Nature of mechanical instabilities and their effect on kinetic friction

Martin H. Müser
Institut für Physik, WA 331; Johannes Gutenberg Universität; 55099 Mainz; Germany
(March 22, 2002)

It has long been recognized that the key to understand kinetic friction force $F_k$ is the analysis of microscopic instabilities that lead to sudden irreversible "pops" of certain degrees of freedom. In this Letter, the nature of such instabilities is characterized with an emphasis on boundary lubricants. It is shown that there are certain critical values of the parameters defining our model Hamiltonian, where the behavior of the instabilities changes qualitatively. Simultaneously, the functional dependence of $F_k$ on the sliding velocity $v_0$ changes. The relevant parameters studied here are dimensionality of the interface, degree of commensurability, first higher harmonic in the lubricant wall potential, and temperature. Molecular dynamics simulations are carried out to test whether the predictions made on the basis of the simple model also hold in less idealized circumstances.

When a solid slider is moved laterally with respect to a substrate, the kinetic friction $F_k$ is usually almost independent of the sliding velocity $v_0$ with leading corrections in the order of $\ln v_0$. This so-called Coulomb friction differs from drag or Stokes friction that states a linear relation between $F_k$ and $v_0$ and that can be understood from equilibrium statistical mechanics as a special case of the fluctuation dissipation theorem. For instance, the drag force experienced by a Brownian particle in solution arises from the many collisions between the Brownian particle and the solvent molecules. In general, the condition for a linear friction force to occur is the (anharmonic) coupling of a central degree of freedom like the Brownian particle or a phonon to (infinitely) many other discrete degrees of freedom. In this Letter, the question will be addressed what the condition is for Coulomb friction to occur.

It has long been recognized that Coulomb friction must be related to instabilities that occur on a microscopic scale. When a slider is moved laterally with respect to the substrate, fast motion (pops) of certain degrees of freedom become unavoidable even if the sliders center of mass velocity is extremely small. The microscopic peak velocities in such pops are rather independent of $v_0$ and consequently the energy dissipated via a Stokes-type mechanism also becomes almost independent of $v_0$. The prototypical instability leading to Coulomb friction was suggested by Prandtl and Tomlinson. In their one-dimensional model, a surface atom in the slider is coupled with a spring of stiffness $k$ to its ideal lattice site which moves at constant velocity $v_0$. Interactions with the rigid substrate are modeled with a potential energy surface $V(x)$ that is periodic in the substrate’s lattice constant plus some drag force linear in the atom’s velocity $\dot{x}$. If $k$ is sufficiently small, pops become unavoidable and neglecting thermal fluctuations, $F_k$ remains finite in the limit of zero $v_0$. Instabilities and small-velocity kinetic friction in more complex model systems have been investigated since the Prandtl Tomlinson model was introduced. In particular, the $F_k(v_0)$ relationship of elastic manifolds sliding in ordered and disordered media has been studied extensively. The functional dependence is commonly found to be

$$F_k(v) = F_k(0) + cv^\beta.$$ (1)

While the elastic instabilities considered in those models are important in various contexts, this does not seem to be the case for the atomistic explanation of solid friction: Many detailed calculations and atomistic computer simulations reveal that in almost all cases, interbulk interactions are too weak to lead to instabilities at the atomic scale and as a consequence $F_k(0) = 0$. If interbulk interactions are very strong, irreversible processes like plastic deformation, material mixing, cold-welding, etc. usually occur and prevent the instabilities from being elastic.

It has been suggested that the presence of adsorbed particles, i.e. a boundary lubricant, confined between two surfaces is a more likely explanation for the commonly observed presence of solid friction. The main argument is that molecules that are only weakly bound to either surface can accommodate the surface corrugation of both walls simultaneously, which locks the walls together. This argument leads to static friction, which is the minimum force to initiate sliding between two solids. However, in order to explain kinetic friction, it is necessary to analyze the adiabatic solution $x_{ad}(t)$ of the lubricant atoms. $x_{ad}(t)$ is the athermal trajectory of an atom that always relaxes to the closest mechanical equilibrium position at every instant of time. The analysis of $x_{ad}(t)$ has become common practice in the context of the motion of elastic manifolds in disordered media. In the impurity limit, interactions between lubricant atoms can be neglected and consequently $x_{ad}(t)$ merely depends on the initial condition and the relative motion of top and bottom wall. In the following, $x_{ad}(t)$ and its connection to kinetic friction will be examined. To the best of the author’s knowledge such an analysis has not yet been done, although the present model has already been used extensively to predict successfully various tribological phenomena.
The equation of motion for a lubricant atom in the boundary regime reads:

\[ \ddot{x} = -\gamma_b \dot{x} - \gamma_t (x - v_0) + \frac{1}{m} \Gamma(t) - \frac{1}{m} \frac{\partial}{\partial x} \{ V_b(x) + V_t(x - v_0 t) \}, \]

where \( x \) denotes the atom's position, \( m \) is the atom's mass, \( \gamma_b \) and \( \gamma_t \) parametrize the damping forces from the top and the bottom wall, and \( V_t \) and \( V_b \) denote the interaction of the confined atom with slider and the substrate. \( \Gamma(t) \) is a Langevin type stochastic random force defining temperature. For the lubricant wall interactions, various calculations are thus the degree of lattice mismatch \( b - b_0 \), the value of the first higher harmonic \( V_1 = V_{t,b}^{(1)} \), and temperature \( T \).

We start the discussion of a commensurate (com.) system \( (b_t = b_0) \) without higher harmonics in the absence of thermal fluctuations. In that case, the net time-dependent potentialconst is simply given by \( V(t) = 2V_0 \cos \left( \frac{2\pi}{\lambda_b x(t)} \right) \cos \left( \frac{\pi}{k_B} (x - vt/2) \right) \). Thus, for times \( \cos \left( \frac{2\pi}{\lambda_b x(t)} \right) \neq 0 \), the atoms move at velocity \( v_0/2 \) as shown in Fig. 1b. An infinitely small moment after a situation where this inequality was not satisfied, an atom will not be able to find a stable position in the immediate vicinity of the previous stable position. As the slider moves on with respect to the substrate, the atoms should therefore slide rapidly towards a new mechanical equilibrium. However, in order for this to happen, one needs a symmetry breaking element such as thermal fluctuations, \( \gamma_b \neq \gamma_t, b_t \neq b_0 \), or round-off errors in numerical calculations. Otherwise all stable trajectories simply are \( x = x_n t + v_0 t/2 \) where \( n \) is an integer number and the average (conservative) force of the lubricant atom acting on either wall will average to zero. For the athermal com. system, we chose to break symmetry by violating Galilei invariance and set \( \gamma_t = 0 \). This choice is arbitrary but convenient, and is a better-controlled procedure than relying on round-off errors. We note also that for inc. walls, there is no physical reason for assuming the equality \( \gamma_t = \gamma_b \).

Owing to broken symmetry \( (\gamma_t = 0) \), the atom can now slide to the next minimum indicated by the gray lines in Fig. 1b. However, the peak velocities \( \dot{x}_p \) in this process remain much smaller than during a pop within the Prandtl Tomlinson model. The reason is that due to the symmetry of \( V_t \) and \( V_b \), the pops occur between equivalent positions in the limit of arbitrarily small \( v_0 \). Since no lower bound for the dissipated energy can be given, the zero-velocity \( F_k \) will be zero. At the same time, there is no upper bound for the ratio \( \dot{x}_p/v_0 \), so that \( F_k \) cannot simply vanish linearly with \( v_0 \) but only with some power \( \beta \) smaller than unity.

The nature of the instabilities changes qualitatively when the first higher harmonic is different from zero. Hence, in the sense of Morse theory [12], which contains Landau’s theory of phase transition as a special case, the com. system without higher harmonics can be considered a (multi-/tri-) critical point. If \( V_1 < 0 \), the adiabatic solution \( x(t) \) becomes continuous as shown in Fig. 1, however, the time derivative \( \dot{x}(t) \) diverges. If \( V_1 > 0 \), the adiabatic solution is discontinuous and the pops occur between inequivalent positions as shown in Fig. 1c. In analogy to phase transitions, the pops occurring for \( V_1 > 0 \) shall be called first-order instabilities, those for \( V_1 \leq 0 \) second-order instabilities. Only for first-order instabilities can one expect finite energy dissipation and thus finite \( F_k \) as \( v_0 \) approaches zero. A numerical analysis shows that all three cases can be described with Eq. 4. The results are shown in Fig. 2 and the expected trend is confirmed: The more discontinuous the adiabatic solution, the larger the kinetic friction. It is important to emphasize that the exponent \( \beta \) (as determined for sufficiently small \( v_0 \)) only depends on the sign of \( V_1 \) but not on its precise value as long as \( |V_1| \) is not too large.

For 1-dimensional, inc. surfaces, the basic picture is similar. If \( V_1 \) is larger than a (positive) critical value \( V_1^c \), whose precise value depends on the lattice mismatch, then pops between inequivalent positions are present and \( F_k \) remains finite as \( v_0 \) tends to zero. For \( V_1 < V_1^c \), however, the time derivative of the (continuous) adiabatic solution remains finite at all times. Hence the
microscopic (peak) velocities \( v_p \) scale linearly with \( v_0 \), which implies Stokes-type friction in that regime (1-d, inc.). Again, the exponent \( \beta \) only depends on the sign of \( V_t - V_t^* \). More detailed results including an analysis of significantly more complex systems will be presented in a separate paper [13].

The reason is that in 2-d, atoms can circumnavigate the points of maximum longitudinal force. In 2-d com. surfaces, the behavior remains qualitatively similar as in 1-d, because the interference of \( V_t \) and \( V_b \) remains similar. Large-scale molecular dynamics simulations by He and Robbins support this argument even if the boundary lubricant is not any longer in the impurity regime. They find small \( F_s \) and large \( F_k \) between com. surfaces, while no such gap is observed for inc. systems [14]. Also experimentally, signs for the effects of increased static friction of com. surfaces in the presence of a lubricant were reported [15].

This has potentially measurable implications for the transition from stick-slip motion to smooth sliding. In the stick-slip regime, friction is dominated by \( F_s \), while in the smooth sliding regime, only \( F_k \) is relevant. We have extended previous simulations [16] to support this point further. For this purpose the same model has been employed as that in Ref. [1]. A schematic of the simulation is shown in Fig. 3 together with the average friction, as defined by the energy dissipated per slid distance. The verification of this prediction requires smooth surfaces, because rough surfaces automatically lead to inhomogeneous energy landscapes [17]. The data shown in Fig. 3 was produced at a normal pressure of 0.4 GPa and a velocity of about 1 m/s using the same conversion of units as in Ref. [1]. Note that the exceedingly small inertia of the slider as compared to experiment moves the transition from stick-slip to smooth sliding to large velocities.

We will now turn to the discussion of the effects of thermal fluctuations. He and Robbins found that velocity dependent corrections in a 2-dimensional, lubricated, inc. interface satisfy [14]:

\[
F_k(v_0) = F_k(v_{\text{ref}}) + \mathcal{O}(\ln(v_0/v_{\text{ref}}))
\]

over several orders of magnitude in \( v_0 \). This is different from the behavior found in the Prandtl Tomlinson model. Although similar temperature corrections have been suggested, for instance by Prandtl himself, more rigorous treatments yield corrections of order \((T \ln v)^{2/5} [18]\). While these corrections describe atomic force microscope experiments of nanoscale single-asperity contacts fairly accurately, it seems that they cannot provide an explanation of the usually observed \( v_0 \) corrections in a straightforward manner.

Here it will be shown that simple logarithmic corrections are obeyed even in the impurity limit. Moreover, the crossover to linear response at extremely small sliding velocities will be included in the discussion. Fig. 3 shows the normalized friction force obtained at thermal energy \( T = 0.07 \) for the com. \( V_t > 0 \) model. Three regimes can be identified. At very small velocities, friction is linear in \( v_0 \) and one may associate this regime with the creep regime. At intermediate \( v_0 \), Eq. [18] is rather well satisfied. At “large” velocities, thermal fluctuations become less relevant and the motion is close to that of the athermal system. The data obtained at different temperatures can be collapsed on a master curve. The collapse requires two dimensionless scaling functions \( r(T) \) and \( s(T) \) that both depend on temperature \( T \) only. The collapse is done via \( F_k(v, T) = r(T^*)F_k(v^*, T^*)/r(T) \) with \( s(T) \ln(v^*(T^*)/v_1) = s(T^*)\ln(v(T)/v_1) \) where \( v_1 \)}
is a constant, \( r(T) \) is almost constant \( [r(0.02) = 0.98, r(0.2) = 1.2] \) and \( s(T) \approx k_B T / \Delta E \) where \( \Delta E \) can be interpreted as an effective (free) energy barrier. Qualitatively similar crossover from the linear response regime to the activated regime are observed in many other systems such as single particles in a static periodic potential [19], driven thermal elastic manifolds [20], and shear-thinning fluids [21].

In conclusion, this Letter provides a classification scheme for instabilities that can occur when two solids are in relative sliding motion. First-order instabilities are defined as pops of atoms (or other degrees of freedom) between inequivalent positions. They lead to kinetic friction that remains finite when the sliding velocity \( v_0 \) goes to zero provided the system is athermal. The exponent \( \beta \) of the velocity corrections \( v^\beta \) depends on the details of the model, however, \( \beta \) only changes its value at certain critical points in the parameter space defining interactions and geometry. At finite temperature, corrections in the order of \( \ln v_0 \) apply. Second-order instabilities are defined as pops between equivalent positions. They lead to a sub-linear power law \( F_k \propto v^\beta \). If, however, the adiabatic solution \( x_{ad} \) of the boundary lubricant moves with finite velocity at all times, then simple Stokes friction follows. Thus an important result of this analysis is the identification of critical points where the kinetic friction law changes qualitatively as a parameter describing the interactions or the geometry is varied.

While the present study is primarily concerned with dilute boundary lubricants, the concept itself seems to be more general. For instance \( x_{ad} \) can be a collective order parameter that fluctuates back and forth between two values. Such quasi-periodic phase transitions have been observed in computer simulations of Ni asperities moving over a Cu substrate [22]. Of course, the situation in those simulations was more complex, because wear occurred as a side effect of the motion. In the other extreme, \( x_{ad} \) may merely denote the position of an electronic orbital.

I thank K. Binder for useful discussions. Support from the BMBF through Grant 03N6015 and from the Materialwissenschaftliche Forschungszentrum Rheinland-Pfalz is acknowledged.

[1] D. Dowson, History of Tribology (Longman, New York, 1979); F. P. Bowden and D. Tabor, The Friction and Lubrication of Solids, (Clarendon Press, Oxford, 1986).
[2] J. H. Dieterich, J. Geophys. Res. 84, 2161 (1979); A. Ruina, J. Geophys. Res. 88, 10359 (1983).
[3] J. P. Hansen and I. R. McDonald, Theory of simple liquids, (Academic Press, London, 1986).
[4] M. Brillouin, Notice sur les Travaux Scientifique, (Gauthier-Vilars, Paris, 1909); C. Caroli and Ph. Nozières, Eur. Phys. J. B, 4, 233 (1998).
[5] L. Prandtl, ZS. f. angew. Math. u. Mech., 8, 85 (1928); G. A. Tomlinson, Phil. Mag. Series, 7, 905 (1929).
[6] D. S. Fisher, Phys. Rev B 31, 1396 (1985); Phys. Rep. 301, 113 (1998).
[7] P. Chauve, P. Le Doussal, and K. J. Wiese, Phys. Rev. Lett. 86, 1785 (2001).
[8] M. O. Robbins and M. H. Müser, in Modern Tribology Handbook, ed. B. Bhushan (CRC Press, Boca Raton, 2001).
[9] G. He, M. H. Müser, and M. O. Robbins, Science 284, 1650 (1999); M. H. Müser, L. Wenning, and M. O. Robbins, Phys. Rev. Lett. 86, 1295 (2001).
[10] M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. Lett. 77, 683 (1996); Phys. Rev. E 54, 6485 (1996).
[11] M. G. Rozman, M. Urbakh, J. Klafter, and F. J. Elmer, J. Phys. Chem. B 102, 7924 (1998).
[12] J. Mihno, Morse Theory (Princeton, Princeton University Press, 1970).
[13] M. Aichele and M. H. Müser (in preparation).
[14] G. He and M. O. Robbins, Tribol. Lett. 10, 7 (2001).
[15] M. Raths and S. Granick, Langmuir 16, 8368 (2000).
[16] M. H. Müser, in Fundamentals of Tribology and Bridging the Gap between Macro- and Micro/Nanoscales, ed. B. Bhushan (Kluwer Academic Publishers, Netherlands, 2001).
[17] J. P. Gao, W. D. Luedtke, and U. Landman, Tribol. Lett. 9, 3 (2000).
[18] Y. Sang, M. Dubé, and M. Grant, Phys. Rev. Lett. 87, 174301 (2001); O. K. Dudko, A. E. Filippov, J. Klafter, and M. Urbakh, Chem. Phys. Lett. 352, 499 (2002).
[19] H. Risken and H. D. Vollmer, Z. Phys. B, 33, 297 (1979).
[20] P. Chauve, T. Giamarchi, and P. Le Doussal, Europhys. Lett. 44, 110 (1998).
[21] S. Granick (private communication); S. Bair, C. McCabe, and P. T. Cummings, Phys. Rev. Lett. 88, 058302 (2002).
[22] A. Buldum and S. Ciraci, Phys. Rev. B 55, 12892 (1997).