© 2022 Institute of Theoretical Physics CAS, Chinese Physical Society and IOP Publishing Printed in China and the UK Communications in Theoretical Physics

Commun. Theor. Phys. 74 (2022) 125601 (6pp) https://doi.org/10.1088/1572-9494/ac936c

Escape rate of an active Brownian particle in a rough potential

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Received 14 August 2022, revised 20 September 2022
Accepted for publication 21 September 2022
Published 30 November 2022

Abstract

We discuss the escape problem with the consideration of both the activity of particles and the roughness of potentials. We derive analytic expressions for the escape rate of an active Brownian particle in two types of rough potentials by employing the effective equilibrium approach and the Zwanzig method. We find that activity enhances the escape rate, but both the oscillating perturbation and the random amplitude hinder escaping.

Keywords: escape rate, active Brownian particle, rough potential, effective potential

(Some figures may appear in colour only in the online journal)

1. Introduction

The escape problem has attracted much attention from researchers in various fields [1–10]. The Arrhenius formula indicates that the rate of a chemical reaction depends exponentially on inverse temperature [3, 4]. Kramers presented the transition state method for calculating the rate of chemical reactions by considering a Brownian particle escaping over a potential barrier [5]. Subsequent studies on escape rate are summarized in [10]. All of the above studies merely involve passive particles. The research theme has been transferred to active particles with self-propulsion in recent years [11–24]. Active systems are intrinsically non-equilibrium since the detailed balance is broken. An effective equilibrium method has been developed to investigate active Brownian particles [25–28]. By using this method, Sharma *et al* discussed an escape problem of active particles in a smooth potential [29]. They found that introducing activity increases the escape rate.

The escape problem in the research mentioned above is simplified as a Brownian particle climbing over a smooth potential barrier. However, the potential is not always smooth in reality. Interface area scans of proteins imply that the protein surface is not smooth [30, 31]. The hierarchical arrangement of the conformational substrates in myoglobin indicates that the potential surface might be rough [32]. In addition, the inside of the cell is quite crowded. Thus, diffusion of substance in the cell may not be regarded as Brownian motion in smooth potential. From the biochemical point of view, it is valuable to consider the influence of the roughness of potential diffusion behaviors. The study of diffusion in rough potential offers insight into fields from the transport process in disordered media [33, 34] to protein folding [35, 36] and glassy systems [37, 38]. Zwanzig dealt with diffusion in a rough potential and found that the roughness slows down the diffusion at low temperatures [39]. Roughness-enhanced transport was also observed in ratchet systems [40–42]. Hu *et al* discussed diffusion crossing over a barrier in a random rough metastable potential [43]. By using numerical simulations, they demonstrate a decrease in the steady escape rate with the an increase of rough intensity. The activity of particles was not considered in these works.

There are a large number of active substances, biochemical reactions, and transport of substances in organisms. Therefore, it is of practical significance to discuss the escape problem with the consideration of both the activity of particles and the roughness of potentials. In order to describe the slow dynamics of a tagged particle in a dense active environment, Subhasish *et al* discussed the escape of a passive particle from an activity-induced energy landscape by using the activity-induced rugged energy landscape approach [44]. In this work, we calculate the escape rate of an active Brownian particle (ABP) in rough potentials by using the effective equilibrium approach [25–29] and the Zwanzig method [39]. The rest of this paper is organized as follows: In section 2, we briefly introduce the effective equilibrium approach. In section 3, we discuss the escape problems of

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ABPs in rough potentials with oscillating perturbation or random amplitude. We derive the effective rough potentials following the effective equilibrium approach. Then we analytically calculate the escape rates of ABPs in the effective rough potentials. We find that activity enhances the escape rate, but both the oscillating perturbation and the random amplitude hinder escaping. The last section is a brief summary.

2. Effective equilibrium approach

In this section, we briefly revisit the main ideas of the effective equilibrium approach [25–29].

The motion of the ABP can be described by the following overdamped Langevin equations

$$\dot{\boldsymbol{r}} = v_0\boldsymbol{n} + \gamma^{-1}\boldsymbol{F} + \boldsymbol{\xi}(t), \tag{1}$$

$$\dot{\boldsymbol{n}} = \boldsymbol{\eta}(t) \times \boldsymbol{n}, \tag{2}$$

where γ is the friction coefficient and $\boldsymbol{F}(t)$ is force on the ABP. $\boldsymbol{r}$ represents the position of the particle. The particle is self-propelling with constant speed v_0 along orientations $\boldsymbol{n}$. The dot '·' above a character represents the derivative with respect to time t. The stochastic vectors $\boldsymbol{\xi}(t)$ and $\boldsymbol{\eta}(t)$ are white noise with correlations $\langle\boldsymbol{\xi}(t)\boldsymbol{\xi}(t')\rangle = 2D_t\boldsymbol{I}\delta(t-t')$ and $\langle\boldsymbol{\eta}(t)\boldsymbol{\eta}(t')\rangle = 2D_r\boldsymbol{I}\delta(t-t')$, where D_t and D_r are the translational and rotational diffusion coefficients, respectively. $\boldsymbol{I}$ is the unit tensor.

We obtain $\langle\boldsymbol{n}(t)\rangle = 0$ and $\langle\boldsymbol{n}(t)\boldsymbol{n}(t')\rangle = (1/3)\boldsymbol{I}\mathrm{e}^{-2D_r|t-t'|}$ from equation (2). By substituting them into equation (1), we derive

$$\dot{\boldsymbol{r}} = \gamma^{-1}\boldsymbol{F} + \boldsymbol{\chi}(t), \tag{3}$$

where $\langle\boldsymbol{\chi}(t)\rangle = 0$ and $\langle\boldsymbol{\chi}(t)\boldsymbol{\chi}(t')\rangle = 2D_t\boldsymbol{I}\delta(t-t') + (v_0^2/3)\boldsymbol{I}\mathrm{e}^{-2D_r|t-t'|}$.

A stochastic process with color-noise in equation (3) is non-Markovian. It is impossible to derive an exact Fokker–Planck equation for the time evolution of the probability distribution. Nevertheless, using the Fox approximate method [45, 46], we may derive an approximate Fokker–Planck equation

$$\frac{\partial\phi(\boldsymbol{r}, t)}{\partial t} = -\nabla\cdot\boldsymbol{J}(\boldsymbol{r}, t), \tag{4}$$

where $\phi(\boldsymbol{r}, t)$ is the probability distribution. The current $\boldsymbol{J}(\boldsymbol{r}, t)$ is expressed as

$$\boldsymbol{J}(\boldsymbol{r}, t) = -D_t D(\boldsymbol{r})[\nabla - \beta\boldsymbol{F}^{\mathrm{eff}}(\boldsymbol{r})]\phi(\boldsymbol{r}, t), \tag{5}$$

where $\boldsymbol{F}^{\mathrm{eff}}(\boldsymbol{r})$ represents the effective force on the particle. $\beta = (k_B T)^{-1}$, in which k_B is the Boltzmann constant and T is the temperature. The dimensionless effective diffusion coefficient $D(\boldsymbol{r}) = 1 + D_a/(1 - \tau\nabla\cdot\beta\boldsymbol{F}(\boldsymbol{r}))$, where $\tau = D_t/(2D_r)$. The activity parameter $D_a = v_0^2/(6D_rD_t)$. The effective force is given by

$$\boldsymbol{F}^{\mathrm{eff}}(\boldsymbol{r}) = \frac{1}{D(\boldsymbol{r})}[\boldsymbol{F}(\boldsymbol{r}) - \beta\nabla D(\boldsymbol{r})]. \tag{6}$$

3. Escape rate of ABP in rough potentials

In this section, we will deduce the effective rough potential and escape rate of ABP in rough potentials. For simplicity, we only consider the case that the bare force depends merely on a one-dimension potential $V = V(x)$. In this case, $\boldsymbol{F} = -V'(x)\boldsymbol{i}$, where $\boldsymbol{i}$ is the unit vector of x-coordinate. The prime '′' on the top right of a character represents the derivative with respect to position x. From equation (6) we can obtain the effective potential

$$\beta V^{\mathrm{eff}}(x) = \ln D(x) + \int_0^x \mathrm{d}y\frac{\beta V'(y)}{D(y)}, \tag{7}$$

with

$$D(x) = 1 + \frac{D_a}{1 + \tau\beta V''(x)}. \tag{8}$$

Now, let us consider a rough potential

$$\beta V(x) = \frac{1}{2}\kappa_0 x^2 - \alpha x^3 + \varepsilon V_1(x), \tag{9}$$

where κ_0 and α are positive constants. The first two terms in equation (9) provide a smooth background with a barrier. The last term in equation (9) is the superposed random or oscillating perturbation. The amplitude ε is assumed to be small, which represents a measure of the 'roughness' of the potential.

Now, we look for the effective rough potential $\beta V^{\mathrm{eff}}(x)$ corresponding to equation (9) from equation (7). Assuming $\kappa_0\tau \ll 1$ and keeping the terms up to the linear order of $\kappa_0\tau$ and ε, we obtain the effective rough potential

$$\beta V^{\mathrm{eff}}(x) \approx \frac{1}{2}\kappa_a x^2 - \alpha' x^3 + g(x) + \frac{\varepsilon V_1(x)}{1 + D_a}, \tag{10}$$

where

$$\kappa_a = \kappa_0\left[\frac{1}{1 + D_a} + \frac{D_a\kappa_0\tau}{(1 + D_a)^2}\right], \tag{11}$$

$$\alpha' = \alpha\left[\frac{1}{1 + D_a} + \frac{3D_a\kappa_0\tau}{(1 + D_a)^2}\right], \tag{12}$$

$$g(x) = \frac{6D_a\alpha\tau}{1 + D_a}x + \frac{9D_a\alpha^2\tau}{2(1 + D_a)^2}x^4. \tag{13}$$

The above three equations and the first three terms in equation (10) have been derived in [29].

The bare and effective rough potentials are schematically depicted in figure 1. x_a and x_b correspond to the minimum and maximum of the potential, respectively. x_c is a point on the right of x_b. Passing x_c, the particle will not return. In the other words, it is an absorbing boundary condition at x_c. In a stationary state, the current (5) can be rewritten as

$$J_{\mathrm{act}}^{\mathrm{rou}} = -D_t D(x)\mathrm{e}^{-\beta V^{\mathrm{eff}}(x)}\frac{\mathrm{d}}{\mathrm{d}x}[\mathrm{e}^{\beta V^{\mathrm{eff}}(x)}\phi(x)]. \tag{14}$$

Following Kramers's approach [5, 47], we obtain the inverse of the escape rate of ABP:

$$\frac{1}{r_{\mathrm{act}}^{\mathrm{rou}}} = \int_{x_1}^{x_2}\mathrm{d}y\mathrm{e}^{-\beta V^{\mathrm{eff}}(y)}\int_{x_a}^{x_c}\mathrm{d}z\frac{1}{D_t D(z)}\mathrm{e}^{\beta V^{\mathrm{eff}}(z)}, \tag{15}$$

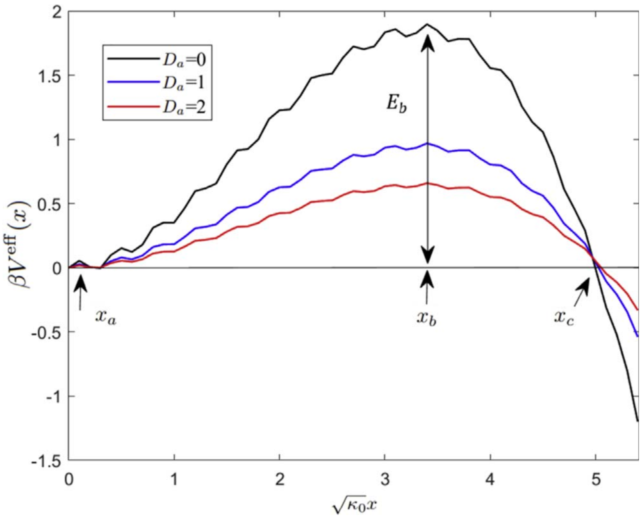

Figure 1. Bare potential and analytic effective potential $\beta V^{\rm eff}(x)$, equation (28), for different values of D_a. For the given parameter $\alpha\kappa_0^{-3/2}=0.1$, $\tau\kappa_0=0.02$, $\varepsilon=0.05$ and $q\kappa_0^{-1/2}=17$.

where $x_1\leqslant x_a\leqslant x_2\leqslant x_b$. The detailed derivation of this equation is shown in appendix A.

Considering the rough character of the potential, we use the Zwanzig method [39] to simplify equation (15). The rough potential (10) may be decomposed into two parts. One is the smooth skeleton

$$\beta V_0^{\rm eff}(x)=\frac{1}{2}\kappa_a x^2-\alpha' x^3+g(x), \tag{16}$$

the other is the rough perturbation

$$\beta V_1^{\rm eff}(x)=\frac{\varepsilon V_1(x)}{1+D_a}. \tag{17}$$

Since $V_1^{\rm eff}(x)$ varies quickly with x, we consider its average effect on escape rate in equation (15). Define $\psi^+(x)$ and $\psi^-(x)$ such that

$$e^{\psi^{\pm}(x)}=\langle e^{\pm\beta V_1^{\rm eff}(x)}\rangle, \tag{18}$$

where $\langle\ \rangle$ denotes the spatial average during a small interval $(x-\Delta/2,\ x+\Delta/2)$. Then equation (15) is transformed into

$$\frac{1}{r_{\rm act}^{\rm rou}}=\int_{x_a}^{x_c}{\rm d}y e^{-\beta V_0^{\rm eff}(y)}e^{\psi^-(y)}\times\int_{x_a}^{x_c}{\rm d}z\frac{e^{\beta V_0^{\rm eff}(z)}e^{\psi^+(z)}}{D_t D(z)}. \tag{19}$$

Next we discuss the spacial situation that $\psi^{\pm}(x)$ happens to be independent of x. In this case, the above equation is transformed into

$$\frac{1}{r_{\rm act}^{\rm rou}}=e^{\psi^-}e^{\psi^+}\int_{x_a}^{x_c}{\rm d}y e^{-\beta V_0^{\rm eff}(y)}\int_{x_a}^{x_c}{\rm d}z\frac{e^{\beta V_0^{\rm eff}(z)}}{D_t D(z)}. \tag{20}$$

By using the saddle-point approximation and considering $\kappa_0\tau$ is small, we derive the escape rate

$$r_{\rm act}^{\rm rou}=\frac{D_t(1+D_a)\sqrt{|\kappa_a\kappa_b|}\,e^{-(\beta E_b-\frac{D_a\kappa_0\tau}{1+D_a})}}{2\pi e^{\psi^-}e^{\psi^+}}, \tag{21}$$

where

$$\kappa_b=\kappa_0\left[-\frac{1}{1+D_a}+\frac{D_a\kappa_0\tau}{(1+D_a)^2}\right], \tag{22}$$

and

$$\beta E_b=\frac{\kappa_0^3}{54\alpha^2(1+D_a)}+\frac{2D_a\kappa_0\tau}{1+D_a}. \tag{23}$$

The detailed derivation of equation (21) is displayed in appendix B.

For a passive Brownian particle moving in a smooth potential, equation (21) is degenerated into

$$r_{\rm pass}=\frac{D_t\kappa_0}{2\pi}e^{-\beta E_0}, \tag{24}$$

where $\beta E_0=\kappa_0^3/(54\alpha^2)$. This is exactly the Kramers rate for the passive particle escaping from a smooth barrier [5]. The escape rate of ABP in rough potential may be further expressed as

$$r_{\rm act}^{\rm rou}=r_{\rm pass}e^{\frac{D_a(\beta E_0-\kappa_0\tau)}{1+D_a}}[e^{\psi^-}e^{\psi^+}]^{-1}. \tag{25}$$

Obviously, the above equation implies the escape rate

$$r_{\rm act}=r_{\rm pass}e^{\frac{D_a(\beta E_0-\kappa_0\tau)}{1+D_a}}, \tag{26}$$

for APB in a smooth potential [29] since $\psi^+=\psi^-=1$ for the smooth potential. Then, equation (25) can be further expressed as

$$r_{\rm act}^{\rm rou}=r_{\rm act}[e^{\psi^-}e^{\psi^+}]^{-1}. \tag{27}$$

3.1. Oscillating perturbation of rough potential

We consider the oscillating perturbation, $V_1(x)=\sin(qx)$ where $q\gg\sqrt{\kappa_0}$. Using equation (10), the effective rough potential may be expressed as

$$\beta V^{\rm eff}(x)\approx\frac{1}{2}\kappa_a x^2-\alpha' x^3+g(x)+\frac{\varepsilon\sin(qx)}{1+D_a}. \tag{28}$$

In figure 1, we plot the effective potential for different values of activity parameter D_a. We find that the effective barrier decreases with the increase of the activity parameter. Thus, the introduction of activity lowers the effective barrier height so that the particle easily escapes the barrier.

From equation (18), we obtain

$$e^{\psi^{\pm}(x)}=I_0\left(\frac{\varepsilon}{1+D_a}\right), \tag{29}$$

where I_0 is the modified Bessel function [36]. Substituting equation (29) into equation (25), we obtain the escape rate

$$r_{\rm act}^{\rm rou}=r_{\rm pass}e^{\frac{D_a(\beta E_0-\kappa_0\tau)}{1+D_a}}\left[I_0\left(\frac{\varepsilon}{1+D_a}\right)\right]^{-2}. \tag{30}$$

Since the modified Bessel function is always larger than 1, we have $r_{\rm act}^{\rm rou}<r_{\rm act}=r_{\rm pass}e^{D_a(\beta E_0-\kappa_0\tau)/(1+D_a)}$. That is, the roughness due to oscillating perturbation hinders escaping. Figure 2 shows the dependence of $r_{\rm act}^{\rm rou}/r_{\rm pass}$ on activity and

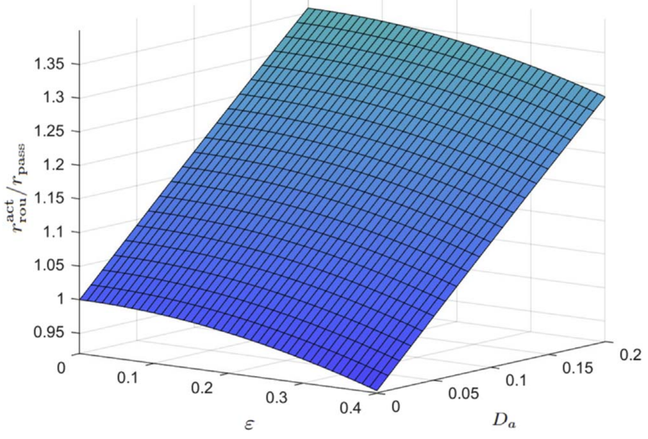

Figure 2. Dependence of $r^{\mathrm{act}}_{\mathrm{rou}}/r_{\mathrm{pass}}$ on amplitude ε and active parameter D_a, where $\alpha\kappa_0^{-3/2} = 0.1$, $\tau\kappa_0 = 0.02$.

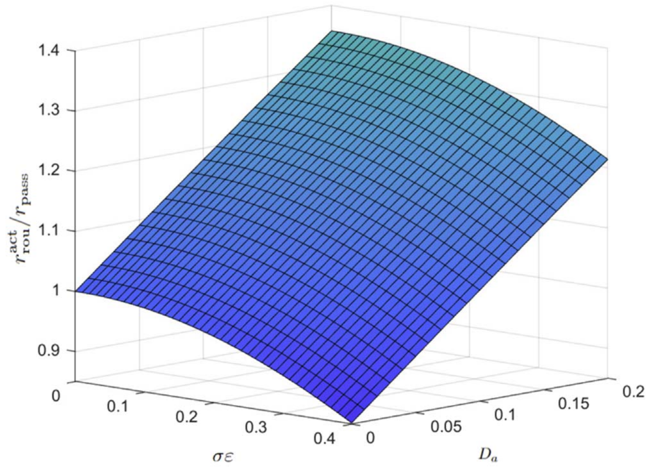

Figure 3. Dependence of $r^{\mathrm{act}}_{\mathrm{rou}}/r_{\mathrm{pass}}$ on amplitude $\sigma\varepsilon$ and active parameter D_a, where $\alpha\kappa_0^{-3/2} = 0.1$, $\tau\kappa_0 = 0.02$.

roughness. $r^{\mathrm{rou}}_{\mathrm{act}}/r_{\mathrm{pass}}$ increases with the increase of activity, but decreases with the increase of roughness.

3.2. Random amplitude of rough potential

Considering the random amplitude of rough potential V_1 with a Gaussian distribution

$$\rho(V_1) = \frac{1}{\sqrt{2\pi\sigma^2}}\mathrm{e}^{-\frac{V_1^2}{2\sigma^2}}, \tag{31}$$

where σ is the standard deviation. The effective rough potential $\beta V^{\mathrm{eff}}(x)$ is

$$\beta V^{\mathrm{eff}}(x) \approx \frac{1}{2}\kappa_a x^2 - \alpha' x^3 + g(x) + \frac{\varepsilon V_1}{1 + D_a}. \tag{32}$$

From equation (18), we obtain

$$\mathrm{e}^{\psi^{\pm}(x)} = \mathrm{e}^{-\frac{\varepsilon^2\sigma^2}{(1+D_a)^2}}. \tag{33}$$

Substituting equation (33) into equation (25), we obtain the escape rate

$$r^{\mathrm{rou}}_{\mathrm{act}} = r_{\mathrm{pass}}\mathrm{e}^{\frac{D_a(\beta E_0 - \omega_0\tau)}{1+D_a}}\mathrm{e}^{-\frac{\varepsilon^2\sigma^2}{(1+D_a)^2}}. \tag{34}$$

Since $\mathrm{e}^{-\varepsilon^2\sigma^2/(1+D_a)^2}$ is always less than 1, we have $r^{\mathrm{rou}}_{\mathrm{act}} < r_{\mathrm{act}} = r_{\mathrm{pass}}\mathrm{e}^{D_a(\beta E_0 - \kappa_0\tau)/(1+D_a)}$. That is, the random amplitude hinders escaping.

Figure 3 shows the dependence of $r^{\mathrm{rou}}_{\mathrm{act}}/r_{\mathrm{pass}}$ on activity and roughness. $r^{\mathrm{rou}}_{\mathrm{act}}/r_{\mathrm{pass}}$ increases with the increase of activity, but decreases with the increase of roughness.

4. Conclusions

In this work, we have discussed the escape rate of ABPs in rough potentials by using the effective equilibrium approach and the Zwanzig method. We find that activity usually enhances the escape rate. Both the oscillating perturbation and the random amplitude of rough potential hinder escaping. We only discussed the influence of two types of rough potential on the escape rate of ABP. According to equation (21), 'rough potential hinders the escape' may not hold in all cases. However, 'activity enhances the escape rate' should be generally applicable. In the theoretical derivation, we need the amplitude ε and $\kappa_0\tau$ are small. Our theory is not applicable to large ε and $\kappa_0\tau$. We will develop a new theoretical approach to deal with these situations in the future.

Acknowledgments

The authors are grateful for financial support from the National Natural Science Foundation of China (Grant No. 11975050 and No. 11735005). We are very grateful for the help of Xiu-Hua Zhao.

Appendix A. Detailed derivation of equation (15)

Following the Kramers method in [47], we derive the inverse escape rate of ABP in the effective rough potential.

Assume $\beta E_b \gg 1$. In this situation, the system stays the quasi-stationary state such that the probability current $J^{\mathrm{rou}}_{\mathrm{act}}$ is approximately independent of x. By integrating equation (14) between x_a and x_c and considering an absorbing boundary condition $x = x_c$, we obtain

$$J^{\mathrm{rou}}_{\mathrm{act}} = \frac{D_t \mathrm{e}^{\beta V^{\mathrm{eff}}(x_a)}\phi(x_a)}{\int_{x_a}^{x_c}\frac{\mathrm{e}^{\beta V^{\mathrm{eff}}(x)}}{D(x)}\mathrm{d}x}. \tag{A1}$$

Because the barrier is high, $\phi(x)$ near x_a may be approximately given by the stationary distribution

$$\phi(x) = \phi(x_a)\mathrm{e}^{-[\beta V^{\mathrm{eff}}(x) - \beta V^{\mathrm{eff}}(x_a)]}. \tag{A2}$$

The probability p to find ABP near x_a is

$$p = \int_{x_1}^{x_2}\phi(x)\mathrm{d}x = \phi(x_a)\mathrm{e}^{\beta V^{\mathrm{eff}}(x_a)}\int_{x_1}^{x_2}\mathrm{e}^{-\beta V^{\mathrm{eff}}}\mathrm{d}x, \tag{A3}$$

where $x_1 \leqslant x_a \leqslant x_2 \leqslant x_b$. Finally, we can derive equation (15) by using $p/J^{\mathrm{rou}}_{\mathrm{act}}$.

Appendix B. Saddle-point approximation

The integral expression in equation (20) may be obtained via the saddle-point approximation at x_a and x_b, respectively.

The effective smooth potential of nearly x_b can be expanded nearby x_b as:

$$\beta V_0^{\mathrm{eff}}(x) = \beta V_0^{\mathrm{eff}}(x_b) - \frac{1}{2}\kappa_b(x - x_b)^2. \tag{A4}$$

The second integral of smooth potential on the right-hand side of equation (20) is expressed as

$$\int_{x_a}^{x_c} \mathrm{d}x \frac{\mathrm{e}^{\beta V_0^{\mathrm{eff}}(x)}}{D(x)} = \int_{x_a}^{x_c} \mathrm{d}x \times \frac{1}{D(x)} \mathrm{e}^{\beta V_0^{\mathrm{eff}}(x_b) - \frac{1}{2}\kappa_b(x-x_b)^2}. \tag{A5}$$

According to the spirit of saddle-point approximation, equation (A5) is transformed into

$$\int_{x_a}^{x_c} \mathrm{d}x \frac{1}{D(x)} \mathrm{e}^{\beta V_0^{\mathrm{eff}}(x_b) - \frac{1}{2}\kappa_b(x-x_b)^2} = \sqrt{\frac{2\pi}{|\kappa_b|}} \mathrm{e}^{\beta V_0^{\mathrm{eff}}(x_b)} \frac{1}{D(x_b)}. \tag{A6}$$

Substituting x_b into equation (8) and considering $\kappa_0 \tau$ is small, we obtain

$$\int_{x_a}^{x_c} \mathrm{d}x \frac{\mathrm{e}^{\beta V_0^{\mathrm{eff}}(x)}}{D(x)} = \sqrt{\frac{2\pi}{|\kappa_b|}} \frac{\mathrm{e}^{\beta V_0^{\mathrm{eff}}(x_b)} \mathrm{e}^{-\frac{D_a \kappa_0 \tau}{1+D_a}}}{(1 + D_a)}. \tag{A7}$$

Similarly, the first integral of smooth potential on the right-hand side of equation (20) may also be obtained by a saddle-point approximation at x_a.

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