Analytical expressions for the kinetic friction in the Prandtl-Tomlinson model

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Analytical expressions are presented for the motion of a point mass driven on a periodic potential by a lateral spring, approximating an atomically sharp tip rubbing over a crystal surface. The tip position before and after jumping between two consecutive minima, the kinetic friction force $F_{\rm kin}$, and the energy barrier ΔE preventing the tip jumps are expressed in terms of a parameter η, which is the ratio between the maximum curvature of the substrate potential and the elastic spring constant. In the two limiting cases of $\eta \to 1$ (*superlubric transition*) and $\eta \gg 1$, we demonstrate that $F_{\rm kin} \propto (\eta - 1)^2$ and $F_{\rm kin} \propto \eta$, respectively. We also show that the relation $\Delta E \propto (F_c - F)^{3/2}$, which is valid in the case of a strong interaction, is replaced by $\Delta E \propto (F - F_c)^3$ close to the superlubric transition. The proportionality coefficients are determined in all cases. The case of multiple jumps is also studied, and numerical results reproducing the influence of the finite temperature and the viscous damping accompanying the tip slippage are shown.

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I. INTRODUCTION

The development of friction force microscopy[1] (FFM) made clear that the motion of a sharp tip elastically driven on a crystal surface can be ultimately interpreted in the framework of the so-called Prandtl-Tomlinson (PT) model.[2,3] In its basic version, the PT model describes the stick-slip motion of a point mass transversally pulled by a spring on a potential $V_{\rm int}$ with the symmetry of the surface lattice. The point mass represents the tip apex of the FFM, whereas the spring combines the torsion of the microcantilever supporting the tip with the lateral deformation of the contact region.[4,5] If the ratio between the sliding velocity and the lattice constant is well below the characteristic vibrational frequencies of the tip in the minima of the potential $V_{\rm int}$, the average tip position moves quasistatically until the spring elongation reaches a critical value, and the tip suddenly jumps into (usually) the closest minimum defined by the scan direction. Remarkable formal analogies with this problem can be recognized in the dynamics of driven charge-density waves.[6]

The previous picture is modified at a finite temperature T. In such a case, a tip jump can be thermally activated when the energy barrier ΔE preventing it becomes comparable to $k_B T$, where k_B is Boltzmann's constant. Thermal activation was invoked to predict the dependence of friction on the temperature and the sliding velocity already in the seminal work by Prandtl.[2] Experimental confirmations of Prandtl's predictions have come from high-resolution FFM measurements in ultrahigh vacuum.[7,8] In order to get further understanding of these processes, one has to know how the barrier ΔE changes with time t and/or with the lateral force F acting on the tip. As long as the tip-surface interaction is strong enough, the dependence of the energy barrier on the lateral force is given by $\Delta E \propto (\text{const} - F)^{3/2}$ (*ramped creep*). Regarding the coefficient of proportionality, different expressions have been reported.[9–12] Alternatively, the linear approximation $\Delta E \propto (\text{const} - F)$ (*linear creep*) is also in a certain agreement with experimental studies at low speed.[7] Compared to the ramped creep, the choice of the time t (or the force F) around which the energy barrier can be linearly approximated is arbitrary, and no specific expressions for the coefficient of proportionality have been reported to our knowledge.

Even more surprisingly, analytical expressions for the tip location x_c' immediately after jump are not discussed in the literature. As shown below these expressions are required to relate the average value of the kinetic friction force to the amplitude of the interaction potential $V_{\rm int}$, which is essential for the theoretical foundations of nanotribology. These observations motivated the development of the present article. After a brief review of the PT model in one dimension (1D) in Sec. II, analytical approximations are obtained for the position x_c' and the kinetic friction $F_{\rm kin}$ in the limiting cases of high tip-surface interaction and close to the opposite regime of continuous sliding or superlubricity (Sec. III). In Sec. IV the energy barrier ΔE is estimated as a function of t and F. Original formulas are derived for the energy barrier close to superlubricity (in the ramped regime) and in the linear regime. Finally, Sec. V addresses the case of jumps over several lattice constants, which has been recently described in experimental studies on graphite and alkali-metal halide crystal surfaces.[13,14] Here, analytical results are complemented by numerical calculations relating the appearance of multiple jumps to the lateral damping of the tip oscillations.

II. THE MODEL

In a first approximation, a sharp asperity (*tip*) sliding on a crystal lattice moves like a point mass driven by an elastic spring on a sinusoidal potential $V_{\rm int}$. In this case, it is convenient to introduce the parameter

$$\eta = \frac{4\pi^2 V_0}{ka^2}, \tag{1}$$

where V_0 and a are the amplitude and periodicity of the potential $V_{\rm int}$, and k is the spring constant. If $\eta < 1$ the

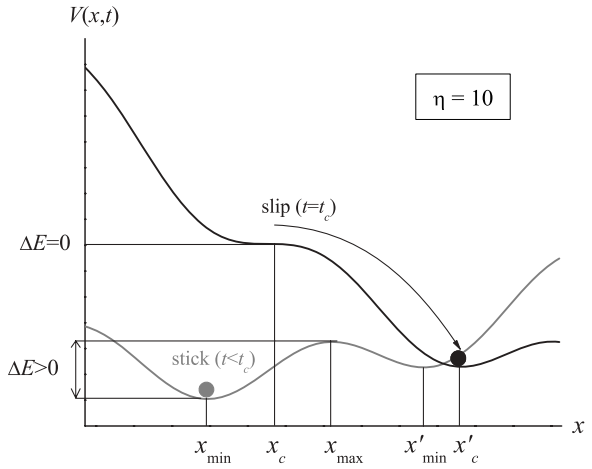

FIG. 1. The equilibrium of a particle driven by a lateral spring on a sinusoidal potential is broken at a critical time t_c when the tip suddenly jumps from the minimum position x_c to the next one, x_c'.

motion is continuous (*superlubric*), whereas a series of abrupt jumps with fast recovery of the tip equilibrium (*stick-slip*) are observed when $\eta > 1$. A typical situation in FFM experiments, corresponding to the value $\eta = 10$, is shown in Fig. 1. It is important to observe that, if the interaction potential $V_{\rm int}$ is not sinusoidal, the definition (1) is not well posed and the stick-slip condition becomes $-V_{\rm int}''^{(\max)}/k > 1$.[9]

To simplify our calculations, we substitute $a \to 2\pi$ and $k \to 1$. In the new units the forces are expressed in multiples of $ka/2\pi$, and the interaction potential $V_{\rm int}$ has an amplitude $V_0 = \eta$, so that

$$V(x,t) = -\eta \cos x + \tfrac{1}{2}(x - vt)^2 \tag{2}$$

is the total potential experienced by the tip. Standard units will be adopted only in the formulas describing the final results. The tip position $x_{\rm min}$ is given by the equilibrium condition $\partial V/\partial x = 0$, which, in our case, becomes

$$\eta \sin x + x - vt = 0. \tag{3}$$

In a first approximation (when $t \to 0$ or $\eta \gg 1$):

$$x_{\rm min} \simeq \frac{vt}{1+\eta}, \qquad F \simeq \frac{\eta}{1+\eta} vt. \tag{4}$$

The equilibrium position $x_{\rm min}$ slightly moves forwards when the pulling spring is elongated along the direction x. When the tip reaches the critical position x_c defined by $\partial^2 V/\partial x^2 = 0$, the equilibrium becomes unstable. This position is given by

$$x_c = \arccos\left(-\frac{1}{\eta}\right),$$

and the corresponding critical time is

$$vt_c = \sqrt{\eta^2 - 1} + \arccos\left(-\frac{1}{\eta}\right) \equiv f(\eta). \tag{5}$$

At this point the (*static*) lateral force $F = vt - x_{\rm min}$ acting on the tip is

$$F_{\rm stat} = \frac{ka}{2\pi}\sqrt{\eta^2 - 1}. \tag{6}$$

Note that this value is lower than the maximum value $F_{\rm max} = \eta$ of the lateral force.[15] The value $F_{\rm max}$ is reached shortly before jumping, when the tip, which is strongly accelerated, overcomes the velocity v of the spring support.

When $t = t_c$ the tip jumps towards the next minimum $x'_{\rm min} = x_c'$ (multiple jumps with $n > 1$ are discussed in Sec. V). In the limiting cases $\eta \to 1$ and $\eta \gg 1$ the quantity x_c' takes the values $x_c'(1) = \pi$ and $x_c'(\infty) = 5\pi/2$, respectively. At each jump the energy amount $\Delta V = V(x_c) - V(x_c')$ is released from the contact region in the form of phonons. The average (*kinetic*) friction force can be easily estimated from this quantity as $F_{\rm kin} = \Delta V/2\pi$, whereas the variation of the lateral force in the jump is given by $\Delta F = x_c' - x_c$ (in reduced units). Furthermore, the energy barrier ΔE preventing the jump is defined as $\Delta E = V(x_{\rm max}) - V(x_{\rm min})$, where $x_{\rm max}$ is the position of the first maximum next to $x_{\rm min}$ (see Fig. 1).

In the following, the tip positions x_c and x_c', the kinetic friction force $F_{\rm kin}$, and the energy barrier ΔE are estimated by Taylor expansions in the limiting cases $\eta \to 1$ and $\eta \gg 1$.

III. CRITICAL POSITIONS AND KINETIC FRICTION

A. Case $\eta \to 1$

If $\eta \to 1$ we expand the function $f(\eta)$ defined by (5), introducing the variable $\nu = \sqrt{\eta - 1}$:

$$f(\eta) = \pi + \frac{2\sqrt{2}}{3}\nu^3 - \frac{3}{5\sqrt{2}}\nu^5 + \frac{23}{56\sqrt{2}}\nu^7 + \cdots. \tag{7}$$

Next we assume that

$$x_c' = \pi + \alpha.$$

From the minimum condition $\partial V/\partial x = 0$ we obtain

$$-(\nu^2 + 1)\sin\alpha + \pi + \alpha = f. \tag{8}$$

Taking into account that the Taylor expansion of $\sin\alpha$ contains only odd powers of α, we assume that $\alpha = \sum_k a_k \nu^k$, with $k = 1,3,5,\ldots$. Substituting and expanding in (8), and using the expression (7) for the function f, we find two series of values for the coefficients a_k, which describe the tip position before and after jumping, respectively. Retaining the first three terms in the expansion of α, we have,

$$x_c = \pi - \sqrt{2}\nu + \frac{5}{6\sqrt{2}}\nu^3 - \frac{43}{80\sqrt{2}}\nu^5 + \cdots, \tag{9}$$

$$x_c' = \pi + 2\sqrt{2}\nu - \frac{19}{15\sqrt{2}}\nu^3 + 0.5237\nu^5 + \cdots. \tag{10}$$

The energy variation in the jump, ΔV, can be estimated by substituting the expressions (9) and (10) into (2), with $t = t_c$, and expanding.

The kinetic friction force, obtained as described in Sec. II, is

$$F_{\rm kin} = \frac{ka}{2\pi}\left(\frac{9}{4\pi}(\eta-1)^2 - \frac{9}{5\pi}(\eta-1)^3 + 0.4829(\eta-1)^4 - \cdots\right), \tag{11}$$

whereas the variation of the lateral force is given, as a first approximation, by $\Delta F \simeq 3\sqrt{2(\eta-1)}$.

B. Case $\eta \gg 1$

If $\eta \gg 1$ we expand the function $f(\eta)$ introducing the variable $\nu = 1/\sqrt{\eta}$:

$$f(\eta) = \frac{1}{\nu^2} + \frac{\pi}{2} + \frac{\nu^2}{2} + \frac{\nu^6}{24} + \cdots. \tag{12}$$

The positions of the tip before and after jumping are

$$x_c = \frac{\pi}{2} + \beta, \qquad x_c' = \frac{5\pi}{2} + \gamma.$$

The condition $\partial V/\partial x = 0$ gives

$$\frac{\cos\beta}{\nu^2} + \frac{\pi}{2} + \beta = f \tag{13}$$

and, respectively,

$$\frac{\cos\gamma}{\nu^2} + \frac{5\pi}{2} + \gamma = f. \tag{14}$$

Taking into account that the Taylor expansion of $\cos\beta$ contains only even powers of β, we assume that $\beta = \sum_k b_k \nu^k$, with $k = 0,2,4,\ldots$. Substituting and expanding in (14), and using the expression (12) for the function f, we find that

$$x_c = \frac{\pi}{2} + \nu^2 + \frac{\nu^6}{6} + \frac{3}{40}\nu^{10} + \cdots. \tag{15}$$

In the Taylor expansion of γ both odd and even terms need to be considered: $\gamma = \sum_k c_k \nu^k$, with $k = 0,1,2,\ldots$. Substituting and expanding in (14), and using again the expression (12) for the function f, we have

$$x_c' = \frac{5\pi}{2} - 2\sqrt{\pi}\nu + \nu^2 - \frac{\pi^{3/2}}{3}\nu^3 + \cdots. \tag{16}$$

Using again (2), with $t = t_c$, to estimate the energy variation ΔV, we obtain the following expression for the kinetic friction force:

$$F_{\rm kin} = \frac{ka}{2\pi}\left(\eta - \pi + \frac{4}{3}\sqrt{\frac{\pi}{\eta}} - \frac{1}{2\eta} + \cdots\right), \tag{17}$$

whereas ΔF is independent of η and equal to 2π (in a first approximation).

C. Discussion

The relations (11) and (17) lead to the important conclusion that the kinetic friction force $F_{\rm kin}$ is proportional to the parameter η when $\eta \gg 1$, whereas $F_{\rm kin}$ approaches the superlubric transition according to the law $F_{\rm kin} \propto (\eta - 1)^2$. We notice that these laws already appeared (without derivation) in an earlier work by Helman *et al.*[16]

In order to determine the range of validity of the previous results, we have plotted the tip positions $x_c(\eta)$ and $x_c'(\eta)$, as estimated from (9),(10) and (15),(16) together with numerical solutions of the equation $\partial V/\partial x = 0$ with $V(x,t)$ given by (2): See Figs. 2(a) and 2(b). Similarly, the dependence $F_{\rm kin}(\eta)$ given by (11) and (17) is compared to the values obtained numerically in Fig. 2(c). The corresponding errors (not shown) reveal that the analytical approximations hold quite well for x_c, they are less precise for x_c' and they are unsatisfactory for $F_{\rm kin}$ in the region around $\eta = 1.5$–2, where the convergence of the series is slow and the relative error is >10%. Since the parameter η in FFM experiments often takes values in the last range, we have also approximated the dependence $F_{\rm kin}(\eta)$ around $\eta = 2$. This point is not singular and a linear relation holds:

$$F_{\rm kin}(\eta) = 0.4029 + 0.1791(\eta - 2) + \cdots, \tag{18}$$

which can be useful for practical applications (the coefficient of friction once the relation between the normal force F_N and the parameter η is known).

Incidentally, it also makes sense to consider the *ultrasuperlubric* case $\eta \to 0$. In such a case, the tip follows the support without accelerating, so that $x_{\rm min} = vt$ and $F(t) = \eta \sin vt$.

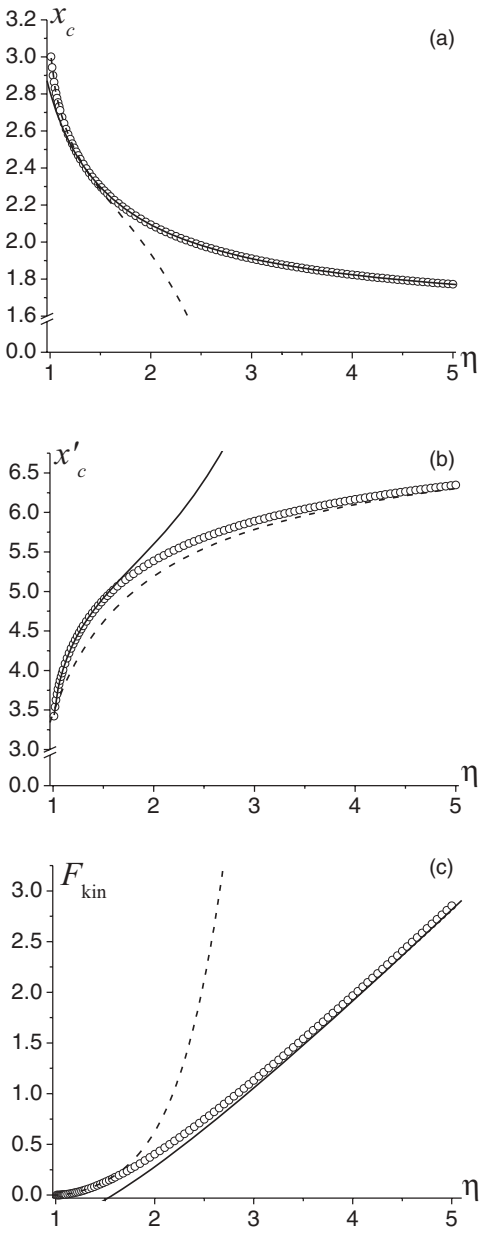

FIG. 2. (a) Tip position x_c before jumping, (b) tip position x_c' after jumping, and (c) kinetic friction force $F_{\rm kin}$ in the overdamped limit vs the parameter η defined by (1). The open circles correspond to numerical solutions of the conditions of stability of the nanotip. The dashed curves represent the approximations (9), (10), and (11) derived in the text when $\eta \to 1$. The continuous curves represent the approximations (15), (16), and (17) when $\eta \gg 1$.

Thus, the force $F(t)$ perfectly reproduces the sinusoidal potential V_{int}. This remains true for an arbitrary shape of the periodic potential, not only in 1D.

IV. ENERGY BARRIER FOR THERMALLY ACTIVATED JUMPS

A. Ramped creep

In order to determine the energy barrier ΔE as a function of the actual lateral force $F(t)$, we write the tip position before jumping as

$$x_{\text{min}} = x_c - \delta.$$

Substituting into the condition $\partial V/\partial x = 0$, we obtain a transcendental equation for δ as a function of time. Expanding it up to the second order in δ and taking into account the definition (5), we find

$$\delta \simeq \pm A\sqrt{f - vt}, \qquad A \equiv \frac{\sqrt{2}}{(\eta^2 - 1)^{1/4}}. \tag{19}$$

The negative solution corresponds to the position of the maximum x_{max}. At the same order in δ we can approximate the energy barrier as $\Delta E \simeq 2(f - vt)\delta$ and, using (19),

$$\Delta E \simeq \frac{2\sqrt{2}}{(\eta^2 - 1)^{1/4}}(f - vt)^{3/2},$$

or, in normal units (in which the energies are expressed as multiples of V_0/η),

$$\Delta E \simeq \frac{8V_0}{\eta(\eta^2 - 1)^{1/4}}\left(\frac{\pi v}{a}\right)^{3/2}(t_c - t)^{3/2}. \tag{20}$$

Note that this result differs by a factor 3/2 from the one derived by Müser[9] and previously reported by Sang *et al.*[10] and Persson *et al.*[11] The result presented in these references can be recovered if ΔE is expanded up to the third order in δ, but this is not consistent with the second-order approximation leading to Eq. (19).

In general it is easy to see that, in reduced units, the following relation holds (since $F_c = \sqrt{\eta^2 - 1}$):

$$F = vt - x_{\text{min}} \simeq F_c - (f - vt) + A\sqrt{f - vt}. \tag{21}$$

Close to the transition the third term on the right-hand side is much larger than the second one. Thus we can assume that $\sqrt{f - vt} \simeq (F - F_c)/A$ and conclude that

$$\Delta E \simeq \frac{(\eta^2 - 1)^2}{\eta}\left(\frac{F}{F_c} - 1\right)^3 V_0. \tag{22}$$

If $\eta \gg 1$, the relation (22) holds only in a very limited range of values close to the transition. Out of this range, $f - vt \simeq F_c - F$ and Eq. (20) implies that

$$\Delta E \simeq 2\sqrt{2}\left(1 - \frac{F}{F_c}\right)^{3/2} V_0. \tag{23}$$

This formula was already used by Dudko *et al.* [Eq. (4) in Ref. 12]. However, Eq. (22) has not been reported to our knowledge. This result can be useful for further theoretical studies on the superlubric transition.

Different situations corresponding to $\eta = 1.1$, 2, 5, and 10 are shown in Fig. 3. Here, numerical solutions for the energy barrier ΔE are plotted as functions of the lateral force (continuous lines). The analytic expressions (22) and (23) are also plotted as functions of the same variable. Note that the critical value of the lateral force when $\eta = 1.1$ ($F_c = 0.458$) is much lower than the maximum value $F_{\text{max}} = 1.1$, so that the decrease of F is well pronounced when the threshold $\Delta E = 0$ is approached. This is not the case when $\eta = 10$, where $F_c = 9.95$ is quite close to $F_{\text{max}} = 10$ and the slight reentrance of the lateral force cannot be appreciated even in a double logarithmic scale.

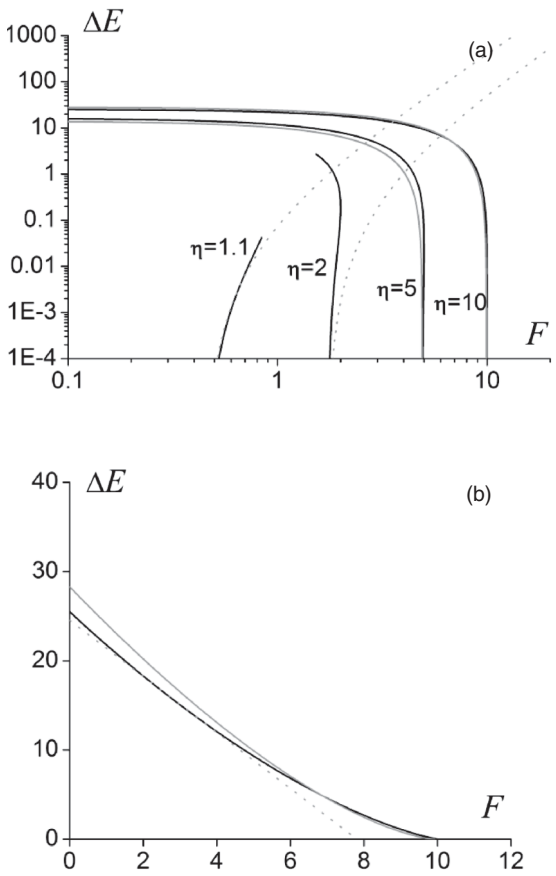

FIG. 3. (a) Energy barrier ΔE (see Fig. 1) as a function of the lateral force F (in double logarithmic scale) when $\eta = 1.1$, 2, 5, and 10. The black lines represent numerical solutions of the equation of motion of the nanotip; the continuous and dotted gray lines correspond to the analytical approximations (23) and (22), respectively. Note that, when $\eta \to 1$, the maximum x_{max} and the energy barrier ΔE are defined only in close proximity to $F = F_c$. (b) Ramped approximation (continuous gray curve) and linear approximation (dotted gray curve) compared to the numerical solution (continuous black curve) for the dependence $\Delta E(F)$ when $\eta = 10$.

B. Linear creep

For estimating the energy barrier in the case of linear creep, we choose the symmetric configuration considered by Tshiprut *et al.*,[17] where the energy barrier for a forward jump $x_{\text{min}} \to x'_{\text{min}}$ equals the energy barrier for a backward jump $x'_{\text{min}} \to x_{\text{min}}$. Assuming that $x_{\text{min}} = x_{\text{max}} - \varepsilon$ and $x'_{\text{min}} = x_{\text{max}} + \varepsilon$, the condition $V(x_{\text{min}}) = V(x'_{\text{min}})$ implies that $x_{\text{max}} - vt =$

$-\eta \sin\varepsilon \sin x_{\max}/\varepsilon$. Since the maximum $x_{\max}$ also satisfies the condition (3) we conclude that $x_{\max} = \pi$. The quantity ε is determined by equating the two derivatives of the total potential V in the minima $x_{\min}$ and $x'_{\min}$, which gives

$$\varepsilon - \eta \sin\varepsilon = 0 \tag{24}$$

for the implicit relation $\varepsilon = \varepsilon(\eta)$, and

$$\Delta E_0 = -\frac{\varepsilon^2}{2} + \eta(1 - \cos\varepsilon) \tag{25}$$

for the energy barrier in the chosen configuration.

It is easy to see that

$$\varepsilon \simeq \sqrt{6(\eta - 1)}, \qquad \Delta E_0 = \tfrac{3}{2}(\eta - 1)^2 - \tfrac{6}{5}(\eta - 1)^3 + \cdots$$

when $\eta \to 1$ and

$$\varepsilon \simeq \frac{\eta}{1 + \eta}\pi, \qquad \Delta E_0 = 2\eta - \frac{\pi^2}{2} + \frac{\pi^2}{2\eta} + \cdots$$

when $\eta \gg 1$.

Let us now assume that the tip position slightly deviates from the symmetric configuration. In this case $x_{\min} = \pi - \varepsilon - \delta$ and $x_{\max} = \pi + \delta'$. Equating the derivative $\partial V/\partial x$ to zero and using (24), we get

$$\delta \simeq \frac{\pi - vt}{1 - \eta\cos\varepsilon}, \qquad \delta' \simeq \frac{\pi - vt}{\eta - 1}$$

and, for the energy barrier,

$$\Delta E \simeq \Delta E_0 + \varepsilon(\pi - vt).$$

When $\eta \gg 1$, using (4),

$$\Delta E \simeq \frac{1 + 5\eta^2 + 4\eta^3}{2\eta^2(1 + \eta)} V_0 - \frac{a}{2} F, \tag{26}$$

which is plotted as the dashed line in Fig. 3(b). The final result is quite simple: The slope of the ΔE vs F curve is equal to $a/2$ (this quantity was referred to as λ in Ref. 7).

V. MULTIPLE JUMPS

Depending on the value of the parameter η, other equilibrium positions are possible beyond x'_c.[13] A jump over κ lattice constants (towards the position $x = x_c^{(\kappa)}$) may appear if the conditions $\partial V/\partial x = 0$ and $\partial^2 V/\partial^2 x > 0$ are satisfied in at least κ points. It is not difficult to see that the appearance of this kind of jump is given by the condition

$$f(\eta_k) = \kappa\pi,$$

corresponding to the values of $\eta_1 = 1$, $\eta_2 = 4.603$, $\eta_3 = 7.790$, etc. Using the same approach as in Sec. III, it can be proven that, when $\eta \gg 1$, the tip position after a jump over k lattice constants is given by

$$x_c^{(\kappa)} = \frac{\pi}{2} + 2\kappa\pi - 2\sqrt{\kappa\pi}\,v + v^2 - \frac{(\kappa\pi)^3}{3} v^3 + \cdots,$$

and the kinetic friction force is given by the expression (17) with π replaced by $\kappa\pi$ everywhere.

The previous derivations were implicitly carried out assuming that the tip motion is *quasistatic*, i.e., the tip is always in mechanical equilibrium, except when it slips. The quasistatic approximation also allows an estimation of the frictional force

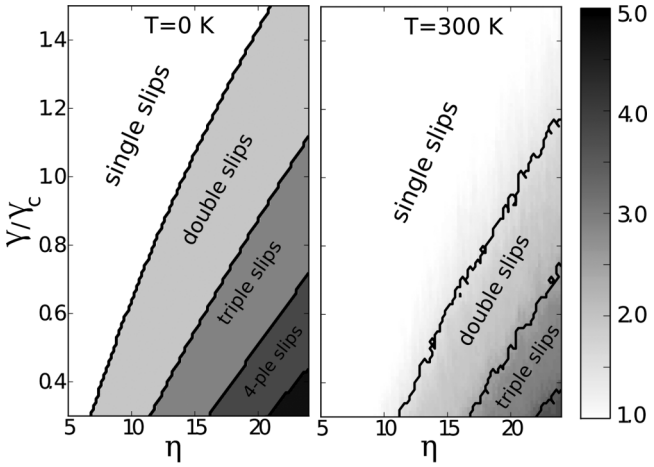

FIG. 4. Depending on the values of the damping coefficient γ in Eq. (27) the nanotip can jump over multiple numbers of the lattice constant a in both overdamped ($\gamma > \gamma_c$) and underdamped ($\gamma < \gamma_c$) regimes. Here, the regions of occurrence of multiple jumps have been estimated (a) at zero temperature and (b) at $T = 300$ K. In both cases the tip response becomes chaotic if $\gamma \lesssim 0.3\gamma_c$.

accompanying a jump over κ lattice constants. However, it cannot predict which value of κ will be experienced in the jump. In order to answer this question, the equation of motion of the nanotip has to be solved. At a finite temperature T, this equation is

$$m\ddot{x} + m\gamma\dot{x} + V'(x) = \xi(t), \tag{27}$$

where the damping coefficient γ describes the coupling with phonon and possible electron oscillations in the substrate, and the term $\xi(t)$ describes the Brownian motion of the tip according to the fluctuation-dissipation theorem: $\langle\xi(t)\xi(t')\rangle = 2m\gamma k_B T\delta(t - t')$. Equation (27) has been solved with $m = 10^{-12}$, $v = 50$ lattice constants per unit time, and γ expressed in units of $\gamma_c = 2\sqrt{k/m}$ for both $T = 0$ and $T = 300$ K. As a result, we observe that the η-γ plane can be divided into

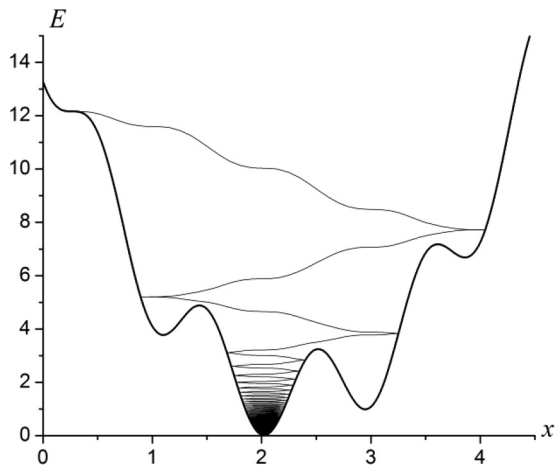

FIG. 5. Potential profile $V(x)$ corresponding to a critical position of the tip (thick curve) and variation of the total tip energy E while jumping in the underdamped case $\gamma = 0.1\gamma_c$ with $\eta = 12.8$ (thin curve). Distances are expressed in terms of the lattice constant a and the energies in multiples of $ka^2/4\pi^2$.

different regions, as shown in Figs. 4(a) and 4(b). At zero temperature, jumps of κ lattice constants occur (for a fixed value of the parameter η) only if $\gamma_{c,\kappa}(\eta) < \gamma < \gamma_{c,\kappa-1}(\eta)$ (when $\kappa > 1$) or $\gamma > \gamma_{c,1}(\eta)$ (when $\kappa = 1$). However, the situation changes if γ is low. If $\gamma \lesssim 0.3\gamma_c$ a chaotic regime is indeed observed, in which the "landing" position of the tip may be several lattice constants away from the "take-off" position and may change significantly with little variation of the parameters η and γ. At finite temperature the curves separating regions corresponding to jumps with different values of κ are smoothed, and overall shifted towards larger values of η.

In order to get better insight into the relaxation process of the tip (at zero temperature), we have also represented the total energy $E = (1/2)m\dot{x}^2 + V(x)$ as a function of the instantaneous tip position when a multiple jump occurs. In Fig. 5, corresponding to $\eta = 12.8$ and $\gamma = 0.1\gamma_c$, it can be seen that the tip bounces back and forth between different equilibrium positions until it is conveyed by the potential profile $V(x)$ two lattice constants beyond the take-off position, where the tip finally accommodates. The actual value of κ is thus determined by the shape of $V(x)$ and, in the underdamped case, is extremely sensitive to the value of the coefficient γ. A detailed analysis of the tip trajectories in this chaotic regime goes beyond the goals of this paper.

VI. CONCLUSION

In conclusion, analytical expressions for the average friction force and the energy barrier in the one dimensional Prandtl-Tomlinson model have been derived analytically in the quasistatic limit. The friction force can be precisely described in the case of very high friction and also at the onset of superlubricity. Previous assumptions for the energy barrier have been confirmed and the coefficients of proportionality have been estimated. Although the range of application of the power laws that we obtained is somewhat limited, due to the slow convergence of the series which appear in their derivation, these results can be used as an important starting point for further experimental and computational work aimed at a better understanding of atomic-scale friction and superlubricity in two dimensions, where the analysis is complicated by the symmetry properties of the crystal lattice.[18,19]

Furthermore, the equation of motion of the tip has been numerically solved for different values of the control parameters η and γ, which describe the curvature of the tip-surface interaction (as compared to the lateral contact stiffness) and the damping coefficient of the lateral tip oscillations. The number of lattice constants crossed in a tip jump has been related to these parameters at both zero and room temperature. A chaotic response is observed in the underdamped limit and associated with the tip bouncing back and forth between the potential walls, causing the stick-slip motion.

Note added in proof. Bistable solutions of (5) appear only in a limited x-range centered about $x_c = \pi$ as long as $x_c' < 3\pi/2$. As discussed in Ref. 13, this occurs for $1 < \eta < 4.603$. This explains why the curves for $\eta = 1.1$ and 2 do not extend back to $F = 0$, whereas those for $\eta = 5$ and 10 do so.

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