Anomalous heat conduction in anharmonic chains with space-reversal symmetry

Yuki Minami (Gifu Univ.)

Collaboration with H. Nakano (Tokyo univ.) and K. Saito (Kyoto univ.)

Introduction

- Anomalous heat conduction in low dimensions

  heat conductivity $\kappa \to \infty$ in system size $L \to \infty$

- Theoretically discussed since the 70s

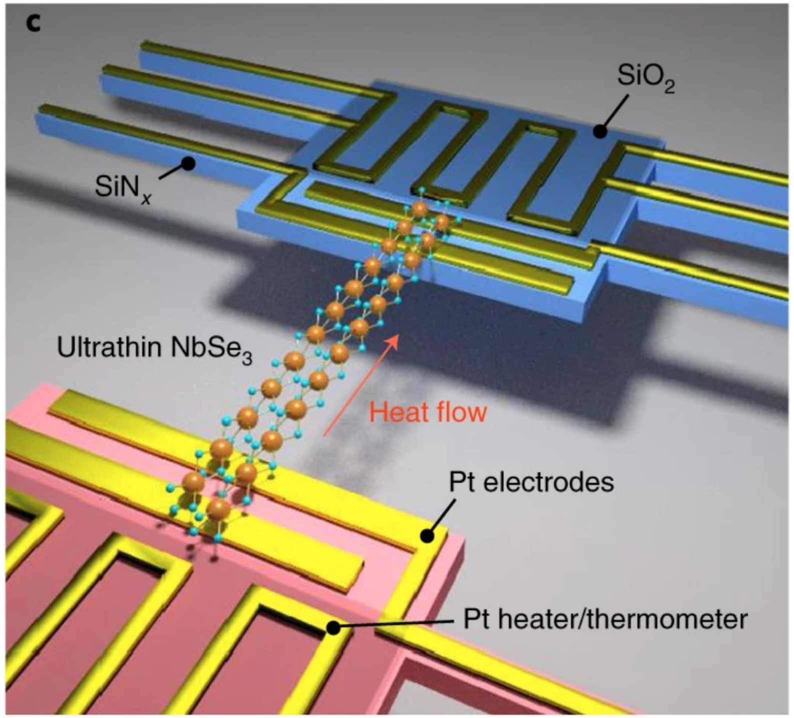
- Becomes possible to experiment in recent years

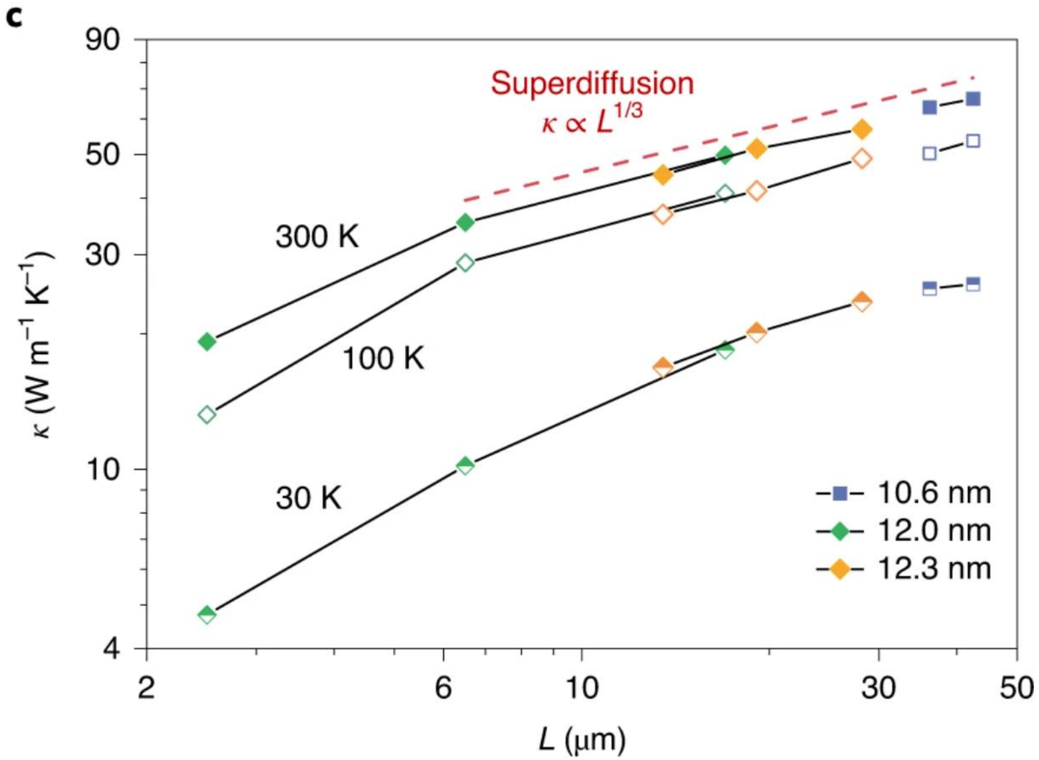
Nanowire

- Pseudo 1D system: Length~μm >> Diameter~nm

$$\kappa \sim L^{1/3}$$

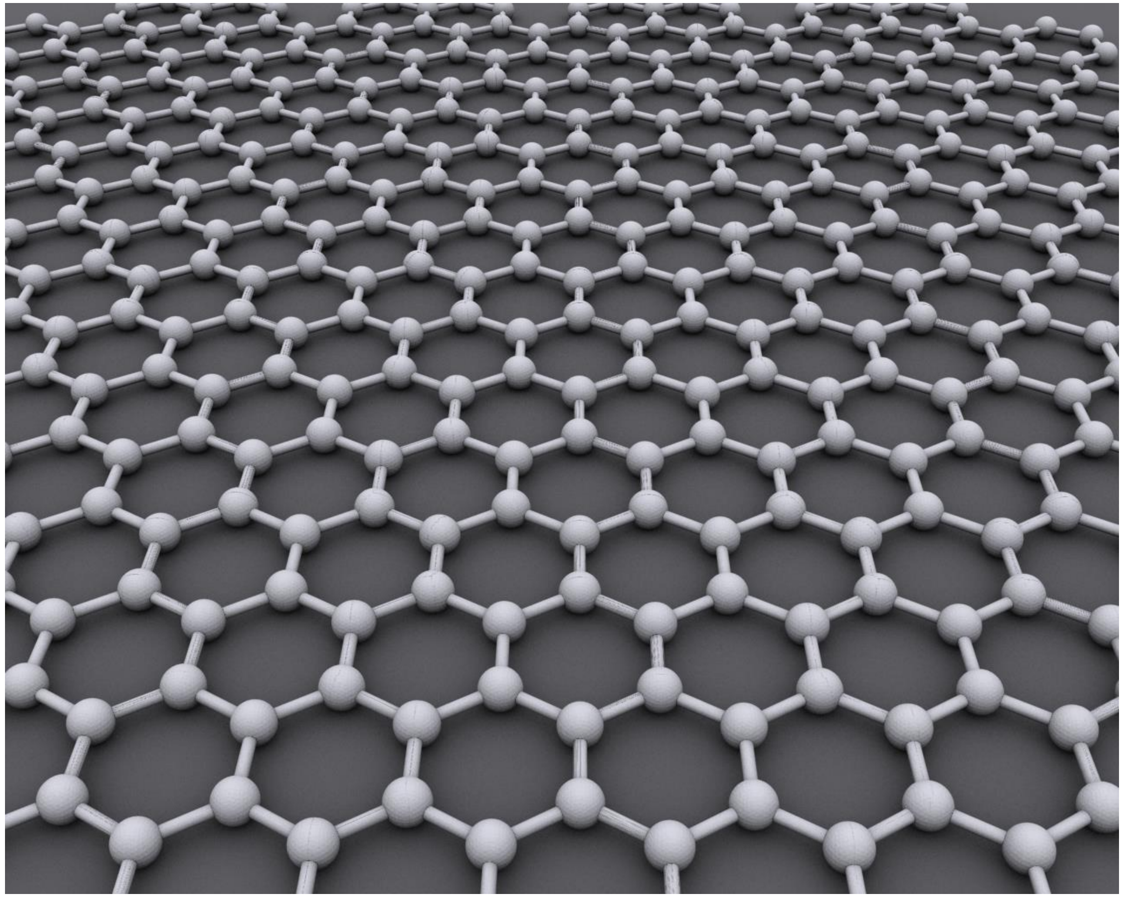
Experiment: L. Yang, et.al., Nature nanotechnology (2021)





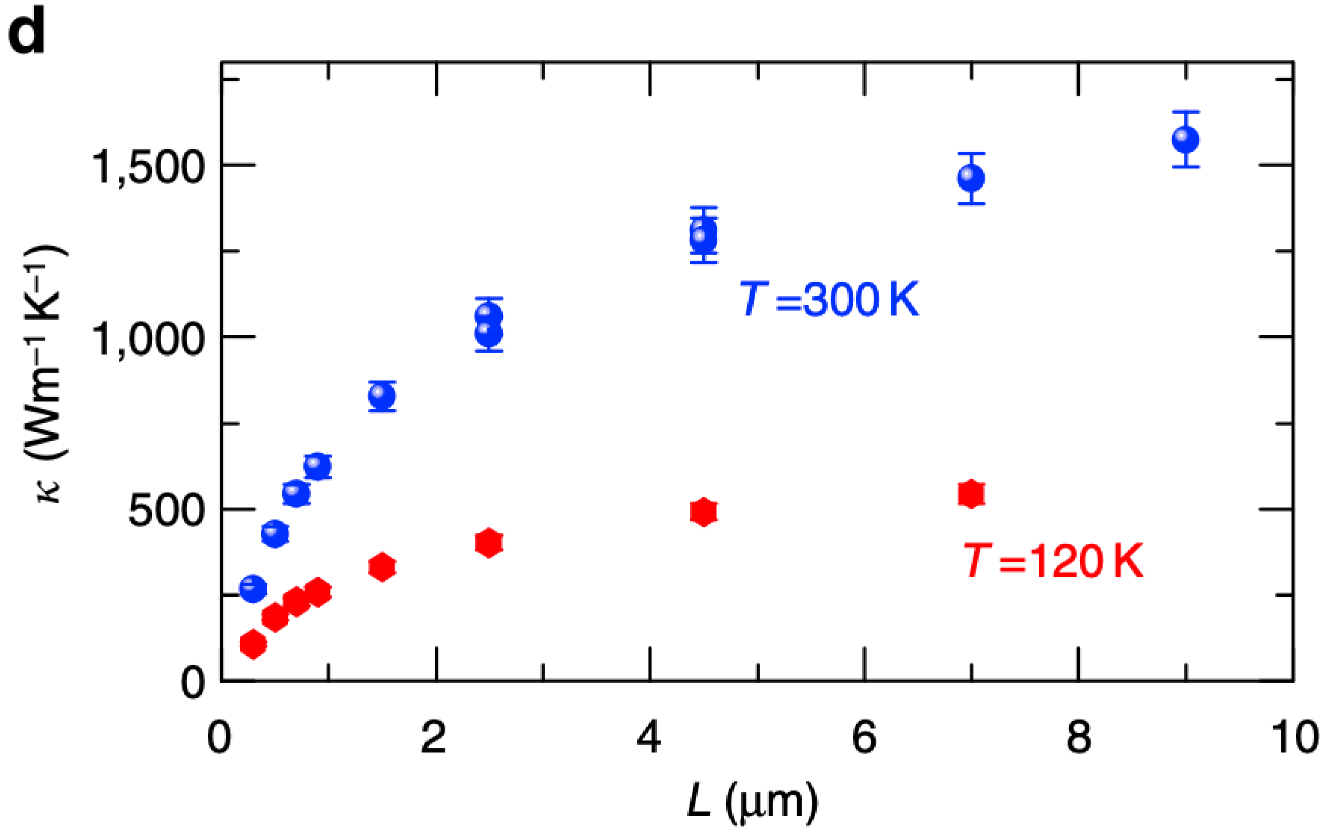
Graphene

- 2D lattice



Heat conductivity of Graphene

Experiment: X. Xu, et.al. Nature Communications(2014)

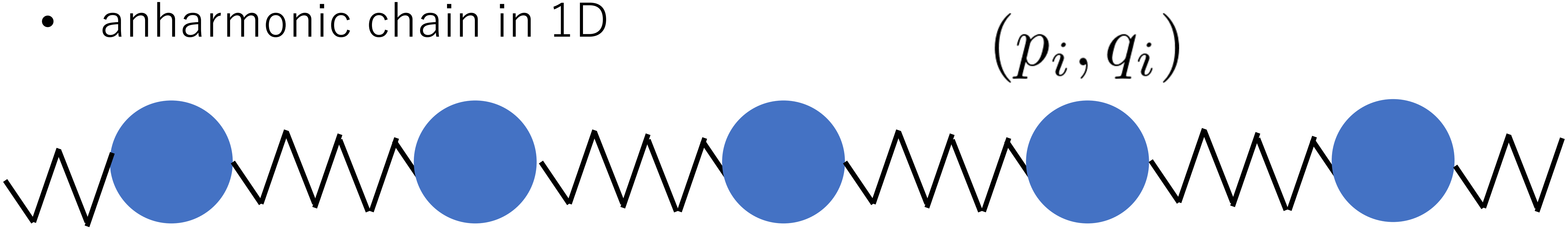


$$\kappa \sim \log L$$

Theory for anharmonic chain

Spohn, J. stat. mech(2014); arXiv:1505.05987v2 [cond-mat.stat-mech]

- anharmonic chain in 1D



Hamiltonian:

$$H = \sum_i \left[\frac{p_i^2}{2m} + V(q_{i+1} - q_i) \right],$$

Example:

$$V(x) = ax^2 + bx^3 + cx^4,$$

Fluctuating hydrodynamics (FHD)

Hydrodynamic variables: energy e, momentum g, stretch l

For $V(x) \neq V(-x)$ and nonzero pressure $P \neq 0$

Dissipation

Conservative noise

$$\partial_t e - \partial_x \left(\underline{-D_e \partial_x e - D_{el} \partial_x l} + Pg + \underline{(\partial_l P) lg + (\partial_e P) eg} \right) = \underline{\xi_e},$$

$$\partial_t g - \partial_x \left(\underline{-D_g \partial_x g} + (\partial_l P) l + (\partial_l P) e + \underline{\frac{1}{2}(\partial_l^2 P) l^2 + \cdots} \right) = \underline{\xi_g},$$

Nonlinear terms

$$\partial_t l - \partial_x g = 0,$$

EOM of Normal modes

Diagonalize

$$(e, g, l) \to (\phi^+, \phi^-, \phi^0)$$

Sound mode

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + \lambda_1 \partial_x(\phi^\sigma \phi^\sigma) + \underline{\lambda_2 \partial_x(\phi^0 \phi^\sigma) + \cdots} = \xi^\sigma,$$

Cross terms

heat mode

$$\sigma = \pm,$$

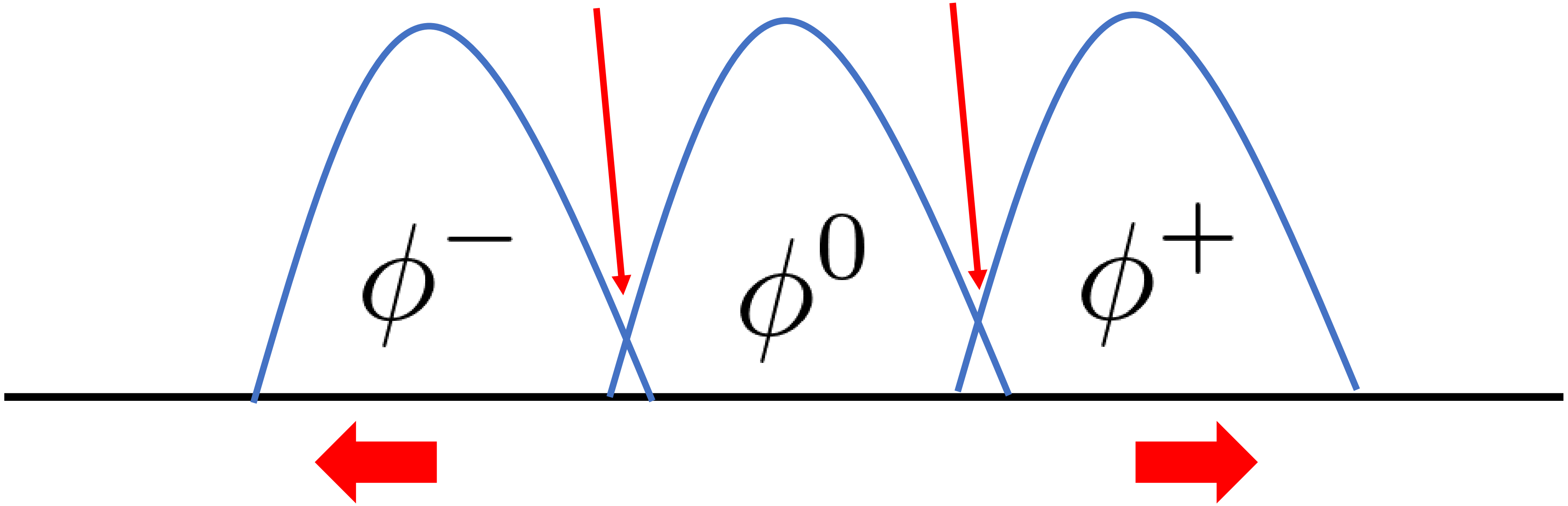
$$(\partial_t - D_0 \partial_x^2)\phi^0 + \sum_\sigma \sigma \lambda \partial_x(\phi^\sigma \phi^\sigma) = \xi^0,$$

Spohn's argument

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + \lambda_1 \partial_x(\phi^\sigma \phi^\sigma) + \lambda_2 \partial_x(\phi^0 \phi^\sigma) + \cdots = \xi^\sigma,$$

Neglect all cross terms

Overlap will be small in long-time limit



Burgers eq. with sound velocity

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + \lambda_1 \partial_x(\phi^\sigma \phi^\sigma) = \xi^\sigma,$$

KPZ class

$$\langle \phi^\sigma(x + \sigma c_s t, t)\phi^\sigma(x, 0)\rangle \sim t^{-1/z},$$

$$z = 3/2,$$

Exponents of heat conductivity and current

Energy current:

$$J_e \propto \phi^\sigma \phi^\sigma \qquad \langle J_e(t) J_e \rangle \sim t^{1/z},$$

Heat conductivity:

$$\kappa \sim \int_0^{L/c_s} dt \langle J_e(t) J_e \rangle \sim L^{1-1/z}, \quad z = 3/2,$$

consistent with the Nanowire experiment

with Space-reversal symmetry

There is discrepancy to observed exponent

For even potential and zero pressure

$$V(x) = V(-x), \qquad P = 0,$$

Distribution function

$$P_{eq}(q) = \frac{1}{Z}\exp\left[-\beta\sum_i\Big(V(q_{i+1}-q_i)+Pq_i\Big)\right],$$

$$P_{eq}(q) = P_{eq}(-q),$$

Some interactions vanish by reversal symmetry

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + \underline{\lambda_1 \partial_x (\phi^\sigma \phi^\sigma)} + \lambda_2 \partial_x (\phi^0 \phi^\sigma) \underline{+ \cdots} = \xi^\sigma,$$

=0

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + 2\sigma\lambda \partial_x (\phi^0 \phi^\sigma) = \xi^\sigma,$$

$$(\partial_t - D_0 \partial_x^2)\phi^0 + \sum_\sigma \sigma\lambda \partial_x (\phi^\sigma \phi^\sigma) = \xi^0,$$

Spohn's argument

No Diagonal term

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + \underline{2\sigma\lambda\phi^0\phi^\sigma} = \eta^\sigma,$$

Still Neglect cross term
(super rough approximation!)

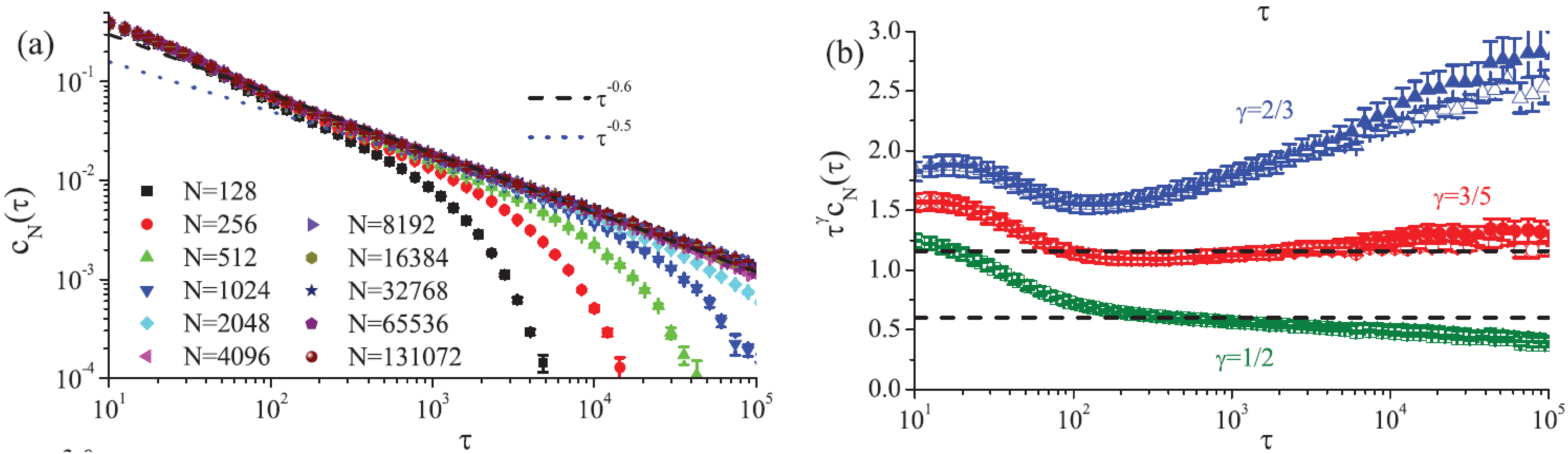
Linear equation→ trivial exponent z=2

Nontrivial exponent from MD

L. Wang, L. Xu, and H. Zhao, Phys. Rev. E **91**, 012110 (2015)

Even potential $V(x)=\frac{1}{4}x^4$ and zero pressure

Energy current correlation $c_N(\tau)=\frac{1}{k_B T^2 N}\langle J(t)J(t+\tau)\rangle \sim \tau^{-0.6}$



Current status

	Observed exponent	Spohn
Without space reversal symmetry	~2/3	2/3
With reversal symmetry	~0.6	1/2

No accountable analysis

What we do

- Wilson Renormalization Group (RG) of Spohn's FHD

- Numerical simulation

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + 2\sigma\lambda\partial_x(\phi^0\phi^\sigma) = \xi^\sigma,$$

$$(\partial_t - D_0\partial_x^2)\phi^0 + \sum_\sigma \sigma\lambda\partial_x(\phi^\sigma\phi^\sigma) = \xi^0,$$

Wilson RG

Integrate out the component in the wavenumber shell

$$\phi^{\alpha}(k) \quad \text{in} \quad \Lambda - \delta\Lambda \leq |k| \leq \Lambda,$$

⬇

RG eq. for parameters

$$-\Lambda \frac{\partial \lambda}{\partial \Lambda} = \cdots, \qquad -\Lambda \frac{\partial D_s}{\partial \Lambda} = \cdots,$$

Path integral action

Free part:

$$I_0 = \frac{1}{2}\int dtdx \begin{pmatrix}\phi^\alpha & \pi^\alpha\end{pmatrix} \begin{pmatrix} 0 & G_A^{-1} \\ G_R^{-1} & -2D_\alpha\partial_x^2 \end{pmatrix} \begin{pmatrix}\phi^\alpha \\ \pi^\alpha\end{pmatrix},$$

π^α : Auxiliary field

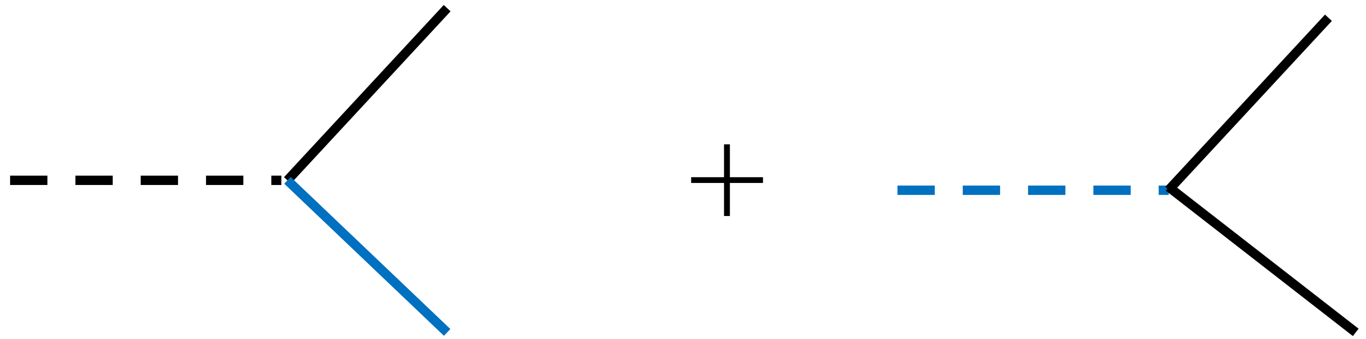
Inverse of Green function:

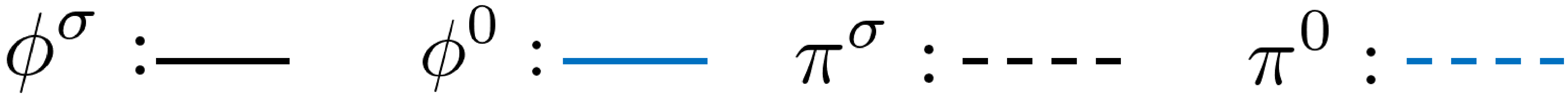
$$G_{R,A}^{-1} = \pm(\partial_t + \alpha c_s \partial_x) - D_\alpha \partial_x^2$$

Interactions and diagram

$$I_{int} = \int dxdt \left[\lambda \sigma \pi^{\sigma} \partial_x (\phi^0 \phi^{\sigma}) + 2\lambda \sigma \pi^0 \partial_x (\phi^{\sigma} \phi^{\sigma}) \right],$$

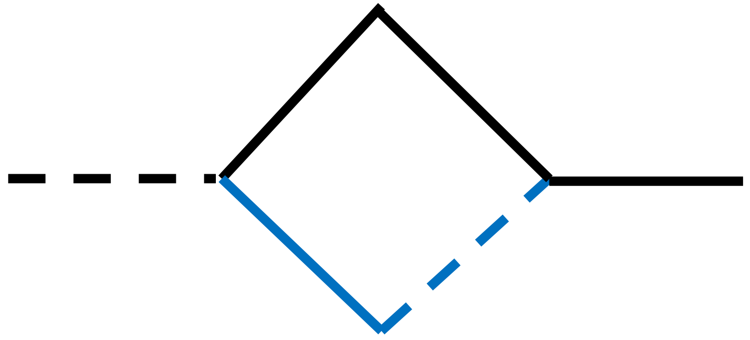
Two vertices:

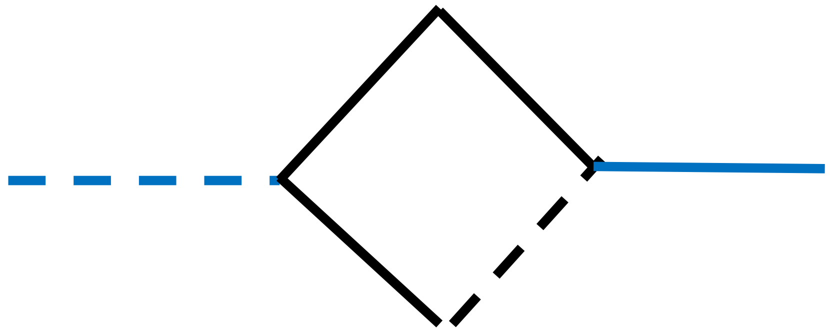




Self energy and vertex correction

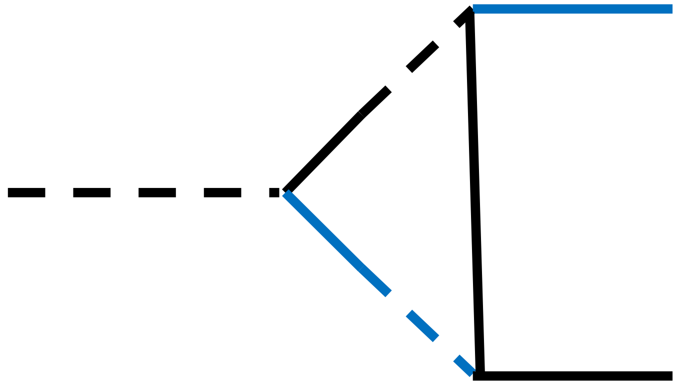
Selfe energy

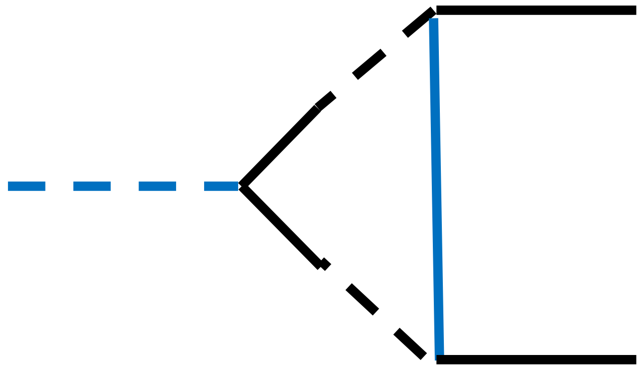




Vertex correction

More diagrams appear





RG equation at 1-loop calculation

$$-\Lambda \frac{\partial \lambda}{\partial \Lambda} =$$ [redacted]

$$-\Lambda \frac{\partial c_s}{\partial \Lambda} =$$ [redacted]

$$-\Lambda \frac{\partial D_0}{\partial \Lambda} = D_0$$ [redacted]

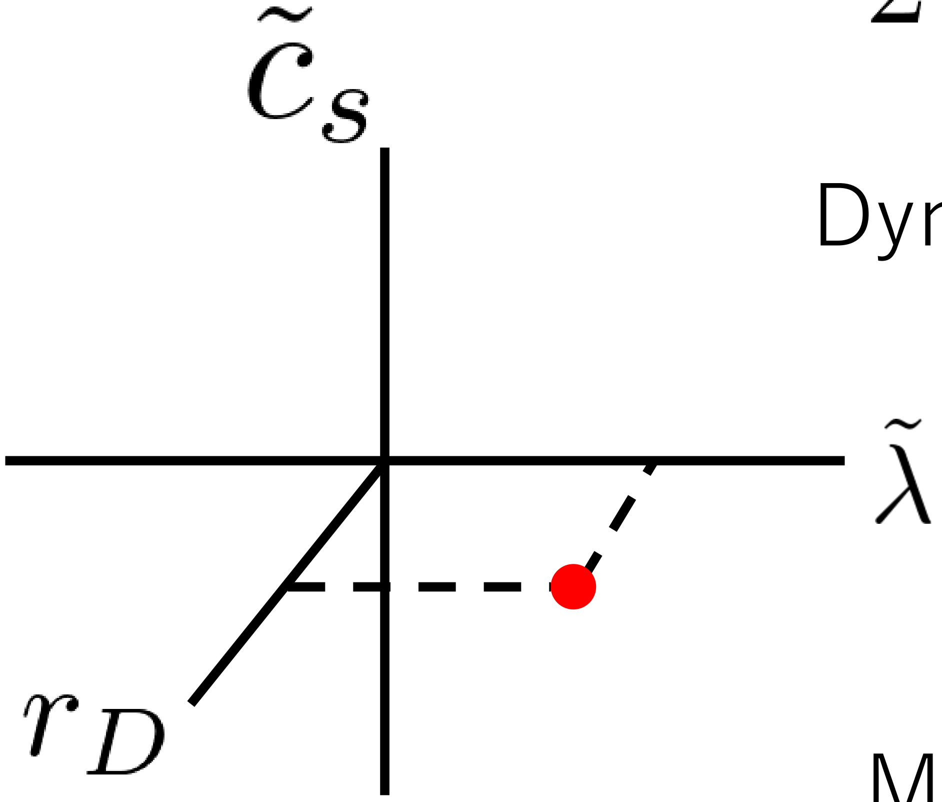
$$-\Lambda \frac{\partial D_s}{\partial \Lambda} = D_s$$ [redacted]

Dimensionless parameters:

$$\tilde{\lambda^2} = \frac{\lambda^2}{\pi D_s^2 \Lambda}, \quad \tilde{c}_s = \frac{c_s}{D_s \Lambda}, \quad r_D = \frac{D_0}{D_s},$$

Nontrivial Fixed point and exponent

$$\tilde{\lambda}^* = \frac{1}{2}, \quad r_D^* = 1, \quad \tilde{c} = 0$$



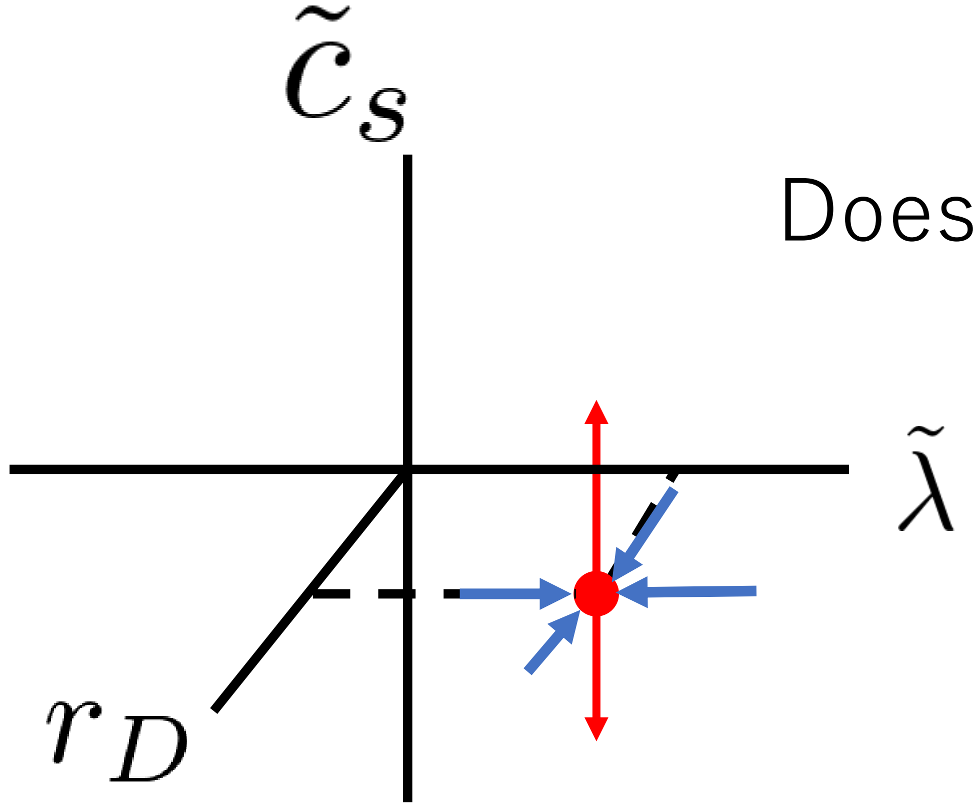
Dynamic exponent $z = \frac{3}{2}$,

$$\langle J_e(t) J_e \rangle \sim t^{-0.66},$$

MD result: $t^{-0.6}$

Parameter flow around fixed point

- Repulsive along sound velocity



Does scaling depend on sound velocity?

Numerical simulation of FHD

$$(\partial_t + \sigma c_s \partial_x - D_s \partial_x^2)\phi^\sigma + 2\sigma\lambda\partial_x(\phi^0\phi^\sigma) = \xi^\sigma,$$

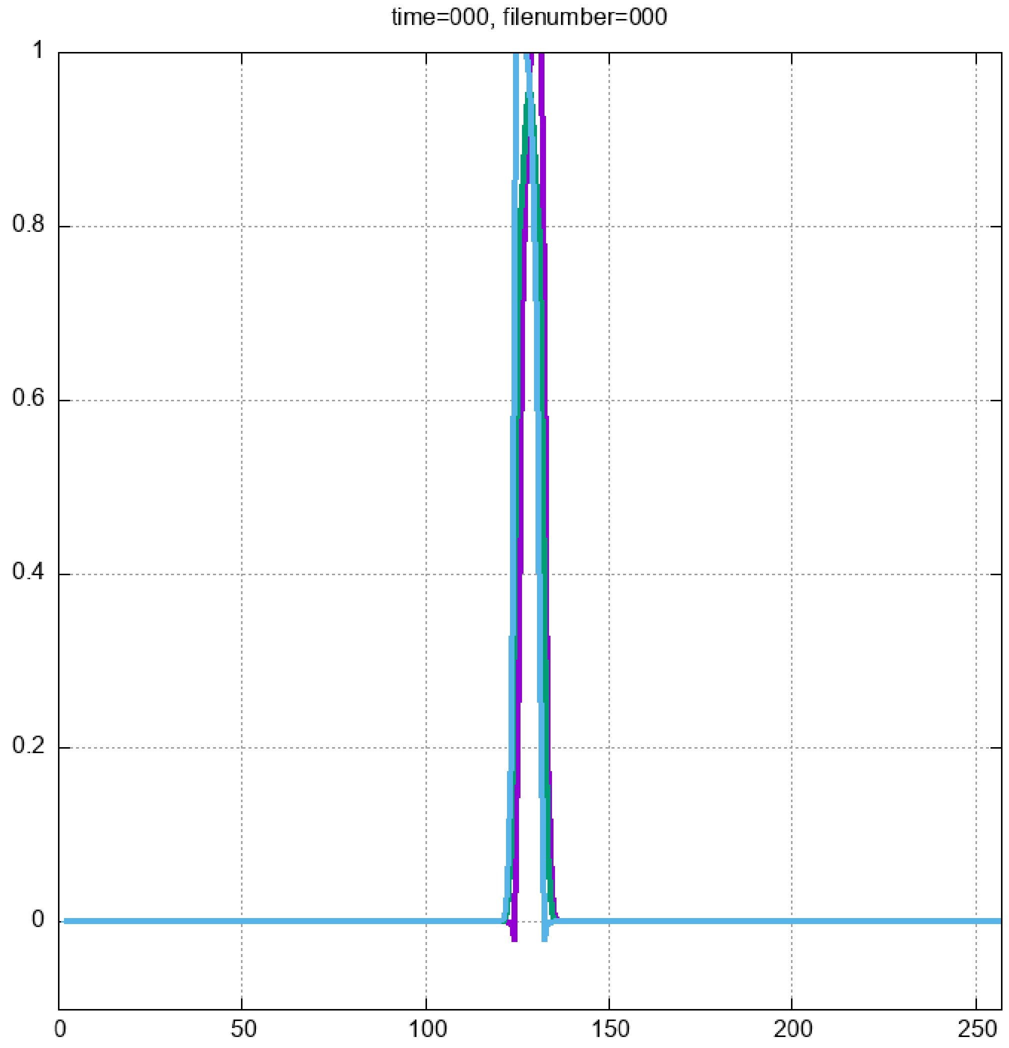
$$(\partial_t - D_0 \partial_x^2)\phi^0 + \sum_\sigma \sigma\lambda\partial_x(\phi^\sigma\phi^\sigma) = \xi^0,$$

$$\Downarrow$$

$$\langle \phi^0(x,t)\phi^0(x,0)\rangle$$

$$\langle \phi^\sigma(x+\sigma c_s t, t)\phi^\sigma(x,0)\rangle$$

Time evolution without noise



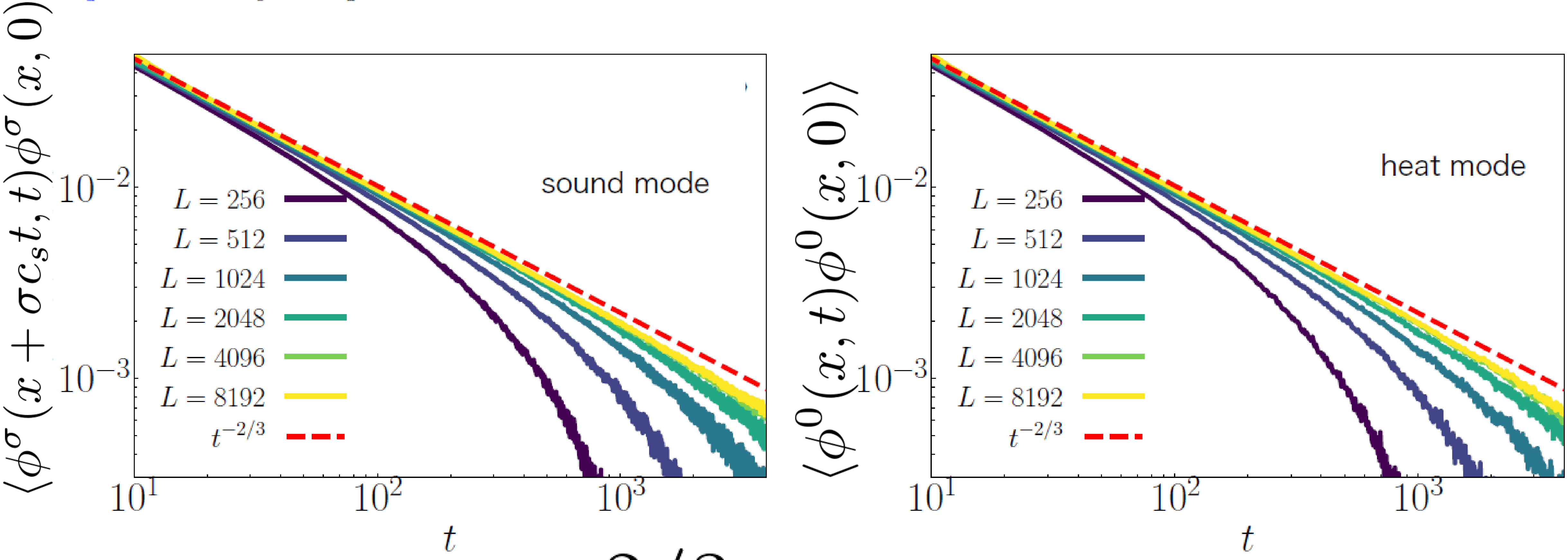
ϕ^0 : (green line) ϕ^σ : (purple and cyan lines)

Part of ϕ^0 propagates by nonlinear interaction

Spohn's argument fails

Scaling at zero sound velocity

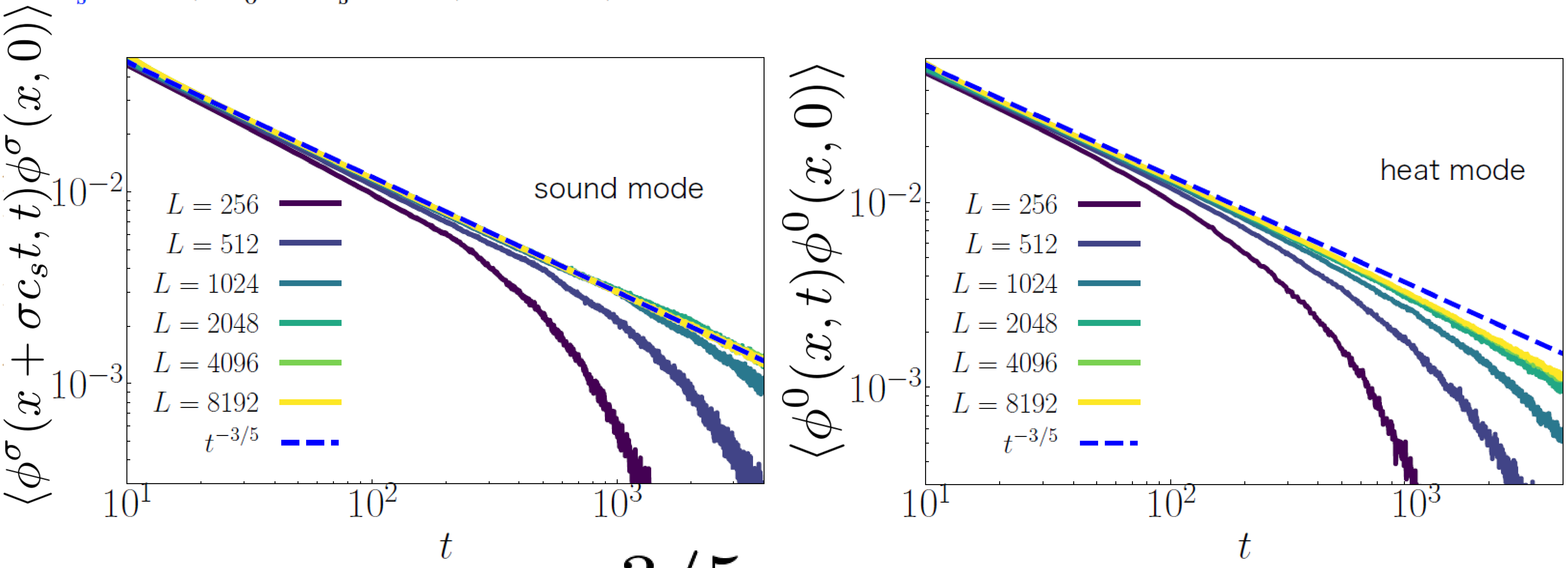
$c_s = 0.0$, $D_0 = D_s = 1.0$, $T = 1.0$, $dt = 0.004$



$t^{-2/3}$:consistent with RG

Scaling at finite sound velocity

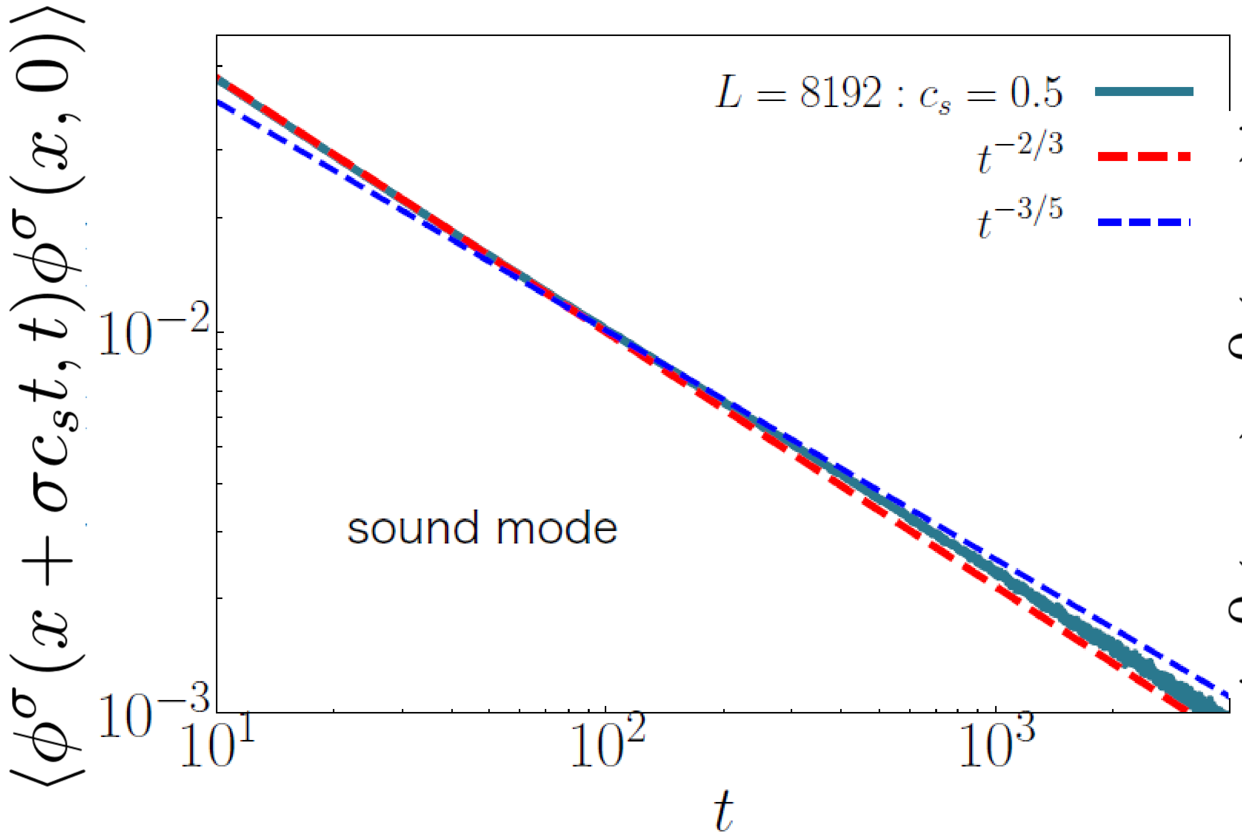
$c_s = 1.0$, $D_0 = D_s = 1.0$, $T = 1.0$, $dt = 0.004$

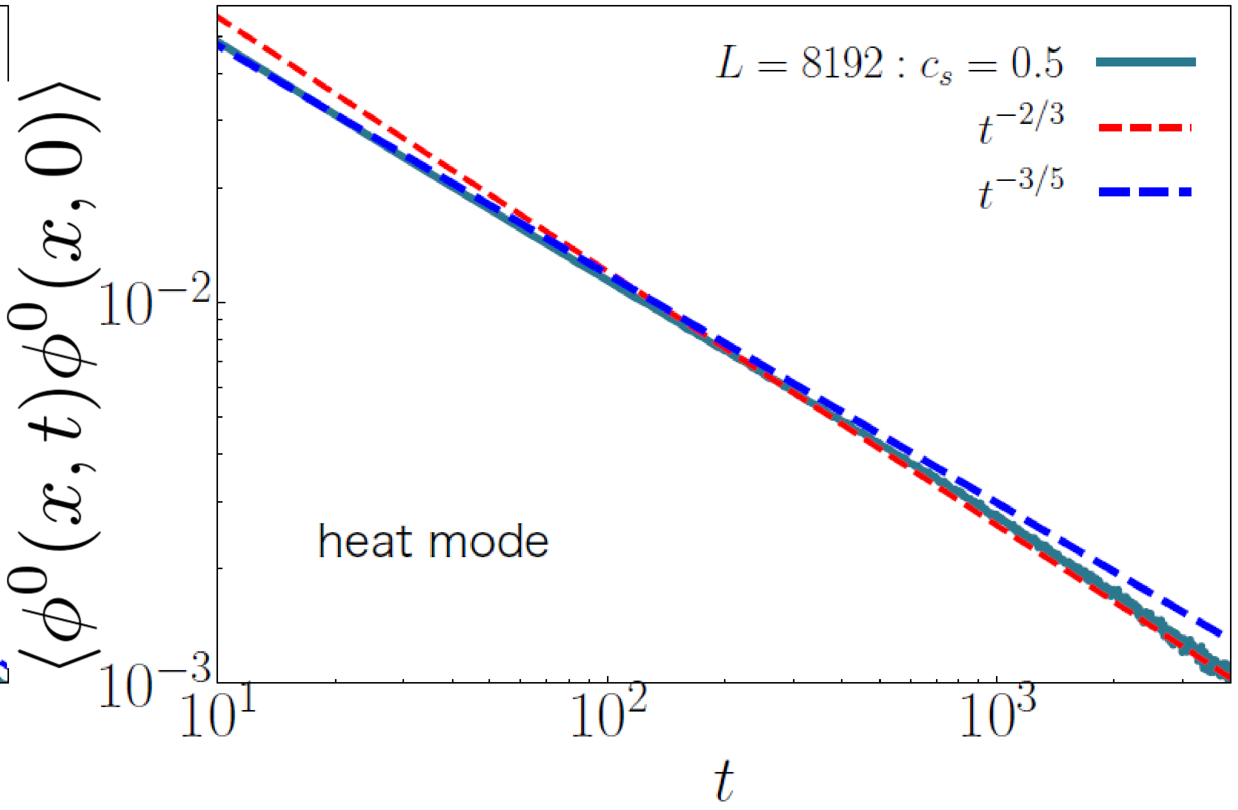


$t^{-3/5}$:consistent with MD

Scaling at intermediate sound velocity

$D_0 = D_s = 1.0$, $T = 1.0$, $dt = 0.004$ $c_s = 0.5$

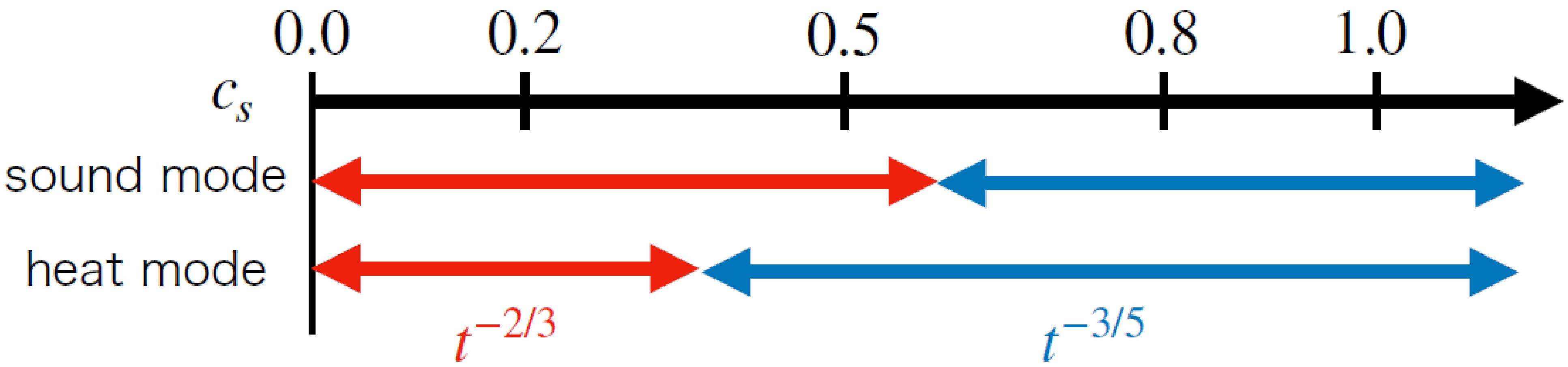




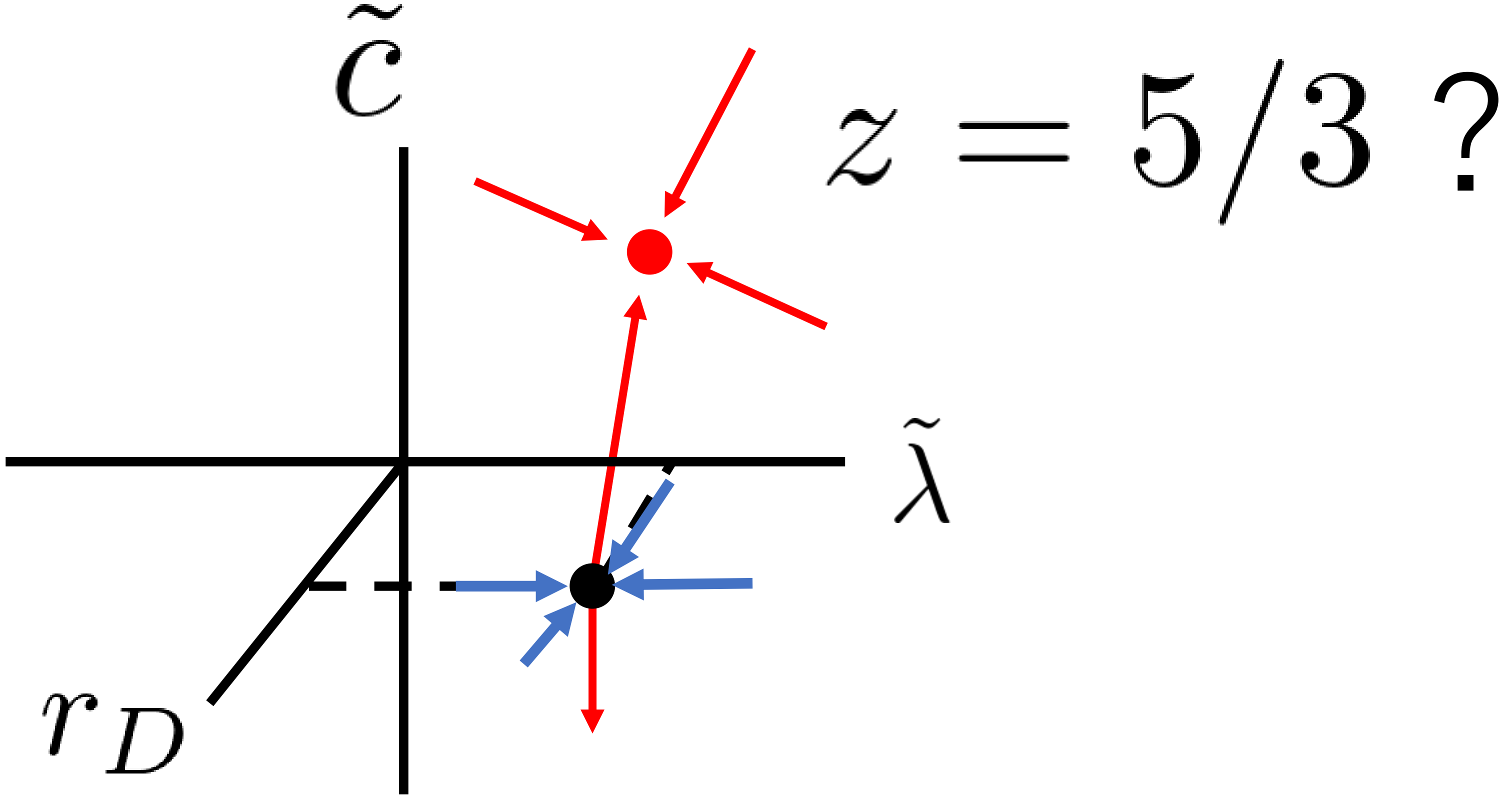
$t^{-2/3}$?

$t^{-3/5}$?

Two scaling exponents



Missing another fixed point?

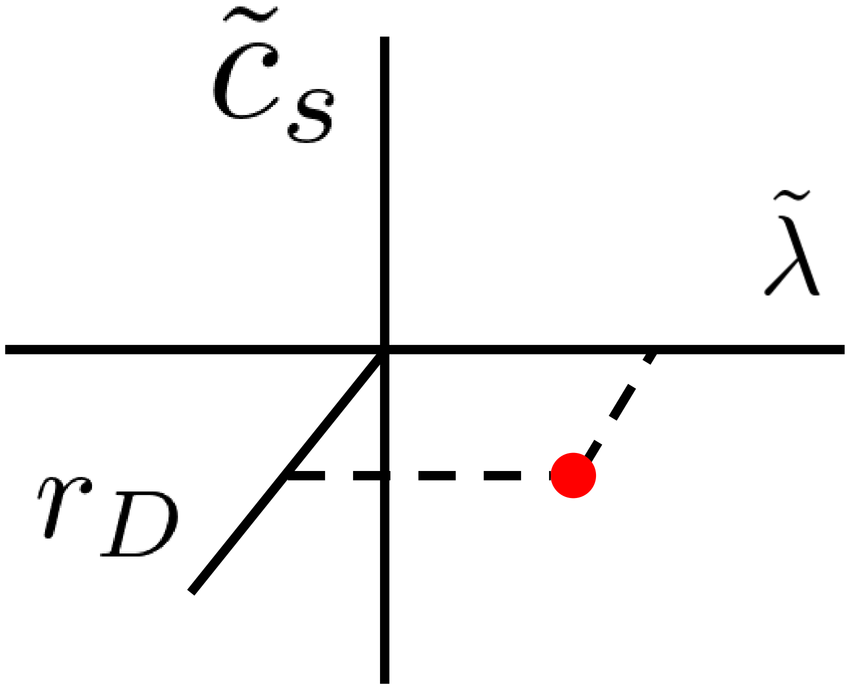


Summary

- Anharmonic chain with space reversal symmetry

- Wilson RG of FHD

$$\langle J_e(t) J_e \rangle \sim t^{-2/3}$$



- Numerical simulation