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Exactly quantized sliding of a confined solid lubricant under shear

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Friction and Adhesion in
Nanomechanical Systems (FANAS)

Exactly Quantized Sliding of a Confined Solid Lubricant under Shear

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in collaboration with:
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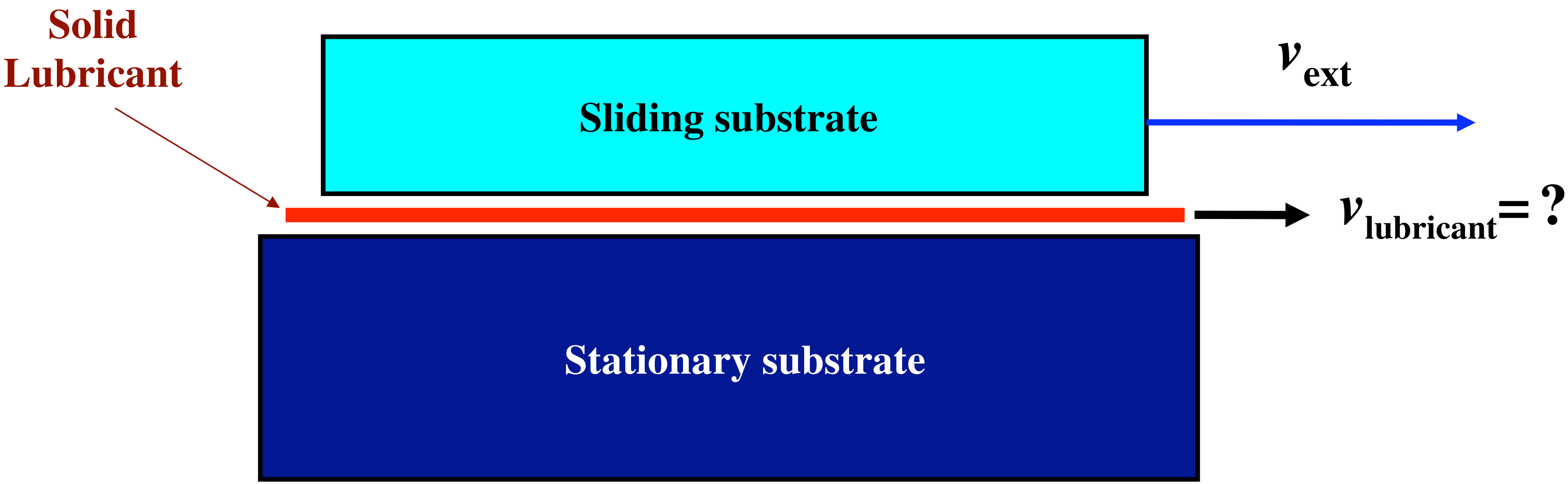
Lubricated Friction

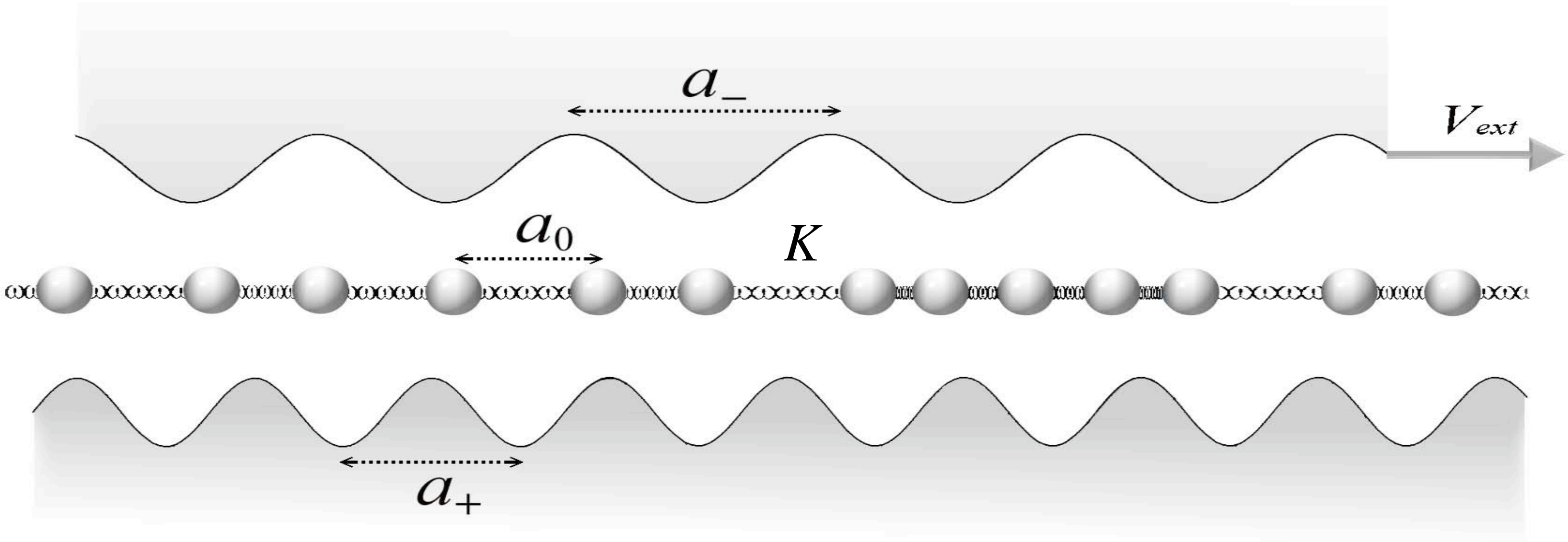


- Macroscopic expectation: $v_{lubricant} = v_{ext}/2$
- **At nanoscale** (boundary-lubrication regime - solid lubricant layer): How do **substrate/lubricant periodicities** & **hardness of lubricant** influence $v_{lubricant}$?

  - 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_{ext}



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

γ = phenomenological viscous damping (*underdamped* regime)

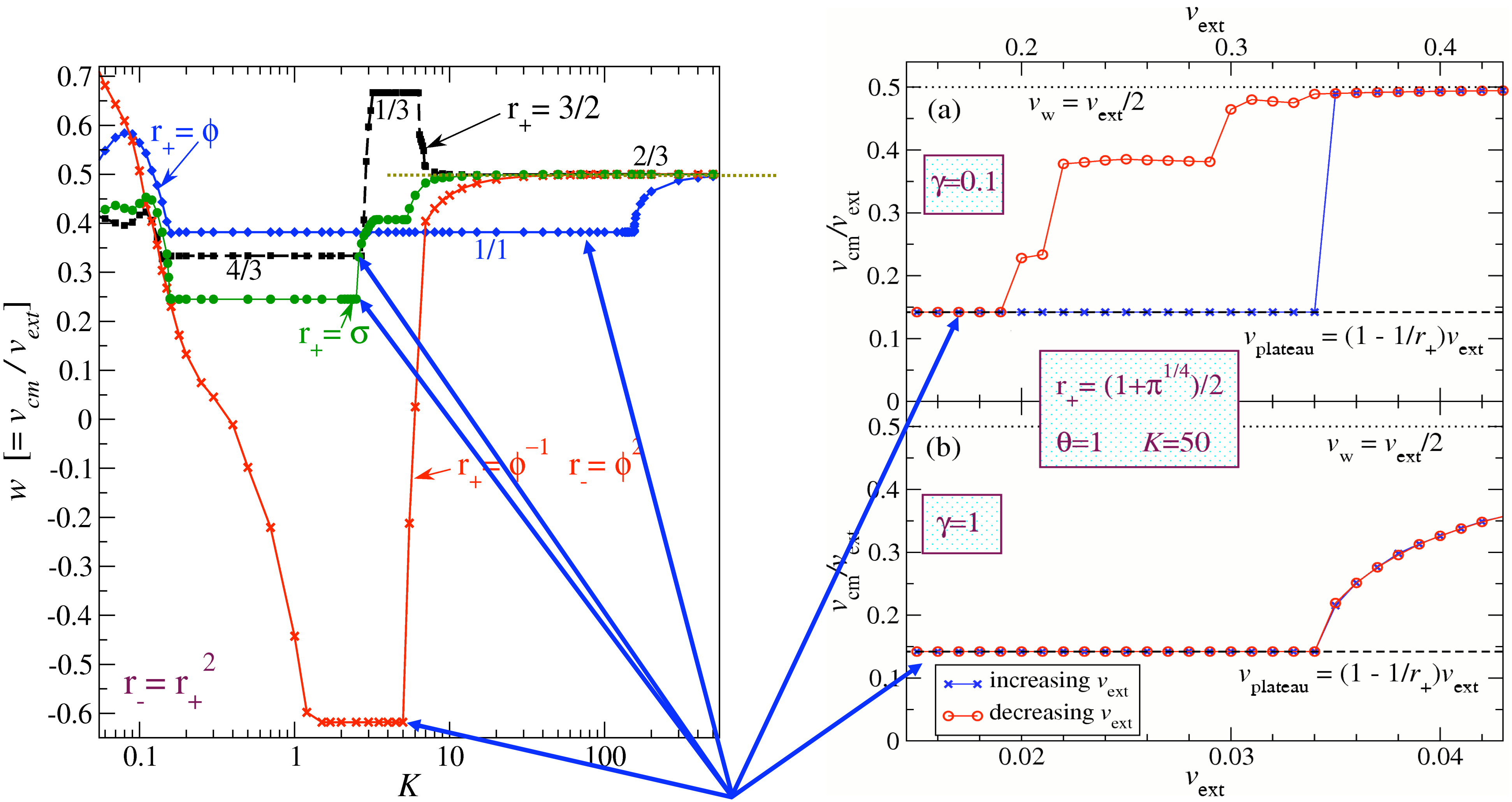
a_0 = average distance between the chain of atoms

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

A. Vanossi, N. Manini, G. Divitini, G.E. Santoro, and E. Tosatti, PRL **97**, 056101 (2006)

A. Vanossi, N. Manini, F. Caruso, G.E. Santoro, and E. Tosatti, PRL **99**, 206101 (2007);

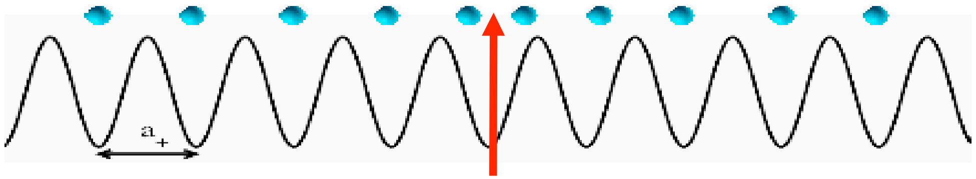
Results for the CM lubricant sliding velocity



Large non-trivial **plateaus**

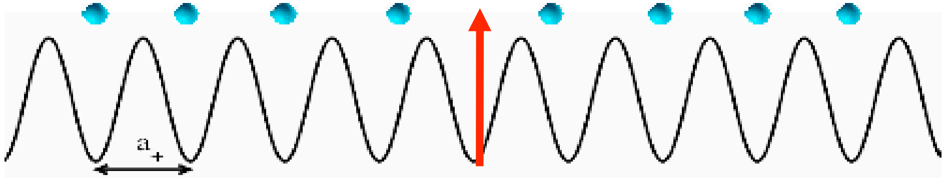
- ***asymmetrical*** ◆ ***infinitely flat*** ◆ ***negative plateaus with backwards motion***
- $\boldsymbol{w = v_{\mathrm{plateau}}/v_{\mathrm{ext}}}$ "***universal***" function of r_+ only (***independent*** of K, v_{ext}, F_+, F_-, …)

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

$$\rho_{sol} = d / a_+ = \frac{r_+ - 1}{a_+} \qquad \rho_{part} = 1 / a_0 = \frac{r_+}{a_+}$$

kinks dragged at full velocity v_{ext}

$$\rho_{sol} v_{ext} = \rho_{part} v_{plateau}$$

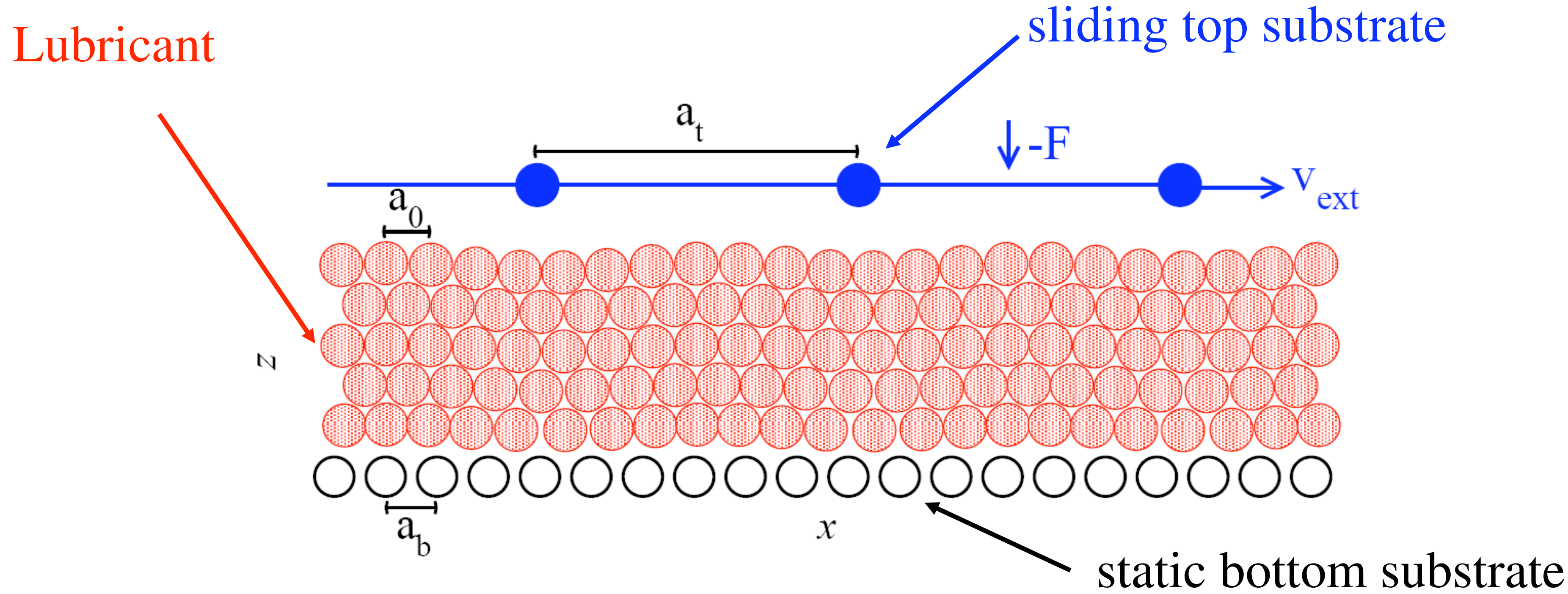
$$\Downarrow$$

$$w = \frac{v_{plateau}}{v_{ext}} = 1 - \frac{1}{r_+}$$

only dependent on r_+ !

A more realistic model

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



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

$\epsilon_{\rm tl} = \epsilon_{\rm ll} = \epsilon_{\rm bl} = \epsilon$ same LJ interactions

$\sigma_{\rm tl} = a_{\rm t}\,,\ \sigma_{\rm bl} = a_{\rm b}\,,\ \sigma_{\rm ll} = a_0\,,$ for simplicity, the 3 LJ radii σ_a coincide with the characteristic spacings a_t, a_b, a_0

I.E. Castelli, N. Manini, R. Capozza, A. Vanossi, G.E. Santoro, and E. Tosatti, J. Phys.: Condens. Matter **20** (2008) 354005

The 2 ***relevant length-ratios*** are defined by with λ_b closer to unity

$$\lambda_{\mathrm{b}} = \frac{a_{\mathrm{b}}}{a_0}\,, \quad \lambda_{\mathrm{t}} = \frac{a_{\mathrm{t}}}{a_0}\,,$$

$$\vec{F}_j = -\frac{\partial}{\partial \vec{r}_j}\Big[\sum_{i=1}^{N_{\mathrm{t}}} \Phi_{\mathrm{tl}}(|\vec{r}_j - \vec{r}_{\mathrm{t}\,i}|) + \sum_{\substack{j'=1 \\ j'\neq j}}^{N_{\mathrm{l}}} \Phi_{\mathrm{ll}}(|\vec{r}_j - \vec{r}_{j'}|) + \sum_{i=1}^{N_{\mathrm{b}}} \Phi_{\mathrm{bl}}(|\vec{r}_j - \vec{r}_{\mathrm{b}\,i}|)\Big]$$

Total force acting on the j-th ***lubricant*** particle

$$r_{\mathrm{t}\,i\,x}(t) = i\,a_{\mathrm{t}} + v_{\mathrm{ext}}\,t\,, \quad r_{\mathrm{t}\,i\,z}(t) = r_{\mathrm{t}\,z}(t)\,,$$ where:

$$N_{\mathrm{t}} m\,\ddot{r}_{\mathrm{t}\,z} = -\sum_{i'=1}^{N_{\mathrm{t}}} \sum_{j=1}^{N_{\mathrm{l}}} \frac{\partial \Phi_{\mathrm{tl}}}{\partial r_{\mathrm{t}\,i'\,z}}(|\vec{r}_{\mathrm{t}\,i'} - \vec{r}_j|) - N_{\mathrm{t}} F$$

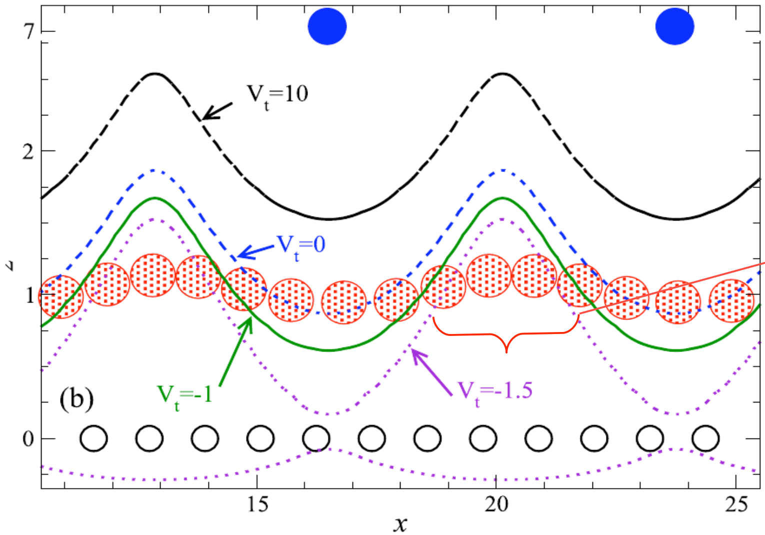
$$\vec{f}_{\mathrm{damp}\ i} = -\eta\,\dot{\vec{r}}_i - \eta\,(\dot{\vec{r}}_i - \dot{\vec{r}}_{\mathrm{t}})$$

$$\langle f_{j\,x}(t)\, f_{j\,x}(t')\rangle = 4\eta k_{\mathrm{B}} T\,\delta(t - t')$$

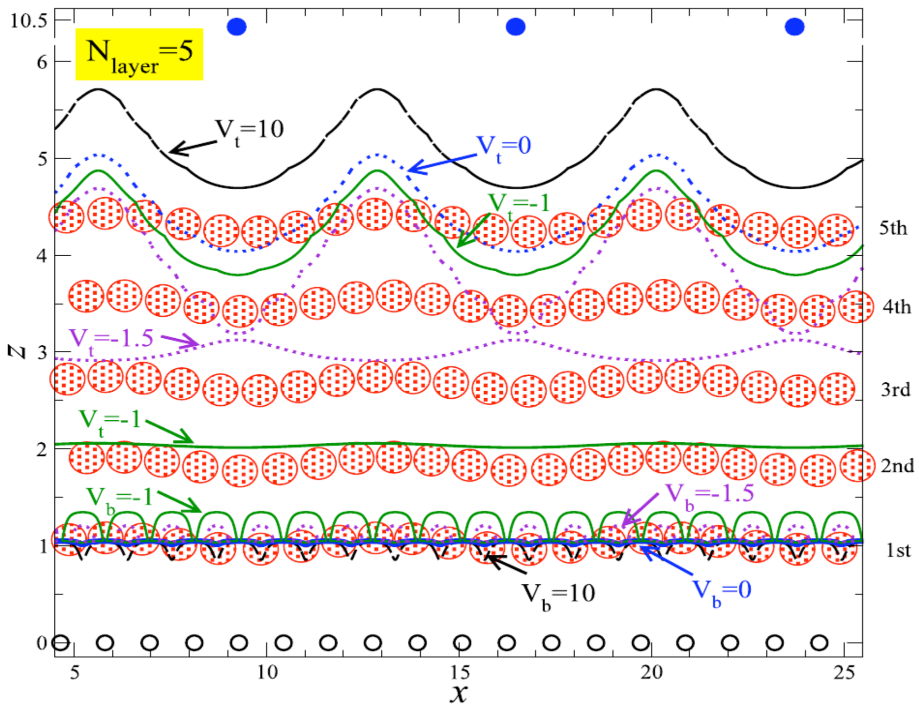
$$\eta \sum_{i}^{N_{\mathrm{l}}} (\dot{\vec{r}}_i - \dot{\vec{r}}_{\mathrm{t}}) = \eta\, N_{\mathrm{l}}\,(\vec{v}_{\mathrm{cm}} - \dot{\vec{r}}_{\mathrm{t}})$$

Standard ***Langevin dynamics***, with the addition of a dissipative damping term plus a Gaussian random force to the Newton equations

Kinks in the2D model

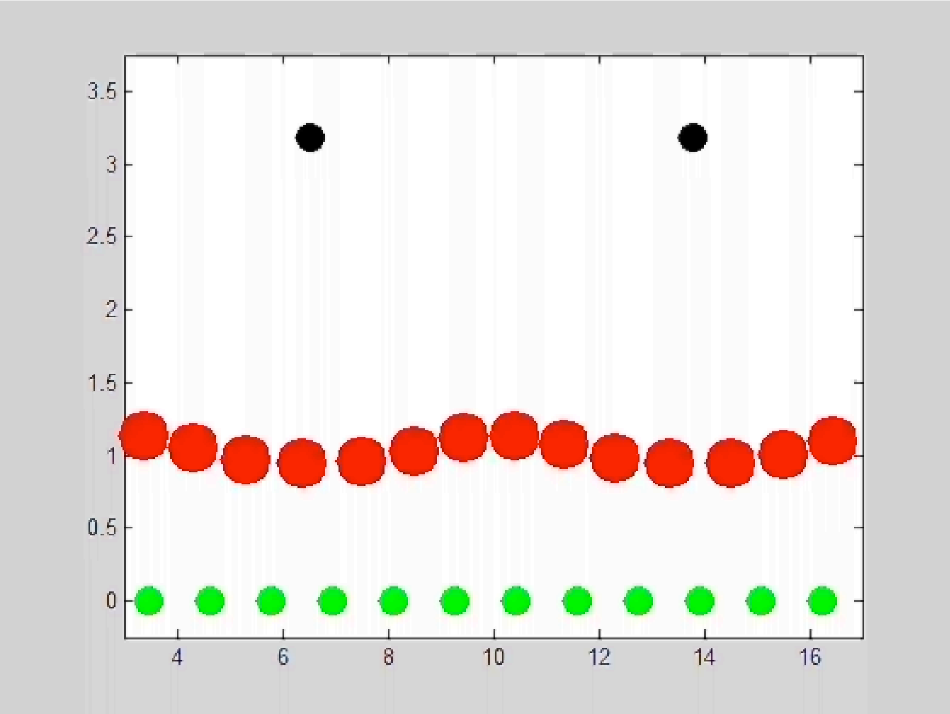


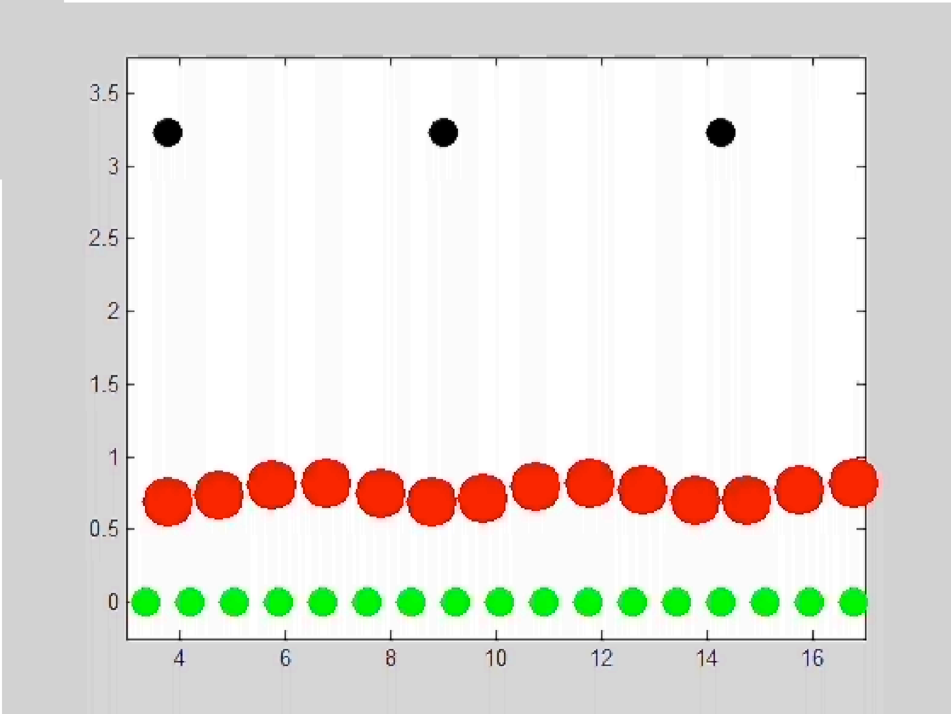
Kinks are visible like more dense and vertically displaced regions (non-uniform distribution of the vertical load)



Kinks are seen only in the horizontal displacement of the two lowest layers, while vertical ondulations of all lubricant layers are apparent.

Results: kink ($a_0 < a_b$) & anti-kink ($a_0 > a_b$) dragging





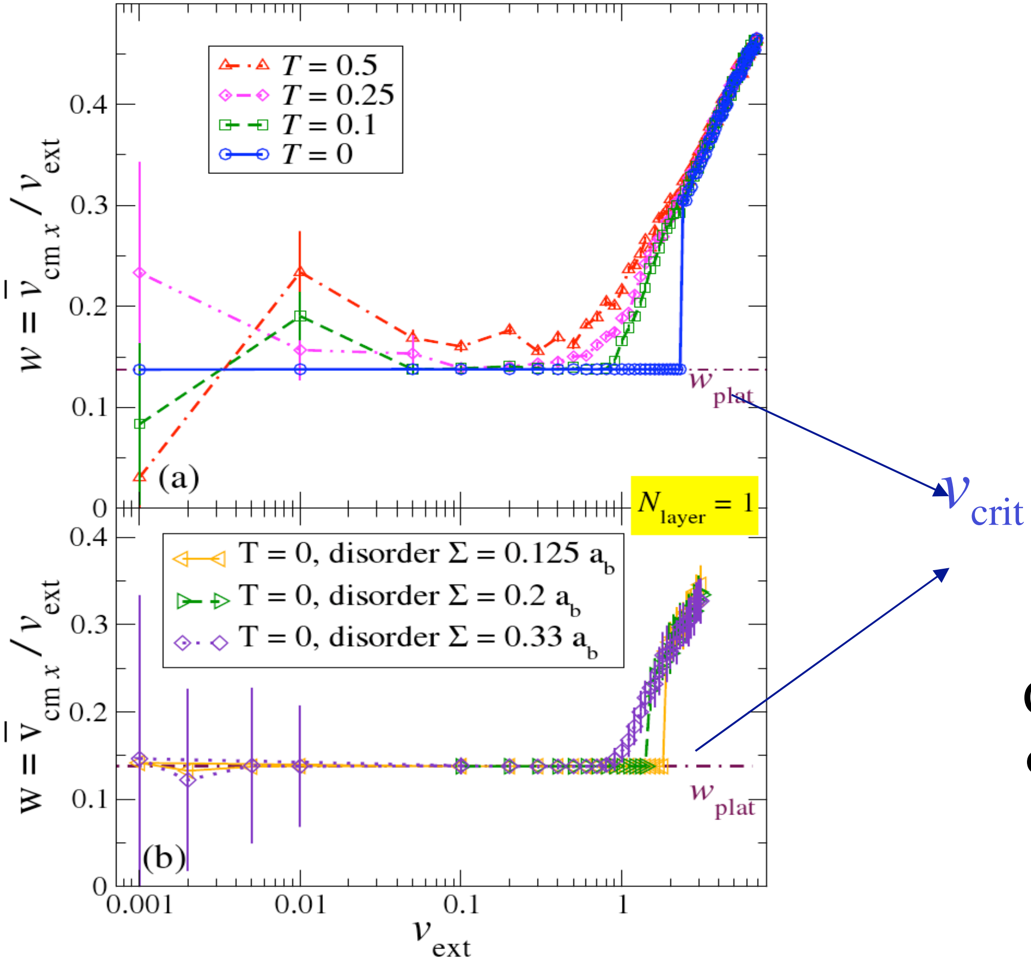
backward lubricant motion at speed
$w = 1 - 1/\lambda_b = -0.19$

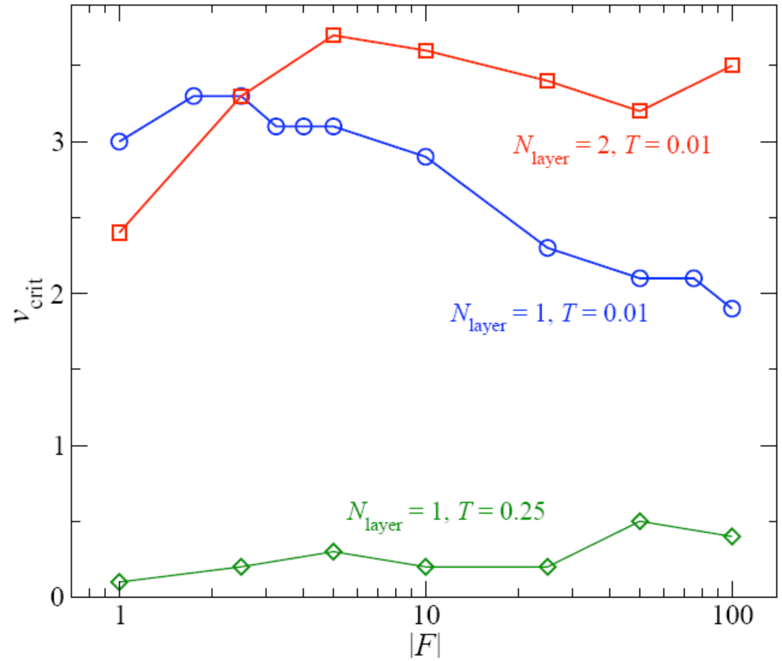
Velocity quantization ($N_{\text{layer}} = 1$)

$$w_{\text{plat}} = \frac{\overline{v_{\text{cm }x}}}{v_{\text{ext}}} = 1 - \frac{1}{\lambda_b}$$

varied v_{ext}

varied load |F|

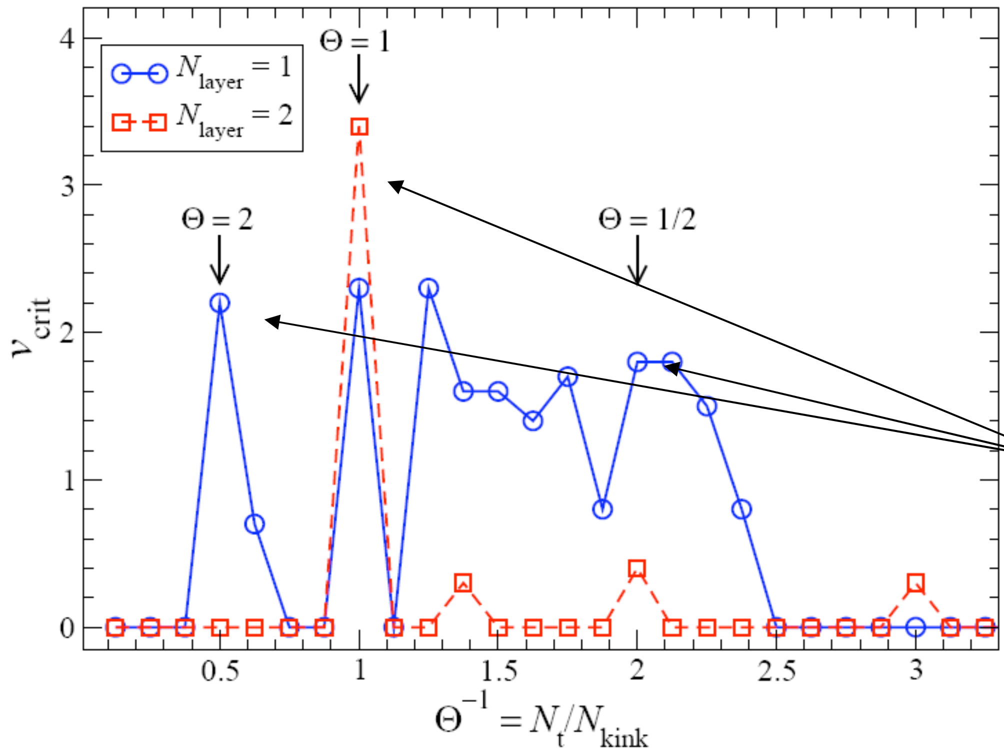




The plateau attractor tends to affect the dynamics even in the presence of large thermal fluctuations and disordered substrates.

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

Role of kink coverage $\theta = N_{kink}/N_t$

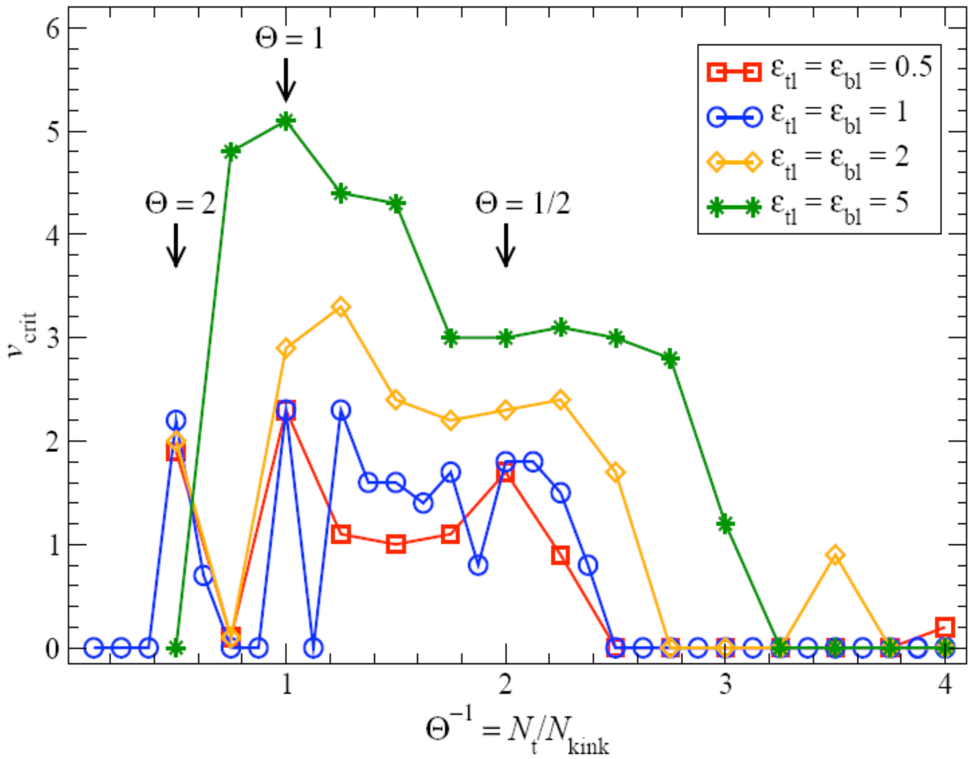


λ_t, not affecting the velocity plateau value, crucially sets the kink coverage:

$$\Theta = N_{\rm kink}/N_{\rm t} = \left(1 - \lambda_{\rm b}^{-1}\right)\lambda_{\rm t}$$

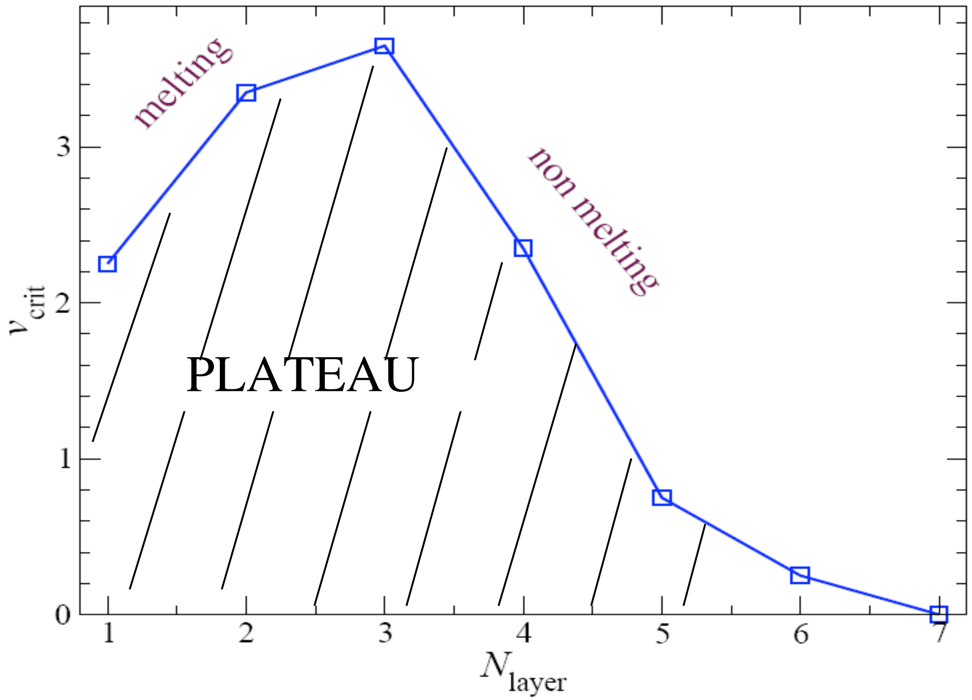
and affects the plateau robustness, v_{crit}

v_{crit}- maxima at well-commensurate coverage θ

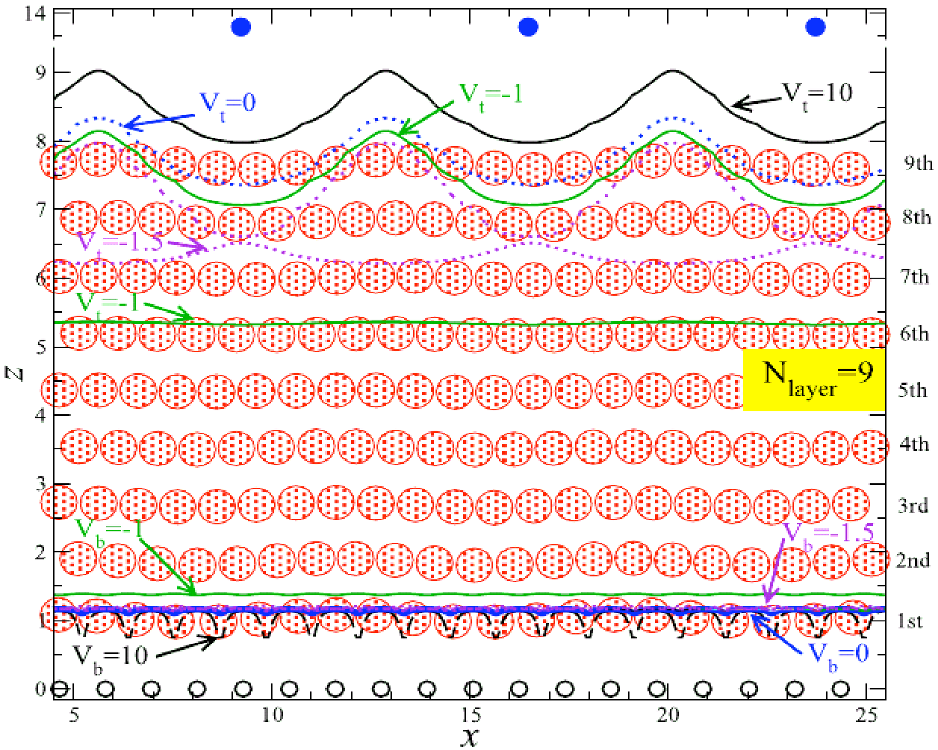


Stronger substrate interactions favour in-register lubricant regions, with narrow kinks being easily dragged by the top corrugations

Lubricant Multilayers

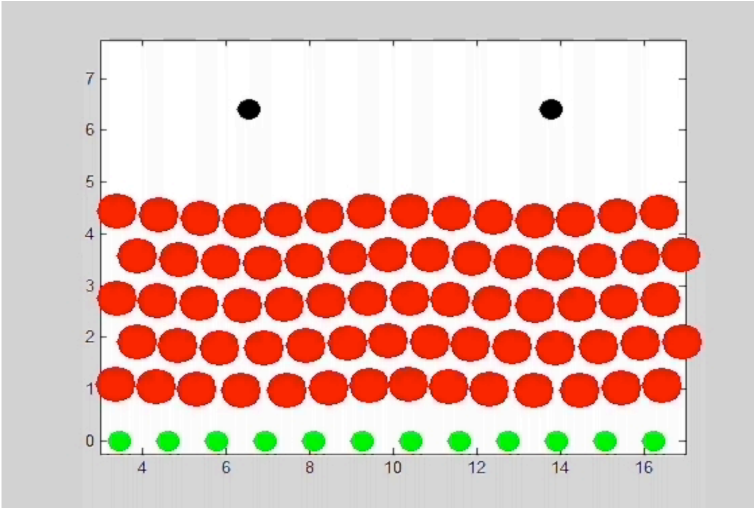


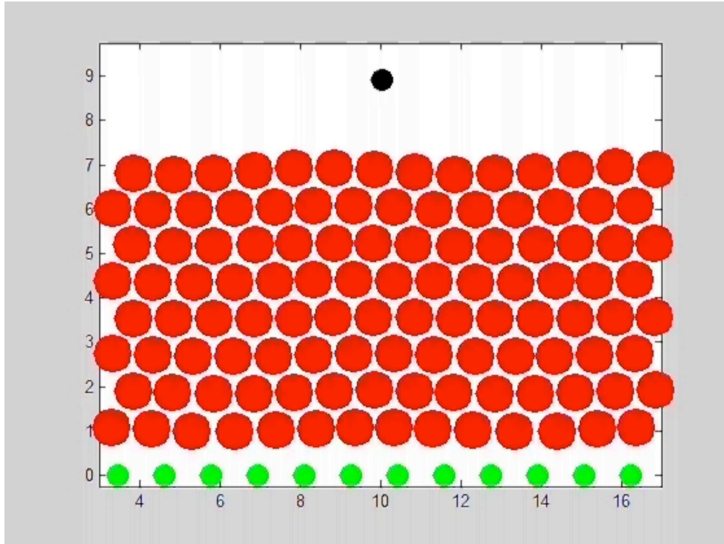
v_{crit} dependence on N_{layer} in fully commensurate $\theta = 1$ condition



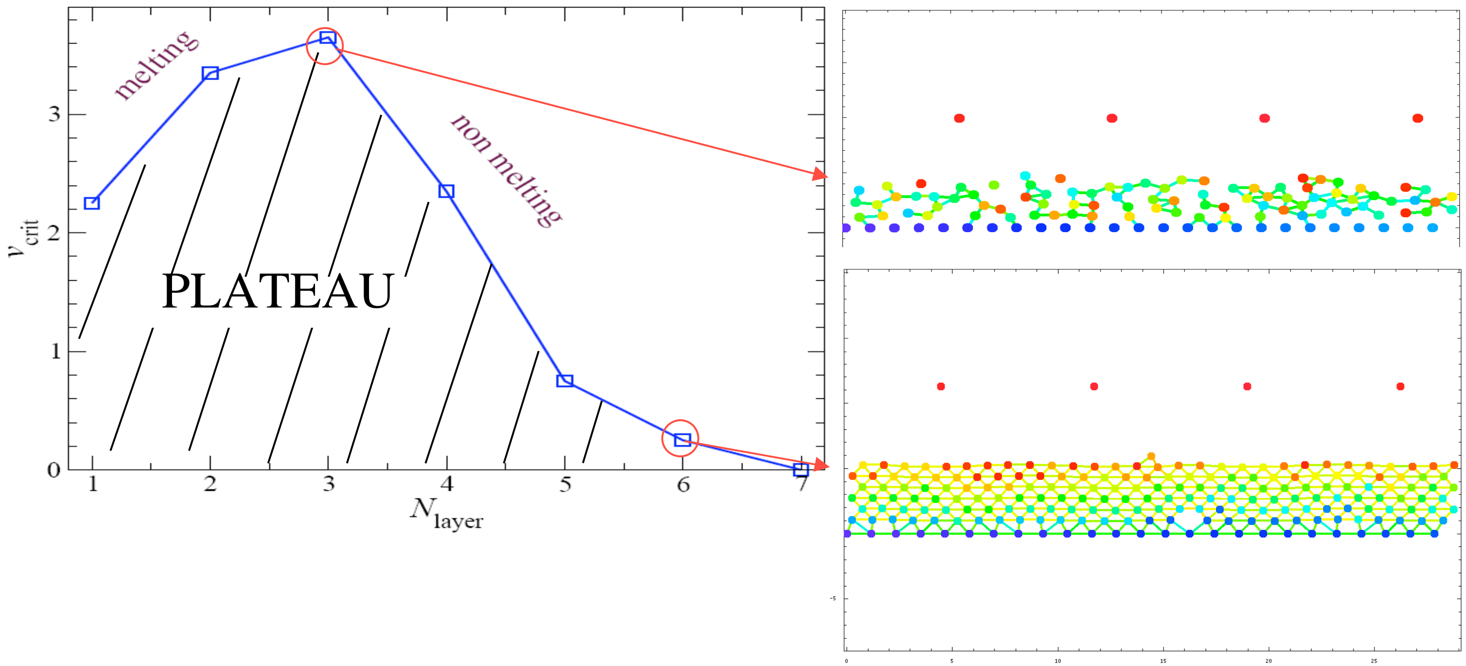
Lubricant vertical corrugation induced by the kinks favors the perfect velocity quantization.

By increasing N_{layer}, z-displacements decay rapidly, and such a mechanism becomes less effective to support the dynamically pinned state.





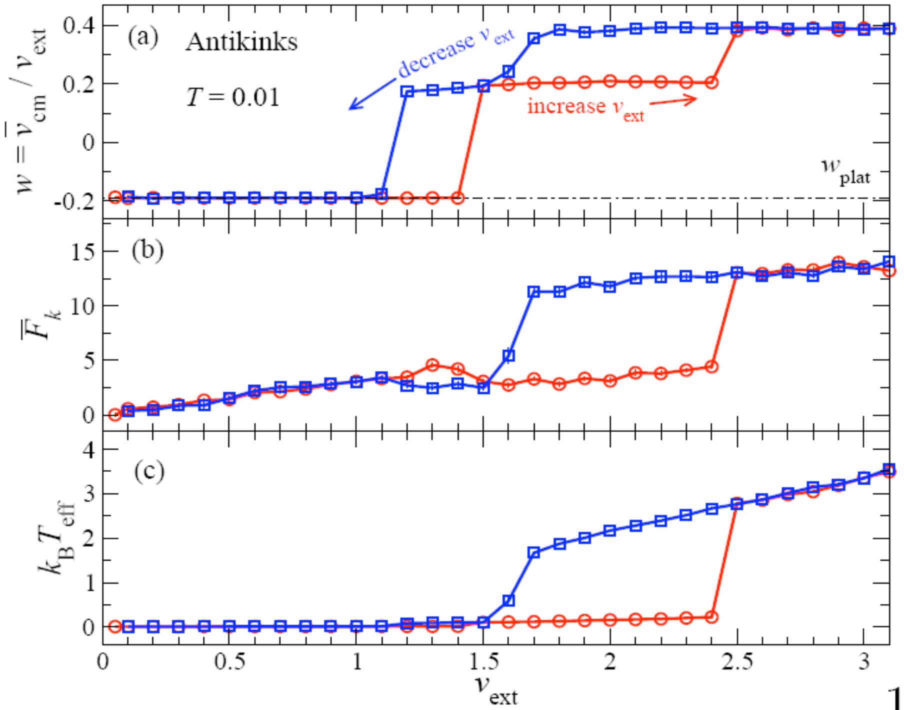
Lubricant Melting at the depinning transition

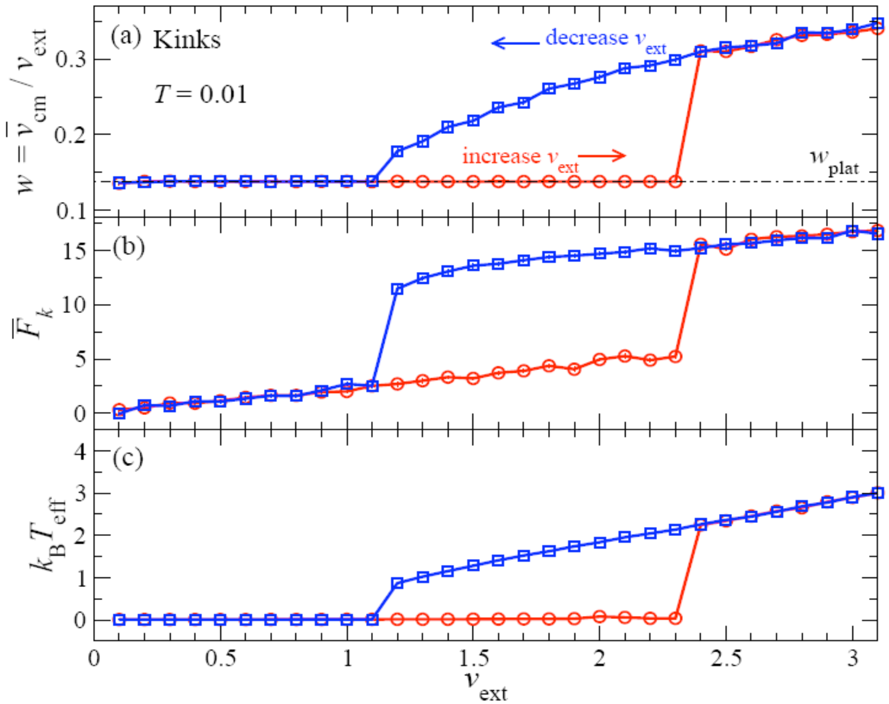


While the plateau occurs due to solitons being driven gently, the transition to the unpinned state may involve the lubricant melting, due to large shear-induced Joule heating.

Hysteresis & Friction

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





F_k = *kinetic friction force*

$$k_B T_{\rm eff} = \frac{1}{N_l}\overline{E_{k\,\rm cm}}$$

$$\overline{F_k} = \frac{4\eta}{m\,v_{\rm ext}}\left(\overline{E_{k\,\rm cm}} - N_l k_B T\right) + \frac{\eta N_l}{v_{\rm ext}}\left[\overline{v_{\rm cm}^2} + \overline{(\dot{\vec{r}}_{\rm t} - \vec{v}_{\rm cm})^2}\right]$$

fluctuations of the particle velocities in the CM frame.

force contribution coming from the lubricant as "rigid body" (..minimum if $v_{{\rm cm}\,x} = \frac{1}{2} v_{\rm ext}$)

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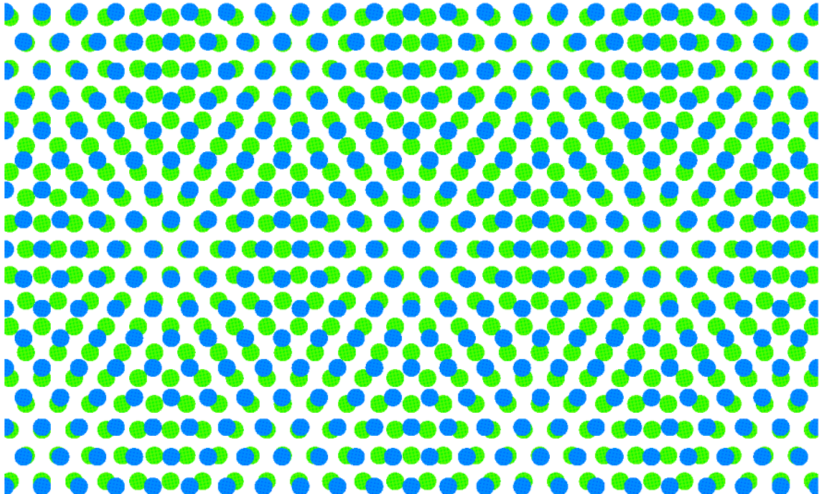
Accepted for publication in J.Chem. Phys

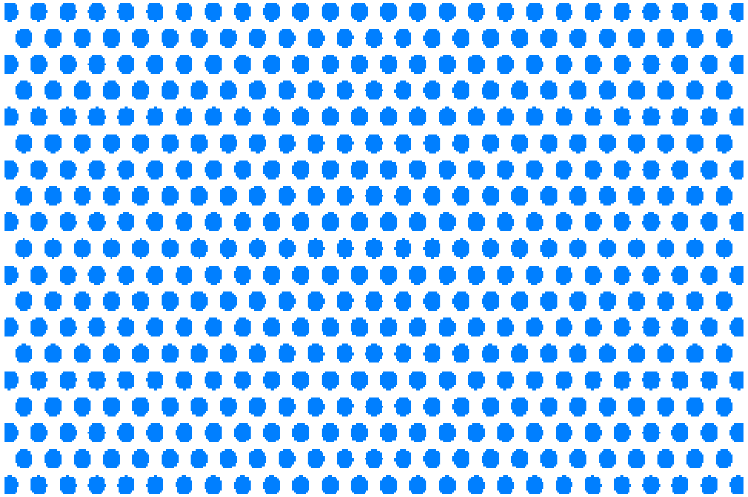
Work in progress

- Role of disorder (preliminary results) and substrate flexibility

- Realistic MD simulations: 3D model



dragging of a moiré pattern



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!!

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

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

standard MD (Newton e.o.m.)

4th-order Runge-Kutta integration

Nose-Hoover thermostat chain

PBC

drop an initial "thermalization" transient ($\sim 10^3$ time units)

pressure –F applied to top