Exactly quantized sliding of a confined solid lubricant under shear

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Lubricated Friction

- Macroscopic expectation: $v_{\text{lubricant}} = v_{\text{ext}} / 2$
- At nanoscale (boundary-lubrication regime - solid lubricant layer): How do substrate/lubricant periodicities & hardness of lubricant influence $v_{\text{lubricant}}$?
  - 1D model
  - 2D model (multilayers)
1D Microscopic Model

**Simplest scheme**: a generalized Frenkel-Kontorova simulating the classic dissipative dynamics of a 1D chain of harmonically interacting atoms confined between two sinusoidal substrate potentials, with the top substrate driven at constant velocity $v_{\text{ext}}$.

\[
m \ddot{x}_i = K(x_{i+1} + x_{i-1} - 2x_i) - \frac{1}{2} \left[ F_+ \sin \frac{2\pi}{a_+} x_i + F_- \sin \frac{2\pi}{a_-} (x_i - v_{\text{ext}} t) \right] - 2\gamma (\dot{x}_i - \frac{v_{\text{ext}}}{2})
\]

$\gamma$ = phenomenological viscous damping (underdamped regime)

$a_0$ = average distance between the chain of atoms

$r = a / a_0$ = two independent relevant length-ratios

A. Vanossi, N. Manini, F. Caruso, G.E. Santoro, and E. Tosatti, PRL 99, 206101 (2007);
Results for the CM lubricant sliding velocity

Large non-trivial plateaus

- asymmetrical
- infinitely flat
- negative plateaus with backwards motion

\[ w = \frac{v_{\text{plateau}}}{v_{\text{ext}}} \]

universal function of \( r_+ \) only (independent of \( K, v_{\text{ext}}, F_+, F_-, \ldots \))
Velocity-plateau mechanism: kinks and anti-kinks

Extra particle: **kink**

\[ a_0 < a_+ \quad (r_+ = 1 + d) \]

Extra “hole”: **anti-kink**

\[ a_0 > a_+ \quad (r_+ = 1 - d) \]

kinks/antikinks explain the geometric “quantized” plateau velocity

\[
\rho_{sol} = \frac{d}{a_+} = \frac{r_+ - 1}{a_+} \quad \rho_{part} = \frac{1}{a_+} = \frac{r_+}{a_+}
\]

kinks dragged at full velocity \( v_{ext} \)

\[
\rho_{sol} v_{ext} = \rho_{part} v_{plateau}
\]

\[
W = \frac{v_{plateau}}{v_{ext}} = 1 - \frac{1}{r_+}
\]

only dependent on \( r_+ \)!
A more realistic model

2D (x,z) lubricant, Lennard-Jones potential, PBC

\[ \Phi_a(r) = \epsilon_a \left[ \left( \frac{\sigma_a}{r} \right)^{12} - 2 \left( \frac{\sigma_a}{r} \right)^{6} \right] \]

\[ \epsilon_{t1} = \epsilon_{l1} = \epsilon_{b1} = \epsilon \quad \text{same LJ interactions} \]

\[ \sigma_{t1} = a_t , \quad \sigma_{b1} = a_b , \quad \sigma_{l1} = a_0 , \quad \text{for simplicity, the 3 LJ radii } \sigma_a \text{ coincide} \]

with the characteristic spacings \( a_t, a_b, a_0 \)

The 2 relevant length-ratios are defined by
\[
\lambda_b = \frac{a_b}{a_0}, \quad \lambda_t = \frac{a_t}{a_0},
\]
with \( \lambda_b \) closer to unity

\[
\vec{F}_j = -\frac{\partial}{\partial \vec{r}_j} \left[ \sum_{i=1}^{N_t} \Phi_{tl}(|\vec{r}_j - \vec{r}_{ti}|) + \sum_{\substack{j'=1\ j' \neq j}}^{N_t} \Phi_{ll}(|\vec{r}_j - \vec{r}_{j'}|) + \sum_{i=1}^{N_b} \Phi_{bl}(|\vec{r}_j - \vec{r}_{b_i}|) \right]
\]
Total force acting on the j-th lubricant particle

\[
r_{tix}(t) = i a_t + v_{ext} t, \quad r_{tiz}(t) = r_{tiz}(t), \quad \text{where:}
\]

\[
N_t m \ddot{r}_{tiz} = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_t} \sum_{j'}^{N_t} \frac{\partial \Phi_{tl}}{\partial \vec{r}_{tiz}} (|\vec{r}_{tiz} - \vec{r}_{ij'}|) - N_t F
\]

\[
\vec{f}_{\text{damp}}_i = -\eta \dot{\vec{r}}_i - \eta (\dot{\vec{r}}_i - \dot{\vec{r}}_t)
\]
Standard Langevin dynamics, with the addition of a dissipative damping term plus a Gaussian random force to the Newton equations

\[
\langle f_{jx}(t) f_{jx}(t') \rangle = 4\eta k_B T \delta(t - t')
\]

\[
\eta \sum_{i} (\vec{r}_i - \vec{r}_t) = \eta N_1 (\vec{v}_{cm} - \vec{r}_t)
\]
Kinks in the 2D model

Kinks are visible like more dense and vertically displaced regions (non-uniform distribution of the vertical load).

Kinks are seen only in the horizontal displacement of the two lowest layers, while vertical undulations of all lubricant layers are apparent.
Results: kink ($a_0 < a_b$) & anti-kink ($a_0 > a_b$) dragging

backward lubricant motion at speed

$w=1-1/\lambda_b = -0.19$
Velocity quantization \((N_{layer} = 1)\) 

\[ w_{plat} = \frac{\bar{v}_{cm,x}}{v_{ext}} = 1 - \frac{1}{\lambda_b} \]

varied \(v_{ext}\)

Competition between the beneficial role of limiting thermal fluctuations, and the detrimental effect of hampering the vertical lubricant movements.

The plateau attractor tends to affect the dynamics even in the presence of large thermal fluctuations and disordered substrates.
Role of kink coverage \( \Theta = \frac{N_{\text{kink}}}{N_t} \)

Stronger substrate interactions favour in-register lubricant regions, with narrow kinks being easily dragged by the top corrugations.

\( \lambda_t \), not affecting the velocity plateau value, crucially sets the kink coverage:

\[
\Theta = \frac{N_{\text{kink}}}{N_t} = \left(1 - \lambda_b^{-1}\right) \lambda_t
\]

and affects the plateau robustness, \( v_{\text{crit}} \) maxima at well-commensurate coverage \( \Theta \)
Lubricant Multilayers

$v_{\text{crit}}$ dependence on $N_{\text{layer}}$ in fully commensurate $\theta = 1$ condition

Lubricant vertical corrugation induced by the kinks favors the perfect velocity quantization.

By increasing $N_{\text{layer}}$, $z$-displacements decay rapidly, and such a mechanism becomes less effective to support the dynamically pinned state.
Lubricant Melting at the depinning transition

While the plateau occurs due to solitons being driven gently, the transition to the unpinned state may involve the lubricant melting, due to large shear-induced Joule heating.
**Hysteresis & Friction**

By cycling here up and down $v_{ext}$, an hysteresis cycle opens, even at finite temperature.

\[ F_k = \text{kinetic friction force} \]

\[ k_B T_{\text{eff}} = \frac{1}{N_1} \bar{E}_{k \text{cm}} \]

\[ \bar{F}_k = \frac{4 \eta}{m v_{ext}} (\bar{E}_{k \text{cm}} - N_1 k_B T) + \frac{\eta N_1}{v_{ext}} \left[ \bar{v}_{cm}^2 + (\bar{r}_t - \bar{v}_{cm})^2 \right] \]

fluctuations of the particle velocities in the CM frame.

force contribution coming from the lubricant as “rigid body”

(\text{..minimum if } v_{cm \times} = \frac{1}{2} v_{ext} \text{ )}

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Conclusions

The observed dynamical pinning of the solid lubricant onto a rigidly quantized sliding state has been understood in terms of solitons being set into motion by the shear due to the moving surfaces.

This kind of soliton dragging can be argued to represent a rather general mechanism, possibly at play in some realistic situations.
Thanks for Your Attention!!
standard MD (Newton e.o.m.)

4\textsuperscript{th}-order Runge-Kutta integration

Nose-Hoover thermostat chain

PBC

drop an initial “thermalization” transient

(\sim 10^3 \text{ time units})

pressure $-F$ applied to top

**model units** | **typical**
---|---
length | $a_0$ | 0.3 nm
mass | $m$ | 50 a.m.u.
energy | $\epsilon$ | 1 eV
force | $\epsilon a_0^{-1}$ | 0.5 nN
velocity | $\epsilon^{1/2} m^{-1/2}$ | 1000 m/s
time | $m^{1/2} \epsilon^{-1/2} a_0$ | 0.2 ps

all equal LJ energies $\epsilon$ ; $\sigma_{tp} = a_t$, $\sigma_{bp} = a_b$, $\sigma_{pp} = a_0$