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Nonlinear response and fluctuation dissipation relations

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Outline

- **Formal Result**: unified derivation of fluctuation dissipation relations (FDR) of arbitrary order for continous and discrete spins

- **Applications**:

  1. detection of a growing length in disordered systems

  2. effective temperature from nonlinear FDR

Vector-Operator formalism for stochastic processes

- Microscopic states $\sigma = (\sigma_1, .., \sigma_N) \Rightarrow$ basis vectors $|\sigma\rangle$ of a vector space

- Macroscopic states $P(\sigma, t)$ go into vectors $|P(t)\rangle \Rightarrow$ $\langle\sigma|P(t)\rangle = P(\sigma, t)$

- Transition probabilities $P(\sigma, t|\sigma', t') \Rightarrow$ matrix elements of the propagator $\langle\sigma|\, \widehat{P}(t|t')\, |\sigma'\rangle$

  $$|P(t)\rangle = \widehat{P}(t|t')\, |P(t')\rangle\,, \quad t \geq t'$$

- Generator of a stochastically continous Markov process

  $$\widehat{P}(t + \Delta t|t) = \widehat{1} + \widehat{W}(t)\Delta t + \mathcal{O}(\Delta t^2)$$

  Fokker-Planck, Glauber, Kawasaki,...

- The process is completely specified by the pair $\{|P(t_0)\rangle\,, \widehat{W}(t)\}$

What is an FDR?

Stochastic evolution under the action of an external field:

- Experimental protocol $[h_i(t')]$; $t' \in (t_w, t)$
- family of stochastic processes $\{\sigma(t), [h_i(t')]\}$

Problem: reconstruct the generic process $\{\sigma(t), [h_i(t')]\}$ from the unperturbed process $\{\sigma(t), [h_i(t') \equiv 0]\}$

- Generic process $\Rightarrow$ Hierarchy of moments

  $\langle \sigma_{i_n}(t_n)..\sigma_{i_1}(t_1)\rangle_h, \quad t_n \geq t_{n-1} \geq ... \geq t_1$

  functionals of $[h_i(t')]$

Taylor expansion

$$\langle \sigma_{i_n}(t_n)..\sigma_{i_1}(t_1)\rangle_h = \langle \sigma_{i_n}(t_n)..\sigma_{i_1}(t_1)\rangle_0 +$$
$$\sum_m \frac{1}{m!} \sum_{j_1..j_m} \int_{t_w}^{t} dt'_1 .. \int_{t_w}^{t} dt'_m R^{(n,m)}_{I(n),J(m)}(T(n),T'(m))$$
$$\times h_{j_1}(t'_1)..h_{j_m}(t'_m)$$

$$R^{(n,m)}_{I(n),J(m)}(T(n),T'(m)) = \left.\frac{\delta^m \langle \sigma_{i_n}(t_n)..\sigma_{i_1}(t_1)\rangle_h}{\delta h_{j_1}(t'_1)..\delta h_{j_m}(t'_m)}\right|_{h=0}$$

m-th order response of the n-th moment

Question: is there any relation between $R^{(n,m)}$ and the correlation functions of the unperturbed process?

- At equilibrium and linear order: fluctuation dissipation theorem (FDT)

- What about off equilibrium? $\Rightarrow$ FDR

Result for discrete and continous spins

1. $R^{(n,m)}$ involve $\frac{\delta}{\delta h_j(t')}\langle \cdots \rangle$

2. $\frac{\delta}{\delta h_j(t')}\langle \cdots \rangle = \langle \cdot \cdot \frac{\partial \widehat{W}(t')}{\partial h_j} \cdot \cdot \rangle$

3. $\frac{\partial \widehat{W}(t')}{\partial h_j} = \frac{\beta}{2}\left\{[\widehat{\sigma}_j, \widehat{W}] - \widehat{B}_j\right\}$

   - Continous spins: $\widehat{B}_j$ drift of Langevin equation
     $\frac{\partial \sigma_j}{\partial t} = B_j + \eta_j \quad \Rightarrow \quad \frac{\partial \langle \sigma_j \rangle}{\partial t} = \langle B_j \rangle$

   - Discrete spins: $\widehat{B}_j = \{\widehat{W}, \widehat{\sigma}_j\}$, is an observable and $\frac{\partial \langle \sigma_j \rangle}{\partial t} = \langle B_j \rangle$

4. $\langle \cdot \cdot [\widehat{\sigma}_j, \widehat{W}(t')] \cdot \cdot \rangle = \frac{\partial}{\partial t'}\langle \cdot \cdot \sigma_j(t') \cdot \cdot \rangle$

5. $\frac{\delta}{\delta h_j(t')}\langle \cdots \rangle = \frac{\beta}{2}\frac{\partial}{\partial t'}\langle \cdot \cdot \sigma_j(t') \cdot \cdot \rangle - \frac{\beta}{2}\langle \cdot \cdot \widehat{B}_j(t') \cdot \cdot \rangle$

Response functions of the first moment

First order response function

$$R_{ij}^{(1,1)}(t,t') = \left.\frac{\delta\langle\sigma_i(t)\rangle}{\delta h_j(t')}\right|_{h=0}$$

Linear FDR

$$R_{i,j}^{(1,1)}(t,t') = \frac{\beta}{2}\left[\frac{\partial}{\partial t'}\langle\sigma_i(t)\sigma_j(t')\rangle - \langle\sigma_i(t)B_j(t')\rangle\right]$$

- recover FDT:

  at stationarity from time translation invariance and time inversion invariance (Onsager relation)

  $$\langle\sigma_i(t)B_j(t')\rangle = -\frac{\partial}{\partial t'}\langle\sigma_i(t)\sigma_j(t')\rangle$$

  FDT: $R_{i,j}^{(1,1)}(t,t') = \beta\frac{\partial}{\partial t'}\langle\sigma_i(t)\sigma_j(t')\rangle$

- zero field algorithm for the computation of $R^{(1,1)}$

Second order response function

$$R^{(1,2)}_{ij_1j_2}(t,t_2,t_1) = \left.\frac{\delta^2\langle\sigma_i(t)\rangle_h}{\delta h_{j_2}(t_2)\delta h_{j_1}(t_1)}\right|_{h=0}$$

Second order FDR

$$\begin{aligned} R^{(1,2)}_{ij_1j_2}(t,t_2,t_1) &= (\beta/2)^2\{\frac{\partial^2}{\partial t_2\partial t_1}\langle\sigma_i(t)\sigma_{j_2}(t_2)\sigma_{j_1}(t_1)\rangle \\ &- \frac{\partial}{\partial t_2}\langle\sigma_i(t)\sigma_{j_2}(t_2)B_{j_1}(t_1)\rangle \\ &- \frac{\partial}{\partial t_1}\langle\sigma_i(t)B_{j_2}(t_2)\sigma_{j_1}(t_1)\rangle \\ &+ \langle\sigma_i(t)B_{j_2}(t_2)B_{j_1}(t_1)\rangle\} \end{aligned}$$

- second order FDT: at stationarity

$$\begin{aligned} R^{(1,2)}_{ij_1j_2}(t,t_2,t_1) &= (\beta^2/2)\{\frac{\partial^2}{\partial t_2\partial t_1}\langle\sigma_i(t)\sigma_{j_2}(t_2)\sigma_{j_1}(t_1)\rangle \\ &- \frac{\partial}{\partial t_1}\langle\sigma_i(t)B_{j_2}(t_2)\sigma_{j_1}(t_1)\rangle\} \end{aligned}$$

- zero field algorithm for the computation of $R^{(1,2)}$

Growing length scale

Usually $L(t)$ is revealed through the decay of

$C_{ij}(t) = \langle \sigma_i(t)\sigma_j(t)\rangle$.

Problem: in glassy systems $C_{ij}(t)$ is short ranged even if $L(t)$ grows.

Space heterogeneities are revealed by

$$\begin{aligned} C_{ij}^{(4)}(t,t_w) &= \langle \sigma_i(t)\sigma_i(t_w)\sigma_j(t)\sigma_j(t_w)\rangle \\ &- \langle \sigma_i(t)\sigma_i(t_w)\rangle\langle \sigma_j(t)\sigma_j(t_w)\rangle \end{aligned}$$

but hard to measure.

Connect $C_{ij}^{(4)}(t,t_w)$ to measurable susceptibilities via FDR.

- second order response of the second moment

$$R^{(2,2)}_{ijj_1j_2}(t,t_2,t_1) = \left.\frac{\delta^2\langle\sigma_i(t)\sigma_j(t)\rangle_h}{\delta h_{j_2}(t_2)\delta h_{j_1}(t_1)}\right|_{h=0}$$

- FDR

$$\begin{aligned} & R^{(2,2)}_{ijij}(t,t_2,t_1) = \\ & (\beta/2)^2\{\frac{\partial^2}{\partial t_2 \partial t_1}\langle\sigma_i(t)\sigma_j(t)\sigma_i(t_2)\sigma_j(t_1)\rangle \\ - & \frac{\partial}{\partial t_2}\langle\sigma_i(t)\sigma_j(t)\sigma_i(t_2)B_j(t_1)\rangle \\ - & \frac{\partial}{\partial t_1}\langle\sigma_i(t)\sigma_j(t)B_i(t_2)\sigma_j(t_1)\rangle \\ + & \langle\sigma_i(t)\sigma_j(t)B_i(t_2)B_j(t_1)\rangle\} \end{aligned}$$

- integrated response function

$$\begin{aligned} & -\chi^{(2,2)}_{ij}(t,t_w) = \int_{t_w}^{t} dt_1 \int_{t_w}^{t} dt_2 R^{(2,2)}_{ijij}(t,t_2,t_1) \\ - & \int_{t_w}^{t} dt_1 R^{(1,1)}_{ii}(t,t_1) \int_{t_w}^{t} dt_2 R^{(1,1)}_{jj}(t,t_2) \end{aligned}$$

- Equilibrium statistical mechanics

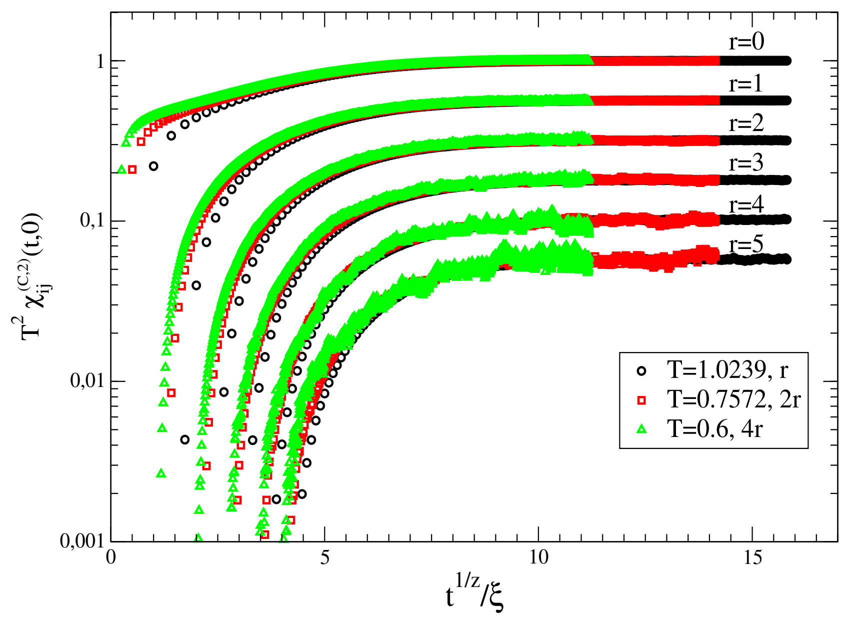
$$\lim_{t\to\infty} \chi_{ij}^{(2,2)}(t,t_w) = (\beta C_{ij,eq})^2$$

- Equilibrium scaling

$$C_{ij,eq}^2 = \xi^{4-2d-2\eta} \widetilde{F}\left(\frac{|i-j|}{\xi}\right)$$

- Finite time scaling

$$T^2 \chi_{ij}^{(2,2)}(t,t_w) = \xi^{4-2d-2\eta} F\left(\frac{|i-j|}{\xi}, \frac{L(t)}{\xi}, \frac{t_w}{t}\right)$$



Ising $d = 1, \eta = 1, r = |i-j|/\xi, L(t) \sim t^{1/2}, t_w = 0$

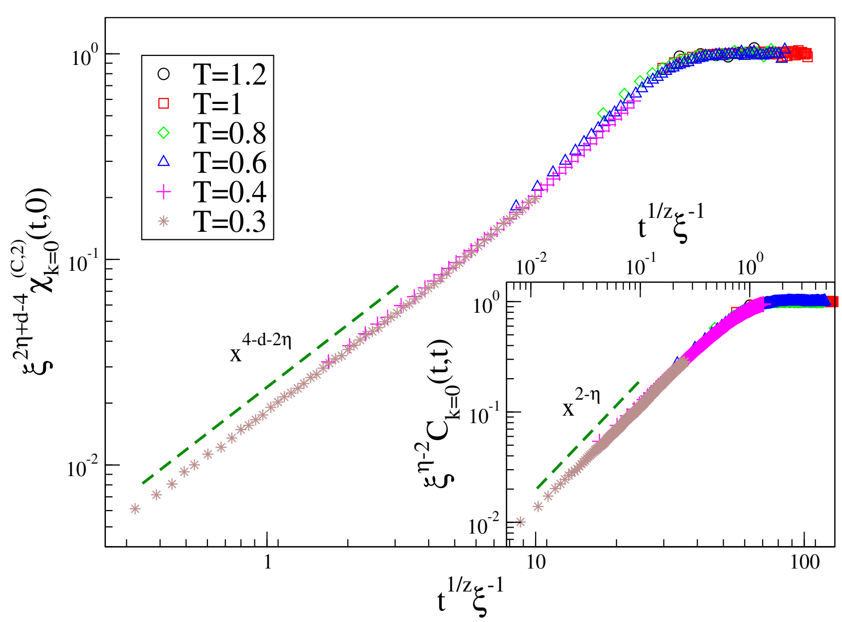
Measurement of $L(t)$ in the Edwards-Anderson model

$$\chi^{(2,2)}_{\vec{k}=0}(t, t_w) = \xi^{4-d-2\eta} \mathcal{F}\left(\frac{L(t)}{\xi}, \frac{t_w}{t}\right)$$

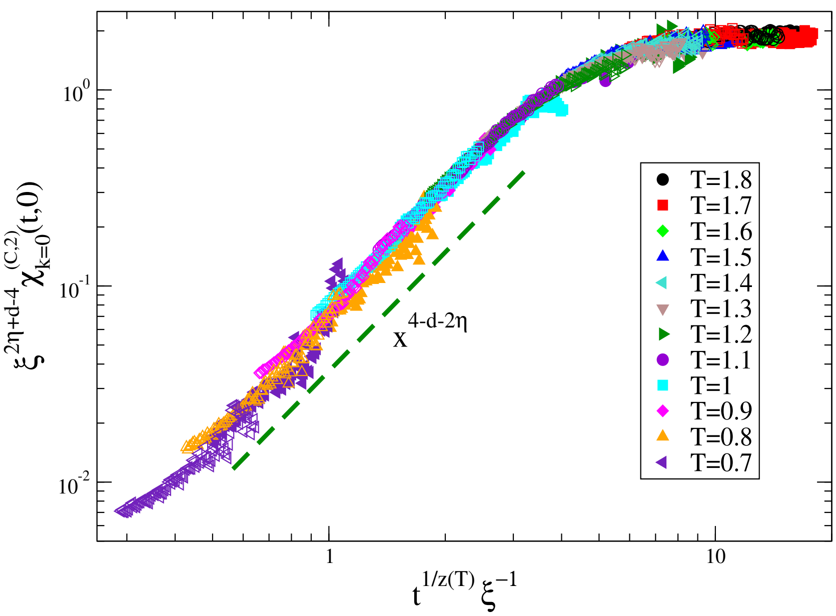
1. for $L(t) \ll \xi$, $\quad \chi^{(2,2)}_{\vec{k}=0}(t, 0) \sim L(t)^{4-d-2\eta}$

2. collapse of $\xi^{-4+d+2\eta}\chi^{(2,2)}_{\vec{k}=0}(t, 0)$ vs $L(t)/\xi$

$d = 1$, $\quad L(t) \sim t^{1/2}$

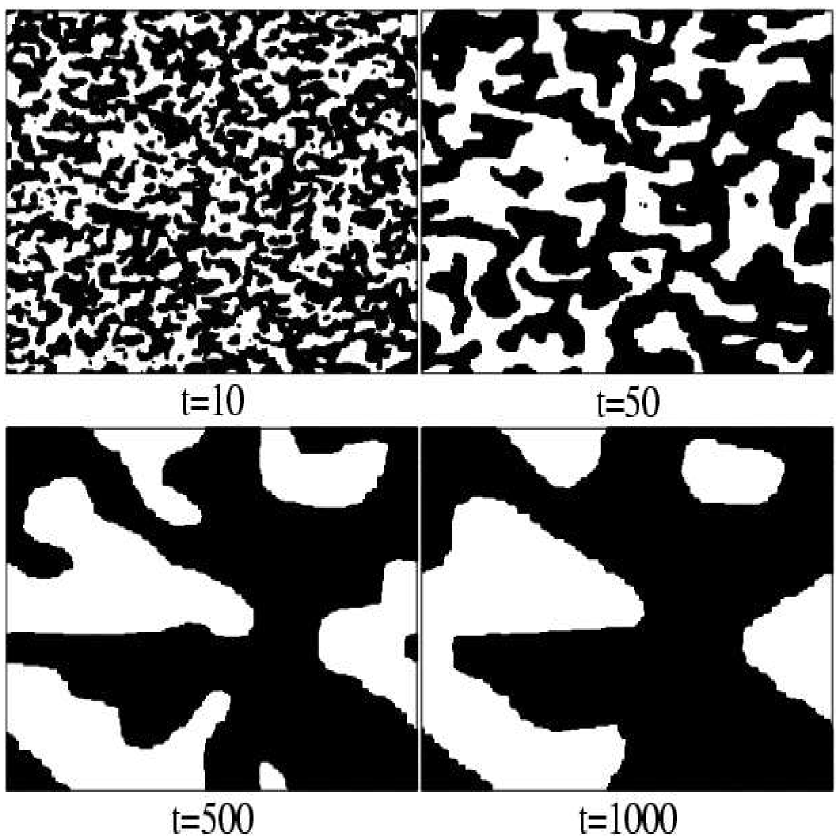


$d = 2, \quad \eta = 0, \quad L(t) \sim t^{1/z(T)}, \quad z(T) \simeq 4/T$



Effective temperature in the quench of non disordered systems below T_C

$d = 2$ Ising model quenched from $T = \infty$ to $T/T_C = 0.88$



Effective temperature from the linear FDR

$$\chi_{ii}^{(1,1)}(t,t_w) = \frac{\beta}{2}\int_{t_w}^{t} dt' \left[\frac{\partial}{\partial t'}\langle\sigma_i(t)\sigma_i(t')\rangle - \langle\sigma_i(t)B_i(t')\rangle\right]$$

$$\psi^{(1)}(t,t_w) = \int_{t_w}^{t} dt' \frac{\partial}{\partial t'}\langle\sigma_i(t)\sigma_i(t')\rangle = 1 - \langle\sigma_i(t)\sigma_i(t_w)\rangle$$

- Equilibrium: $0 \le \psi^{(1)} \le 1 - M^2$

  $\chi_{ii}^{(1,1)}(t,t_w) = \beta\psi^{(1)}(t,t_w)$

  $\beta = \frac{d\chi_{ii}^{(1,1)}}{d\psi^{(1)}}$

- Off equilibrium: $0 \le \psi^{(1)} \le 1$

  time reparametrization

  $\chi_{ii}^{(1,1)}(t,t_w) = \chi_{ii}^{(1,1)}(\psi^{(1)},t_w)$

  $\beta_{eff}(\psi^{(1)}) = \lim_{t_w\to\infty} \frac{\partial\chi_{ii}^{(1,1)}(\psi^{(1)},t_w)}{\partial\psi^{(1)}}$

Large t_w behavior of $\chi_{ii}^{(1,1)}$

From domain coarsening:

- $\chi_i^{(1,1)}(\psi^{(1)}, t_w) = \chi_{st}^{(1,1)}(\psi^{(1)}) + \chi_{ag}^{(1,1)}(\psi^{(1)}, t_w)$

- $\chi_{ag}^{(1,1)}(\psi^{(1)}, t_w) = t_w^{-a} F(\psi^{(1)}), \quad a > 0$

- $\lim_{t_w \to \infty} \chi_{ag}^{(1,1)}(\psi^{(1)}, t_w) = 0$

$$\beta_{eff}(\psi^{(1)}) = \begin{cases} \beta, & \text{for } 0 \leq \psi^{(1)} \leq 1 - M^2 \\ 0, & \text{for } 1 - M^2 < \psi^{(1)} \leq 1 \end{cases} \tag{1}$$

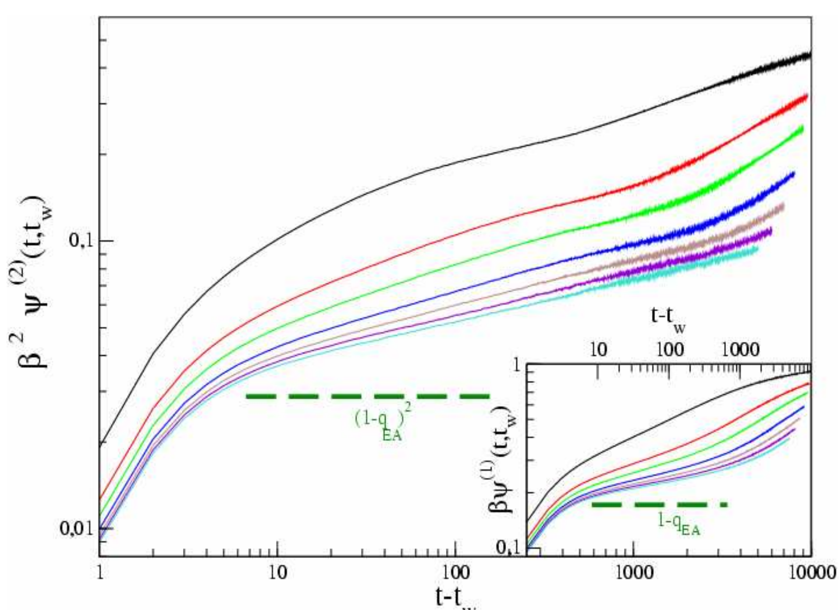
Effective temperature from the second order FDR

$$\chi^{(2,2)}_{\vec{k}=0}(t,t_w), \quad \psi^{(2)}(t,t_w)$$

- Equilibrium: $\psi^{(2)} \leq (1-M^2)^2$

$$\chi^{(2,2)}_{\vec{k}=0}(t,t_w) = \beta^2 \psi^{(2)}(t,t_w), \quad \beta^2 = \frac{d\chi^{(2,2)}_{\vec{k}=0}}{d\psi^{(2)}}$$

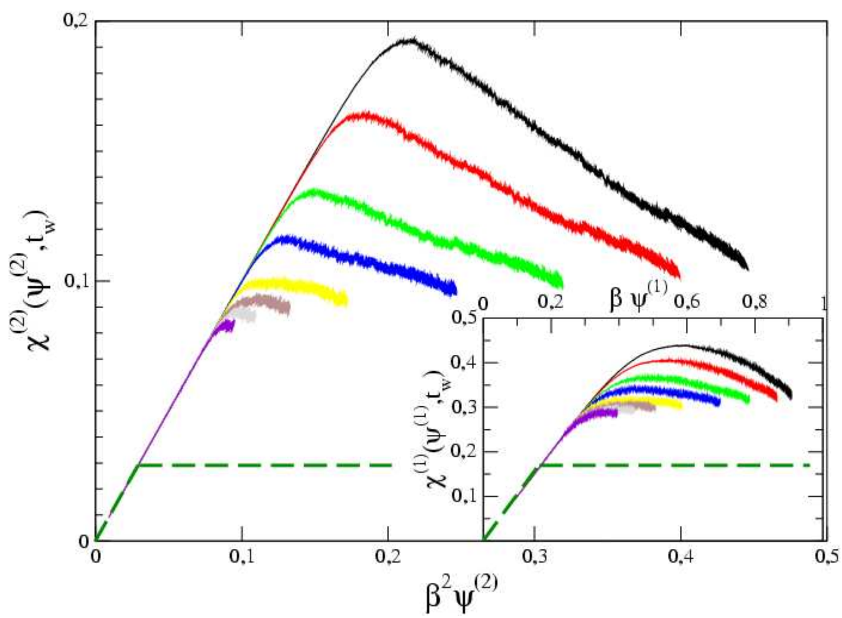
- Off equilibrium



- time reparametrization: $\chi^{(2,2)}_{\vec{k}=0}(\psi^{(2)}, t_w)$

- domain coarsening:

$$\chi^{(2,2)}_{\vec{k}=0}(\psi^{(2)}, t_w) = \chi^{(2,2)}_{st}(\psi^{(2)}) + \chi^{(2,2)}_{ag}(\psi^{(2)}, t_w)$$

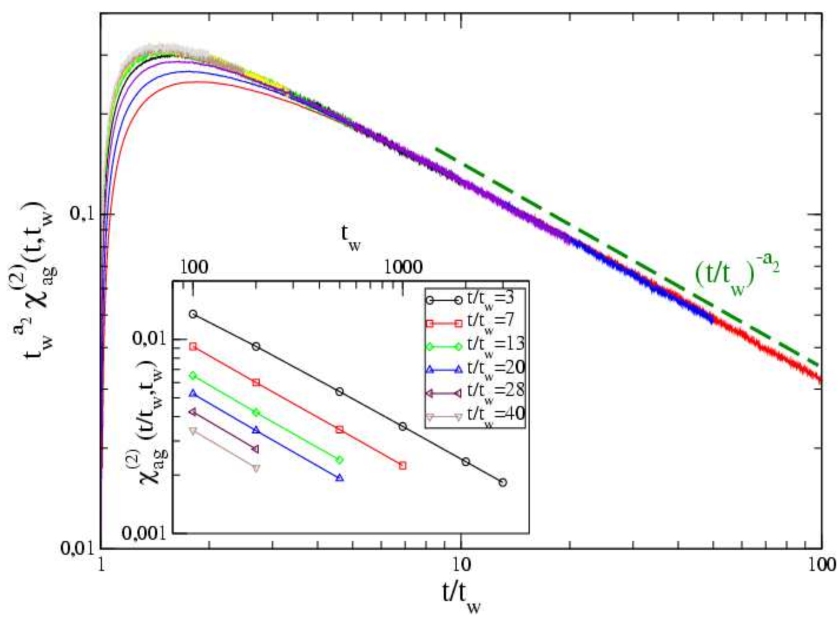


$$\beta^2_{eff}(\psi^{(2)}) = \lim_{t_w\to\infty} \frac{\partial\chi^{(2,2)}_{\vec{k}=0}(\psi^{(2)},t_w)}{\partial\psi^{(2)}}$$

Question: is $\beta_{eff}(\psi^{(2)}) = \beta_{eff}(\psi^{(1)})$?

Large t_w behavior of $\chi_{ag}^{(2,2)}$

- $\chi_{ag}^{(2,2)}(\psi^{(2)}, t_w) = t_w^{-a_2} F_2(t/t_w), \quad a_2 \simeq 0.6$



- $\lim_{t_w\to\infty} \chi_{ag}^{(2,2)}(\psi^{(2)}, t_w) = 0$

- $$\beta_{eff}(\psi^{(2)}) = \begin{cases} \beta, & \text{for } \psi^{(2)} \leq (1-M^2)^2 \\ 0, & \text{for } (1-M^2)^2 < \psi^{(2)} \end{cases} \qquad (2)$$