On the asymptotic expressions of critical energy barrier in Prandtl-Tomlinson model

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ABSTRACT

The Prandtl-Tomlinson (PT) model is the most widely used and successful minimalistic model to describe atomistic scale friction. It can describe the thermally activated, stress assistant process which shows stick-slip frictional behavior. The relationship between the energy barrier and lateral force is critical to determine how the frictional force depends on velocity and temperature. There is some confusion in the literature to derive such relationship. The underlying assumption and approximations are not stated in a clear way and the rigorous derivations are missing. This study discusses the asymptotic behavior of the energy barrier as the support-spring coupling lowers it to zero and gives a detailed derivation of the asymptotic expression of the energy barrier within the framework of PT model.

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1. Introduction

Da Vinci, Amonton and Coulomb stated the fundamental law of friction as following:

\[ F = \mu N \tag{1} \]

where \( N \) is the normal force, \( F \) is frictional force, and \( \mu \) is the friction coefficient. It works for static as well as kinetic friction. From this simple expression, we can conclude: (1) friction is proportional to the applied load, (2) kinetic friction does not depend on the velocity, (3) friction is independent of the apparent contacting area between the two sliding objects \([1,2]\). This law can describe a wide range of phenomenon commonly observed at the macroscopic scale. It has been believed that macroscopic friction comes from the collective detachment and reattachment of many microscopic asperities between two sliding surfaces \([3]\).

The invention of the friction force microscope (FFM) in 1987 \([4]\) (one year after the birth of atomic force microscope (AFM) \([5]\)) makes it possible to study atomic friction in a single asperity contact. With the help of FFM measurements \([4,6,7]\), people commonly believed that the nanoscale friction exhibits stick-slip behavior in a sawtooth pattern which is fundamentally different from macroscopic friction laws.

The Prandtl-Tomlinson (PT) model \([8,9]\) (usually only referred to as the Tomlinson model) is the most widely used and successful minimalistic model to describe atomistic
scale friction, which can be experimentally investigated by dragging an AFM tip along a crystalline surface. It is shown schematically in Figure 1. The motion of the AFM tip can be described by a thermally activated hopping process on a periodic potential. Within the framework of the PT model, the tip is represented by a point mass $m$ pulled by a harmonic spring of effective elastic constant $k$ over a sinusoidal corrugation potential which describes the interactions between the tip and substrate. The time-dependent interaction between the AFM tip and substrate can be expressed by the PT potential

$$V(x, R(t)) = -U \cos \left( \frac{2\pi x}{a} \right) + \frac{k}{2} [R(t) - x]^2$$

(2)

where $a$ is the lattice constant of substrate, $k$ is the effective elastic constant of the spring between the point mass $m$ and the support, and $U$ is the surface barrier potential height. $R(t) = vt$ is the position of support moving at a constant speed $v$ and $x$ is the position of point mass. The energy barrier $\Delta E$ is defined as $\Delta E(t) = V(x_{\text{max}}(t), t) - V(x_{\text{min}}(t), t)$. Here $x_{\text{max}}(t)$ and $x_{\text{min}}(t)$ are the first minimum and maximum of potential $V$ at time $t$, respectively. Initially, at $t = 0$ and $x = 0$, the energy barrier $\Delta E$ is $2U$.

Consider the stick-slip movement of the point mass in PT model without thermal activation ($T = 0$). Initially, the point mass is in the stick state with the energy barrier $2U$. As the support moves forward, the energy barrier would be lowered due to the extension of the spring. This process can be seen in Figure 2. Until the instability induced by the spring, the slip movement can start to occur. Such a critical point is so called inflection point, which

![Figure 1. Schematic representation of the PT model, by which the FFM is modeled by an AFM tip connected by a spring. The tip is represented by a point mass $m$ pulled by a harmonic spring of effective elastic constant $k$ over a sinusoidal corrugation potential which describes the interactions between the tip and substrate. $R(t) = vt$ is the position of support moving at a constant speed $v$ and $x$ is the position of point mass.](image-url)
is corresponding to $\partial V/\partial x = 0$, $\partial^2 V/\partial x^2 = 0$. At higher temperature, on the other hand, thermal activation ($k_B T$ where $k_B$ is Boltzmann’s constant and $T$ is temperature) can make the point mass overcome the energy barrier easier and slip earlier, which leads to decrease in friction with temperature. Also when the support moves at higher velocity, it would take less time for thermal activation to facilitate the slip, which leads to increase in friction with velocity. In the slip process, the corresponding frictional force (i.e. kinetic friction) is smaller than the threshold of friction for initial sliding (i.e. static friction), which can naturally explain why the coefficient of static friction is usually larger than that of kinetic friction.

The dynamics of the tip (or point mass $m$) can be described by the Langevin equation

$$m \frac{d^2 x}{dt^2} + m\gamma \frac{dx}{dt} = -\frac{\partial V(x, R)}{\partial x} + \xi(t)$$

(3)

where $\gamma$ is the damping coefficient and $\xi(t)$ is the random thermal activation force satisfying the fluctuation-dissipation relation $\langle \xi(t_1) \xi(t_2) \rangle = 2 m k_B T \delta(t_1 - t_2)$. In this expression, the angular brackets denote an ensemble average and $\delta$ is the Dirac delta function. It should be noted that PT model does not include the effect of energy dissipation from tip to substrate, which is represented by a course-grained viscous damping term. Numerically solving the Langevin equation is the most common method to include the thermally activation effect and to interpret dry atomistic scale friction.

The first FFM measurement of the velocity dependence of atomic-scale friction [10] revealed that at low velocities the lateral sliding friction force has a logarithmic dependence, i.e.

$$F \propto \text{const} + \ln(v)$$

(4)

Their argument starts with the master equation [10]

$$\frac{dp(t)}{dt} = -f_0 \exp \left( -\frac{\Delta E(t)}{k_B T} \right) p(t),$$

(5)

where $p(t)$ is the probability to find the tip in the local minimum, $\Delta E(t)$ is the time dependent activation energy between the current local minimum and the next maximum, and $f_0$ is the

![Figure 2. Schematic representation of the time-dependent potential energy in PT model. The moving harmonic potential is superimposed on the sinusoidal potential (left). As the tip is dragged by the spring attached with the support, the energy barrier is decreasing with the time. At the inflection point, the slip would happen (right).](image-url)
characteristic frequency. It should be noted here that the backward slips are not taken into account. Since we are interested in the frictional force associated with the maximum value of \( p(t) \), after the change of variable from \( t \) to \( F \), the master Equation (5) turns to

\[
\frac{dp(F)}{dF} = -f_0 \exp \left( -\frac{\Delta E(F)}{k_B T} \right) \left( \frac{dF}{dt} \right)^{-1} p(F),
\]

(6)

In their derivation [10], two approximations are made. The first one is

\[
\frac{dF}{dt} = \frac{dF}{dx} \frac{dx}{dt} = kv
\]

(7)

Note that \( x \) is the position of the support instead of tip. This approximation is valid because the friction in the stick stage increases linearly with the displacement of the support during which the displacement of the point mass can be neglected. The second one is assuming the linear relationship

\[
\Delta E(F) = \lambda (F^* - F),
\]

(8)

where \( F^* \) is the lateral force which can make a jump at \( T = 0 \). Therefore at maximum

\[
\frac{d^2 p(F)}{dF^2} = 0
\]

(9)

We can obtain

\[
F(v) = F^* + \frac{k_B T}{\lambda} \ln \frac{v}{v_1} = F_0 + \frac{k_B T}{\lambda} \ln \frac{v}{v_1},
\]

(10)

which reproduces Equation (4).

A later investigation [11] argued that the logarithmic dependence on velocity in prior study [10] actually corresponds to linear creep (see Equation (8)) when considering a small constant potential bias. Such logarithmic velocity dependence is only valid over a limited and relatively low range of velocities. They pointed out that the potential bias is continuously ramped up when a tip is dragged across the surface, which is quite different from the above-mentioned study [10]. They demonstrate that \( \Delta E(F) \sim (\text{const} - F)^{3/2} \), so at constant temperature, \( F \propto \text{const} - T^{3/2} \left| \ln v / \ln v_1 \right|^{3/2} \).

From above brief introduction, it is suggested that the relationship between \( \Delta E \) and \( F \) close to critical point is very essential and it should follow 3/2 power law. However, there is some confusion in the literature to derive such relationship [11–15]. The underlying assumption and approximations were not stated explicitly in a clear way and the detailed derivations are missing. The purpose of this article is to focus on the asymptotic behavior of the energy barrier as the support-spring coupling lowers it to zero and to give a rigorous derivation of the asymptotic expression of the energy barrier within the framework of PT model.

2. Results and discussion

2.1. Energy barrier for compliant contact

Due to translational invariance, we can concentrate on one typical minimum for simplicity, viz. \( x = 0 \) and \( R = 0 \) [11]. Following the prior treatment, as the support is moving,
the energy barrier for jumping to next minimum vanishes at critical positions $x_c$ and $R_c$, which corresponds to infecting point as following:

$$\frac{\partial V(x, R(t))}{\partial x}|_{x=x_c, R=R_c} = \frac{2\pi U}{a} \sin\left(\frac{2\pi x_c}{a}\right) - k[R_c - x_c] = 0,$$

(11)

$$\frac{\partial^2 V(x, R(t))}{\partial x^2}|_{x=x_c, R=R_c} = \frac{4\pi^2 U}{a^2} \cos\left(\frac{2\pi x_c}{a}\right) + k = 0$$

(12)

Then we can obtain

$$\frac{2\pi R_c}{a} = \frac{2\pi x_c}{a} + \frac{1}{\Omega^2_k} \sin\left(\frac{2\pi x_c}{a}\right),$$

(13)

$$\cos\left(\frac{2\pi x_c}{a}\right) = -\Omega^2_k,$$

(14)

where

$$\Omega^2_k = \frac{a^2 k}{4\pi^2 U}$$

(15)

Following the method in Ref [15], we can assume

$$x = x_c + \delta x,$$

(16)

$$R = R_c + \delta R$$

(17)

So

$$V(x, R) = V(x_c + \delta x, R_c + \delta R) = V(x_c, R_c) + \delta V(\delta x, \delta R)$$

(18)

On one hand,

$$V(x_c + \delta x, R_c + \delta R) = \frac{k}{2} [(R_c + \delta R) - (x_c + \delta x)]^2 - U \cos\left(\frac{2\pi x_c}{a}\right) \cos\left(\frac{2\pi \delta x}{a}\right)$$

$$- \sin\left(\frac{2\pi x_c}{a}\right) \sin\left(\frac{2\pi \delta x}{a}\right) = \frac{k}{2} (R_c - x_c)^2 + k(R_c - x_c)(\delta R - \delta x) + \frac{k}{2} (\delta R - \delta x)^2 - U \cos\left(\frac{2\pi x_c}{a}\right) \cos\left(\frac{2\pi \delta x}{a}\right)$$

$$+ \frac{k}{2} (\delta R - \delta x)^2 + U \cos\left(\frac{2\pi x_c}{a}\right) \left(\frac{2\pi \delta x}{a}\right)^2 + U \sin\left(\frac{2\pi x_c}{a}\right) \left[\frac{2\pi}{a} \delta x - \frac{(2\pi \delta x)^3}{6}\right]$$

(19)

where we have used $\sin(\delta x) = \delta x - \frac{(\delta x)^3}{6}$ and $\cos(\delta x) = 1 - \frac{(\delta x)^2}{2}$.
So

\[
\delta V(\delta x, \delta R) = k(R_c - x_c)(\delta R - \delta x) + \frac{k}{2}(\delta R - \delta x)^2 + \frac{U}{2} \cos\left(\frac{2\pi x_c}{a}\right) \left(\frac{2\pi}{a} \delta x\right)^2 \]

\[
+ U \sin\left(\frac{2\pi x_c}{a}\right) \left[\frac{2\pi}{a} \delta x - \frac{(2\pi \delta x)^3}{6}\right] = -\frac{1}{6} \left(\frac{2\pi}{a}\right)^3 U\left(1 - \Omega_k^4\right)^{\frac{1}{2}}(\delta x)^3 - k\delta R \delta x \quad (20)
\]

\[
+ a^2 \frac{k}{\Omega_k^2} R C_0 R \left(\frac{1}{C_0 C_1}\right)^{\frac{1}{2}} \delta R + k \left(\frac{\delta R}{a}\right)^2
\]

It can be expressed in a simpler way,

\[
\delta V(\delta x) = -\frac{1}{6} \left(\frac{2\pi}{a}\right)^3 U\left(1 - \Omega_k^4\right)^{\frac{1}{2}}(\delta x)^3 - k\delta R \delta x + \text{const} \quad (21)
\]

According to scaling behavior of energy barrier discussed in Ref [16], PT model is one type of fold catastrophe [17], which describe the topological change in a function induced by external control parameter. It was derived in Ref [16] that when \( U = -Ax^3 - Bx \delta \), the height of the barrier, \( \Delta U = 2A\left(\frac{-\delta R}{3\pi^2}\right)^{\frac{3}{2}} \). In our case, \( A = \frac{1}{6} \left(\frac{2\pi}{a}\right)^3 U\left(1 - \Omega_k^4\right)^{\frac{1}{2}} \), \( B = k \), and \( \delta = \delta R \). So the asymptotic expression of energy barrier in PT model is

\[
\Delta E = \frac{2}{3} U\left(\frac{4\pi R_c}{a}\right)^{\frac{3}{2}} \frac{\Omega_k^3}{\left(1 - \Omega_k^4\right)^{\frac{1}{2}}} \left(\frac{\delta R}{a}\right)^3 \quad (22)
\]

To lowest order in the bias \( f(t) = 1 - \frac{[R(t) - R_c]}{\Delta R} \ll 1 \) [11], then we can obtain

\[
\Delta E = \frac{2}{3} U\left(\frac{4\pi R_c}{a}\right)^{\frac{3}{2}} \frac{\Omega_k^3}{\left(1 - \Omega_k^4\right)^{\frac{1}{2}}} (f)^3, \quad (23)
\]

which exactly reproduces Equation (7) in Ref [11]. However, Ref [11] does not explicitly give the relationship between \( \Delta E \) and \( F \). Substitute Equation (13–15) into Equation (22), we have

\[
\Delta E = \frac{2 \sqrt{2} a}{3\pi} \frac{[k(R_c - R)]^3}{\sqrt{k(R_c - x_c)}} \quad (24)
\]

Since \( F = k(R - x) \) and \( F_c = k(R_c - x_c) \), \( F_c - F = k([R_c - x_c] - (R - x)) \). For a real FFM system, it is reasonable to assume that the tip-support spring stiffness is much smaller than the stiffness of tip-substrate periodic sinusoidal interaction [18], which means that \( R_c - R >> x_c - x \), so that

\[
F_c - F \approx k(R_c - R), \quad (25)
\]

Then Equation (24) becomes

\[
\Delta E = \frac{1}{\beta} (F_c - F)^{\frac{1}{2}} = \frac{2 \sqrt{2} a (F_c - F)^{\frac{1}{2}}}{3\pi \sqrt{F_c}} \quad (26)
\]

Thus, we obtain the commonly used expression of \( \beta \),
\[ \beta = \frac{3\pi \sqrt{F_c}}{2\sqrt{2a}} \]  

(27)

It is worth noting that

\[ F_c = \frac{2\pi U}{a} \sin \left( \frac{2\pi x_c}{a} \right), \]

(28)

\[ x_c = \frac{a}{2\pi} \cos^{-1}(-\Omega_k^2) \]

(29)

2.2. Energy barrier for constant force sliding

In the other scenario for constant force sliding [15], which is an analogous approach by Eyring [19],

\[ V(x, F) = -\frac{E_0}{2} \cos \left( \frac{2\pi x}{a} \right) - Fx, \]

(30)

In order to compare directly with original paper [12], we use Equation (30) here instead of Equation (2), where \( U = \frac{E_0}{2} \). Following the same procedure as above [15],

\[ \frac{\partial V(x, F)}{\partial x} \bigg|_{x=x_c, F=F_c} = \frac{\pi E_0}{a} \sin \left( \frac{2\pi x_c}{a} \right) - F_c = 0, \]

(31)

\[ \frac{\partial^2 V(x, F)}{\partial x^2} \bigg|_{x=x_c, F=F_c} = \frac{2\pi^2 E_0}{a^2} \cos \left( \frac{2\pi x_c}{a} \right) = 0 \]

(32)

Then we can obtain

\[ x_c = \frac{a}{4}, \]

(33)

\[ F_c = \frac{\pi E_0}{a}, \]

(34)

which is Equation (7) in Ref [12]. So Ref [12] have assumed that \( V(x, R(t)) = -\frac{E_0}{2} \cos \left( \frac{2\pi x}{a} \right) + \frac{k}{2} |R(t) - x|^2 \approx -\frac{E_0}{2} \cos \left( \frac{2\pi x}{a} \right) - Fx = V(x, F). \)

Then we can obtain

\[ V(x_c, F_c) = -\frac{\pi E_0}{4} \]

(35)

Using same expression as (16), (17) and (18)

\[ x = x_c + \delta x, \]

(36)

\[ F = F_c + \delta F \]

(37)

\[ V(x, F) = V(x_c + \delta x, F_c + \delta F) = V(x_c, F_c) + \delta V(\delta x, \delta F) \]

(38)
\[ \delta V(\delta x, \delta F) = -\frac{1}{12} \left( \frac{2\pi}{a} \right)^3 E_0 (\partial x)^3 - \partial F \partial x - \frac{a}{4} \partial F \]  

Equation (39)

Since \( \delta V(\delta x, \delta F) \) can be expressed as \(-A\delta^3 - B\delta\) where \( A = \frac{1}{12} \left( \frac{2\pi}{a} \right)^3 E_0 \), \( B = 1 \), and \( \delta = \delta F \), following the same procedure as above, we can obtain

\[ \Delta E = \frac{1}{\beta} (F - F_c)^{\frac{3}{2}}, \]

where

\[ \beta = \frac{3\pi}{2\sqrt{2}} \frac{\sqrt{F_c}}{a}, \]

Equation (41)

which is the same as Equation (27) and also recovers Equation (9) in Ref [12].

3. Conclusion and discussion

In this report, we rigorously derived the analytical expression of the asymptotic behavior of the energy barrier within the framework of PT model. It has been accepted that the relationship between energy barrier and the lateral frictional force near the critical point should follow 3/2 power law instead of linear correlation. For both of above two scenarios: compliant contact and constant force sliding, it can be concluded that: (1) 3/2 power law are valid (Equation (26) and (40)), (2) the expression of \( \beta \) (Equation (27) and (41)) are the same, (3) the difference lies in the value of \( x_c \) (Equation (29) and (33)) and \( F_c \) (Equations (28) and (34)).

Ref [14] has argued that the expression of Equation (41) does not agree with their results of the Monte Carlo simulations. In their model, the thermal effect on the hopping process of the contact atoms is included and both forward and backward jumps are allowed to occur. They propose that

\[ \beta = \frac{(F_c)^{\frac{3}{2}}}{\left( \frac{kT}{8} + \frac{\tau_{ar}}{\pi} \right)}, \]

Equation (42)

which can extend the application range of Equation (40) away from the critical point. Ref [18] have supplemented the prior work and demonstrated the derivation of \( \beta \) for an arbitrary potential and showed that \( \beta \) depends on the third derivative of potential relative to tip position \( x \), which can explain why the expression of \( \beta \) for compliant contact (Equation (27)) and constant force sliding (Equation (41)) are the same. They show that the expression of \( \beta \) extracted from asymptotic analysis works well only in the regime near the critical point and could significantly underestimates the energy barrier. In order to achieve more accurate predictions if Equation (40) still holds true, \( \beta \) need to be adopted as a fitting parameter.

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