Kramers problem is such a process that a Brownian particle subjected to thermal fluctuation escapes from the barrier of a metastable potential. As early as 1940, Kramers published his seminal paper "Brownian motion in force fields and chemical reaction diffusion model" [1], in which he proposed a formula for the reaction rate constant for a general-damped particle escaping from a metastable potential well and used this model to explain the mechanism of excited nuclear fission. The problem of the nuclear fission rate was studied from the point of view of Brownian motion by Wu et al. [2, 3]. Abe is the first researcher who used a Langevin Monte-Carlo simulation to numerically calculate the nuclear fission rate [4]. In 1990, Hänggi et al. [5] summarized the works fifty years after Kramers, including various improvements and extensions for the Kramers rate theory. Then, the description of fusion of heavy and heavy-ion-induced fission in the frame work of Langevin equations was reviewed by Fröbrich and Gontchar in 1998 [6]. Ye et al. [7] probed the nuclear dissipation with particle multiplicity in heavy-ion-induced light fissioning systems which was described by the Langevin equation expressed by entropy in 2014.

Now a reverse problem appears timely, i.e., a Brownian particle with initial velocity passes over the saddle point to enter into the well of a metastable potential and finally escapes from the saddle point. In fact, molecular collision, atom cluster and heavy-ion fusion are such barrier passage problems [8–16]. The fusion probability was obtained by the passing probability of a Brownian particle over the top of an inverse harmonic potential [17, 18]; the latter has been generalized to include the effects of quantum fluctuation [19], initial distribution [20], anomalous diffusion [21] as well as colored noise [22].

In the previous works, the fusion probability was studied in one dimension and the fission barrier was low in the study of the cross section of a superheavy nucleus, so that the reflection boundary was always ignored. As one knows that the fusion probability has been estimated by the stationary value of the time-dependent passing probability in terms of the fusion by the diffusion model [18], it has a simple form of error function. There is no need to consider the shell correction of potential energy and neutron emission in the fusion phase. Actually, the transient process is very important for the asymptotical passing probability being regarded as the fusion probability. The inverse harmonic potential approximation is suitable only for the near barrier fusion and high fission barrier cases. In this case, the fission life or the mean

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first passage time from the ground state to the barrier is much longer than the transient time of the passing probability over the saddle point. However, the super-heavy element cases should be treated carefully, because the component inside the barrier of time-dependent spatial distribution function (SDF) decays quickly and opposes the process of passing over the barrier. Therefore, it is necessary to consider the influence of the metastable potential structure upon the passing probability over the barrier. Of course, competition between neutron emission and fission decay needs to be investigated; the former decreases the temperature of a compound nucleus, but only occurs in the survival-evaporation phase. At present, we focus on the time-dependent dynamical fusion probability modified by the effect of the reflection boundary of a metastable potential.

The paper is organized as follows. In Section 2, we describe the barrier passage dynamics and propose an approximate expression for the probability of passing and against escaping over the barrier of a metastable potential. In this section, we also analyze the error for the stationary passing probability over the saddle point of an inverse harmonic potential regarded as the fusion probability. Finally, concluding remarks are given in Section 3.

2 Modified barrier passing probability and fusion-fission dynamics

The dynamics of a Brownian particle of mass m subjected to a fluctuation force $\xi(t)$ in a potential $U(x)$ is described by the following Langevin equation:

$$m\ddot{x}(t)+\gamma\dot{x}(t)+U'(x)=\xi(t), \tag{1}$$

where $\xi(t)$ is the Gaussian white noise satisfying $\langle\xi(t)\rangle=0$ and $\langle\xi(t)\xi(t')\rangle=2\gamma k_{\rm B}T\delta(t-t')$, $k_{\rm B}$ is the Boltzmann constant, T is the temperature and γ is the damping coefficient. In order to present an approximate expression for the time-dependent passing probability and against escaping over the barrier in a metastable potential, we consider an inverse harmonic potential linking smoothly with a harmonic potential,

$$U(x)=\begin{cases} U_{\rm g}(x)=\dfrac{1}{2}\omega_{\rm g}^2(x-x_{\rm g})^2, & x\leqslant x_{\rm c}; \\ U_{\rm s}(x)=U_{\rm b}-\dfrac{1}{2}\omega_{\rm s}^2x^2, & x\geqslant x_{\rm c}. \end{cases} \tag{2}$$

where $x_{\rm g}$ denotes the coordinate of the ground state, $\omega_{\rm g}$ and $\omega_{\rm s}$ are the circular frequencies of the potential at the ground state and the saddle point, respectively. The linking point of the two potentials is determined by $x_{\rm c}=x_{\rm g}\omega_{\rm g}^2/(\omega_{\rm g}^2+\omega_{\rm s}^2)$ through $U_{\rm g}(x_{\rm c})=U_{\rm s}(x_{\rm c})$ and $U'_{\rm g}(x_{\rm c})=U'_{\rm s}(x_{\rm c})$, $U_{\rm b}$ is the barrier height given by $U_{\rm b}=\dfrac{1}{2}\omega_{\rm s}^2x_{\rm c}x_{\rm g}$. In the calculations, all the parameters are chosen to be dimensionless forms and $m=k_{\rm B}=1.0$. We choose $x_{\rm s}=0$ to be the coordinate of the saddle point.

Firstly, in Fig. 1, we use the Langevin Monte-Carlo simulation to plot the time evolution of SDF of the particle in the inverse harmonic potential and the metastable

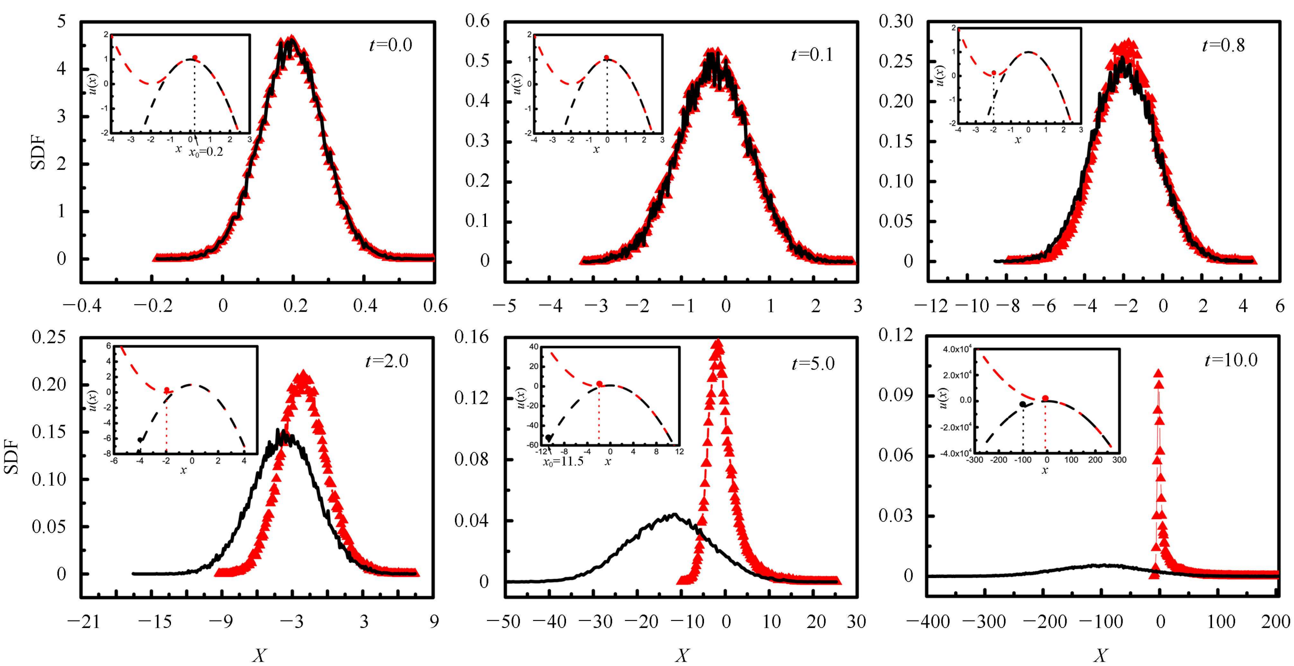

Fig. 1. (color online). Time evolution of SDF of a particle. The black-solid and red-triangle lines are the SDFs of the particle in the inverse harmonic and metastable potentials, respectively. Each inset shows the potential with dots representing the positions where the peak of the distributions locate. The parameters used are: $T=0.4$, $\gamma=1.0$, $U_{\rm b}=1.0$, $\bar{v}_0=-5.0$ and $\bar{x}_0=0.2$. Note that each subgraph has a different scale.

potential, respectively. It is seen that the two SDFs are the same at the beginning, because the metastable well does not have an effect; however, some test particles have come into the saddle point and then they display a different behaviour as time goes on. Due to the reflection boundary of the metastable potential, the SDF in this potential shows a quasi-stationary Boltzmann distribution around the well and its right-tail escapes continually from the barrier; of course, all the test particles escape from the barrier in the long time limit. Nevertheless, the SDF in the inverse harmonic potential case remains Gaussian all along, but its center tends towards infinity after crossing over the potential top when the initial conditions are larger than the critical conditions [18]. On the other hand, we find that the descent time of the particles from the barrier to the bottom of the well is fast enough, so that the influence of this process upon the modified passing probability is not important.

Let us reconsider the time-dependent process for passing over the saddle point of an inverse harmonic potential. In this case, the first equation in Eq. (2) is ignored. This model has been used widely in the calculations of fusion probability. The Brownian particle is located initially at the position $x_0>0$ and has a negative velocity $v_0<0$. The phase distribution function $W(x,v,t)$ of the particle at time t is also a Gaussian one due to both linear equation and Gaussian noise. It is written as [20, 21, 23–25]:

$$W(t;x,v) = \frac{1}{2\pi\sigma_x(t)\sigma_{v(t)}}\exp\left(-\frac{[x(t)-\langle x(t)\rangle]^2}{2\sigma_x^2(t)}\right)\times\exp\left(-\frac{[v(t)-\langle v(t)\rangle]^2}{2\sigma_v^2(t)}\right), \tag{3}$$

where $\langle x(t)\rangle$ is the average position of the particle and $\sigma_x^2(t)$ is the coordinate variance, they are respectively [20]

$$\begin{aligned}\langle x(t)\rangle &= x_0A(t)+v_0B(t),\\ \sigma_x^2(t) &= \frac{T}{m\omega_s^2}\left\{\exp(-\gamma t)\left[\frac{2\gamma^2}{4\omega_s^2+\gamma^2}\sinh^2\left(\frac{t}{2}\sqrt{4\omega_s^2+\gamma^2}\right)+\frac{\gamma}{\sqrt{4\omega_s^2+\gamma^2}}\sinh\left(t\sqrt{4\omega_s^2+\gamma^2}\right)+1\right]-1\right\},\end{aligned} \tag{4}$$

where $A(t)$ and $B(t)$ are given by

$$\begin{aligned}A(t) &= \exp(-\gamma t)\left[\cosh\left(\frac{t}{2}\sqrt{4\omega_s^2+\gamma^2}\right)+\frac{\gamma}{\sqrt{4\omega_s^2+\gamma^2}}\sinh\left(\frac{t}{2}\sqrt{4\omega_s^2+\gamma^2}\right)\right],\\ B(t) &= \frac{2}{m\sqrt{4\omega_s^2+\gamma^2}}\exp(-\gamma t)\times\sinh\left(\frac{t}{2}\sqrt{4\omega_s^2+\gamma^2}\right).\end{aligned} \tag{5}$$

The time-dependent passing probability $P_{\rm pass}(t, x_0, v_0)$ of the particle over the saddle point of an inverse harmonic potential is determined by

$$P_{\rm pass}(t;x_0,v_0) = \int_{-\infty}^{\infty}\int_{-\infty}^{0}W(t;x,v)\mathrm{d}v\mathrm{d}x = \frac{1}{2}\mathrm{erfc}\left(\frac{\langle x(t)\rangle}{\sqrt{2}\sigma_x(t)}\right), \tag{6}$$

which depends on the initial conditions of the coordinates and velocity of the particle.

In the case of heavy-ion fusion, a dispersion of the initial conditions should be considered with a different width, assuming a Gaussian distribution [20],

$$W_0(\bar{x}_0,\sigma_{x_0},\bar{v}_0,T_0) = \frac{1}{2\pi\sigma_{x_0}\sqrt{mT_0}}\exp\left(-\frac{[x_0-\bar{x}_0]^2}{2\sigma_{x_0}^2}\right)\times\exp\left(-\frac{[v_0-\bar{v}_0]^2}{2mT_0}\right). \tag{7}$$

Thus the time-dependent passing probability $\bar{P}_{\rm pass}(t,x_0,v_0)$ over the saddle point of an inverse harmonic potential is written as

$$\begin{aligned}\bar{P}_{\rm pass}(t;\bar{x}_0,\sigma_{x_0},\bar{v}_o,T_0) &= \int_{-\infty}^{\infty}\mathrm{d}x_0\int_{-\infty}^{\infty}\mathrm{d}v_0P_{\rm pass}(t;x_0,v_0)\times W_0(\bar{x}_0,\sigma_{x_0},\bar{v}_0,T_0)\\ &= \frac{1}{2}\mathrm{erfc}\left(\frac{\langle\bar{x}(t)\rangle}{\sqrt{2}\sigma'_x(t)}\right),\end{aligned} \tag{8}$$

where $\langle\bar{x}(t)\rangle$ is the same as in Eq. (5), provided that x_0 and v_0 are replaced by $\bar{x}_0$ and $\bar{v}_0$, respectively. The variance becomes

$$\sigma_x'^2(t)=\sigma_x^2(t)+\sigma_{x_0}^2(t)A^2(t)+mT_0B^2(t). \tag{9}$$

In these equations, T_0 is a parameter for the initial distribution that could be interpreted as the temperature of the nuclei at contact [20]. Naturally, the SDF of the particle under fluctuation force becomes wider and wider and its center moves along the direction of initial velocity as time goes on. After the transient time, a part of the SDF has passed over the saddle point and then the passing probability converges to a finite value with $0\leqslant\bar{P}_{\rm pass}\leqslant1$, because of $\lim_{t\to\infty}\langle\bar{x}(t)\rangle/\sigma'_x(t)$=constant in Eq. (10).

We can find that the descent time of the particle from the barrier to the bottom of the well increases with the increase of the initial temperature of thermalization, as shown in Fig. 2. As a consequence, the initial kinetic energy should be considered and this result is similar to Ref. [20] for a sharp initial condition.

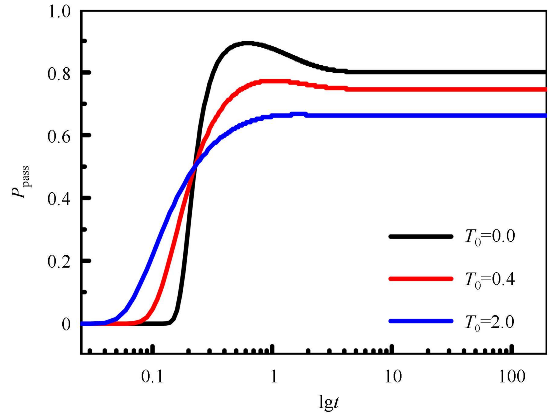

Fig. 2. (color online). The time-dependent passing probability with logarithmic of the time. Here, $T=0.4$, $\gamma=1.0$, $U_{\rm b}=1.0$, $\sigma_{x_0}=0.0$, $\bar{v}_0=-5.0$ and $\bar{x}_0=0.2$.

We now address the modified passing probability taking into account the influence of the reflection boundary of a potential by a reasonable assumption. According to the Kramers rate theory, the particle subjected to thermal fluctuation in the metastable potential will finally decay over the barrier [24, 26]. We multiply the exponential decay factor into the passing probability which has been coupled with the fusion and fission processes, so that the modified passing probability, namely, the time-dependent probability of the particle staying inside the saddle point, is assumed to be

$$P_{\text{m-pass}}(t;x_0,v_0) = \bar{P}_{\text{pass}}(t;\bar{x}_0,\sigma_{x_0},\bar{v}_0,T_0)\exp(-r_{\rm e}t) = \frac{1}{2}\text{erfc}\left(\frac{\langle\bar{x}(t)\rangle}{\sqrt{2}\sigma'_x(t)}\right)\exp(-r_{\rm e}t), \quad (10)$$

where $r_{\rm e}$ is the steady escape rate [1, 5, 27–31]. This approximation implies that once the particle passes over the barrier top, it should finally escape over the barrier with the Kramers decay form. In Fig. 2, it is obvious that the transient time can be ignored in the calculation of the time-dependent modified passing probability. If $r_{\rm e}\to 0$, $\exp(-r_{\rm e}t)\approx 1$ after a finite time, the modified passing probability (Eq. (10)) approaches the passing probability (Eq. (8)) for the inverse harmonic potential.

The Kramers rate formula [1, 5, 29] produces a better stationary result of time-dependent escape rate when the barrier height of the metastable potential is larger than the temperature, as shown in Fig. 3(a). However, when the temperature is larger than the barrier height, the Kramers rate formula is not applicable. We use the inverse of the mean first passage time (MFPT) [30] across an exit $x_{\rm ex}$ given by

$$\tau_{\rm MFPT}(x_0\to x_{\rm ex}) = \left(\frac{\sqrt{\frac{\gamma^2}{4}+\omega_{\rm s}^2}-\frac{\gamma}{2}}{\omega_{\rm s}}\right)^{-1}\frac{\omega_{\rm s}}{T} \times\int_{x_0}^{x_{\rm ex}}{\rm d}y\exp\left[\frac{U(y)}{T}\right] \times\int_{-\infty}^{y}{\rm d}z\exp\left[-\frac{U(z)}{T}\right] \quad (11)$$

to replace the stationary escape rate of the particle in a metastable potential well, i.e., $r_{\rm e}=(\tau_{\rm MFPT})^{-1}$ [5, 31]. Notice that we introduce here a correction factor of general damping to the previous overdamped result. Indeed, Eq. (11) is in agreement with the result of Refs. [30, 32–36] in the overdamped case ($\gamma\gg\omega_{\rm s}$). At low temperature, Eq. (11) can be evaluated within the steepest-descent approximation [5] as the following

$$\tau_{\rm MFPT}(x_0\to x_{\rm ex}) = \left(\frac{\sqrt{\frac{\gamma^2}{4}+\omega_{\rm s}^2}-\frac{\gamma}{2}}{\omega_{\rm s}}\right)^{-1} \times\frac{2\pi}{\omega_{\rm g}}\exp\left(\frac{U_{\rm b}}{T}\right); \quad (12)$$

its inverse coincides with the Kramers rate formula [37].

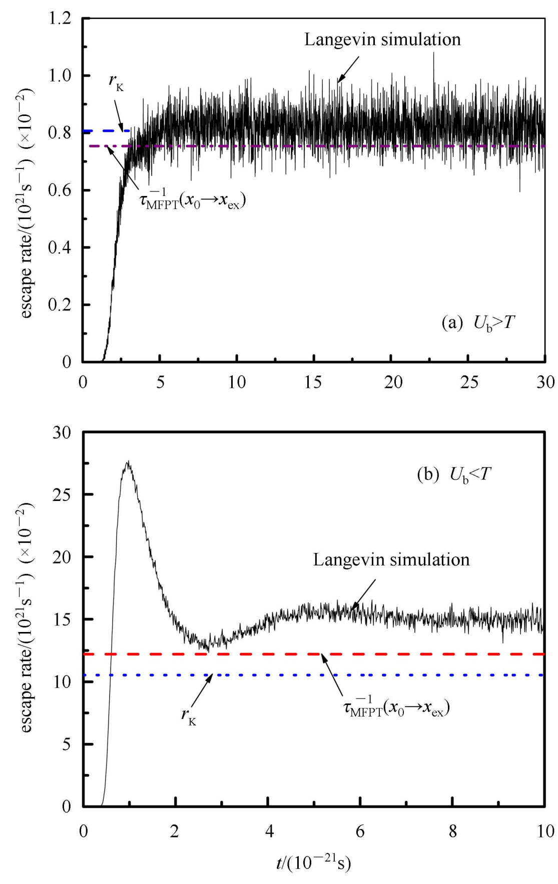

Fig. 3. (color online). Time-dependent escape rate calculated by Langevin simulation and compared by the analytical formula of two kinds. (a) is the low-temperature case ($U_{\rm b}=1.0$, $T=0.4$) and (b) is the high-temperature case ($U_{\rm b}=0.25$, $T=2.0$).

Furthermore, the advance of MFPT or the mean last passage time (MLPT) [35] is not restricted to smooth metastable potentials. Eq. (11) is still suitable even if the nuclear shell correction is taken into account in the deformation potential energy of super-heavy elements. A statistical proof for the relation between the Kramers rate constant and the MFPT or the MLPT was presented in Ref. [36].

As is known, the fusion probability can be defined as the transmission coefficients for central collisions which are calculated by counting for each energy the number of Langevin trajectories which fuse and dividing it by the total number of trajectories [6]. In Figs. 4 and 5, we compare the time-dependent modified passing probability (Eq. (10)) with the Langevin Monte-Carlo simulation for Eqs. (1) and (2) and the passing probability (Eq. (8)) over the saddle point of the inverse harmonic potential, respectively, where three typical initial velocities are used. It is evident from Eq. (10) that the modified passing probability over the barrier of the metastable potential approaches zero in the long-time limit.

It is seen from Fig. 4 that the modified passing probability calculated by our theoretical formula is in agreement with the Langevin Monte-Carlo simulation when $U_b > T$. In particular, the maximal value of the time-dependent modified passing probability is close to the stationary value of the passing probability over the saddle point of the inverse harmonic potential. This means that the influence of the reflection boundary of the metastable potential upon the transient part of the time-dependent passing probability is weak in the case of low temperature or high barrier. Fig. 5 shows the calculated result at high temperature, in which the barrier height of the metastable potential is $U_b = 1.0$ and the temperature $T = 2.0$.

If the barrier height is low, the particle under influence of the reflection boundary of potential can more easily escape over the saddle point, so that the time required for the modified passing probability arriving at the maximum is earlier than that of the passing probability approaching its stationary value. This concludes that the reflection boundary of the metastable potential plays a decreasing role to the transient result of the passing probability.

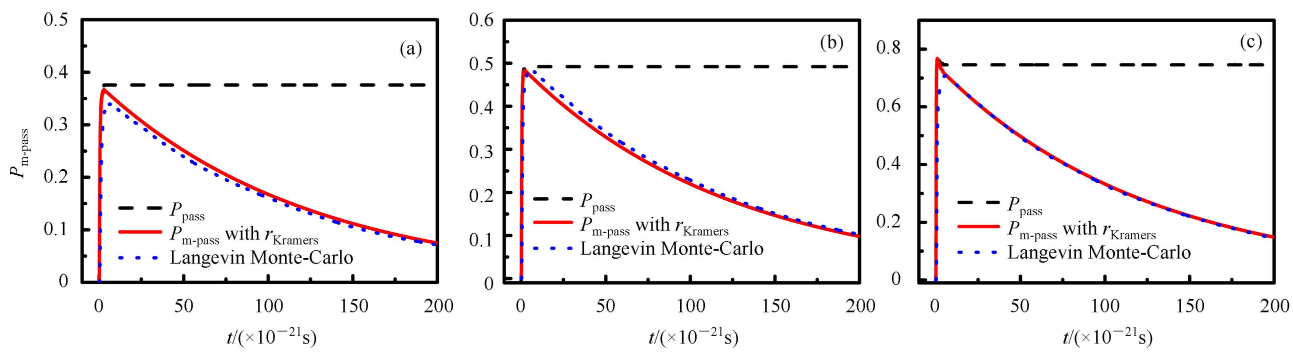

Fig. 4. (color online). The time-dependent modified passing probability over the barrier of the metastable potential and the passing probability over the saddle point of the inverse harmonic potential with three typical initial velocities: (a) $v_0 = 0$, (b) $v_0 = -0.3$, (c) $v_0 = -1.0$. The parameters used are: $U_b = 1.0$, $T = 0.4$, $T_0 = 0.4$, $\sigma_{x_0} = 0$, $\gamma = 1.0$, $x_0 = 0.2$.

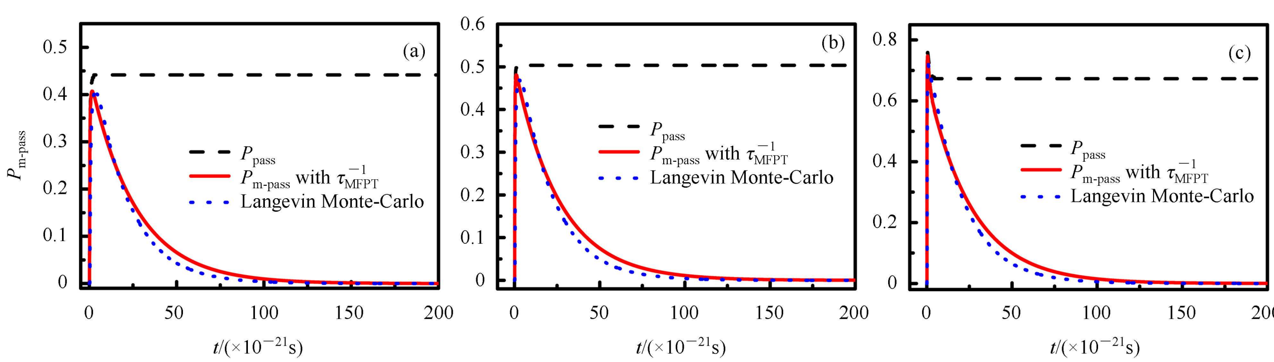

Fig. 5. (color online). Comparison of the time-dependent modified passing probability over the barrier of the metastable potential and the passing probability over the saddle point of the inverse harmonic potential with three typical initial velocities: (a) $v_0 = 0$, (b) $v_0 = -0.5$, (c) $v_0 = -2.0$. The parameters used are: $U_b = 1.0$, $T = 2.0$, $T_0 = 2.0$, $\gamma = 2.0$, $\sigma_{x_0} = 0$, $x_0 = 0.2$.

We have proposed the expression of the time-dependent modified passing probability against escaping over the barrier of the metastable potential, i.e., Eq. (10); the time leading to $P_{\text{m-pass}}$ becomes the maximum that is determined by the positive real root of the following equation:

$$\frac{\mathrm{d}P_{\text{m-pass}}}{\mathrm{d}t} = \frac{1}{2}\exp(-r_{\mathrm{e}}t)J(t) - \frac{1}{2}r_{\mathrm{e}}\exp(-r_{\mathrm{e}}t) \times \mathrm{erfc}\left(\frac{\langle\bar{x}(t)\rangle}{\sqrt{2}\sigma'_x(t)}\right) = 0, \tag{13}$$

where $J(t)$ is the derivative of $\mathrm{erfc}[\langle\bar{x}(t)\rangle/(\sqrt{2}\sigma'_x(t))]$ given by

$$J(t) = -\frac{2}{\sqrt{\pi}}\exp\left(-\frac{\langle\bar{x}(t)\rangle^2}{\sigma'^2_x(t)}\right)\left[\frac{M(t)}{\sqrt{2}\sigma'_x(t)} - \frac{T}{2\sqrt{2}m\omega_{\mathrm{s}}^2}\frac{\langle\bar{x}(t)\rangle G(t)}{\sigma'^3_x(t)}\right], \tag{14}$$

where $M(t)$ and $G(t)$ are

$$M(t) = \exp(-\gamma t)\left[\left(\frac{\bar{v}_0}{m} - \frac{\bar{x}_0\gamma}{2}\right)\cosh\left(\frac{1}{2}at\right) + \left(\frac{a\bar{x}_0}{2} + \frac{\gamma^2\bar{x}_0}{a} - \frac{2\gamma\bar{v}_0}{ma}\right)\sinh\left(\frac{1}{2}at\right)\right],$$

$$G(t) = 2\gamma\left(1 - \frac{\gamma^2}{a^2}\right)\exp(-\gamma t)\sinh^2\left(\frac{1}{2}at\right), \tag{15}$$

where $a = \sqrt{4\omega_{\mathrm{s}}^2 + \gamma^2}$. Hence the maximum of the time-dependent modified passing probability can be obtained by Eq. (10) through solving numerically Eqs. (13)–(15). Notice that this quantity is defined depending on the model parameters. It is seen from Fig. 2 that the time corresponding to the maximal staying probability is equal approximately to the transient time of the passing probability only in the case of a high barrier.

In Fig. 6, we show the maximal value of the time-dependent modified passing probability over the saddle point of the metastable potential as a function of the barrier height, which is also compared with the stationary passing probability over the saddle point of the inverse harmonic potential. It is seen that with the increase of the barrier height, the maximal value of the time-dependent modified passing probability is close to the stationary value of the passing probability over the saddle point of the inverse harmonic potential, so that one can approximately treat the asymptotical passing probability over the saddle point of the inverse harmonic potential as the fusion probability in a massive nuclear fusion reaction. However, when the fission barrier is low, which occurs in the super-heavy element cases, the stationary value of the time-dependent passing probability over the saddle point of the inverse harmonic potential is no longer applicable for the fusion probability. From the present work, we think that it is better to regard the maximal value of the time-dependent modified passing probability over the saddle point of the metastable potential as the fusion probability, since the modified passing probability is the result of the whole fusion-fission process.

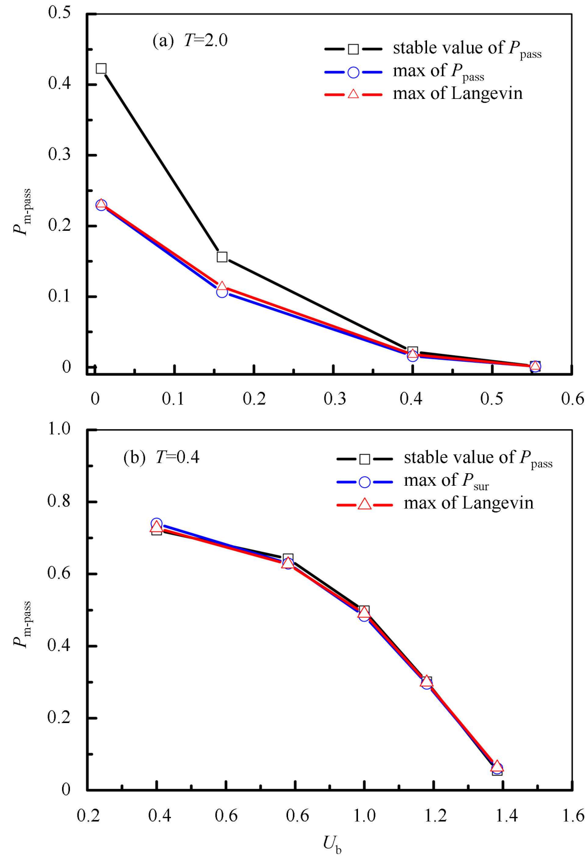

Fig. 6. (color online) The maximum value of the time-dependent modified passing probability (blue-circled-line) over the barrier of the metastable potential and the stationary passing probability (black-squared-line) over the saddle point of the inverse harmonic potential. They are compared with the Langevin Monte-Carlo simulations (red-triangled-line).

3 Conclusion

We have investigated the whole fusion-fission process with the Langevin approach, in which the influence of the reflection boundary of the metastable potential is taken into account in the calculation of the time-dependent passing probability over the saddle point. By the passing probability over the saddle point of the inverse harmonic potential multiplying the exponential decay factor of the particle in the metastable potential, an approximate analytical expression for the modified time-dependent passing probability over the saddle point of the metastable potential has been proposed. Our results have shown that only when the temperature is smaller than the fission barrier of the fusing system, the stationary passing probability over the saddle point of an inverse harmonic potential can be regarded as the fusion probability of the massive nuclei. Nevertheless, at a low fission barrier, the reflection boundary plays a decreasing role for the passing probability over the saddle point. It has been found that the time required for the modified time-dependent passing probability arriving at the maximal value is earlier than the transient time of the passing probability. This is due to the decaying probability against the passing probability.

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