Heat transport in low–dimensional systems

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CSDC-group

A very old problem

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- 1997 - S. Lepri, R.L., A. Politi: FPU revisited

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Simulating lattice heat transport

Chain of N coupled oscillators with n.n. coupling:

$$m\ddot{q}_l = -V'(q_l - q_{l-1}) + V'(q_{l+1} - q_l)$$

$L = Na$ chain length, $V(x)$ nonlinear interparticle potential

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Equilibrium MD: correlation of the heat flux J

$$\kappa_{GK} \;=\; \frac{1}{k_B T^2 d} \lim_{t\to\infty} \int_0^t d\tau \; \lim_{L\to\infty} L^{-d} \langle \mathbf{J}(\tau) \cdot \mathbf{J}(0) \rangle$$

Microscopic expression (in 1d):

$$J = \frac{a}{2} \sum_n (\dot{q}_{n+1} + \dot{q}_n)\, V'(q_{n+1} - q_n)$$

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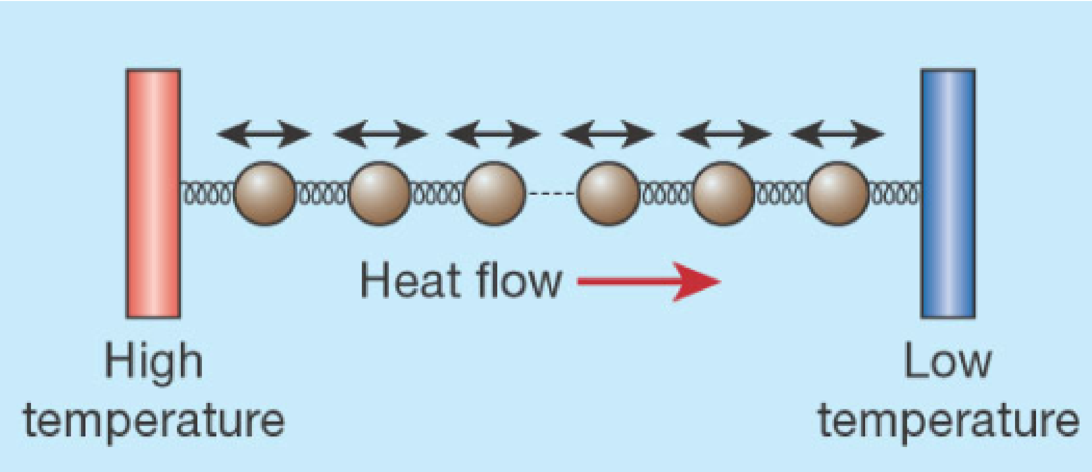
Non-equilibrium MD: $\kappa(L,T) \; = \; \frac{\overline{J}}{(T_+ - T_-)/L}$



Thermostats

Deterministic (Gauss' principle)

Nosé-Hoover, isokinetic, Evans...

$$\ddot{q}_1 = -\zeta_+ \, \dot{q}_1 + \ldots \qquad \ddot{q}_N = -\zeta_- \, \dot{q}_N + \ldots$$

$$\dot{\zeta}_+ = \frac{1}{\Theta^2}\left(\frac{\dot{q}_1^2}{T_+} - 1\right) \qquad \dot{\zeta}_- = \frac{1}{\Theta^2}\left(\frac{\dot{q}_N^2}{T_-} - 1\right)$$

Θ = thermostat response time

Thermostats

Stochastic (infinite reservoirs)

Langevin, “daemon”...

$$t = t_n : \qquad \dot{q}_1 \longrightarrow \dot{q}_1 + \frac{2M}{m+M}(v - \dot{q}_1)$$

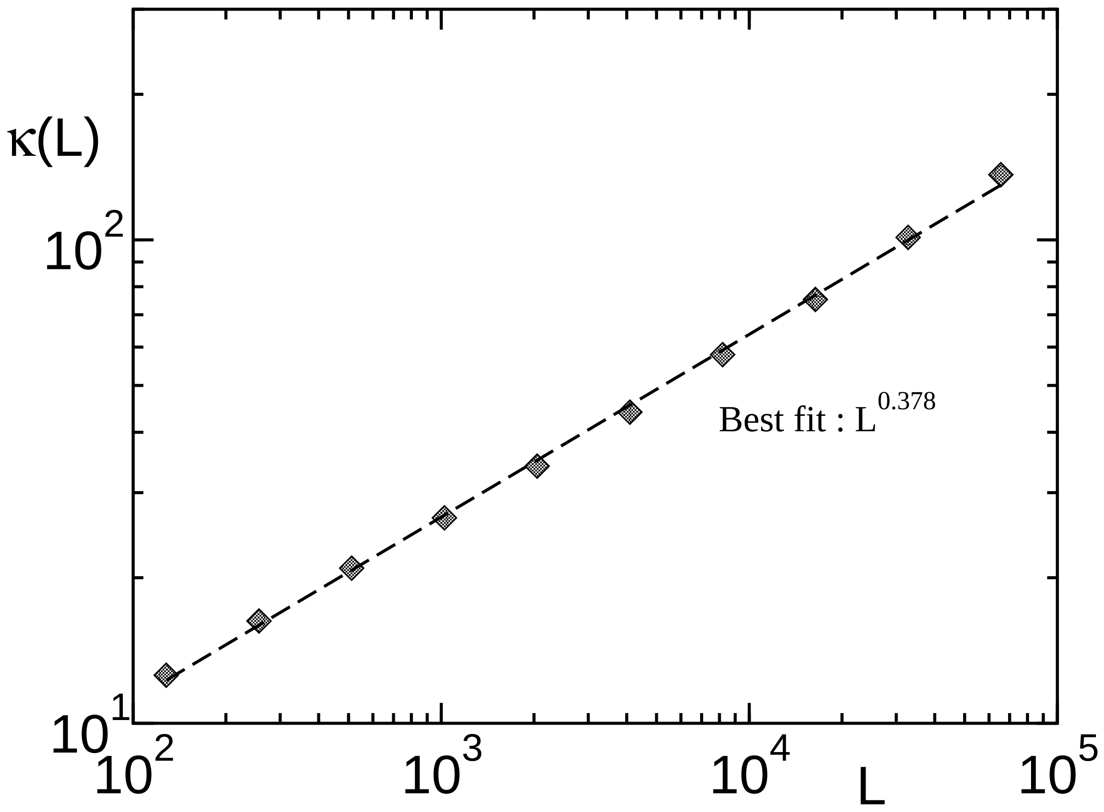
1d Maxwellian distribution:

$$P_\pm(v) = \sqrt{\frac{M}{2\pi k_B T_\pm}} \exp\left(-\frac{Mv^2}{2k_B T_\pm}\right) .$$

Anomalous transport in 1d

Diverging finite-size conductivity

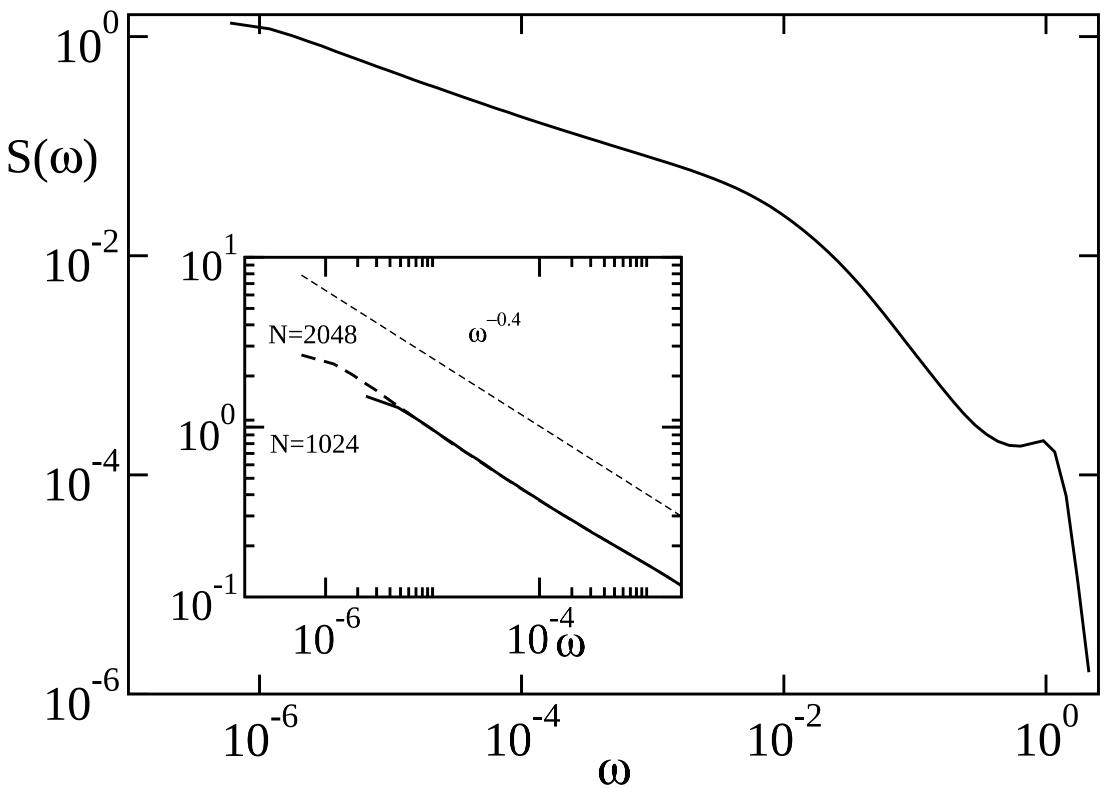
$$\kappa(L) \propto L^{\alpha}$$



Anomalous transport in 1d

Nonintegrable power-law decay of at large t:

$$\langle J(t)J(0)\rangle \propto t^{-(1+\delta)} \quad , \quad -1 < \delta < 0$$



Finite–size scaling

How to compare the two methods?

Cut–off in the Green-Kubo formula:

$$\kappa(L) \;\propto\; \int_0^{L/v_s} \langle J(\tau) J(0) \rangle \, d\tau \;\propto\; L^{-\delta}$$

v_s propagation velocity of excitations (sound waves).

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Consistency with linear response implies $\alpha = -\delta$

Survey of 1d results

Nonequilibrium MD: $\kappa(L) \propto L^{\alpha}$

Model	Reference	α
FPU-β	Lepri et al (1998)	0.37
FPU-α	Lepri (2000)	$\lesssim$ 0.44
Diatomic FPU r=2	Vassalli (1999)	0.43
Diatomic Toda r=2	Hatano (1999)	0.35-0.37
	Vassalli (1999)	0.39
Diatomic Toda r=8	Vassalli (1999)	0.44
Diatomic hard points	Hatano (1999)	0.35
	Grassberger et al. (2002)	0.32

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Equilibrium MD: $S(\omega) \; \propto \; \omega^{\delta}$

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Dynamical RG: $\alpha = -\delta = 1/3$

Mode–coupling theory: $\alpha = -\delta = -2/5$

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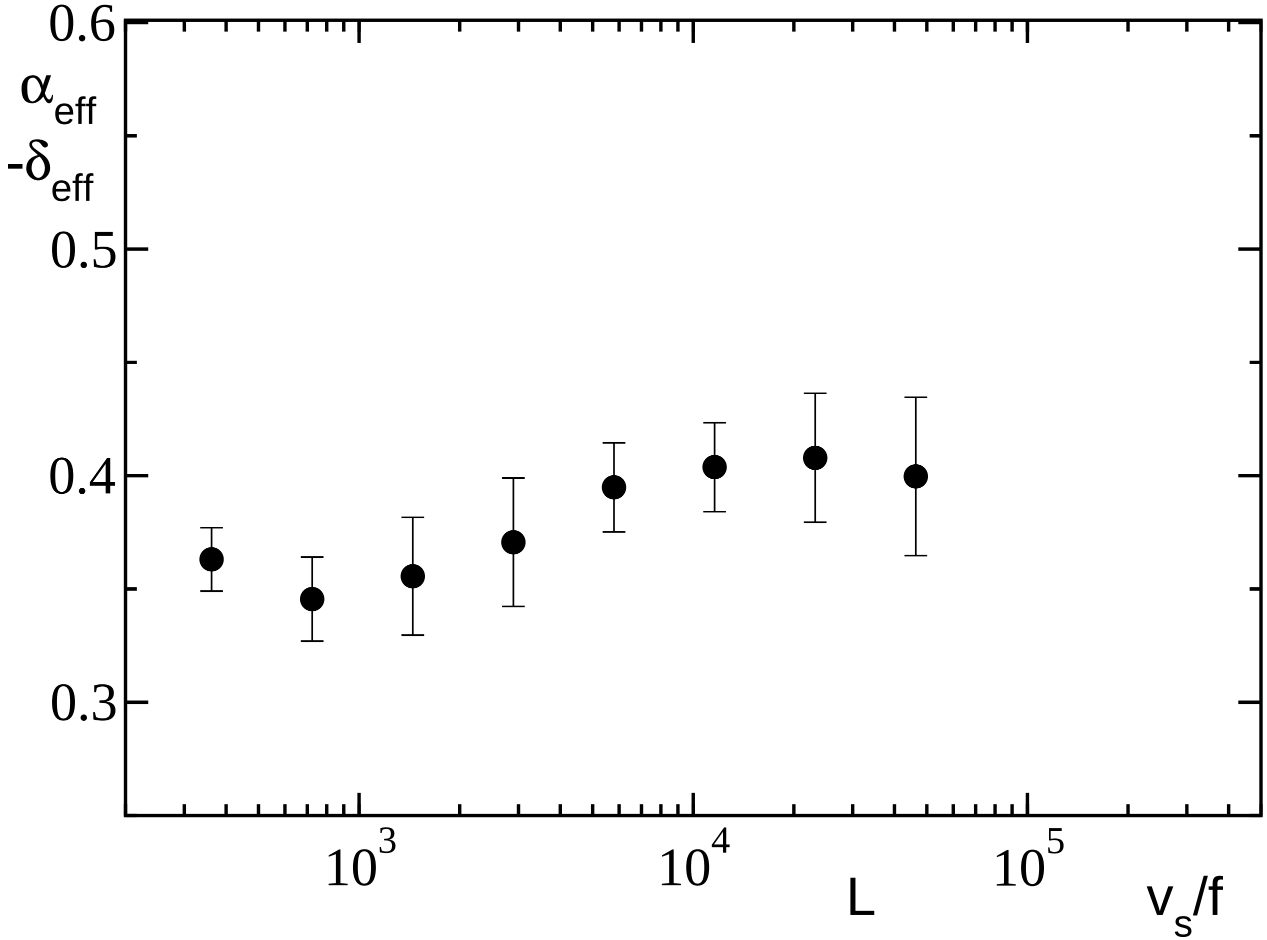
Equilibrium versus nonequilibrium

Effective exponents $\alpha_{eff}(L) = \frac{d\ln\kappa}{d\ln L}$, $\delta_{eff} = \frac{d\ln S}{d\ln\omega}$

"$T=\infty$" FPU $V(x) = x^4/4$



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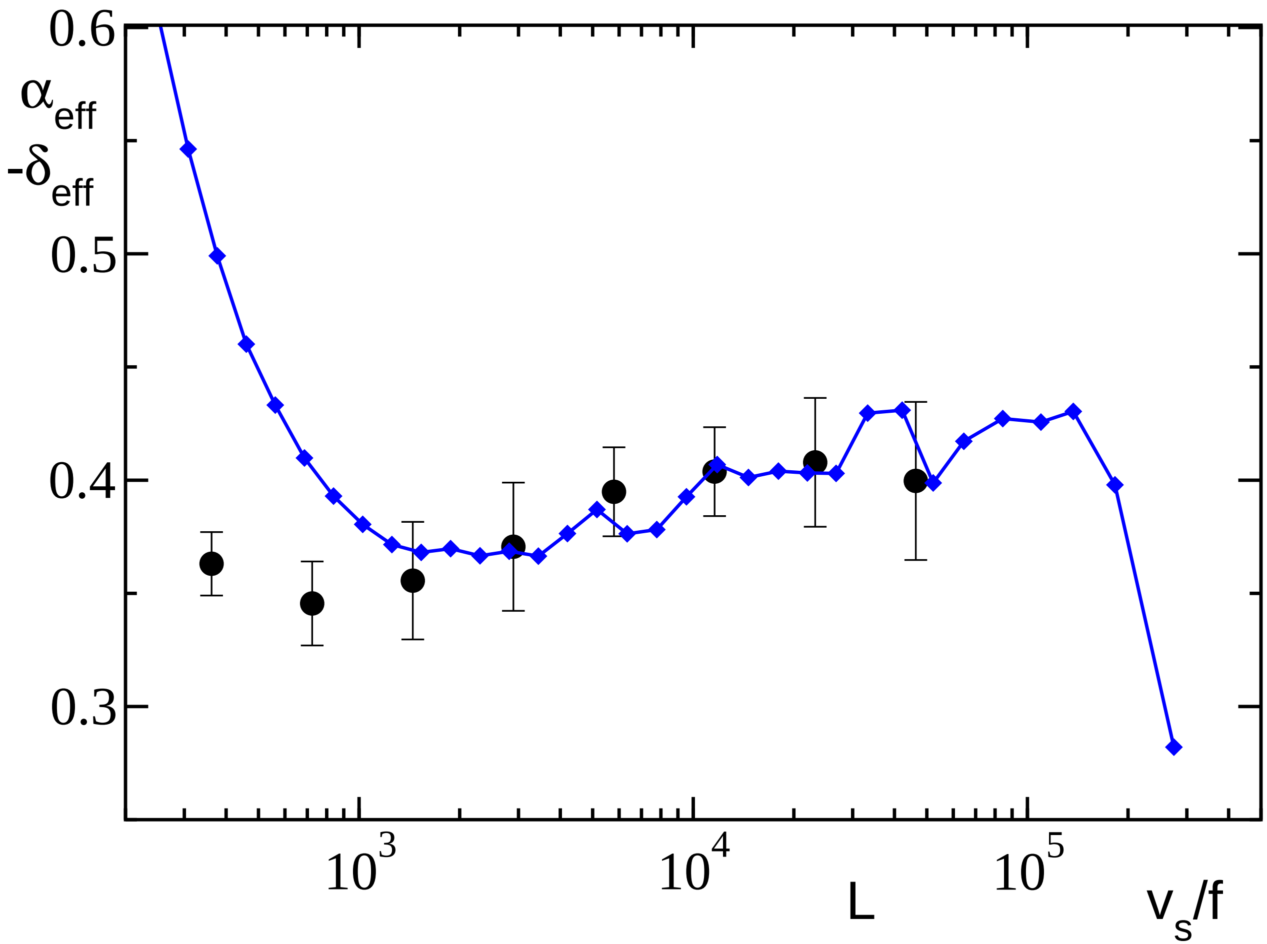

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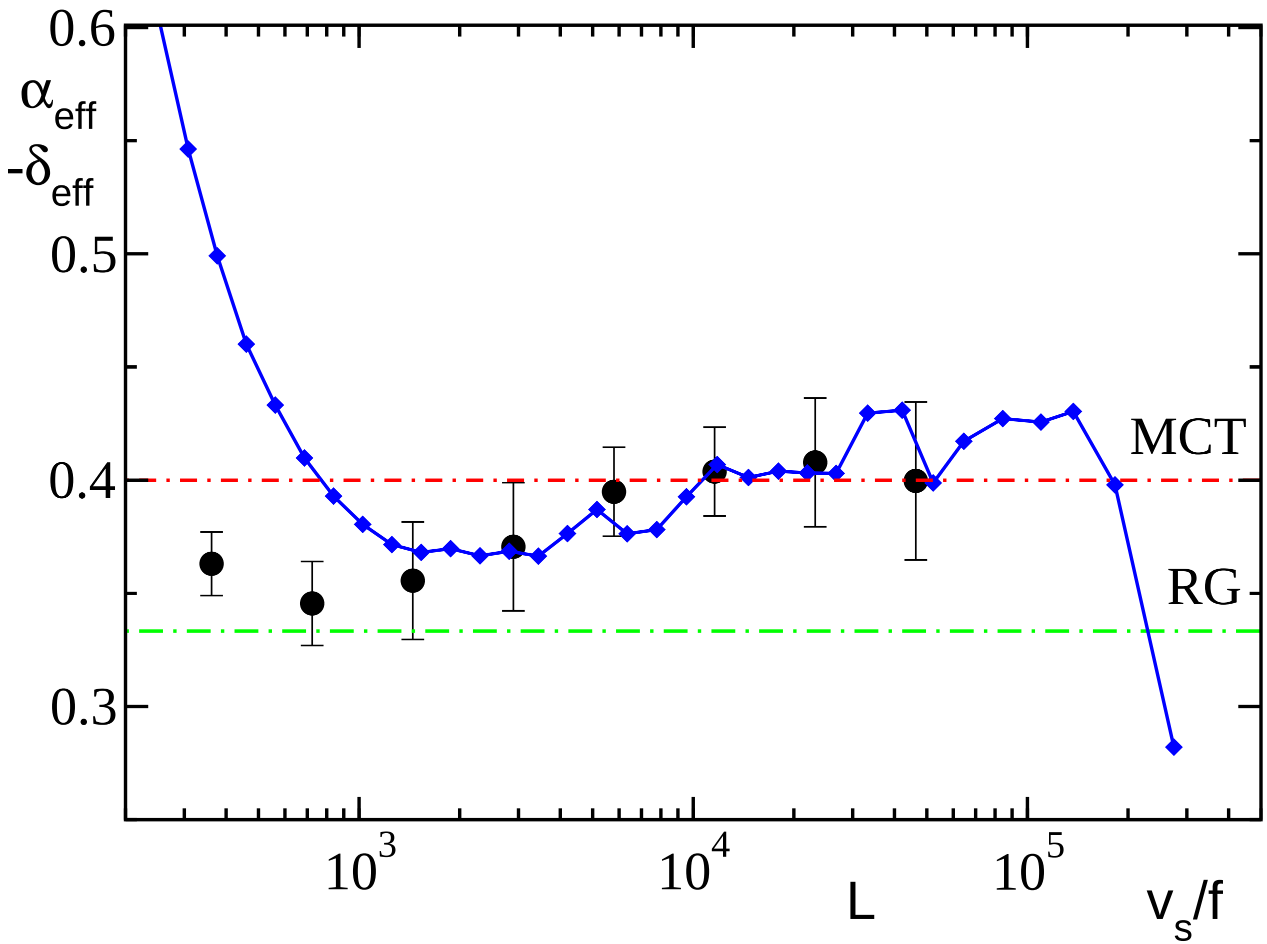
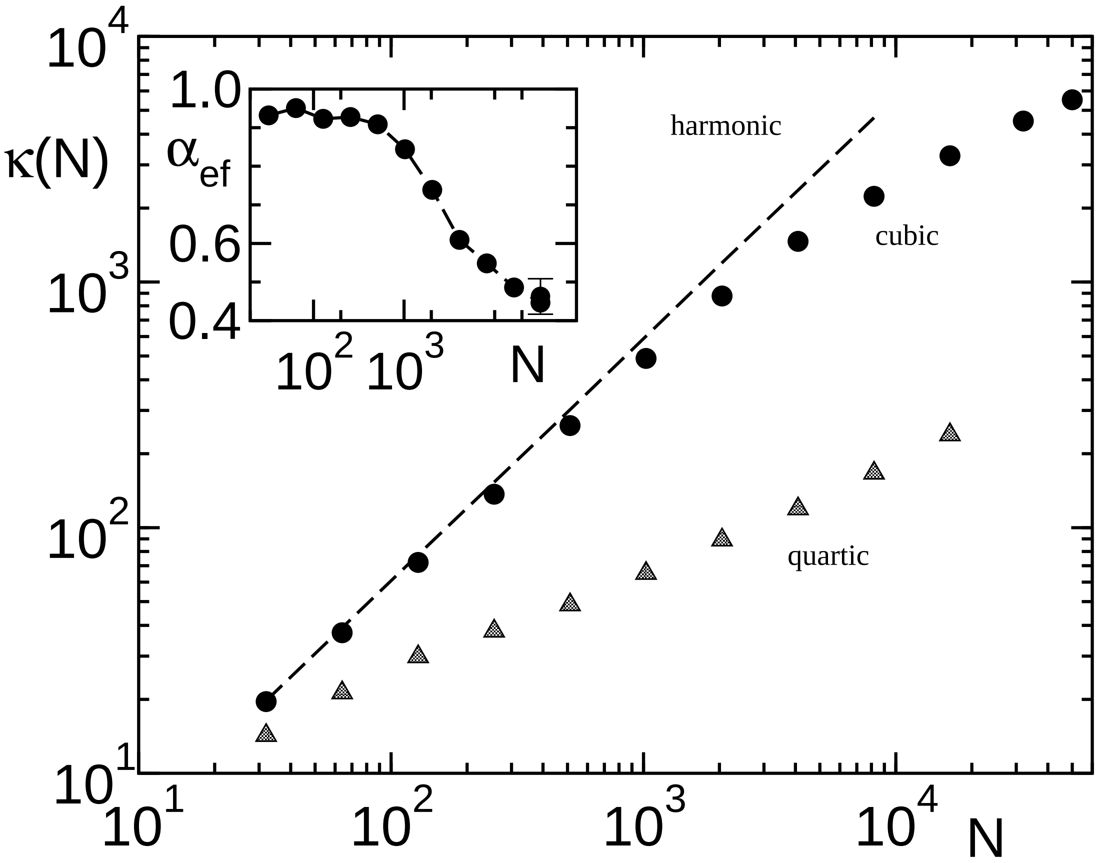


Cubic versus quartic potential

$T_+ = 1.1, T_- = 0.09$, $g = 0.25$, Nosè thermostats, fi xed boundaries



Some news

O. Narayan and S. Ramaswamy, PRL 89, 200601 (2002)
Renormalization group approach predicts

$$\alpha = (2-d)/(2+d) \quad ,\text{i.e.} \quad \alpha = 1/3 \quad \text{for} \quad d = 1$$

irrespectively of the form of the potential.

Some news

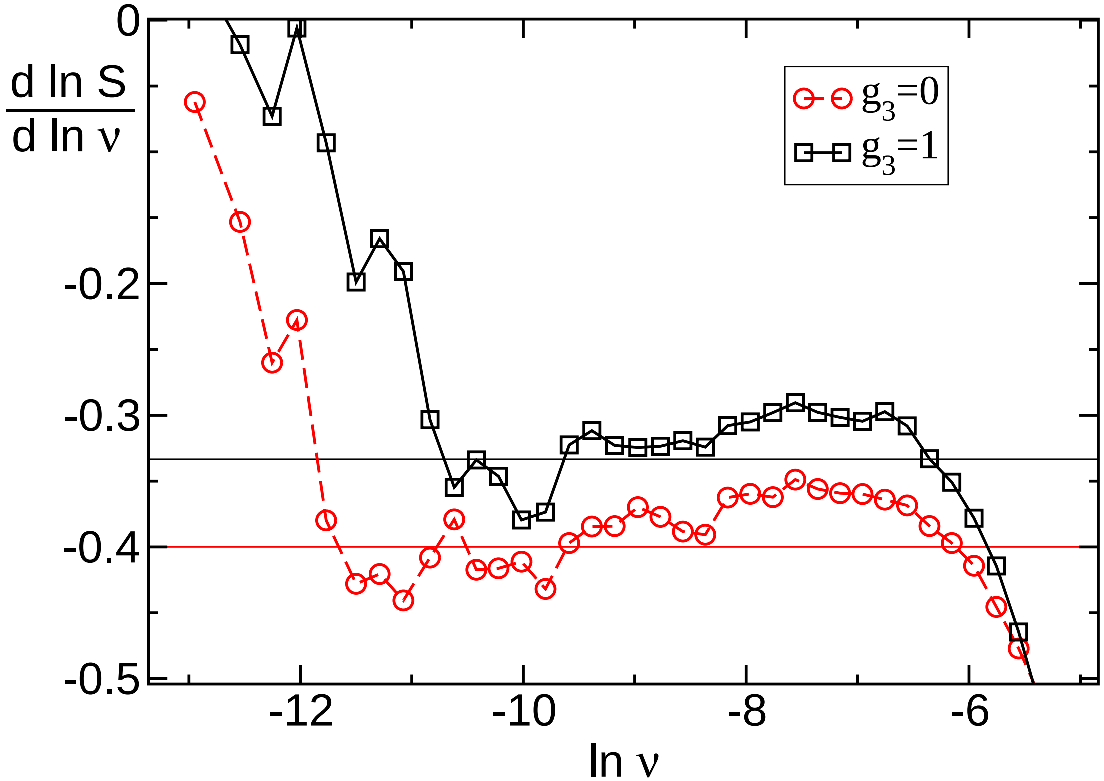
P. Cipriani, S. Denisov and A. Politi, PRL 94, 244301 (2005)

Alternate-mass hard particles 1D gas: $\alpha = 1/3$ (numerical)

Anomalous diffusion

Some news

Further results about FPU : cubic + quartic and purely quartic



Mode-Coupling revisited

with L. Delfini, S. Lepri and A. Politi

- The simplest mode-coupling equations (in dimensionless units $a = m = g_2 = 1$)

$$\ddot{G}(q,t) + \int_0^t \Gamma(q,t-s)\dot{G}(q,s)\,ds + \omega^2(q)G(q,t) \;=\; 0$$

$$\Gamma(q,t) = \epsilon\,\omega^2(q)\int_{-\pi}^{\pi} dp\,G(p,t)G(q-p,t)$$

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- Initial conditions: $G(q,0) = 1$ and $\dot{G}(q,0) = 0$.
- $\omega(q)$ is the *bare* dispersion relation (sound velocity $c = 1$)

$$\omega(q) \;=\; 2\,|\sin\frac{q}{2}|$$

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- The approximate expression of the memory kernel for a monoatomic chain of atoms interacting with a nearest-neighour cubic potential $x^2/2 + g_3 x^3/3$ through the projection method.
- The coupling constant is

$$\epsilon = \frac{3g_3^2 k_B T}{2\pi}$$

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- As a consequence of linear response theory this implies

$$\kappa \;\sim\; L^{\frac{1}{3}}$$

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- Quartic leading nonlinearity

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- Analytic solution yields

$$\kappa \;\sim\; L^{\frac{1}{2}}$$

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- Heat conductivity divergence exponent $\sim 1 - \gamma$

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  - 2) Purely quartic FPU model: $\omega = \alpha = 0 \;\; \beta = 1$,
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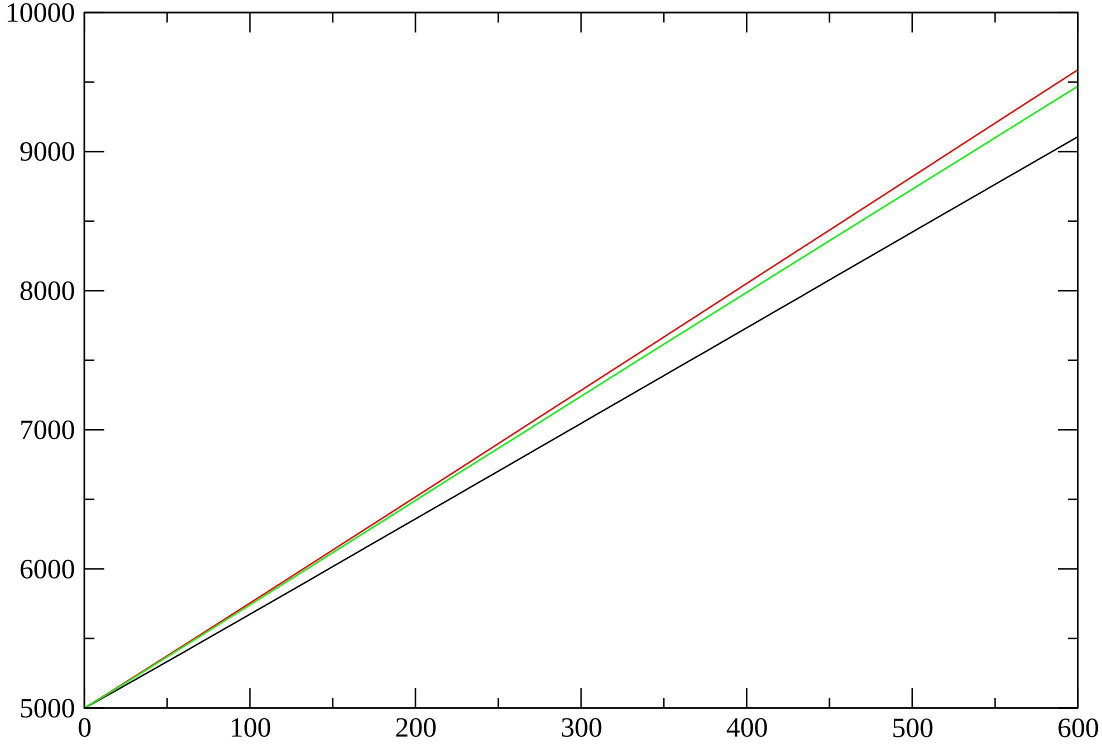
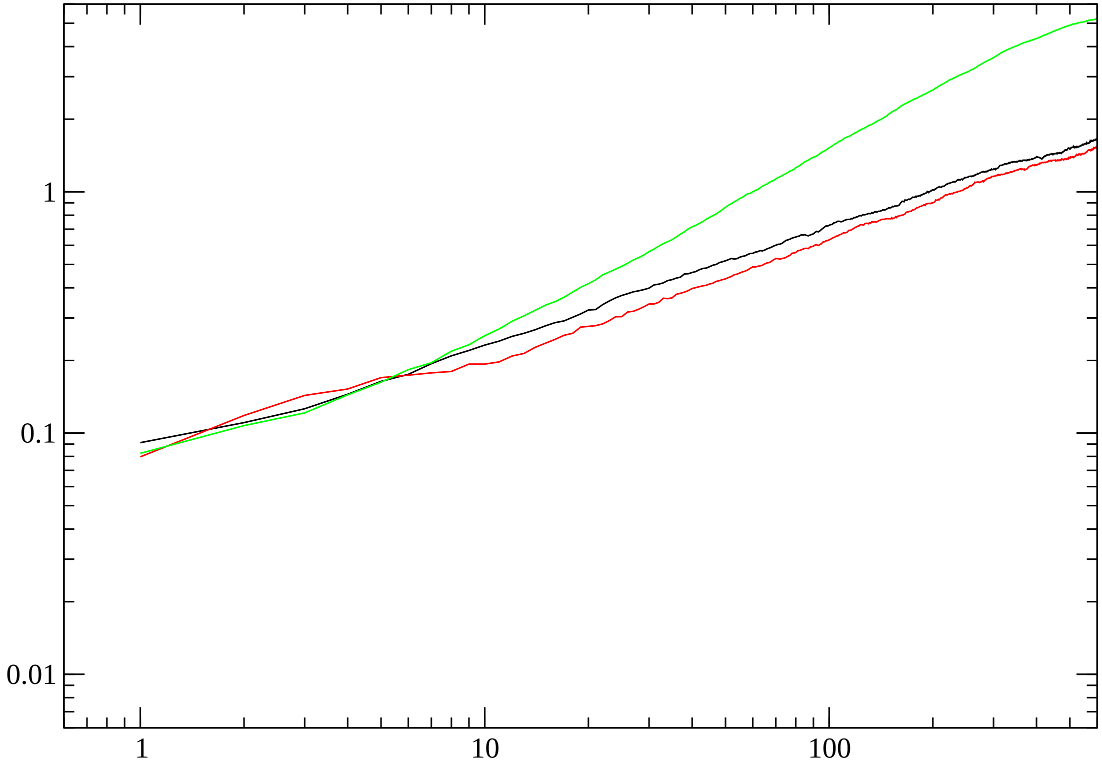
Average front displacement: speed of sound



... Finite Amplitude Perturbations

Square root of the mean square displacement

Cases 1) and 2) $\gamma \approx \frac{1}{2}$; case 3) $\gamma \approx 0.7$



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- Nonlinear excitations

S. Lepri, R. L., A. Politi, *Phys. Rep.* 377, 1 (2003)