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
Modeling stationary energy transport

- Minimal, nonperturbative model
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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
Simulating lattice heat transport

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**Equilibrium MD:** correlation of the heat flux $J$

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

Microscopic expression (in 1d):

$$J = \frac{a}{2} \sum_{n} (\dot{q}_{n+1} + \dot{q}_n) V'(q_{n+1} - q_n)$$
Simulating lattice heat transport

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

Deterministic (Gauss’ principle)
Nosé-Hoover, isokinetic, Evans...

\[
\ddot{q}_1 = -\zeta_+ \dot{q}_1 + \ldots \quad \ddot{q}_N = -\zeta_- \dot{q}_N + \ldots
\]

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

\(\Theta = \text{thermostat response time}\)
Stochastic (infinite reservoirs)
Langevin, “daemon”...

\[ t = t_n : \quad \dot{q}_1 \rightarrow \dot{q}_1 + \frac{2M}{m + M} (v - \dot{q}_1) \]

1d Maxwellian distribution:

\[ P_\pm(v) = \sqrt{\frac{M}{2\pi k_B T_\pm}} \exp \left( -\frac{M v^2}{2k_B T_\pm} \right). \]
Anomalous transport in 1d

Diverging finite-size conductivity

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

![Graph showing the relationship between \(\kappa(L)\) and \(L\)].

Best fit: \(L^{0.378}\)
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).
Finite–size scaling

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Consistency with linear response implies $\alpha = -\delta$
## Survey of 1d results

Nonequilibrium MD: \( \kappa(L) \propto L^\alpha \)

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## Survey of 1d results

### Nonequilibrium MD:

\[ \kappa(L) \propto L^\alpha \]

### 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 \( \alpha_{\text{eff}}(L) = \frac{d \ln \kappa}{d \ln L} \), \( \delta_{\text{eff}} = \frac{d \ln S}{d \ln \omega} \)

“\( T = \infty \)” FPU \( V(x) = x^4/4 \)
Equilibrium versus nonequilibrium

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Heat transport in low-dimensional systems – p. 9/19
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"\( T = \infty \)" FPU \( V(x) = x^4 / 4 \)
Cubic versus quartic potential

\[ T_+ = 1.1, T_- = 0.09, g = 0.25, \text{ Nosè thermostats, fixed boundaries} \]
Renormalization group approach predicts  
\[ \alpha = \frac{(2 - d)}{(2 + d)} \text{, i.e. } \alpha = \frac{1}{3} \text{ for } d = 1 \]  
irrespectively of the form of the potential.
Some news

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

Further results about FPU: cubic + quartic and purely quartic

\[
\frac{d \ln S}{d \ln \nu}
\]

- For \( g_3 = 0 \)
- For \( g_3 = 1 \)

Heat transport in low-dimensional systems – p. 11/19
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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\( \omega(q) \) is the bare dispersion relation (sound velocity \( c = 1 \))

\[
\omega(q) = 2 \left| \sin \frac{q}{2} \right|
\]
The equation consider only the coupling among sound modes (conservation of density and momentum).
... Mode-Coupling revisited

- The equation consider only the coupling *among sound modes* (conservation of density and momentum).

- The approximate expression of the memory kernel for a monoatomic chain of atoms interacting with a nearest-neighbour cubic potential \( x^2/2 + g_3x^3/3 \) through the projection method.
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- The equation consider only the coupling *among sound modes* (conservation of density and momentum).
- The approximate expression of the memory kernel for a monoatomic chain of atoms interacting with a nearest-neighbour cubic potential \( x^2/2 + g_3 x^3 / 3 \) through the projection method.
- The coupling constant is

\[
\epsilon = \frac{3g_3^2 k_B T}{2\pi}
\]
Numerical integration suggests multiscale analysis
... Mode-Coupling revisited

- Numerical integration suggests multiscale analysis
- Analytic solution

\[ \Gamma(q, t) \propto q^2 e^{icqt} + e^{-icqt} / t^{2/3} \]
... Mode-Coupling revisited

- Numerical integration suggests multiscale analysis
- Analytic solution

\[ \Gamma(q, t) \propto q^2 e^{icqt} + e^{-icqt} \]

- As a consequence of linear response theory this implies

\[ \kappa \sim L^{1/3} \]
... Mode-Coupling revisited

- Quartic leading nonlinearity

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

\[
\Gamma(q, t) = \epsilon \omega^2(q) \int_{-\pi}^{\pi} dp' \int_{-\pi}^{\pi} dp \, G(p, t) G(p', t) G(q - p - p', t)
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- Analytic solution yields

\[ \kappa \sim L^{\frac{1}{2}} \]
Finite Amplitude Perturbations

Propagation of localized fronts in nonlinear chains
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- average displacement: $\langle x \rangle \sim t$
Finite Amplitude Perturbations

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  average displacement: $\langle x \rangle \sim t$

  mean square displacement: $\langle \delta x^2 \rangle^{\frac{1}{2}} \sim t^\gamma$
Finite Amplitude Perturbations

- Propagation of localized fronts in nonlinear chains
- average displacement: $\langle x \rangle \sim t$
- mean square displacement: $\langle \delta x^2 \rangle^{\frac{1}{2}} \sim t^\gamma$
- Heat conductivity divergence exponent $\sim 1 - \gamma$
Finite Amplitude Perturbations

FPU model \( \omega x^2 + \alpha x^3 + \beta x^4 \);
...Finite Amplitude Perturbations

- FPU model \( \omega x^2 + \alpha x^3 + \beta x^4 \);

- Cases:
  1) FPU \( \beta \) model: \( \omega = \beta = 1 \ \alpha = 0 \),
  2) Purely quartic FPU model: \( \omega = \alpha = 0 \ \beta = 1 \),
  3) Complete FPU model: \( \omega = \alpha = \beta = 1 \)
...Finite Amplitude Perturbations

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... Finite Amplitude Perturbations

Average front displacement: speed of sound
Square root of the mean square displacement
Cases 1) and 2) $\gamma \approx \frac{1}{2}$; case 3) $\gamma \approx 0.7$
Conclusions & Perspectives

- Correlations in $d \leq 2$ leads to anomalous energy transport
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- Control of finite-size effects in numerical simulations
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