HEAT CONDUCTION IN A MODEL OF DISSOCIATING ATOMIC CHAIN

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SIAM Conference on Dynamical Systems –
DS2015

Fourier Law (1822)

$$\vec{q} = -k\nabla T \qquad \frac{\partial T}{\partial t} = \alpha \Delta T$$

Empiric lowest – order approximation

Fourier Law vs Microstructure

$$\vec{q} = -k\nabla T$$

Diffusive dynamics

k – property of material,

Size – independent heat conduction coefficient

Fourier Law vs Microstructure

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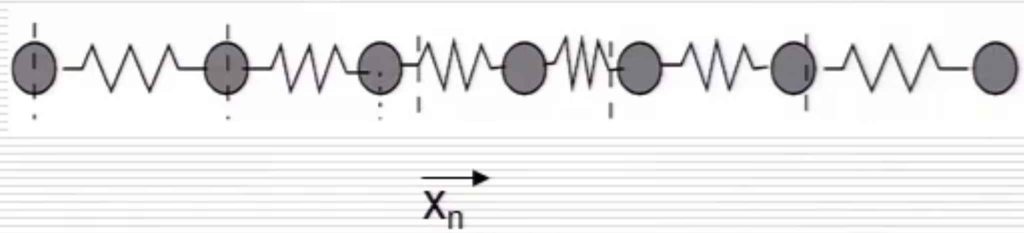


Diffusive dynamics

k – property of material,

Size - independent

$$m\ddot{x}_n + \frac{\partial V(x_n - x_{n-1})}{\partial x_n} + \frac{\partial V(x_n - x_{n+1})}{\partial x_n} = 0$$

$$H = \sum_n \frac{p_n^2}{2m} + V(x_n - x_{n-1}) = const,\ p_n = m\dot{x}_n$$

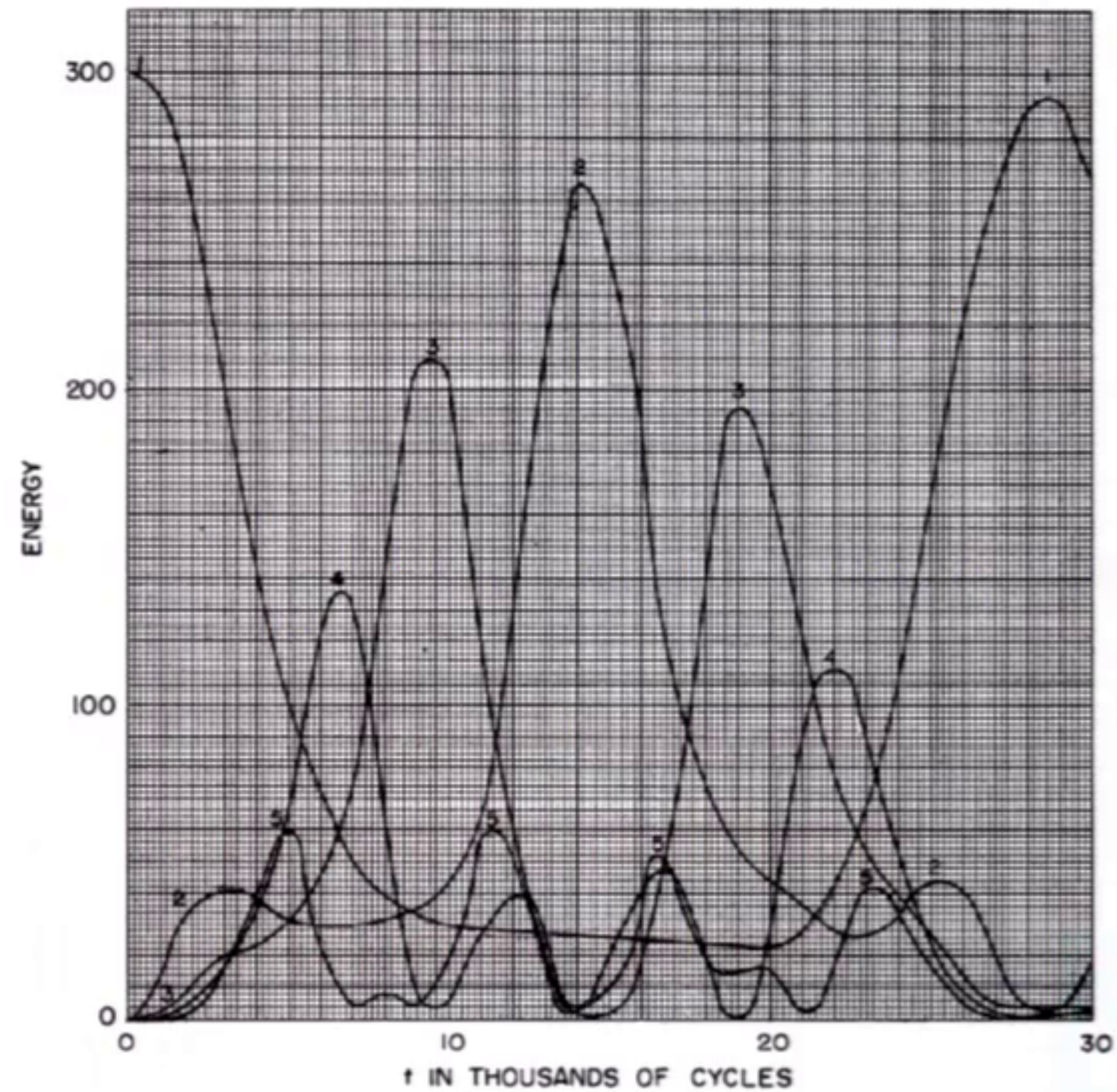
Conservative dynamics

Fermi – Pasta –Ulam (1949)

$$V(z) = \frac{g_2}{2}(z-a)^2 + \frac{g_3}{3}(z-a)^3$$

64 particles , fixed

boundary conditions



Fermi – Pasta –Ulam Experiment (1949)

$$V(z) = \frac{g_2}{2}(z-a)^2 + \frac{g_3}{3}(z-a)^3$$

64 particles , fixed boundary conditions

-lack of mixing and thermalization

-energy remained in few low modes with accuracy of about 4%

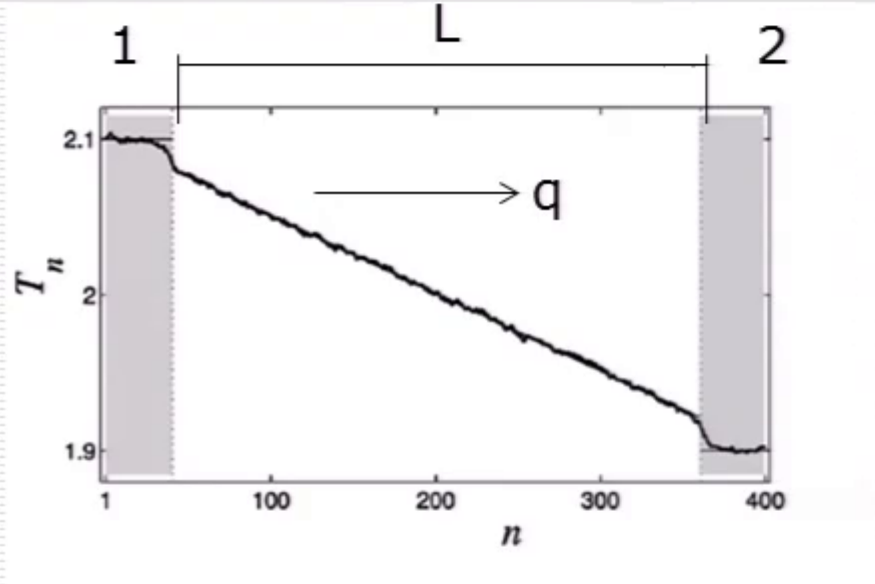
- discovery of integrable continuous models (and numberless other things)

- problem of heat conduction remained unresolved

Fourier Law – what to anticipate in simulation?

$$\frac{\partial T}{\partial t} = \alpha \Delta T$$

$$\vec{q} = -k \nabla T$$



$$\alpha = \frac{qL}{T_1 - T_2}$$

Fourier Law vs Microstructure

Current state of the art

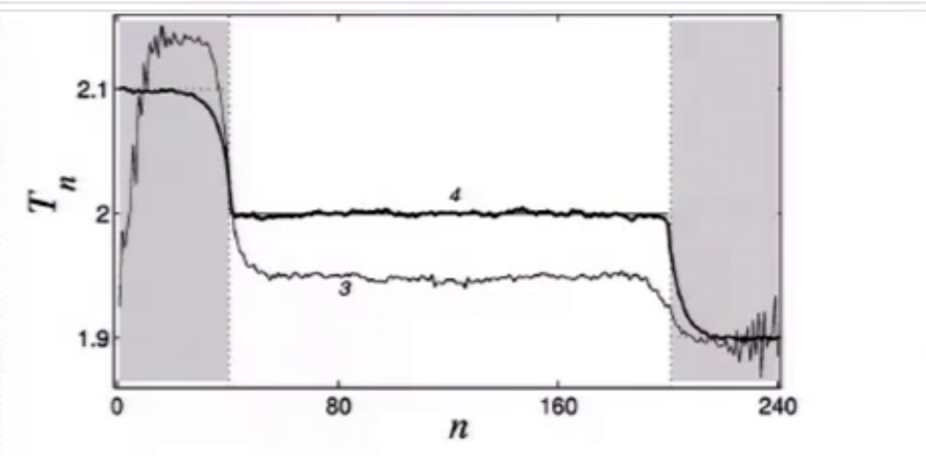
Integrable models (linear, Toda lattice, on-site billiard…)

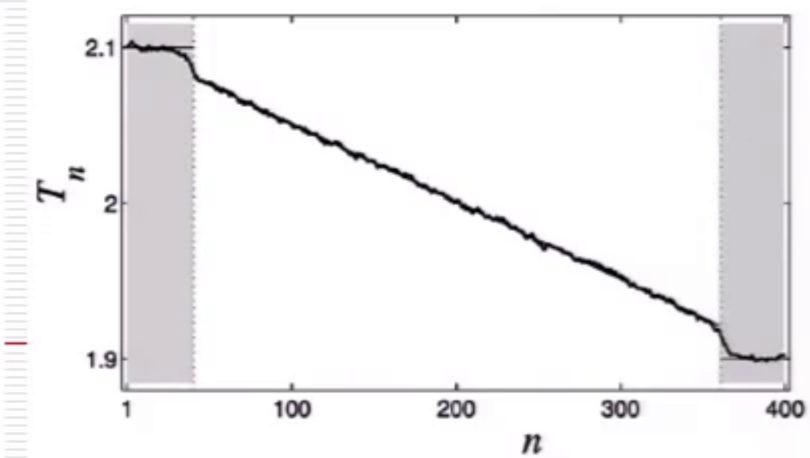
Fourier law wrong!

Non-integrable models:

Linear temperature profile establishes itself.

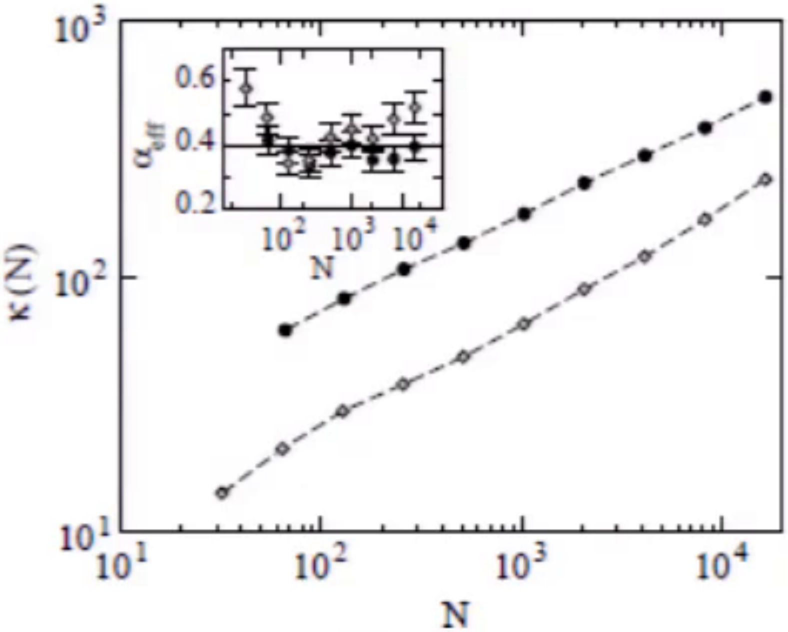
Fourier law correct (?)





β-FPU Model

$$H = \sum_n \left(\frac{1}{2}\dot{u}_n^2 + \frac{1}{2}(u_n - u_{n-1})^2 + \frac{\beta}{4}(u_n - u_{n-1})^4\right)$$



The temperature profile is normal but the thermal conductivity diverges:

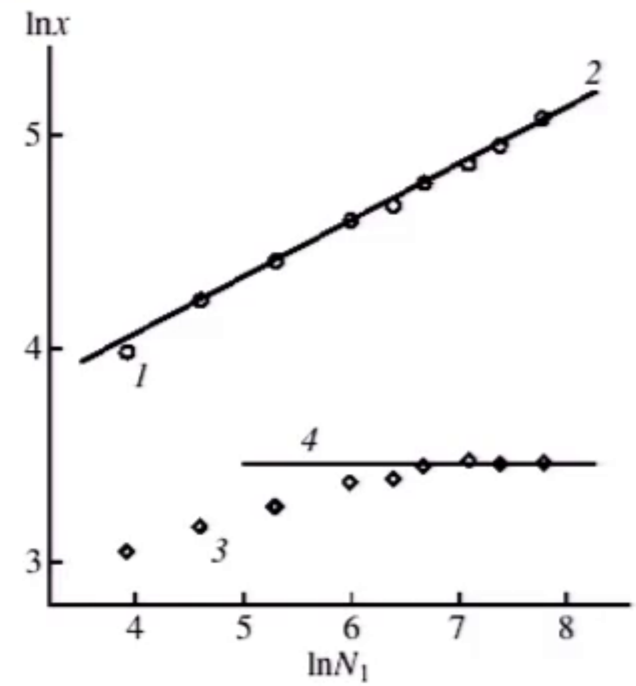
$$\kappa = \frac{JN}{\Delta T} \to \infty \text{ as } N \to \infty,\ \kappa \sim N^{0.32-0.4}$$

S. Lepri, R. Livi, and A. Politi, PRL, **78**, 1896 (1997).
S. Lepri, R. Livi, and A. Politi, Phys. Rep. **311**, 1-80 (2003)

Chain of Coupled Rotators

$$H = \sum_n \left(\frac{1}{2}\dot{\phi}_n^2 + U(\phi_{n+1} - \phi_n)\right)$$

$$U(\phi) = 1 - \cos\phi$$



Normal heat conduction

OVG and A.V. Savin, PR L, 2000
G.Giardina et al, PRL, 2000

Fourier Law vs Microstructure

$$\vec{q} = -k\nabla T$$

k – thermodynamic parameter (independent on the system size)?

1D – "No" for certain models (FPU, diatomic Toda, etc) $k \sim N^{0.35}$

"Yes" for other models (Frenkel – Kontorova, rotators, etc)

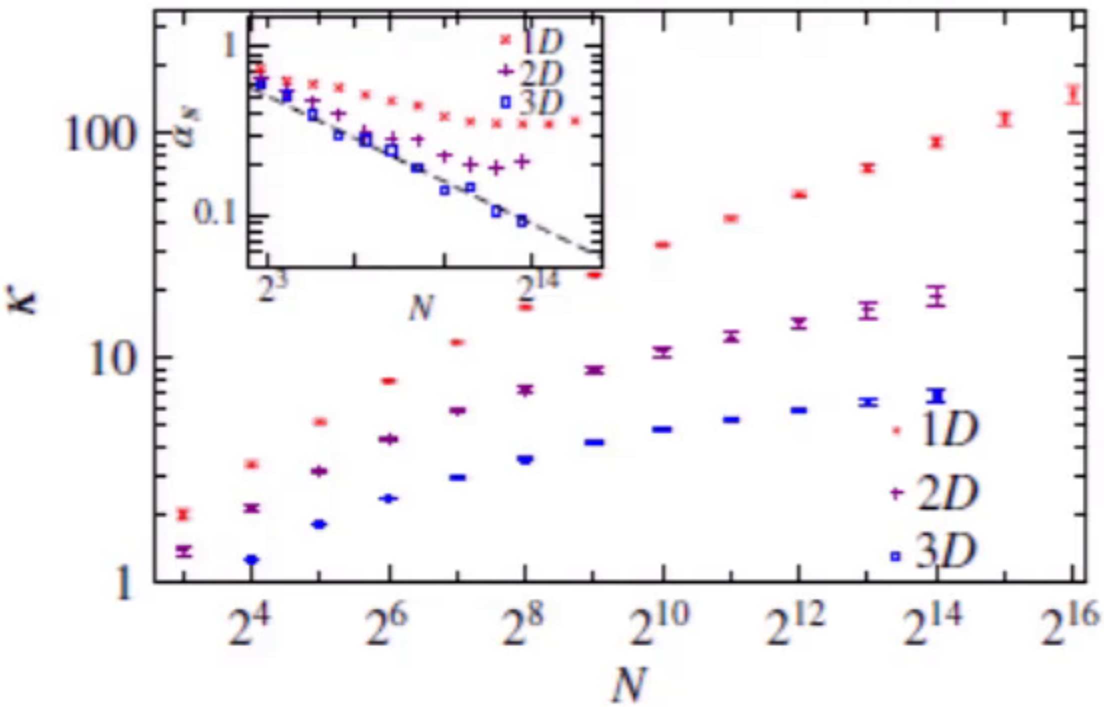
2D - "No" (logarithmic divergence?)

3D - Converges (???) – somewhat doubtful results for relatively small systems

Fourier Law vs Microstructure

3D - Converges (???)

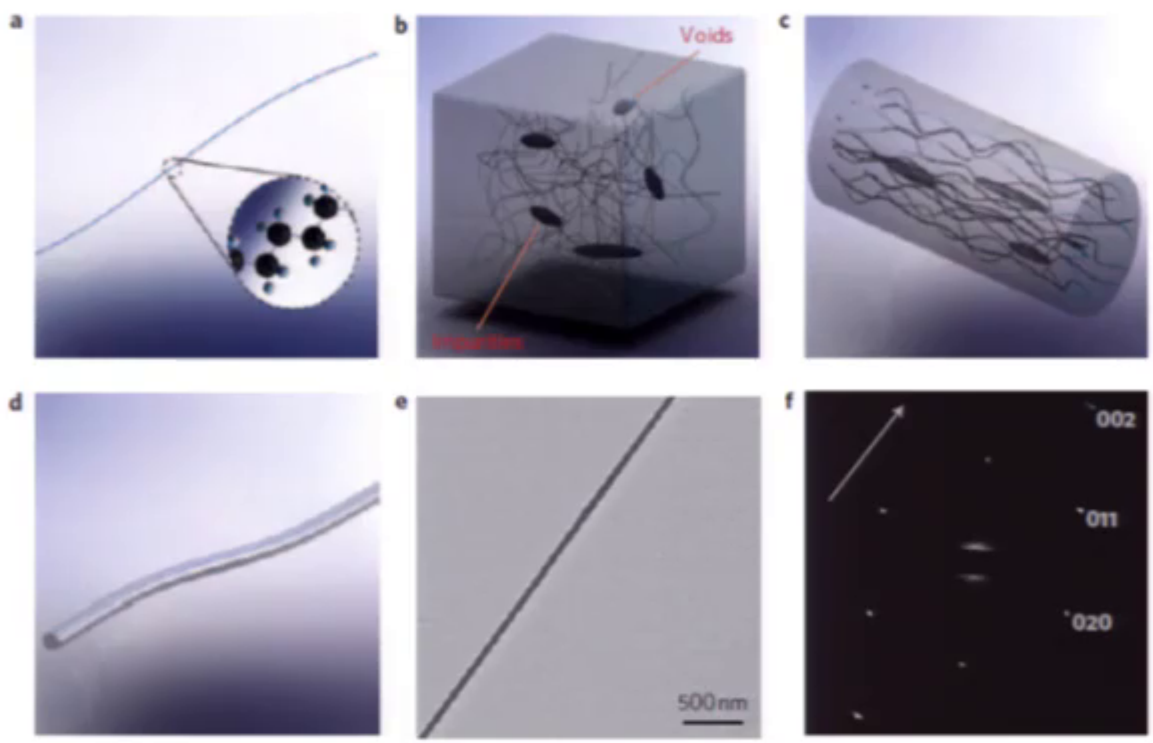
K. Saito and A. Dhar, PRL, **104**, 040601 (2010)



Maximum size:

16x16X8192

Polymer fibres



Ultra – drawn polyethylene nanofibres

S.Shen et al, Polyethylene nanofibres with very high thermal conductivities, Nature Nanotechnology, 5, 251 - 255 (2010)

Analytic approaches that support divergence in 1D case

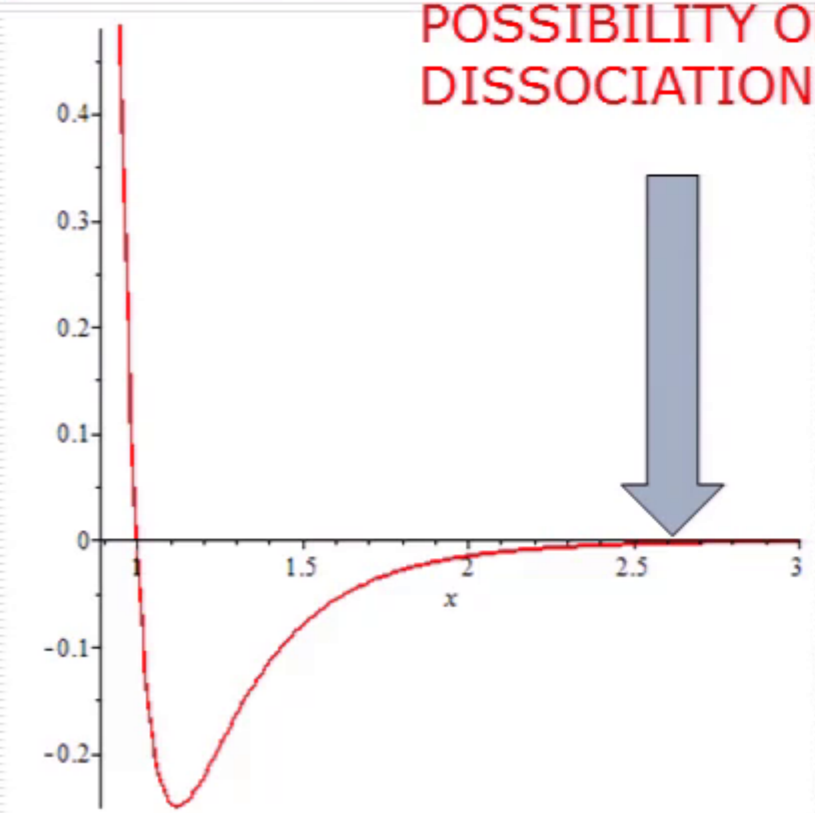
- \- renormalization group (Narayan O. and Ramaswamy S., *PRL* **89** (2002) 200601)
- \- kinetic equations (Lukkarinen J. and Spohn H., *Commun. Pure Appl. Math.*, **61** (2008) 1753.)
- \- mode-coupling theory – analogy with hydrodynamics (Delfini L., Lepri S., Livi R. and Politi A., *PRE*, **73** (2006) 060201(R); van Beijeren H., *PRL*, **108** (2012) 180601; Spohn H., *J. Stat. Phys.*, **154** (2014) 1191)

Model with possibility of dissociation

Common interparticle potential V(r)

FINITE ENERGY ⇔ POSSIBILITY OF DISSOCIATION

$$V(r) = \varepsilon\left(\frac{1}{r^{12}} - \frac{1}{r^{6}}\right)$$

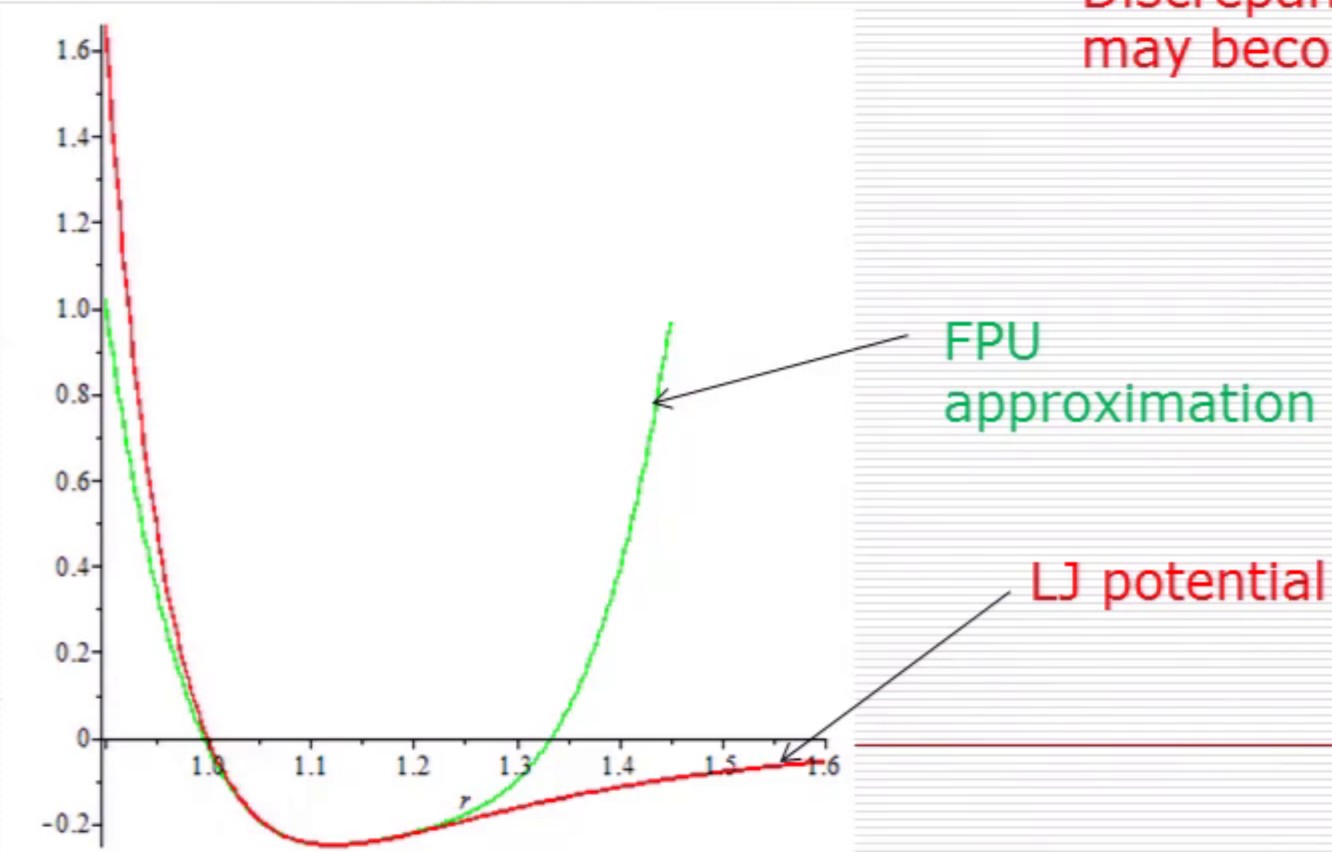


EXAMPLE: Lennard-Jones potential

Model with possibility of dissociation

"Realistic" potential versus common approximation

In thermodynamic limit $N \to \infty$ and time $t \to \infty$. Discrepancy at large r may become crucial!

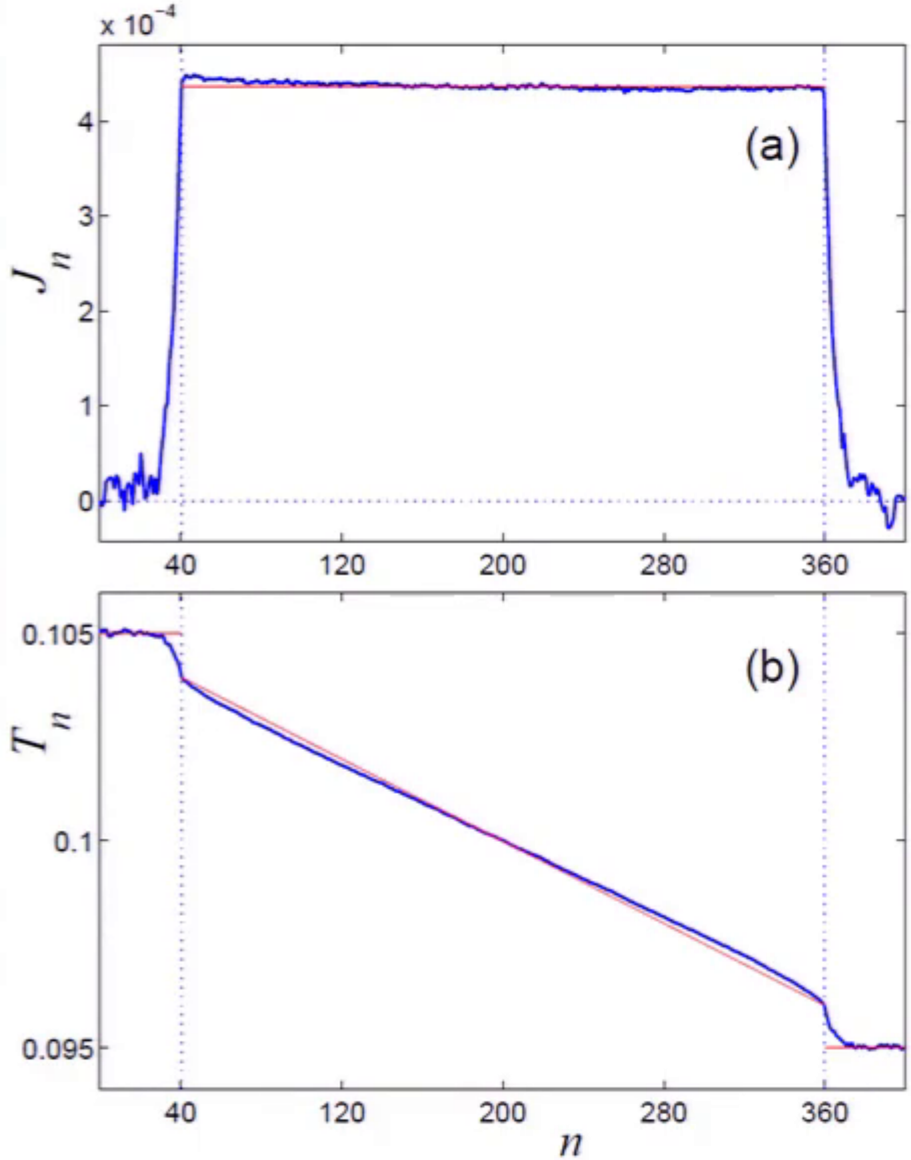


Model with possibility of dissociation

Simplified model of elastic rods

$$V(\rho) = \begin{cases} (\rho - d)^2/2, & \rho < d \\ 0, & \rho \geq d \end{cases} .$$

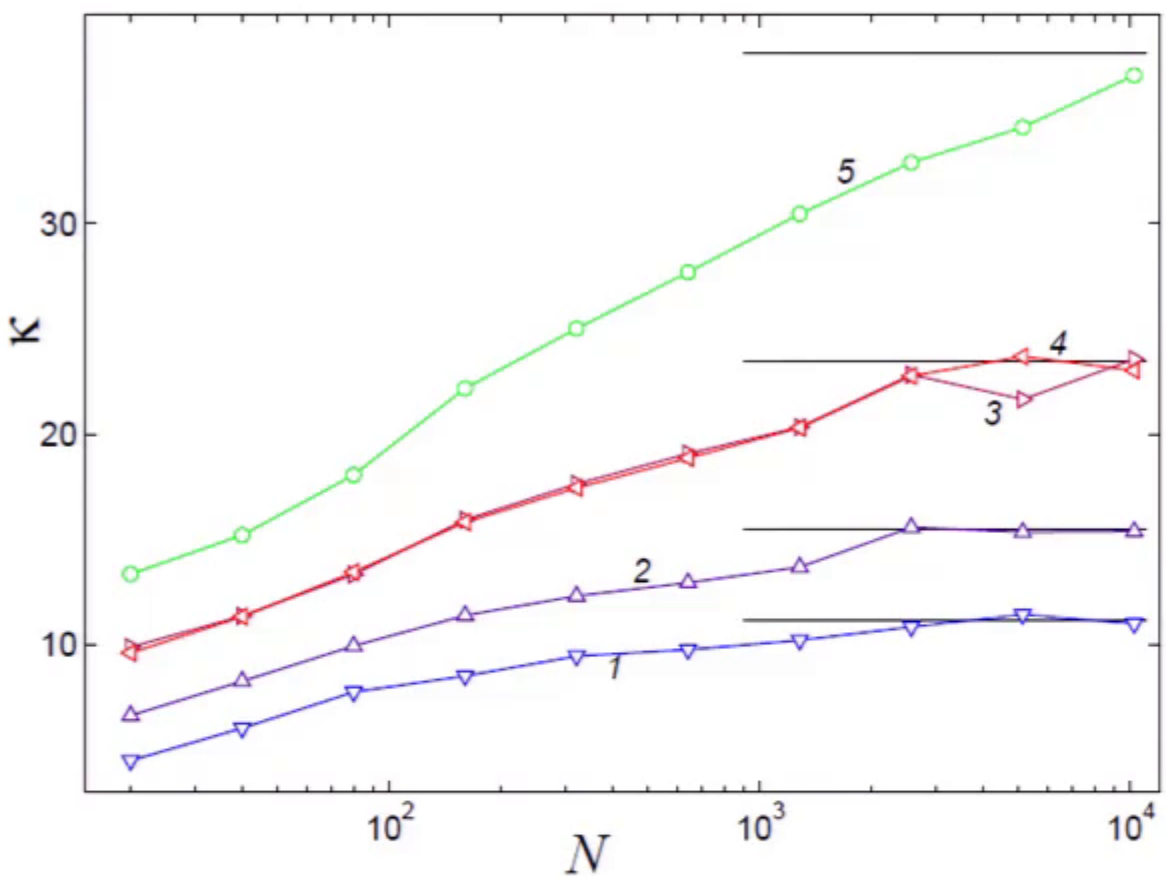
Non-equilibrium simulation



Ends of the chain are imbedded into Langevin thermostats

$$
\begin{aligned}
u_n'' &= -\partial H/\partial u_n - \gamma u_n' + \xi_n^+,\ 1 < n \le N_+, \\
u_n'' &= -\partial H/\partial u_n,\ N_+ < n \le N_+ + N, \\
u_n'' &= -\partial H/\partial u_n - \gamma u_n' + \xi_n^-, \\
& \quad N_+ + N < n < N_+ + N + N_-.
\end{aligned}
$$

Non-equilibrium simulation



OVG and A.V.Savin, EPL, 2014

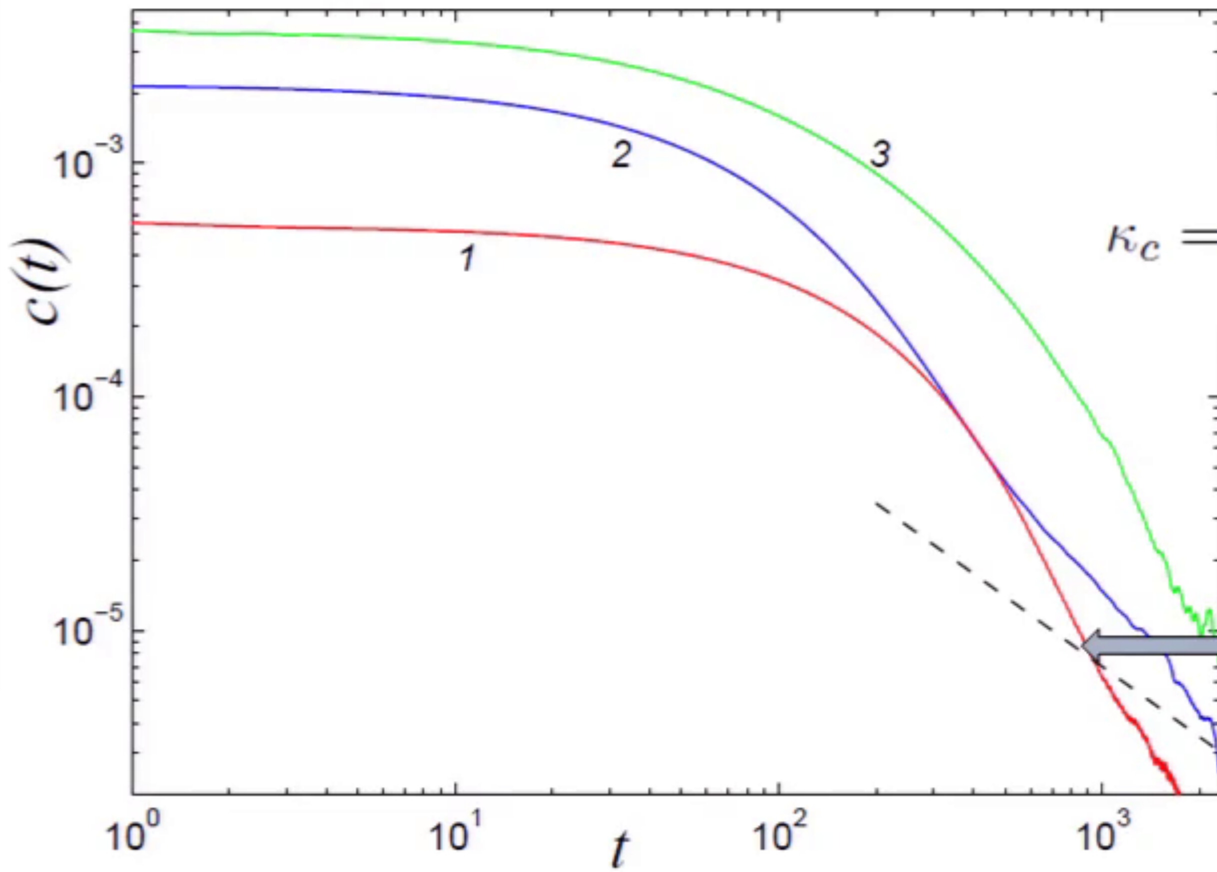
Convergence of heat conductivity

"Arrhenius" approximation for the heat conduction coefficient

For densely packed chain:
Heat conductivity ~ phonon velocity · mean free path
Phonon velocity in linear chain =1
Mean free path is inversely proportional to a probability of thermal fluctuation leading to a dissociation:

$$\kappa \sim \exp[\alpha(d-1)^2/T].$$

Equilibrium simulation

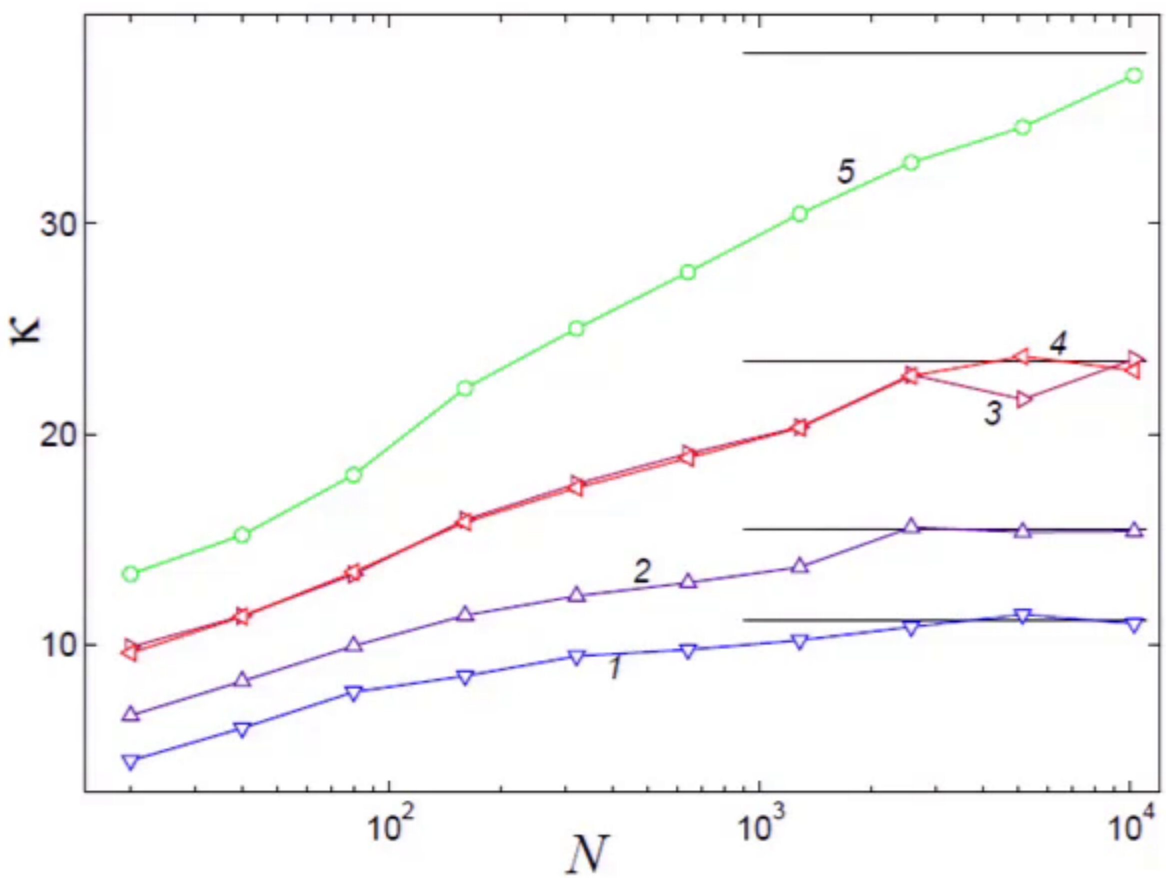


Green-Kubo

$$\kappa_c = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{NT^2}\int_0^{\tau} c(s)ds,$$

All autocorrelation functions decay faster than 1/t

Non-equilibrium simulation



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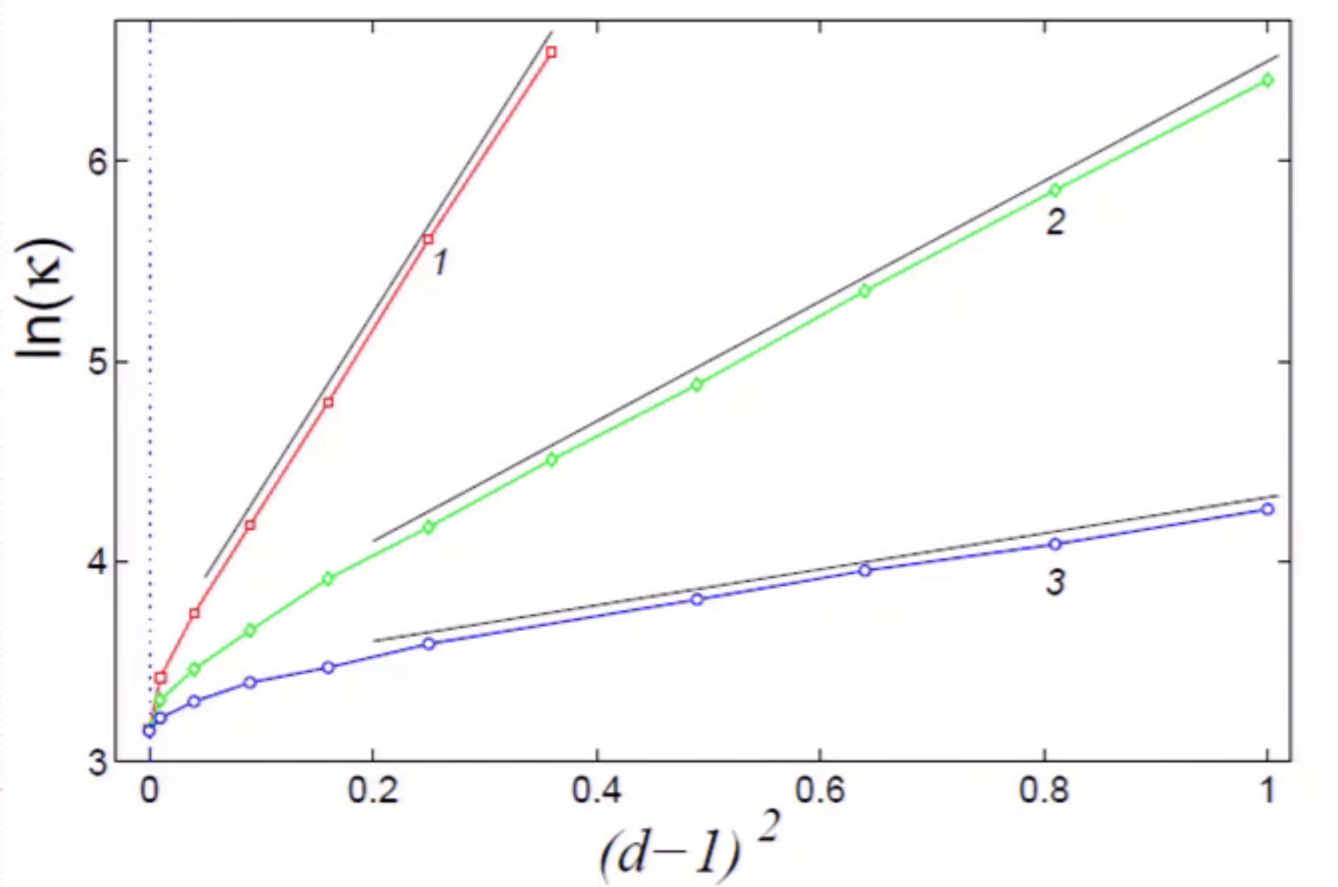
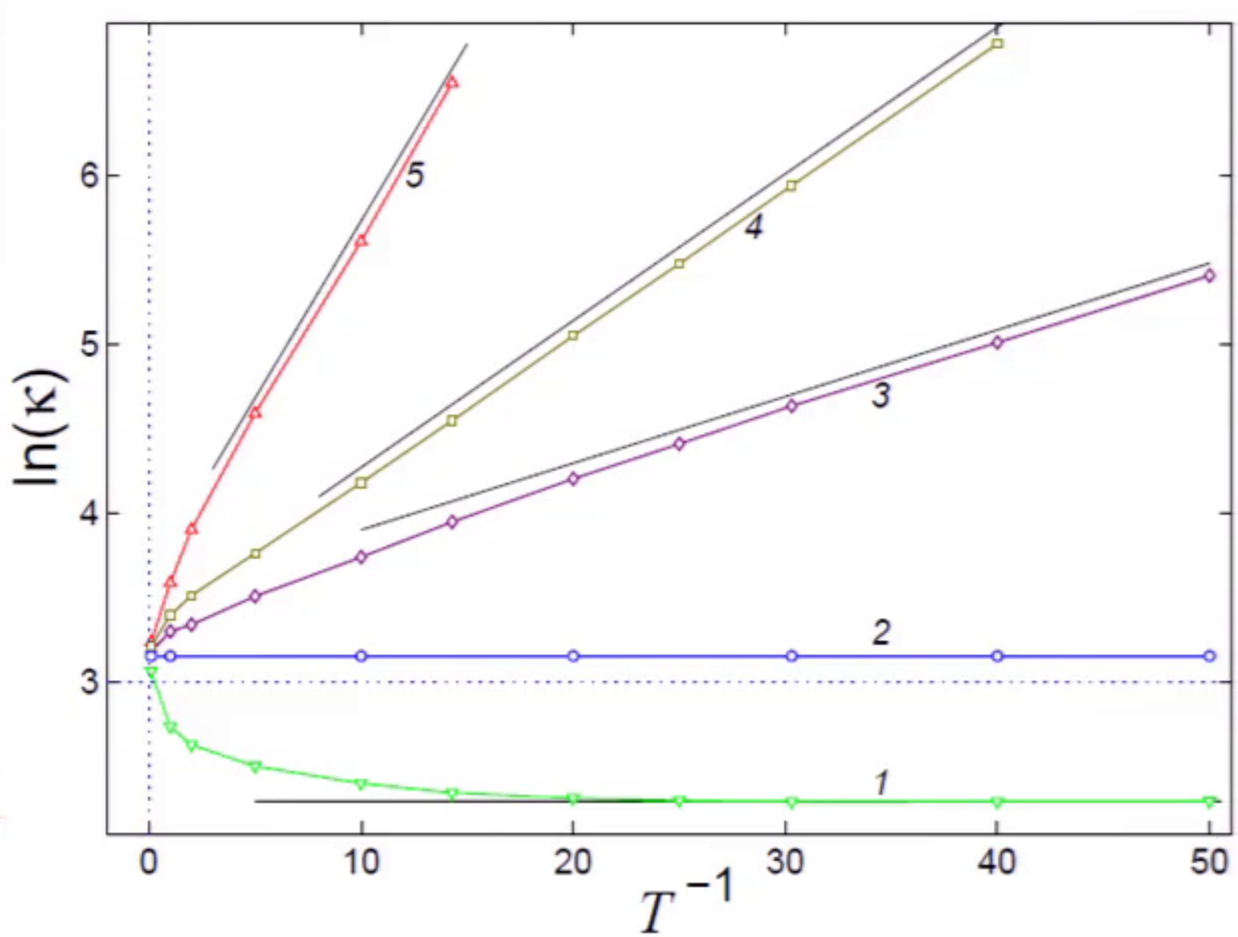


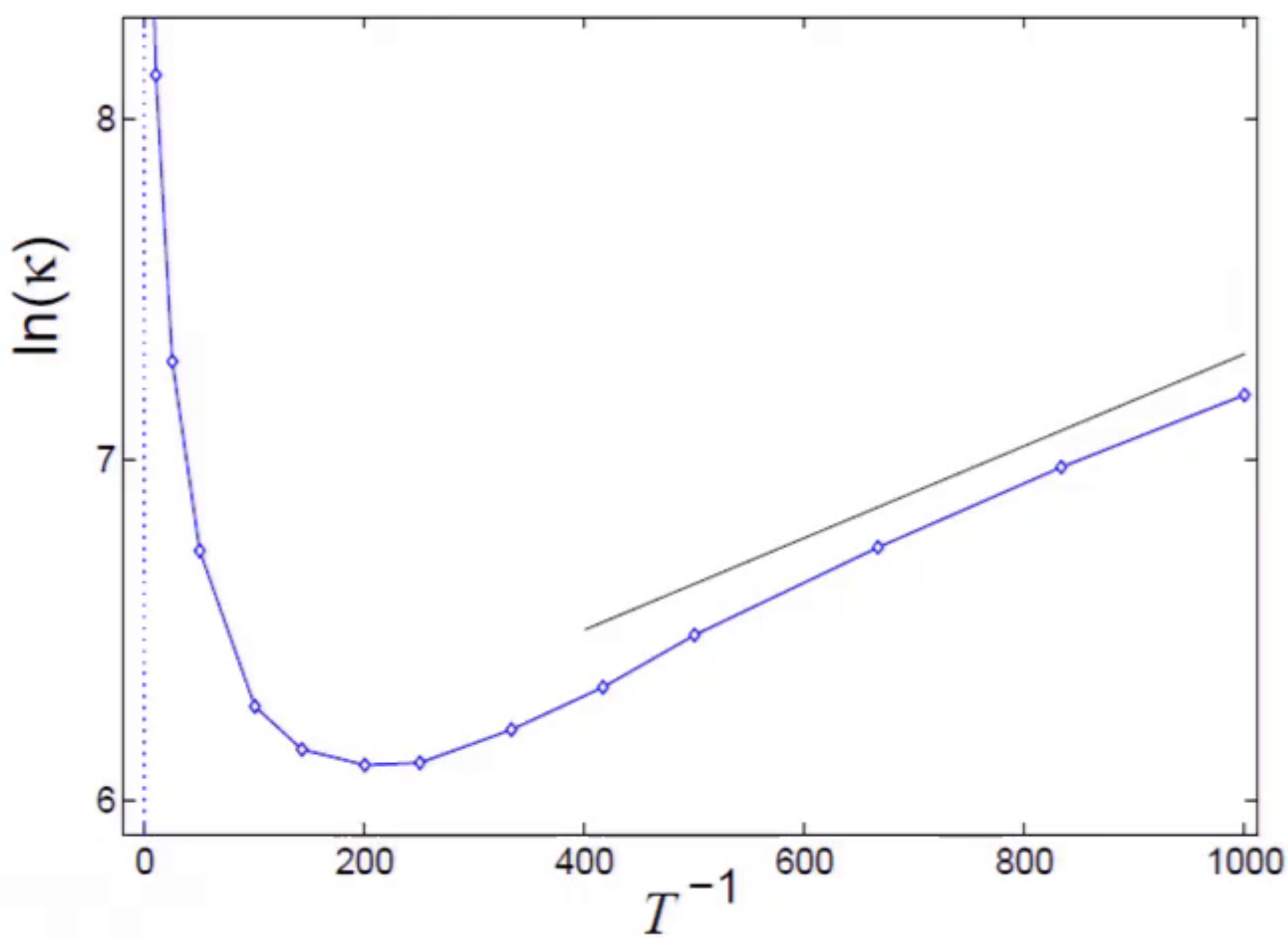
"Arrhenius" approximation for the heat conduction coefficient

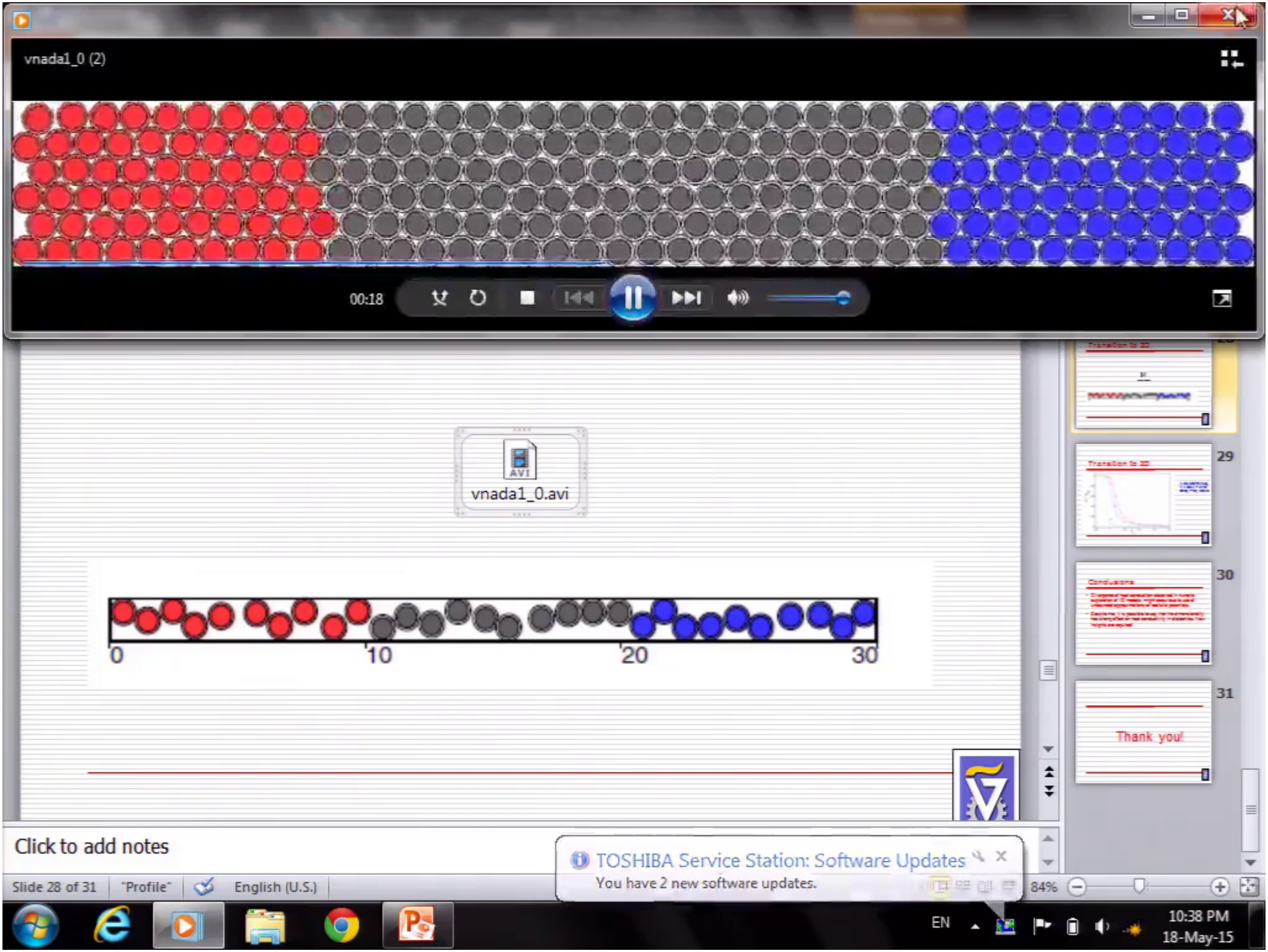
$$\kappa \sim \exp[\alpha(d-1)^2/T].$$

1,2 – low density
3,4,5 – high density (>1)



Generity of "Arrhenius" mechanism: LJ potential

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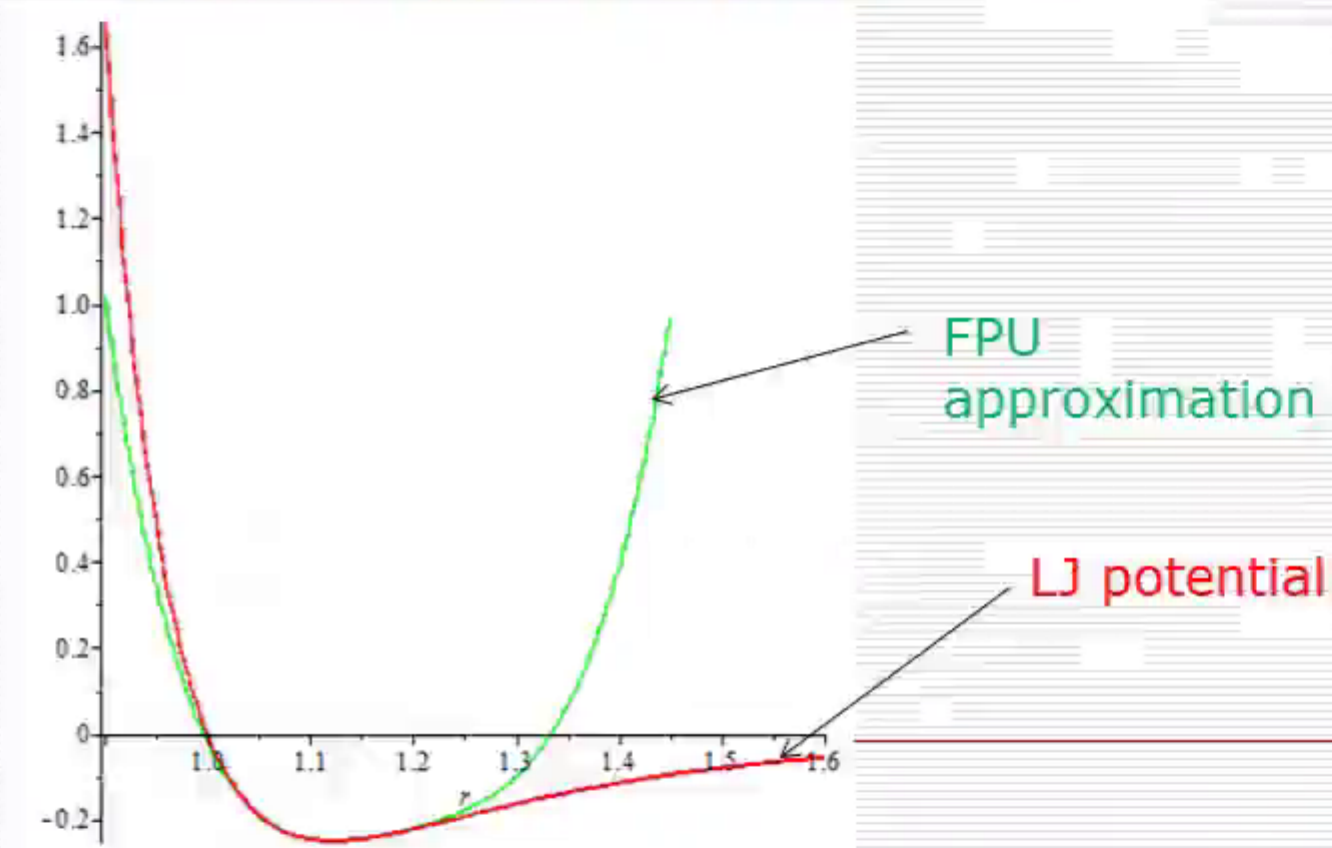

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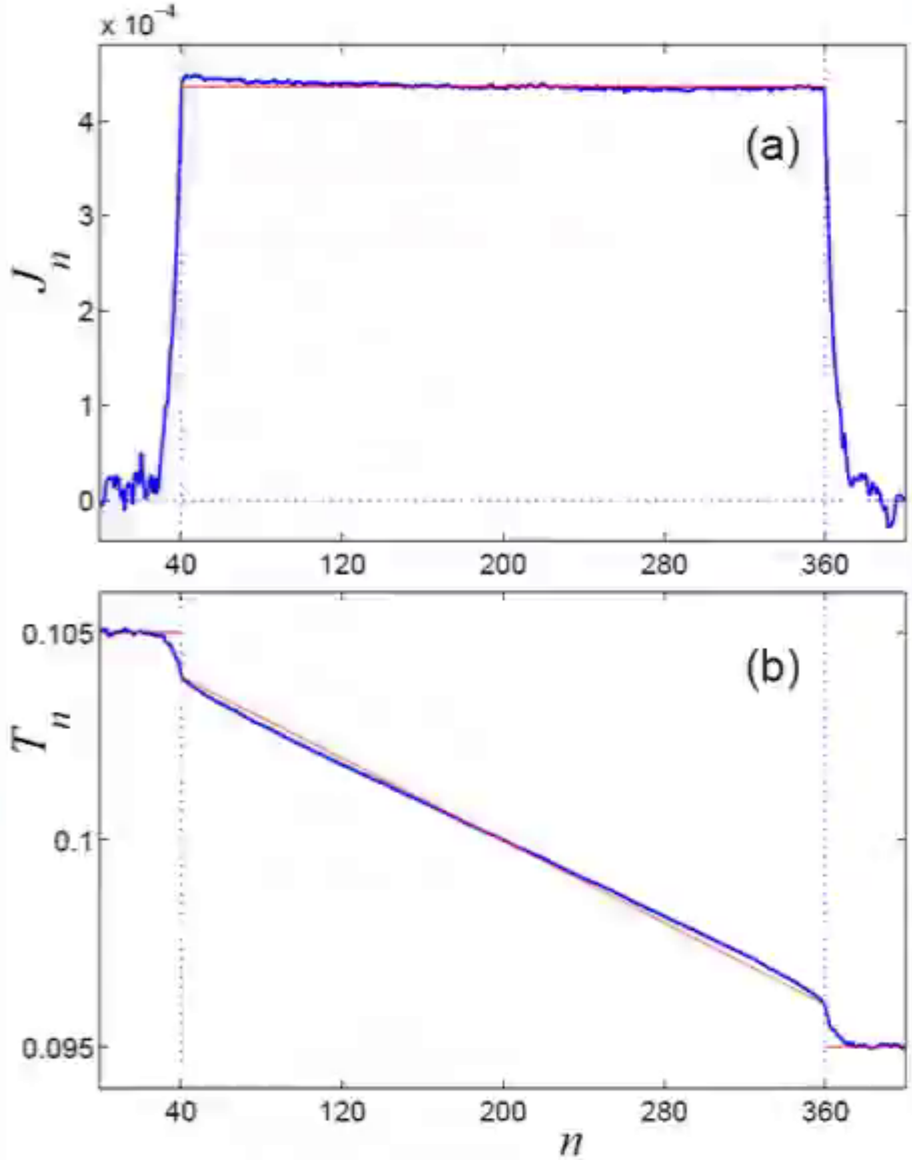

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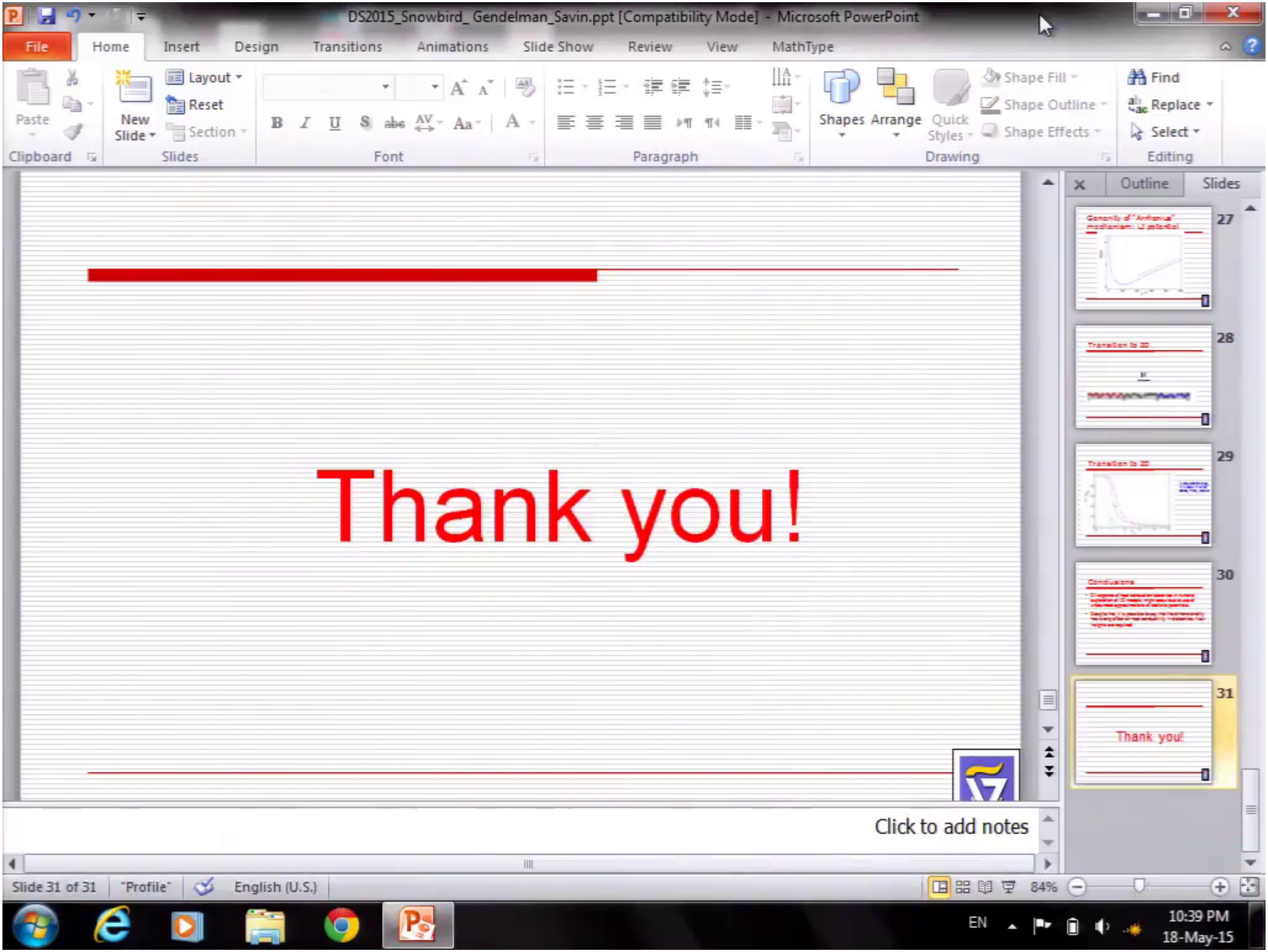
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