

Universal finite-size scaling for a dynamical phase transition in a kinetically constrained model and a quantum phase transition in a ferromagnet.

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Collaboration work with
Vivien Lecomte (Paris VII, LPMA)
Shin-ichi Sasa (Kyoto)
Frédéric van Wijland (Paris VII, MSC)

T. N. V. Lecomte, S. Sasa, F. van Wijland, J. Stat. Mech. (2014) P10001

JSPS Core-to-Core program 2013-2015

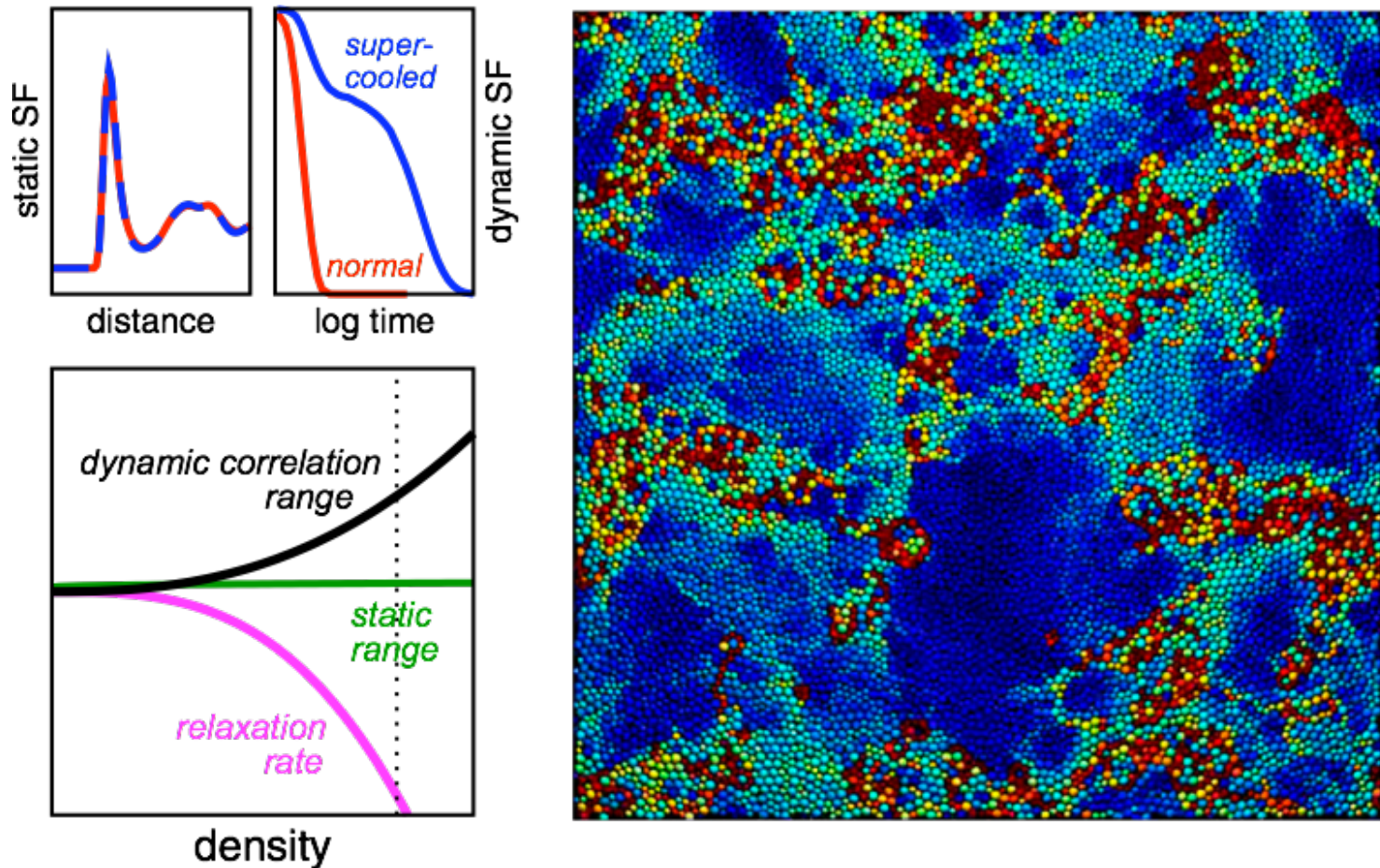
Non-equilibrium dynamics of soft matter and information



Coordinator : Shin-ichi Sasa (Department of Physics, Kyoto University)

dynamical phase transitions in KCMs

Dynamical heterogeneity



J. P. Garrahan, Proc. Natl. Acad. Sci. U. S. A. 2011 108 (12) 4701.

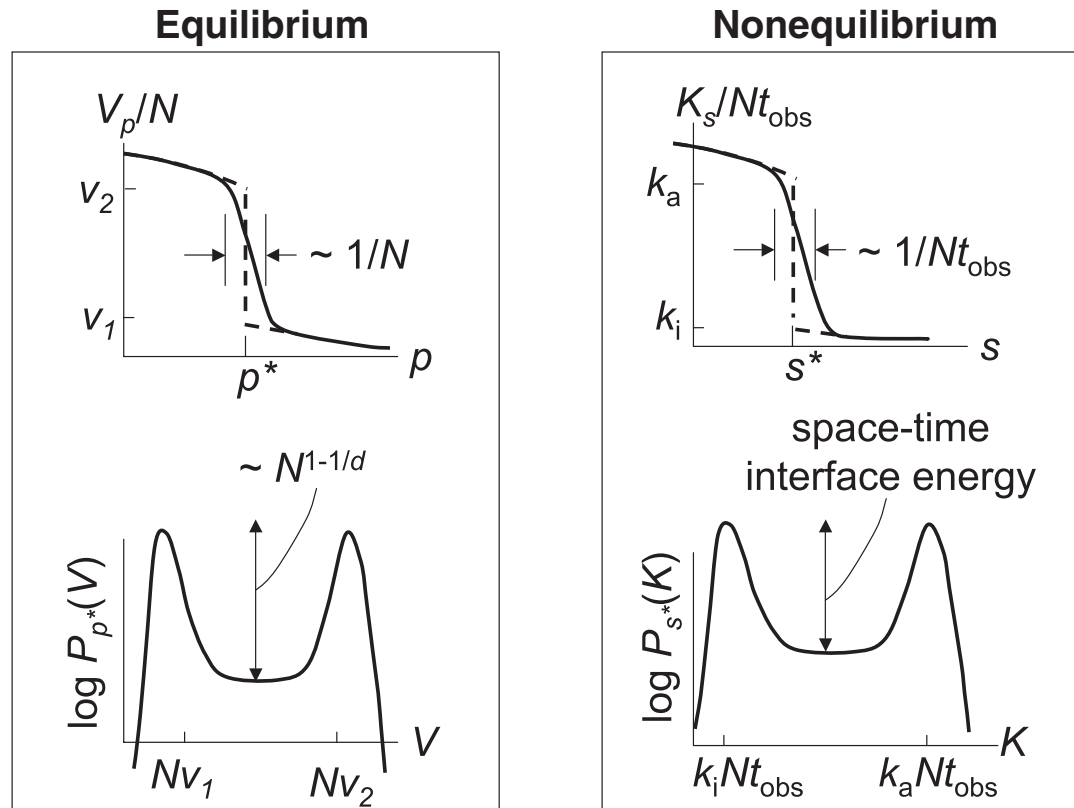
dynamical phase transitions in KCMs

Dynamical phase transition by activity bias

M. Merolle, J. P. Garrahan, D. Chandler, PNAS, 102, 10837 (2005)

R.L. Jack, J.P.Garrahan, D. Chandler, J. Chem. Phys. 125, 184509 (2006)

J. P. Garrahan et al, PRL, **98**, 195702 (20007).



L. O. Hedges, R. L. Jack, J. P. Garrahan, D. Chandler, science, 323, 2009

Finite size scaling in first order transition

Finite size scaling

Second order phase transition

- From small system size simulations,
 - Where is true critical point?
(with finite size simulations)
 - Precise order of the transition

More on first order phase transition

- (i) Scaling speed ?
- (ii) Scaling functions ?

Finite size scaling in first order transition

Finite size scaling: Classical (thermodynamic) transition

M. E. Fisher and A. N. Berker, PRB, **26**, 2507 (1982)

C. Borgs and R. Kotecky, PRL, **68**, 1734 (1992)

In general

Partition function

$$Z_{\text{per}}(h, L) \approx \sum_{q=1}^N \exp\{-f_q(h) \beta L^d\}$$

Number of phases

Index for phases

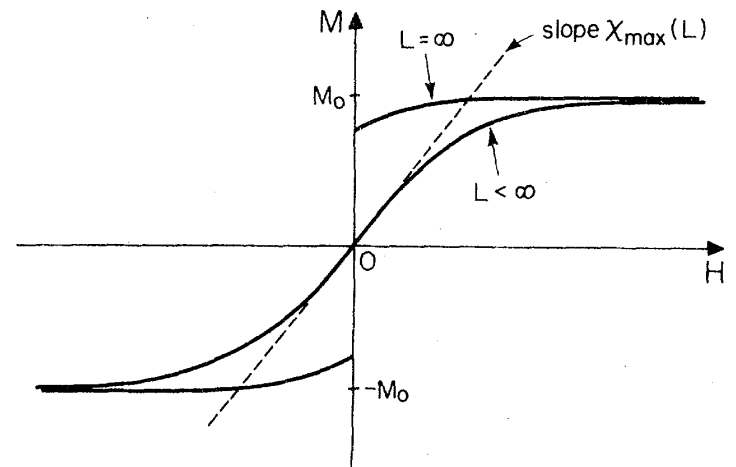
“metastable free energy”

System volume

Ex.) Ising spins (d-dimension)

$$Z_{\text{per}}(h, L) \approx e^{\beta h m L^d} + e^{-\beta h m L^d}$$

$$m_{\text{per}}(h, L) \approx m \tanh(\beta h m L^d)$$



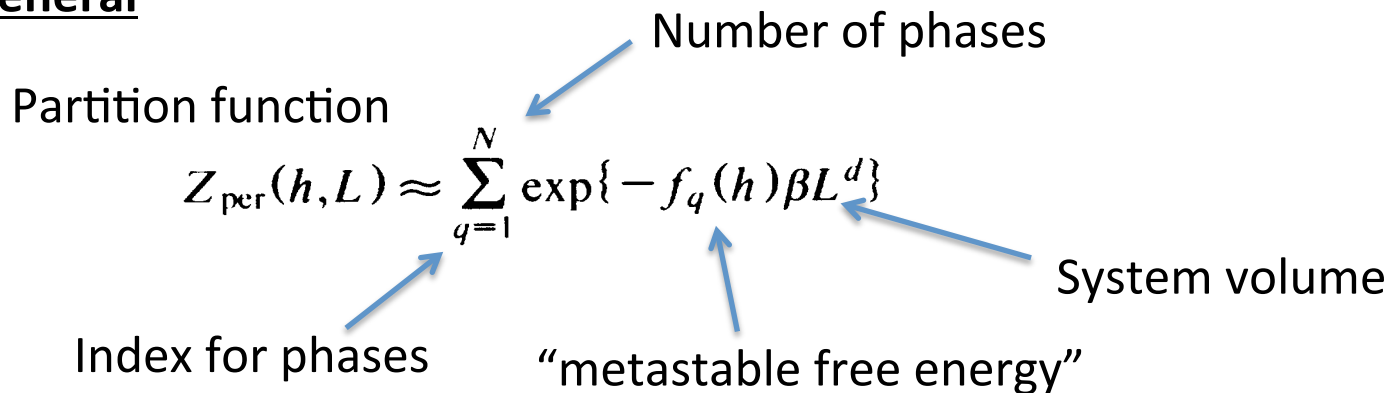
Finite size scaling in first order transition

Finite size scaling: Classical (thermodynamic) transition

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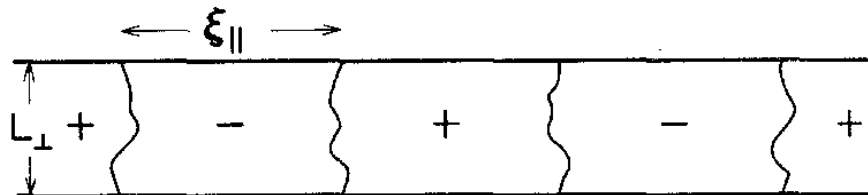
In general



Depending on boundary conditions (2 d, cylinder-shaped)

- Exponentially scaling

V. Privman and M. E. Fisher, J. Stat. Phys. **33**, (1983).



Finite size scaling in first order transition

Finite size scaling: Dynamical phase transition

T. Bodineau and C. Toninelli, Comm. Math. Phys. **311** (2012)

T. Bodineau, V. Lecomte and C. Toninelli, J. Stat. Phys. **147** (2012)

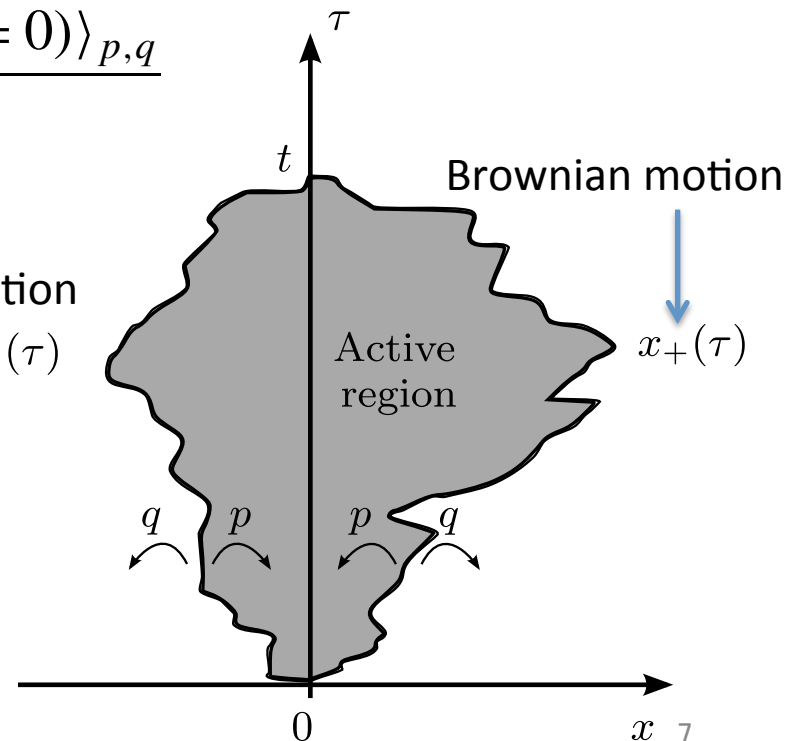
1d-FA → 2 dimensional spin problem?

$$Z_{\text{eff}}(s, t) \equiv \frac{\langle e^{-s\mathbb{K} \int_0^t d\tau [x_+(\tau) - x_-(\tau)]} \delta(x_{\pm}(t) = 0) \rangle_{p,q}}{\langle \delta_{\pm}(x(t) = 0) \rangle_{p,q}}$$

Dynamical free energy

$$\varphi_L(\lambda) = -\Sigma - 4\sqrt{pq} \left(\frac{\lambda\mathbb{K}}{4L\sqrt{pq}} \right)^{\frac{2}{3}} 2^{-\frac{1}{3}} \alpha_1$$

Brownian motion
 $x_-(\tau)$



Finite size scaling in first order transition

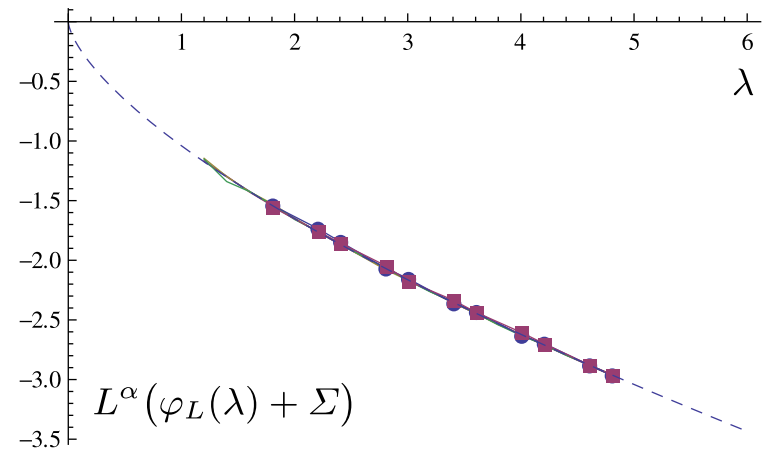
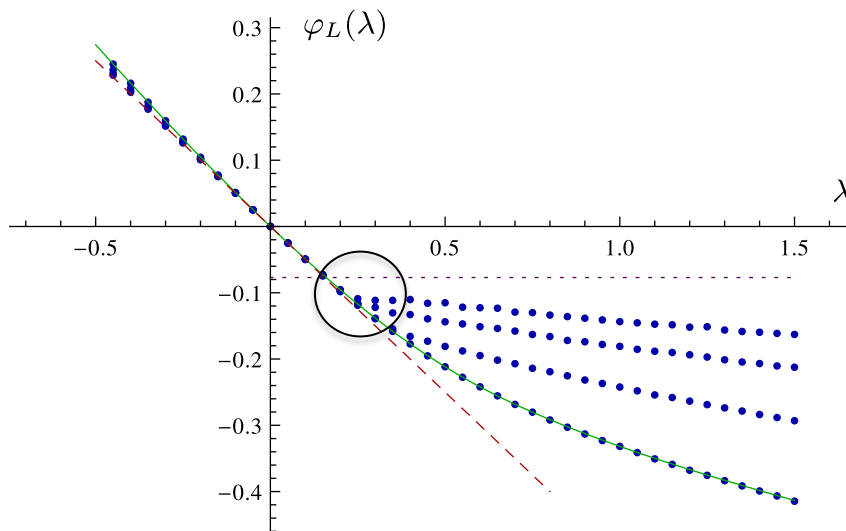
Finite size scaling: Dynamical phase transition

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1d-FA \rightarrow 2 dimensional spin problem?

Dynamical free energy $\varphi_L(\lambda) = -\Sigma - 4\sqrt{pq} \left(\frac{\lambda \mathbb{K}}{4L\sqrt{pq}} \right)^{\frac{2}{3}} 2^{-\frac{1}{3}} \alpha_1$



Finite size scaling in first order transition

Purpose of this talk

On the contrary,

- With **the simplest model** showing dynamical phase transition
- Directly checking if **classical approach** can work

Answer:

- It can work. (But another procedure is needed)
- It is more close to **quantum phase transition**

Construction of this talk

1. Preliminary: Introduction of mean-field FA
2. Problems and how to overcome it
3. Discussions

1. Preliminary: Intro of mean-field FA Model

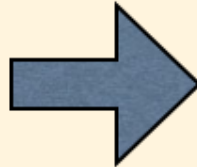
What is KCMs?

KCMs(Kinetically Constrained Models)

F. Ritort and P. Sollich, Adv. Phys., 52, 219 (2003)

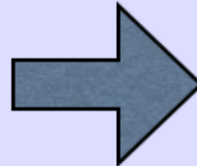
Detailed balance with kinetic constraint

Static property



the same as equilibrium

Kinetic property



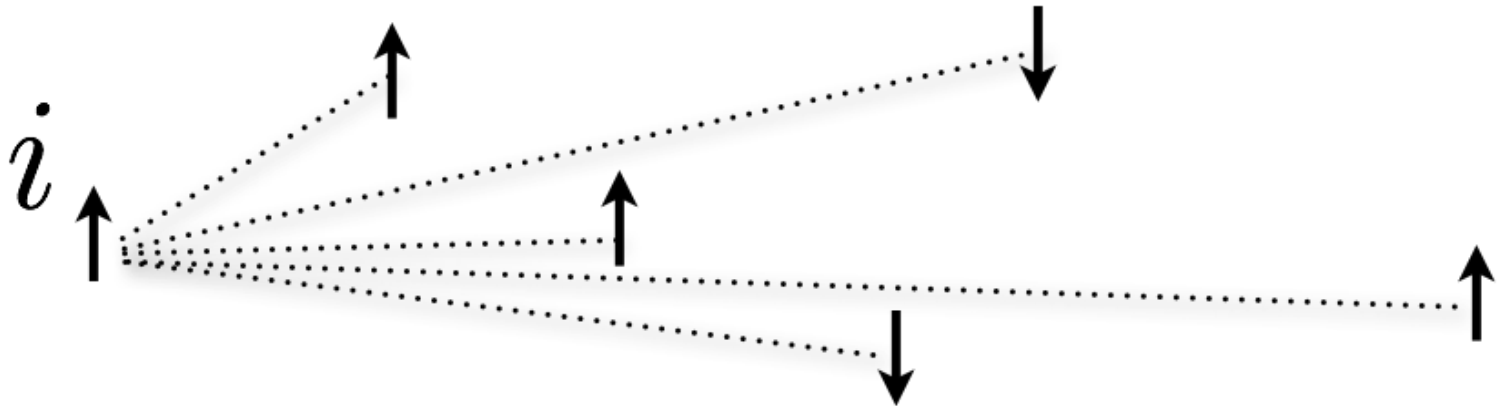
similar to glass?

1. Preliminary: Intro of mean-field FA Model

(e.g. J. P Garrahan et al, J. Phys. A, Math. Theor. 42 (2009) 075007)

Ex.) Frederickson-Andersen Model (FA) on fully-connected lattice:

- L sites (Infinite range) $\mathbf{n} = (n_i)_{i=1}^L$
- each spin takes 0 or 1 $n_i = 1$, or $n_i = 0$

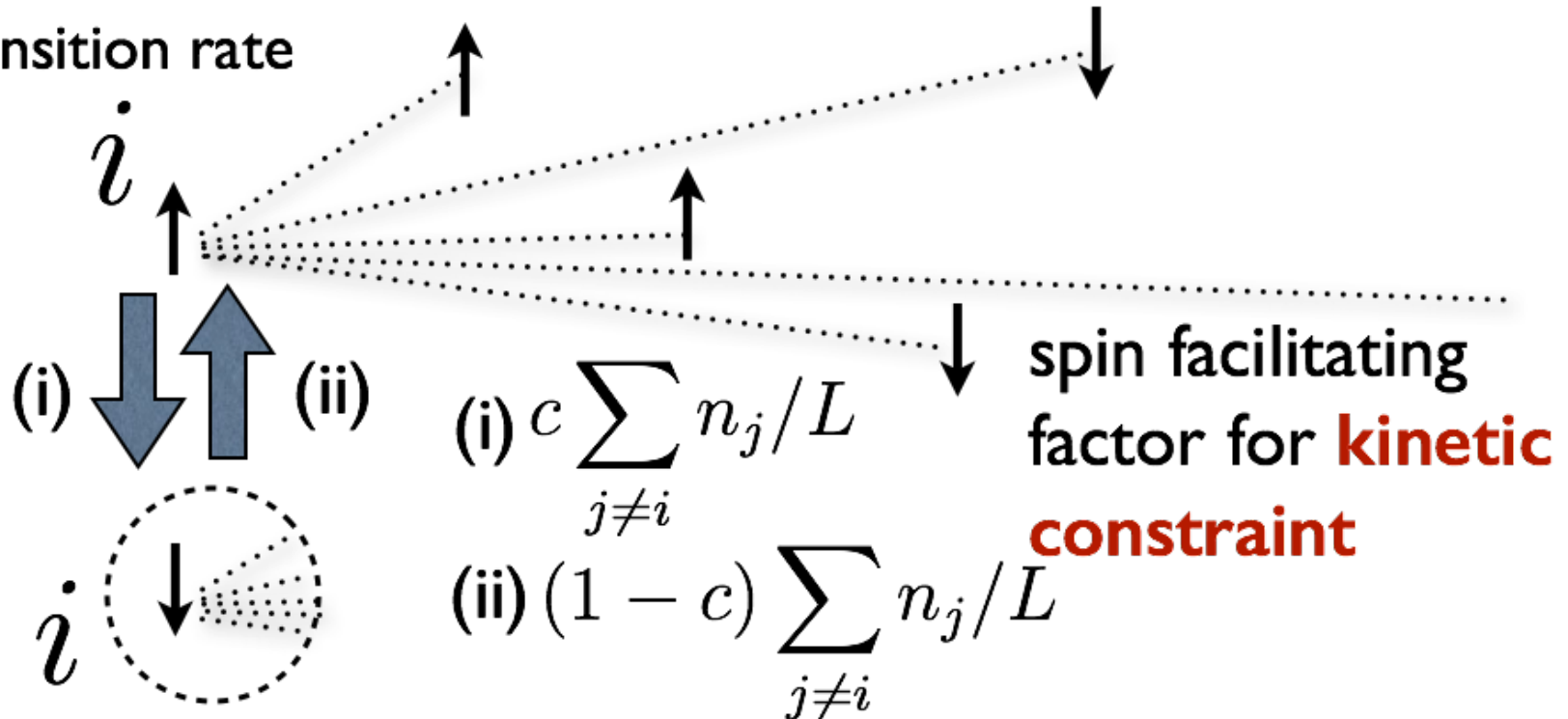


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- L sites (Infinite range) $\mathbf{n} = (n_i)_{i=1}^L$
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- Transition rate

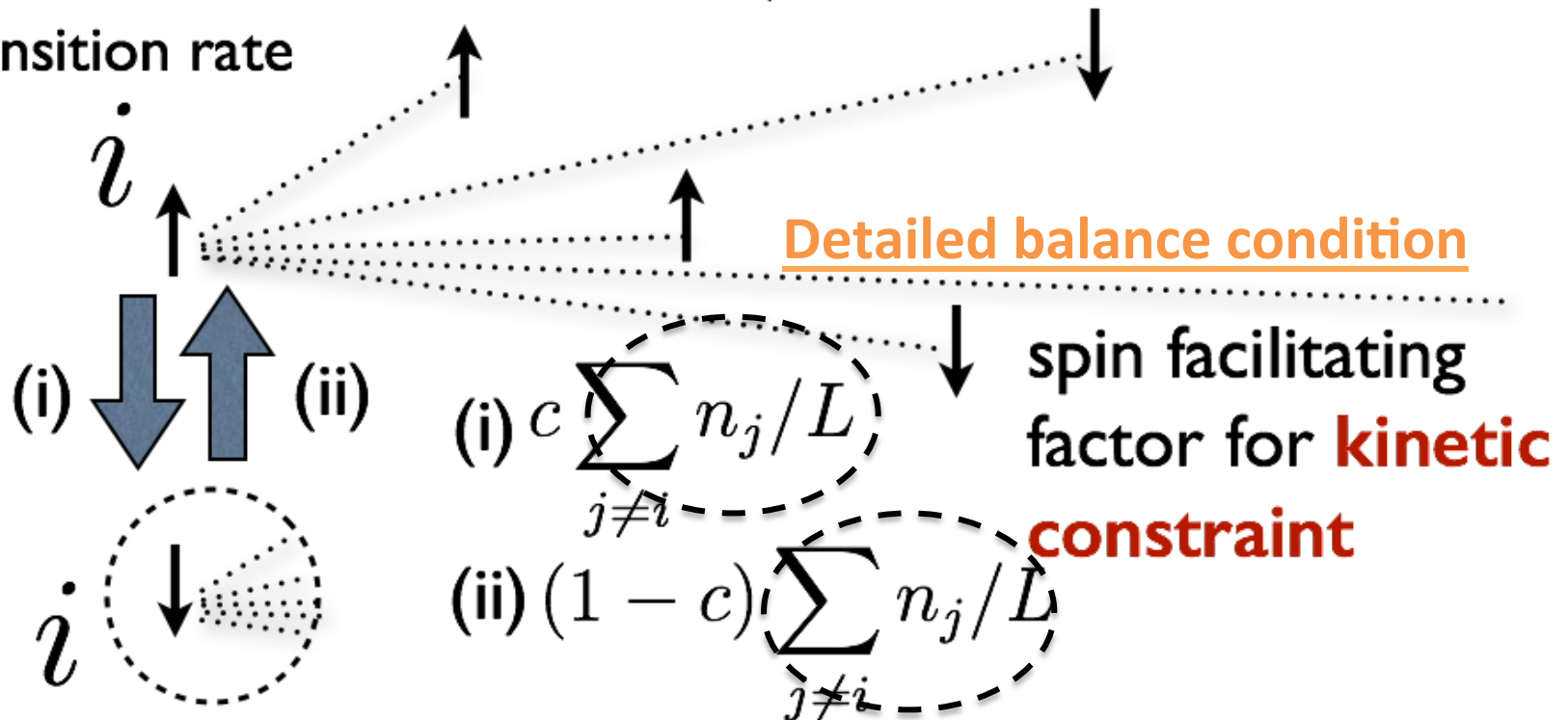


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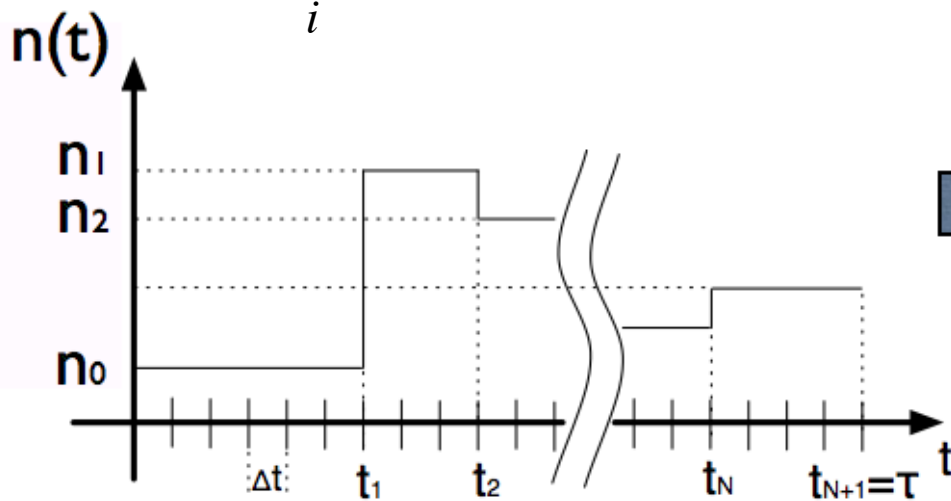
1. Preliminary: Intro of mean-field FA

Dynamical phase transition

s - ensemble

An ensemble biased by a fictitious field s

$$n(t) = \sum_i n_i = 1, 2, \dots, L \quad : \text{state of the system (total spin)}$$



Continuous time Markov dynamics

(i) Path probability density:

$$P(\text{history})$$

(ii) a function of the history:

$$K(\text{history})$$

Ex.) Activity

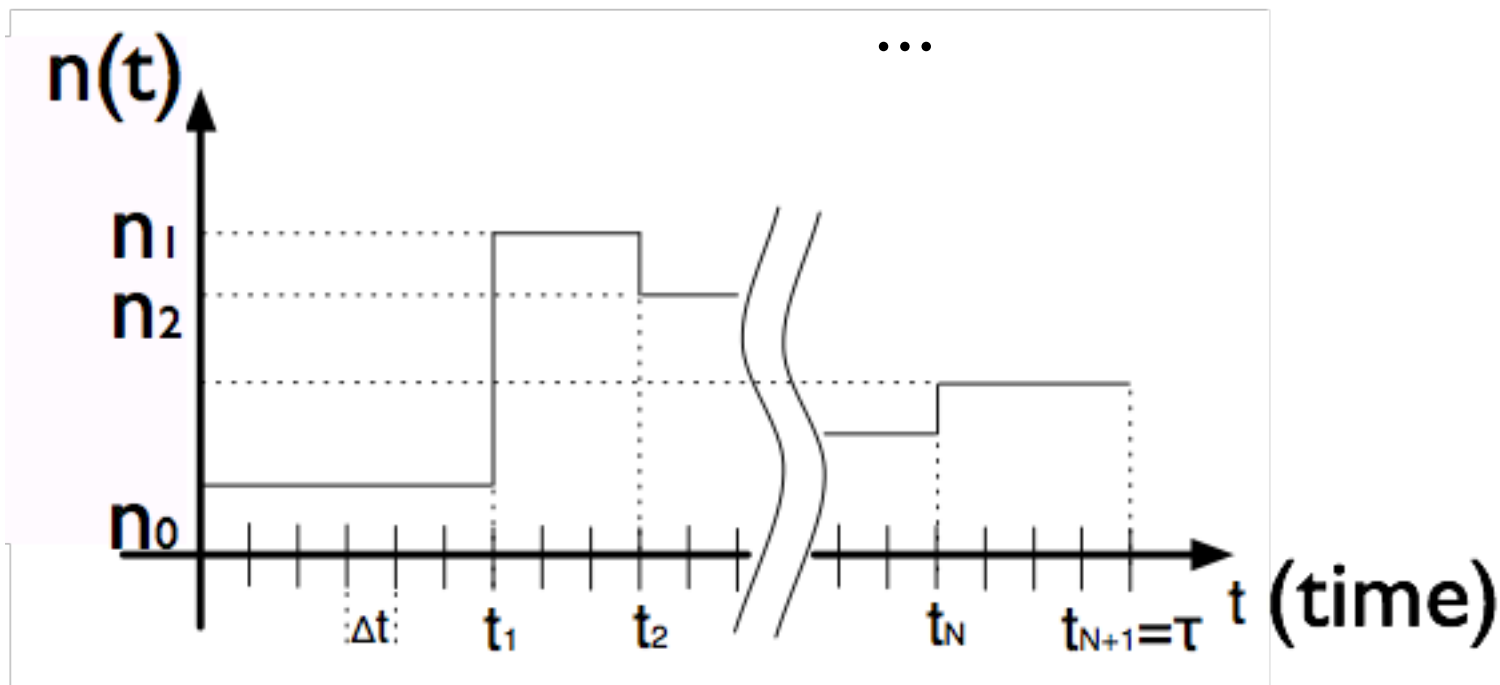
: The total number of the spinflips: N

1. Preliminary: Intro of mean-field FA

Dynamical phase transition

Activity ?

Ex. $K(t_0 \leq t \leq t_2) = 2$
 $K(t_0 \leq t < t_1) = 0$



1. Preliminary: Intro of mean-field FA

Dynamical phase transition

s - ensemble

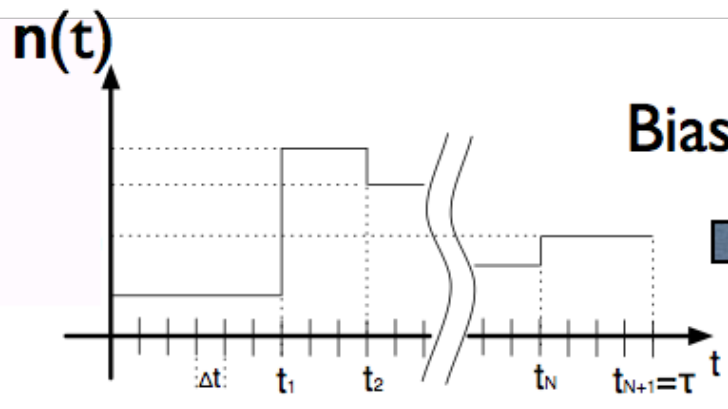
An ensemble biased by a fictitious field s

Path probability of s-ensemble is defined as

$$P_s(\text{history}) \equiv \frac{1}{Z(s)} P(\text{history}) \exp(sK(\text{history}))$$

↑ Dynamical partition function:

$$Z(s) \equiv \sum_{\text{history}} P(\text{history}) \exp(sK(\text{history}))$$



Biased by s

**When $s > 0$ (or $s < 0$),
the path, in which K takes large value,
has larger (or smaller) probability.**

1. Preliminary: Intro of mean-field FA

Dynamical phase transition

s - ensemble An ensemble biased by a fictitious field s

Path probability of s-ensemble is defined as

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↑ Dynamical partition function:

$$Z(s) \equiv \sum_{\text{history}} P(\text{history}) \exp(sK(\text{history}))$$

Dynamical free energy: $f(s) \equiv \frac{1}{\tau} \log Z(s)$

Large deviation function of $x = K / \tau$

$$I(x) = \max_s [xs - f(s)]$$

1. Preliminary: Intro of mean-field FA

Dynamical phase transition

How to calculate dynamical free energy?

- Population dynamics method (In general, numerical method)
C. Giardin`a, J. Kurchan, and L. Peliti, Phys. Rev. Lett. 96, 120603 (2006).
- Transfer matrix (largest eigenvalue problem, solvable model)

1. Preliminary: Intro of mean-field FA

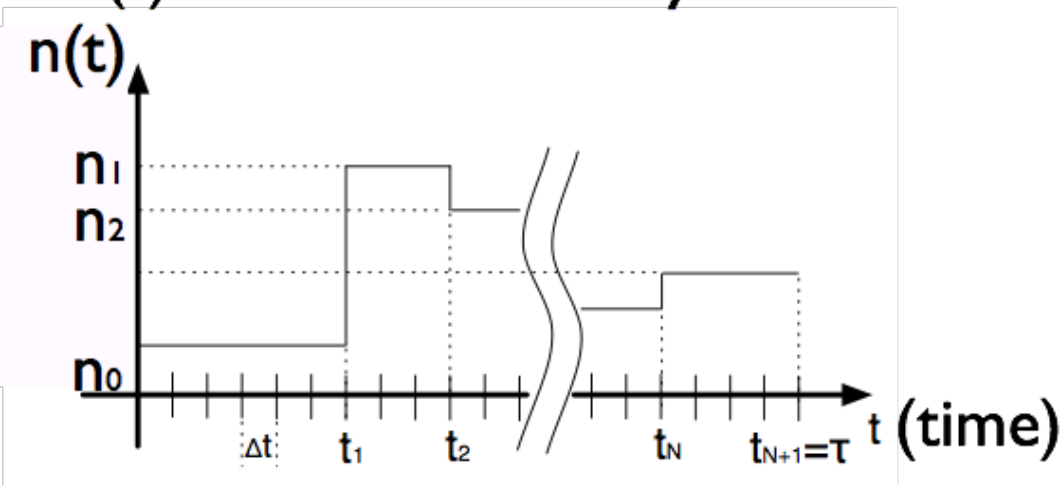
Dynamical phase transition

How to calculate dynamical free energy?

- Transfer matrix (largest eigenvalue problem, solvable model)

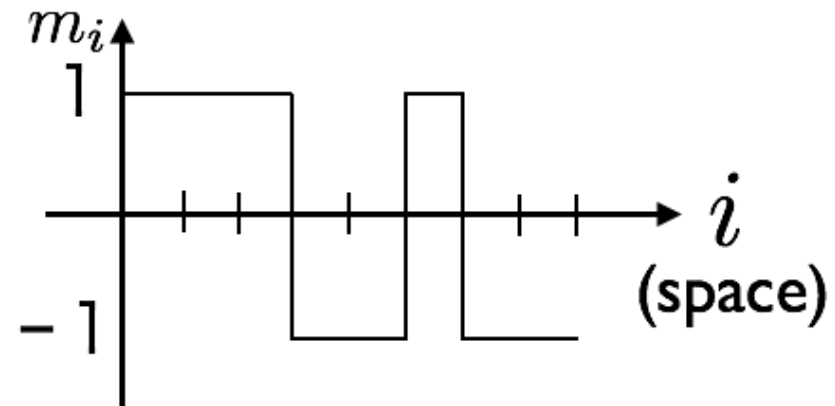
Markov Dynamics corresponds to Ising spins in statistical physics

$n(t)$: the state of the system



Markov dynamics

m_i : realisation of spin



Ising spin (1-dimensional)

1. Preliminary: Intro of mean-field FA

Dynamical phase transition

How to calculate dynamical free energy?

- Transfer matrix (largest eigenvalue problem, solvable model)

Transition rate:

$$w(n \rightarrow n') = \delta_{n',n+1}cn(L-n)/L + \delta_{n',n-1}(1-c)n(n-1)/L$$

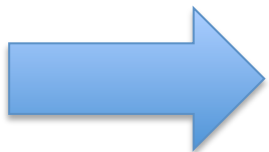
Master operator

$$L_{n,n'} = w(n' \rightarrow n) - \delta_{n,n'}\lambda(n)$$

Escape rate

Modified Master operator by activity

$$L_{n,n'}^s = w(n' \rightarrow n)e^s - \delta_{n,n'}\lambda(n)$$

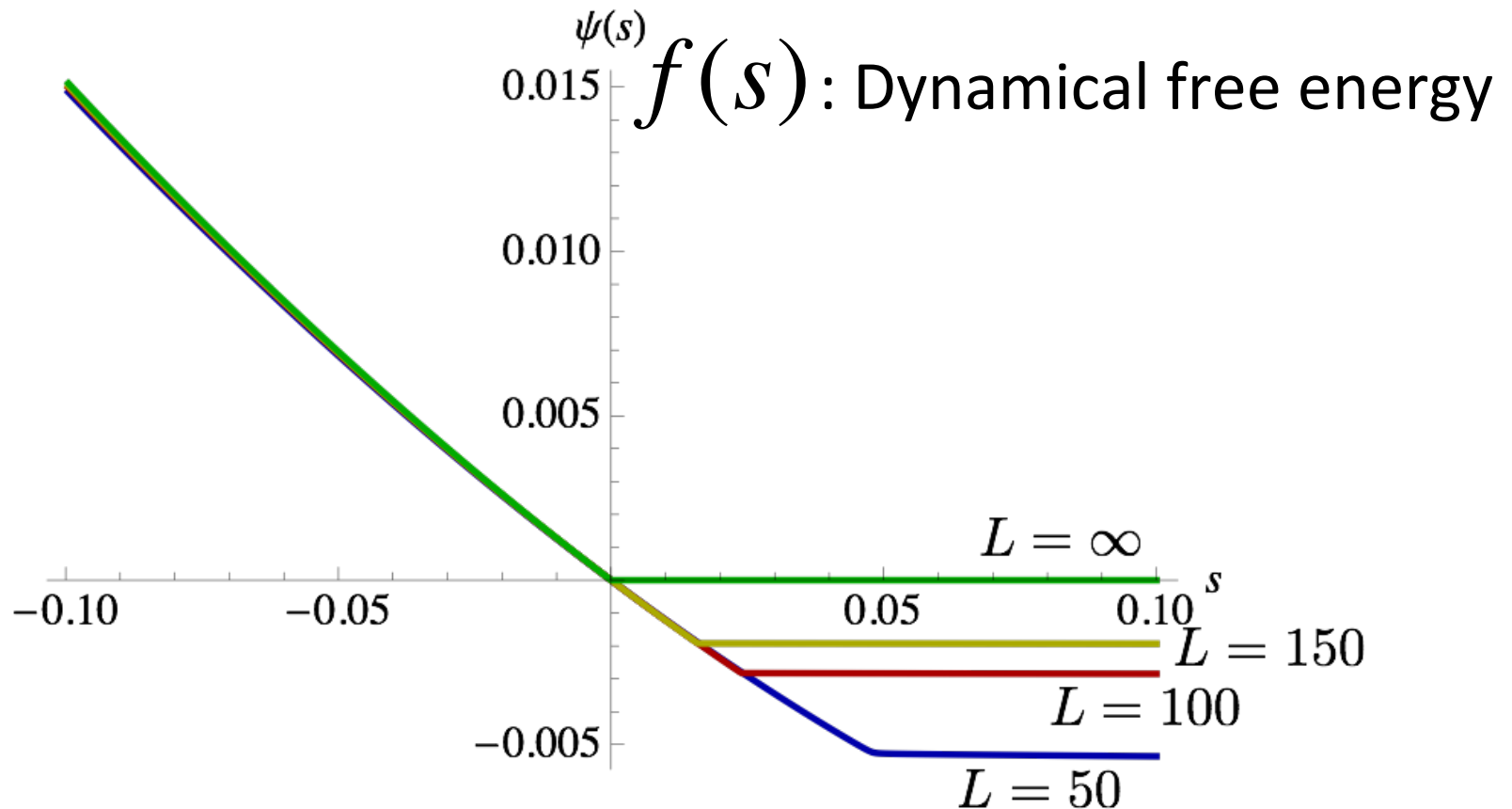


Largest eigenvalue of $L^s = \underline{\text{dynamical free energy}}$

1. Preliminary: Intro of mean-field FA

Dynamical phase transition

Numerical example ($c=0.3$)



1. Preliminary: Intro of mean-field FA

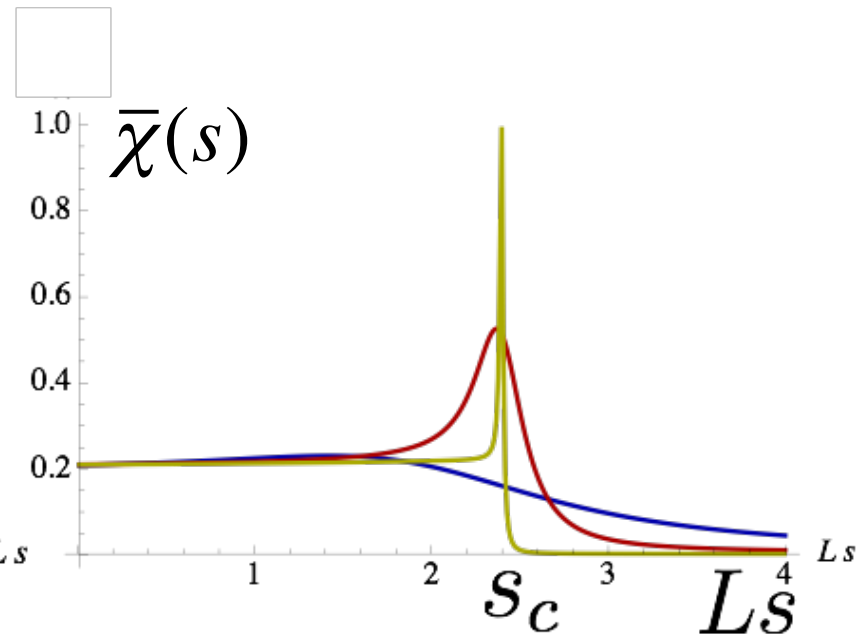
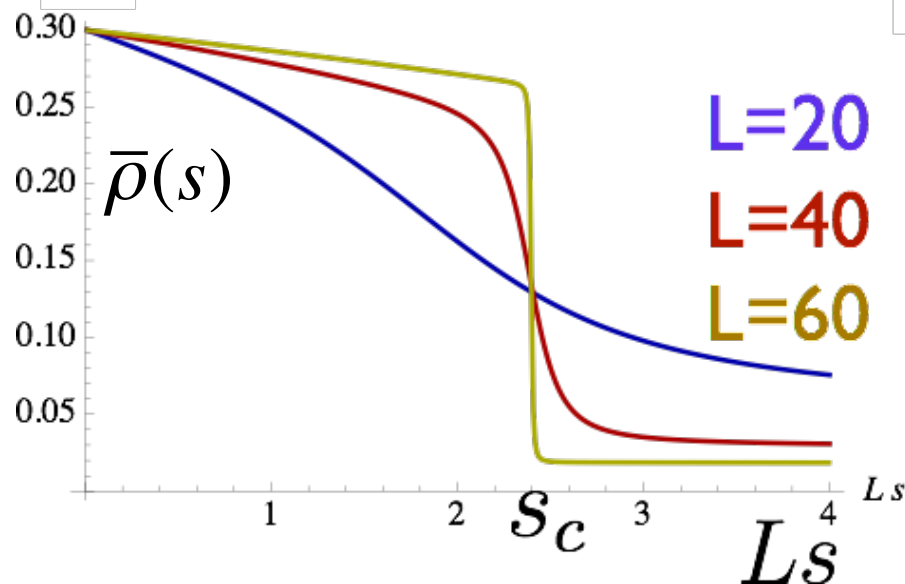
Finite size scaling

Biased total spin, biased susceptibility

Biased total spin (per site) $\bar{\rho}(s) = \sum_{\text{history}} P_s(\text{hist}) \frac{1}{\tau L} \int_0^\tau dt n(t)$

Biased susceptibility $\bar{\chi}(s) = \sum_{\text{history}} P_s(\text{hist}) \frac{1}{\tau L} \int_0^\tau dt [n(t) - L\bar{\rho}(s)]^2$

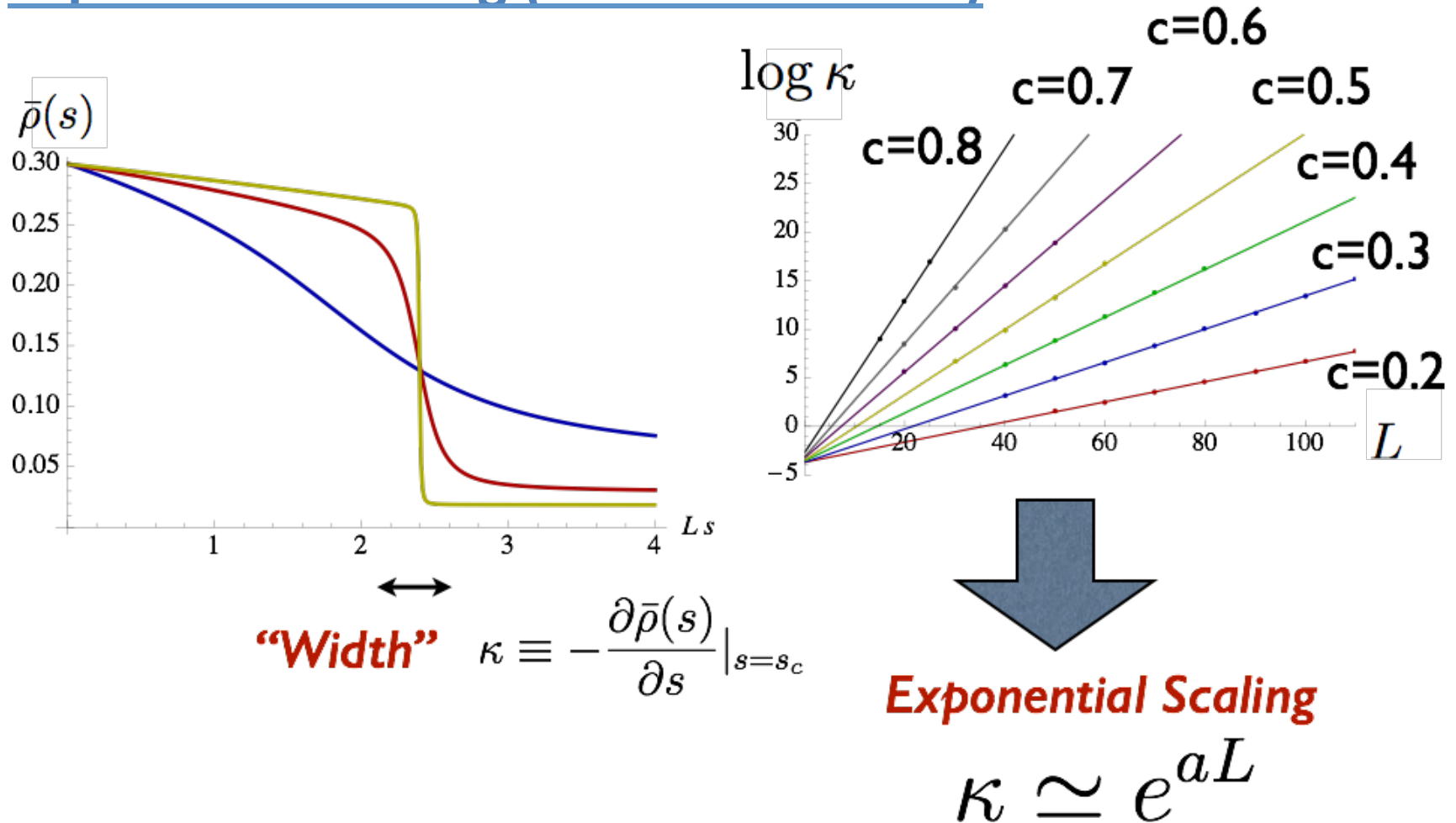
Numerical example (c=0.3)



1. Preliminary: Intro of mean-field FA

Finite size scaling

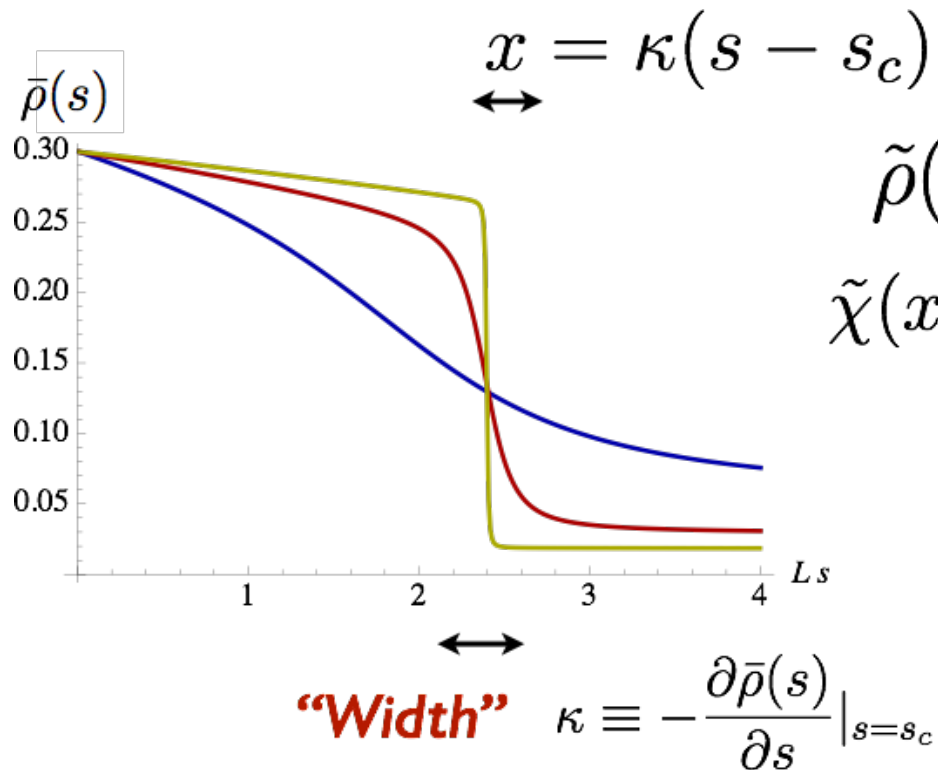
Exponential scaling (numerical check)



1. Preliminary: Intro of mean-field FA

Finite size scaling

Scaling function (numerical check)



1. Preliminary: Intro of mean-field FA

Finite size scaling

Scaling function (numerical check)

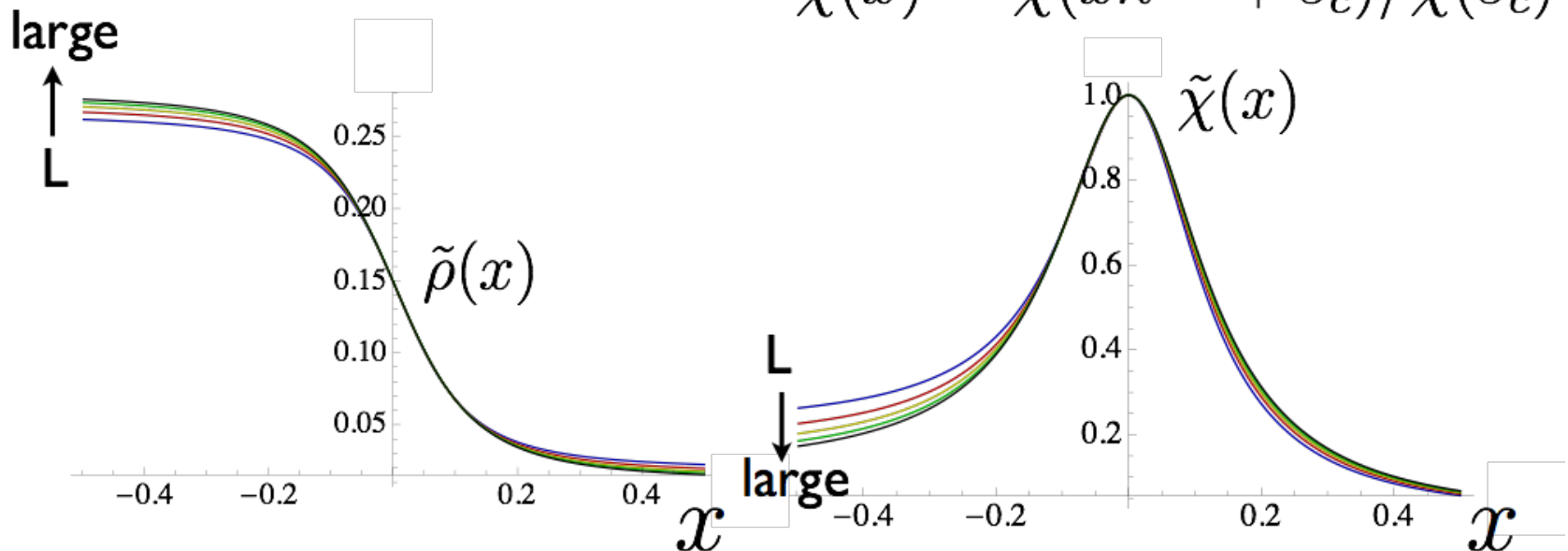
$$x = \kappa(s - s_c)$$

Q1. Analytical expression of these functions?

Q2. How to derive the exponential scaling?

$$\tilde{\rho}(x) = \bar{\rho}(x\kappa^{-1} + s_c)$$

$$\tilde{\chi}(x) = \bar{\chi}(x\kappa^{-1} + s_c) / \chi(s_c)$$



Construction of this talk

1. Preliminary: Introduction of mean-field FA
2. Problems and how to overcome it
3. Discussions

2. Problems and how to overcome it

Problem...?

C. Borgs and R. Kotecky, PRL, 68, 1734 (1992)

Equilibrium
phase transition

Partition function ← Number of phases

$$Z_{\text{per}}(L, h) \cong \sum_{q=1}^N \exp(-f'_q L^d)$$

Index for phases

“metastable free energy”

Dynamical
phase transition

Metastable free energy??
(No canonical distribution)

??

2. Problems and how to overcome it

Idea to solve

- Auxiliary dynamics

R. L. Jack and P. Sollich, Prog. Theor. Phys. Supp. 184, 304 (2010).

- Donsker-Varadhan type variational formula

e.g. J. P Garrahan et al, J. Phys. A, Math. Theor. 42 (2009) 075007

T. N. and S. Sasa, Phys. Rev. E 84, 061113 (2011)

$$P_s(\text{hist}) \approx P_s^{\text{aux}}(\text{hist})$$

s-ensemble \leftrightarrow **Modified system**

(Probability is not conserved)

(Probability is conserved)

$$w_s^{\text{mod}}(\mathbf{n} \rightarrow \mathbf{n}') = w(\mathbf{n} \rightarrow \mathbf{n}') e^{-s - (1/2)[h^*(\mathbf{n}') - h^*(\mathbf{n})]}$$

Modified transition rate Original transition rate

$$h^* \equiv \underset{h}{\text{Argmax}} \langle \lambda^{\text{mod}} - \lambda \rangle_s^{\text{mod}}$$

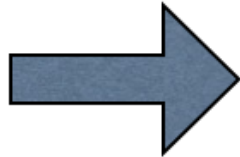
λ : Escape rate

2. Problems and how to overcome it

Idea to solve

- Modifying free energy $h^*(\mathbf{n})$

Original system with Detailed balance condition (DB)



Modified system also satisfies DB

$$w_s^{\text{mod}}(\mathbf{n} \rightarrow \mathbf{n}') = w(\mathbf{n} \rightarrow \mathbf{n}') e^{-s - (1/2)[h^*(\mathbf{n}') - h^*(\mathbf{n})]}$$

The equilibrium distribution function in the **modified system**:

$$P_{\text{eq}}^{\text{mod}}(\mathbf{n}) \propto P_{\text{eq}}(\mathbf{n}) e^{-h^*(\mathbf{n})}$$



Original equilibrium distribution

2. Problems and how to overcome it

Idea to solve

Numerical example of h^* ($L=100$)

$c = 0.3$

Blue: Modifying free energy $h^*(n)/L$

Red: Original free energy (=entropy)

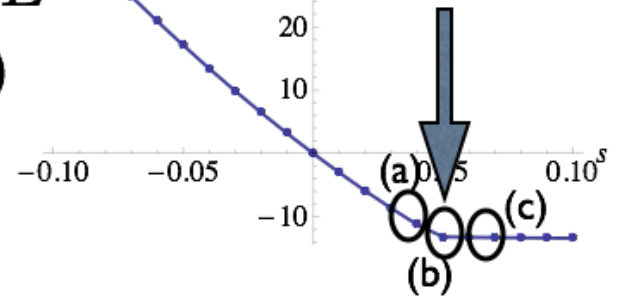
Yellow = **Red** + **Blue**

: Total effective free energy

DYNAMICAL free energy

$\psi_K(s)$

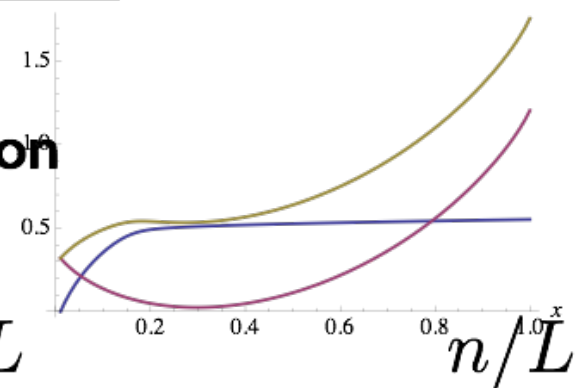
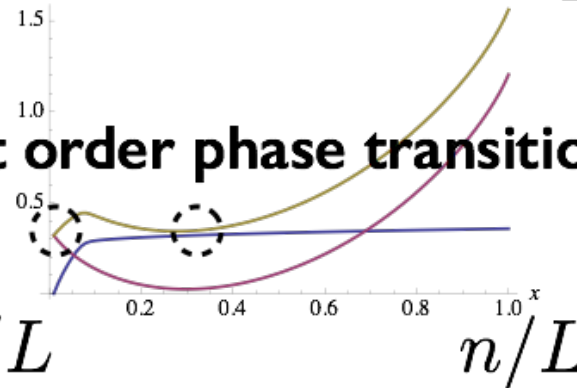
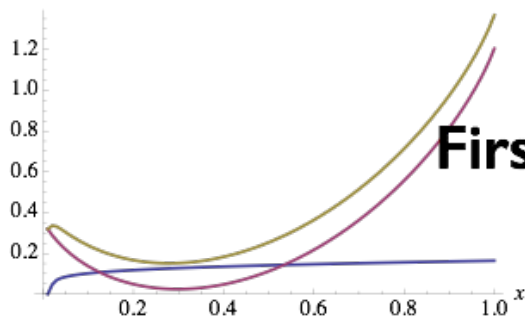
Transition point



(a) $s = 0.95s_c$

(b) $s = s_c$

(c) $s = 1.05s_c$



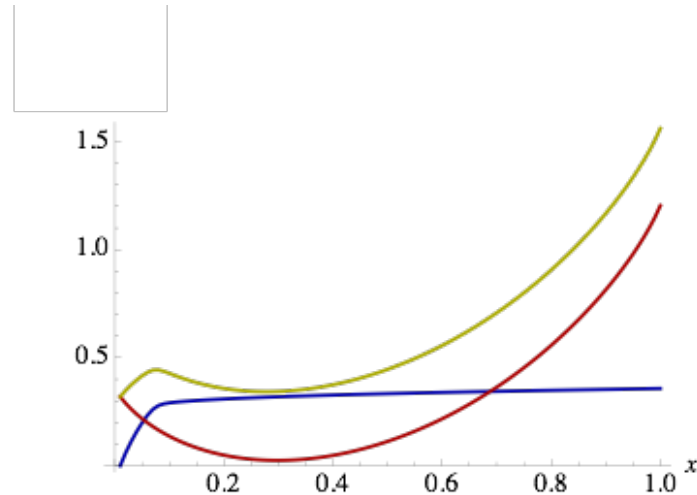
First order phase transition

2. Problems and how to overcome it

Idea to solve

- Non analytic point of h^* at $s = s_c$

For $L = 100$, we got



Blue: Modifying Hamiltonian $h^*(n)/L$

Red: Original Hamiltonian (=entropy)

Yellow = **Red** + **Blue**

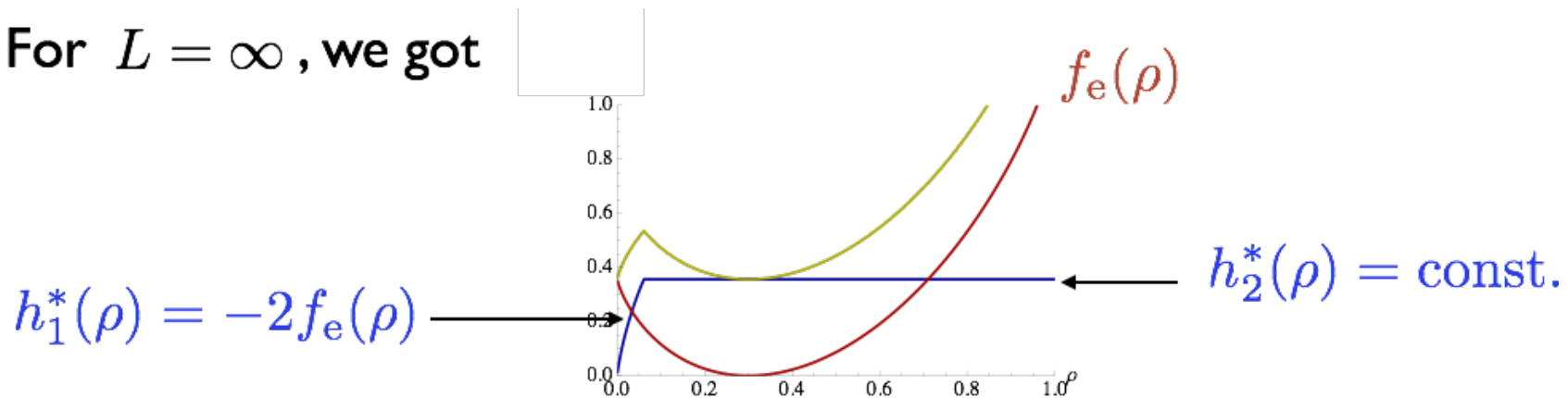
: Total effective Hamiltonian

2. Problems and how to overcome it

Idea to solve

- Non analytic point of h^* at $s = s_c$

For $L = \infty$, we got



Blue: Modifying Hamiltonian $h^*(n)/L$

Red: Original Hamiltonian (=entropy)

Yellow = Red + Blue

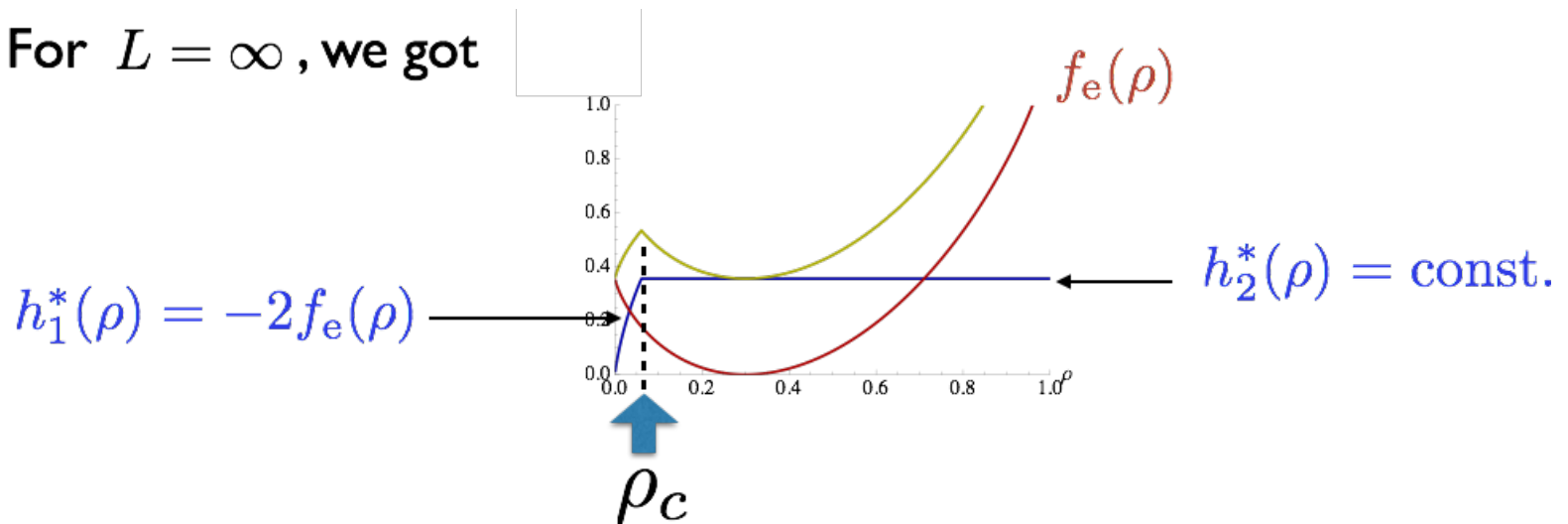
: Total effective Hamiltonian

2. Problems and how to overcome it

Idea to solve

- Non analytic point of h^* at $s = s_c$

For $L = \infty$, we got



ρ_c is determined by a condition of 1-st order phase transition:

$$(\rho_c = \lfloor n_c \rfloor)$$

$$\sum_{n \leq n_c} P_{\text{eq}}^{\text{mod}}(n) \Big|_{s=s_c} = \sum_{n > n_c} P_{\text{eq}}^{\text{mod}}(n) \Big|_{s=s_c}$$

Inactive phase $n \leq n_c$

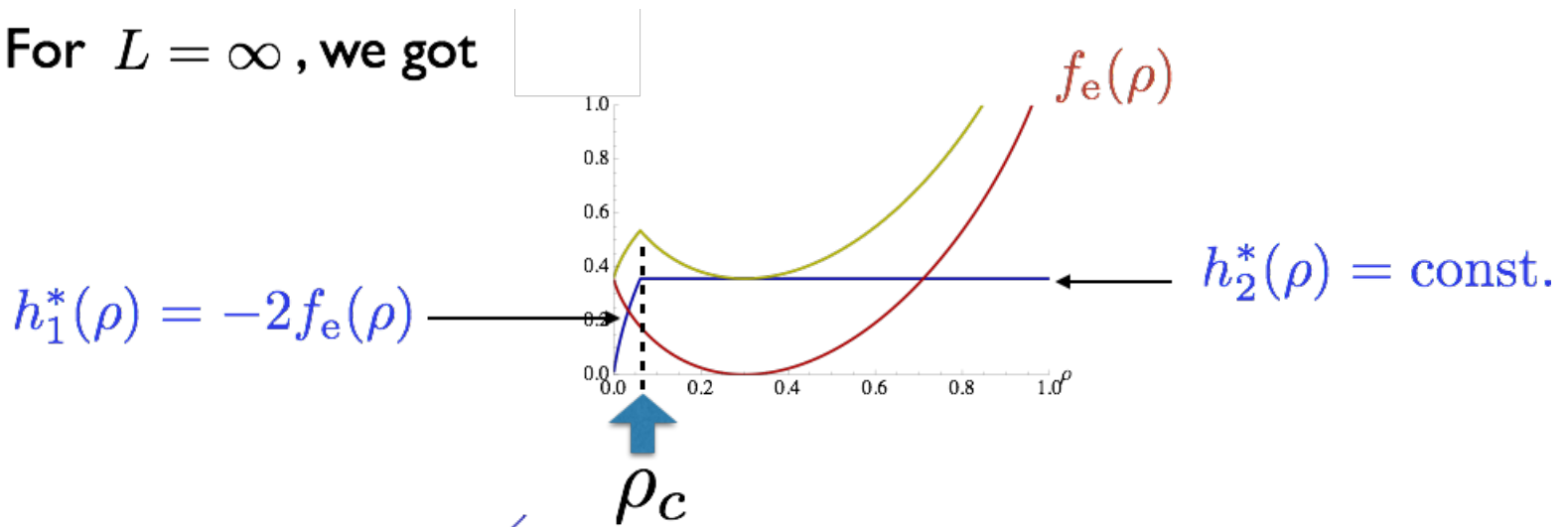
Active phase $n > n_c$

2. Problems and how to overcome it

Idea to solve

- Non analytic point of h^* at $s = s_c$

For $L = \infty$, we got

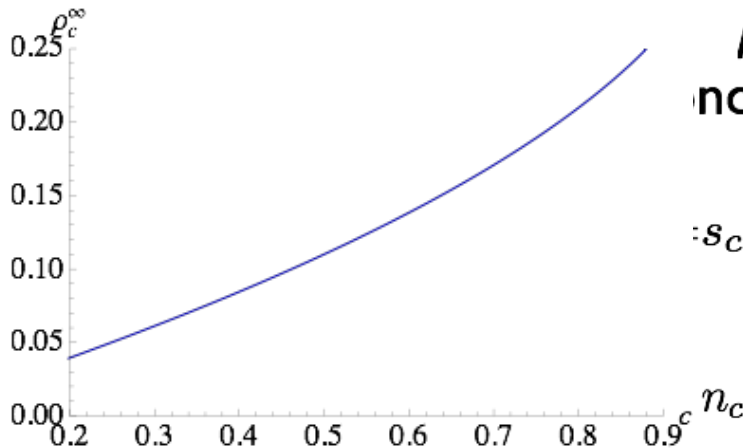


Condition of 1-st order phase transition:

$$(\rho_c = \lfloor n_c \rfloor)$$

$$s_c = \sum_{n > n_c} P_{\text{eq}}^{\text{mod}}(n) |_{s=s_c}$$

Active phase $n > n_c$



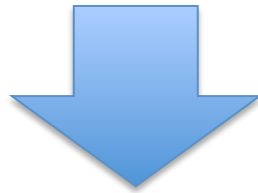
2. Problems and how to overcome it

Idea to solve

- Our ansatz

For finite L , we assume that we know, for $\mathcal{S} = \mathcal{S}_c$

$$\text{Distribution: } P_L^{s_c}(n) \propto \begin{cases} P_i(n) & n \leq n_c(L) \\ P_a(n) & n > n_c(L) \end{cases}$$



For $\mathcal{S} \sim \mathcal{S}_c$ we conjecture

$$P_{\text{eq}}^{\text{mod}}(n)|_{s \sim s_c} = \begin{cases} P_i(n)[1 + a^*(s)] & n \leq n_c \\ P_a(n)[1 - a^*(s)] & n > n_c \end{cases}$$

where $a^*(s)$ is an unknown function.

2. Problems and how to overcome it

Idea to solve

- Our ansatz

$$\bar{\rho}(s) = \frac{\langle \rho \rangle_i}{2} [1 + a^*(s)] + \frac{\langle \rho \rangle_a}{2} [1 - a^*(s)], \quad \rho \equiv n/L$$

$$\chi(s) = L \left\{ \frac{\langle \rho^2 \rangle_i}{2} [1 + a^*(s)] + \frac{\langle \rho^2 \rangle_a}{2} [1 - a^*(s)] - \rho(s)^2 \right\}$$



$$\langle f \rangle_i \equiv 2 \sum_{n \leq n_c} P_i(n) f(n)$$

$$\langle f \rangle_a \equiv 2 \sum_{n > n_c} P_a(n) f(n)$$

For $S \sim S_c$ we conjecture

$$P_{\text{eq}}^{\text{mod}}(n)|_{s \sim s_c} = \begin{cases} P_i(n)[1 + a^*(s)] & n \leq n_c \\ P_a(n)[1 - a^*(s)] & n > n_c \end{cases}$$

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2. Problems and how to overcome it

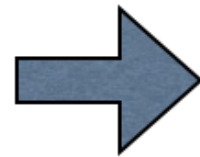
Idea to solve

- Our ansatz

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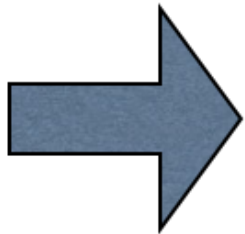
$$\chi(s) = L \left\{ \frac{\langle \rho^2 \rangle_i}{2} [1 + a^*(s)] + \frac{\langle \rho^2 \rangle_a}{2} [1 - a^*(s)] - \rho(s)^2 \right\}$$

How do we determine $a^*(s)$?



Variational formula

$$h^* \equiv \underset{h}{\text{Argmax}} \langle \lambda^{\text{mod}} - \lambda \rangle_s^{\text{mod}}$$



$$a^*(s) = \frac{2x}{\langle \rho \rangle_a - \langle \rho \rangle_i \sqrt{1 + 4x^2 [\langle \rho \rangle_a - \langle \rho \rangle_i]^{-2}}} \Big|_{x=\kappa(s-s_c)}$$

$$\kappa = \frac{1}{\Omega_{\pm}} \left[\left\langle \frac{\rho}{2} \right\rangle_i - \left\langle \frac{\rho}{2} \right\rangle_a \right] \left[\left\langle \frac{r}{2L} \right\rangle_i - \left\langle \frac{r}{2L} \right\rangle_a \right].$$

$$\Omega_{\pm} = 2 \frac{n_c}{L} c \left(1 - \frac{n_c}{L} \right) P_i(n_c) \frac{e^{-Lh_a((n_c+1)/L)/2}}{e^{-Lh_i(n_c/L)/2}} e^{-s}$$

2. Problems and how to overcome it

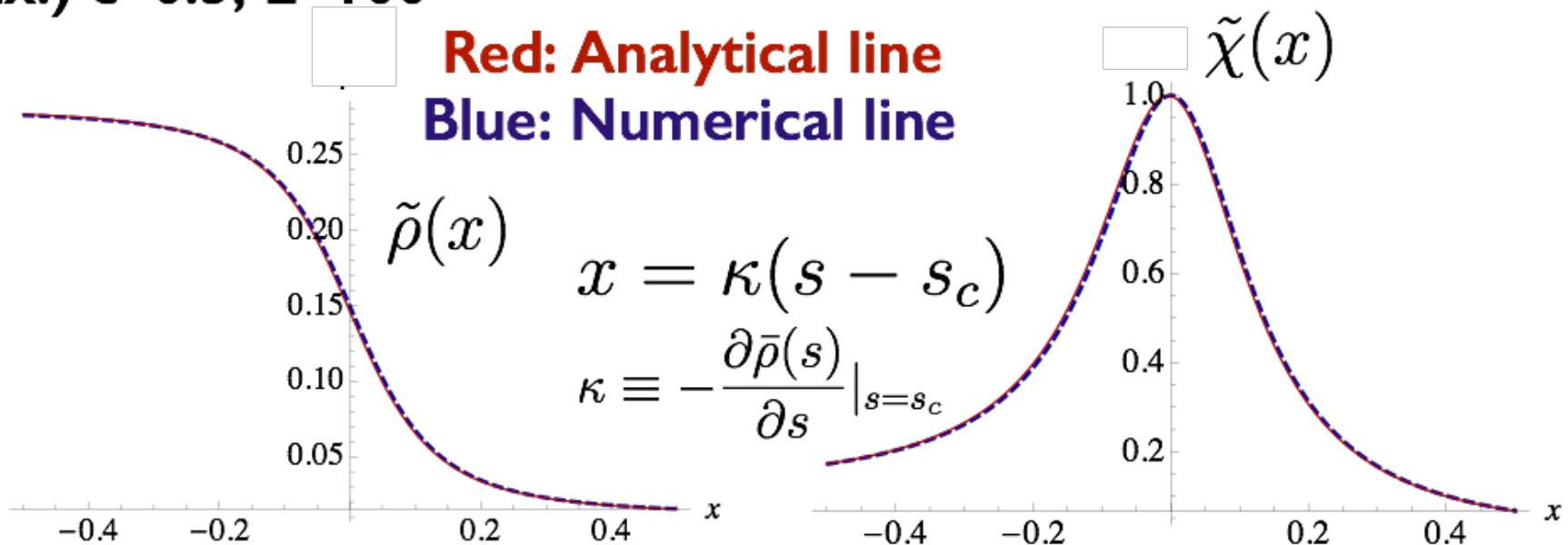
Idea to solve

- Scaling function

$$\tilde{\rho}(x) = \frac{1}{2} \left[\langle \rho \rangle_i + \langle \rho \rangle_a - \frac{2x}{\sqrt{1 + 4x^2 [\langle \rho \rangle_i - \langle \rho \rangle_a]^{-2}}} \right], \quad \rho \equiv n/L$$

$$\tilde{\chi}(x) = \frac{1}{\langle \rho^2 \rangle_i + \langle \rho^2 \rangle_a - [\langle \rho \rangle_i + \langle \rho \rangle_a]^2 / 2} \left[\langle \rho^2 \rangle_i + \langle \rho^2 \rangle_a - \frac{2x [\langle \rho^2 \rangle_i - \langle \rho^2 \rangle_a] [\langle \rho \rangle_i - \langle \rho \rangle_a]^{-1}}{\sqrt{1 + 4x^2 [\langle \rho \rangle_i - \langle \rho \rangle_a]^{-2}}} - 2\tilde{\rho}(x)^2 \right],$$

Ex.) $c=0.3, L=100$



2. Problems and how to overcome it

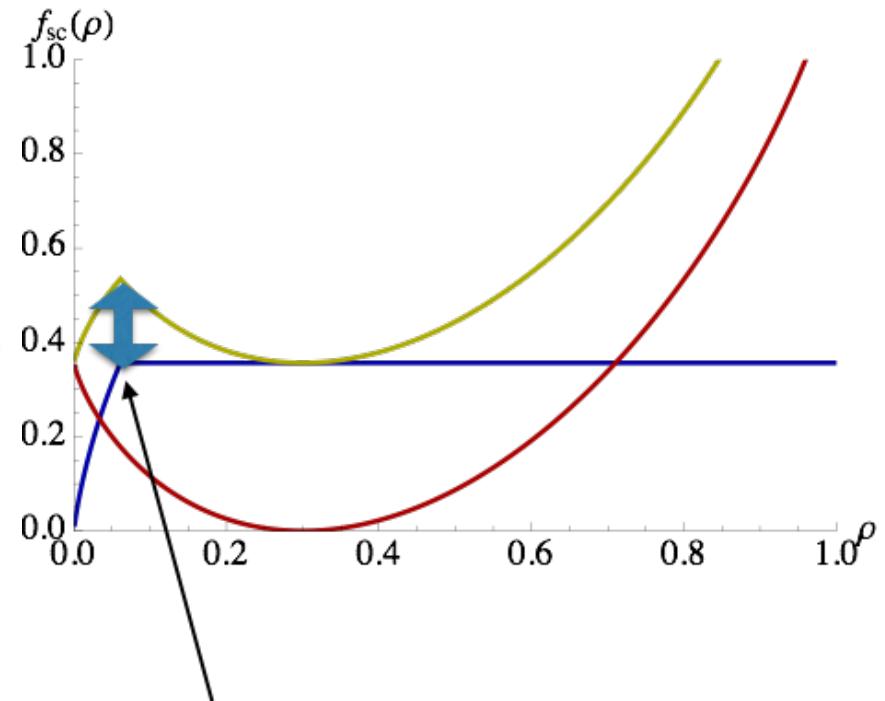
Idea to solve

- Scaling factor

$$K \cong e^{aL}$$



$$a = -\frac{1}{2} \log(1 - c)$$

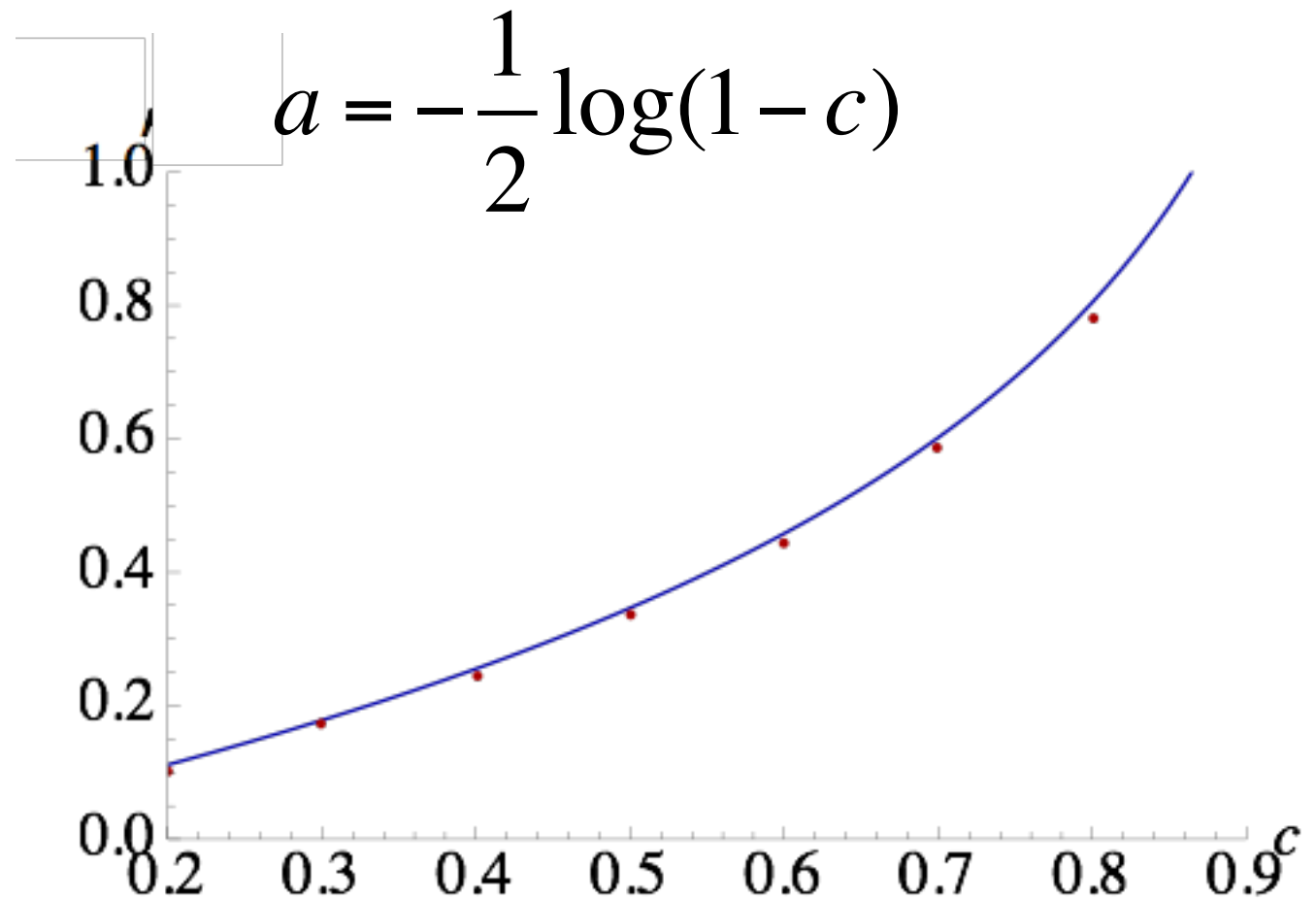


A is the potential height separating two phases

2. Problems and how to overcome it

Idea to solve

- Scaling factor

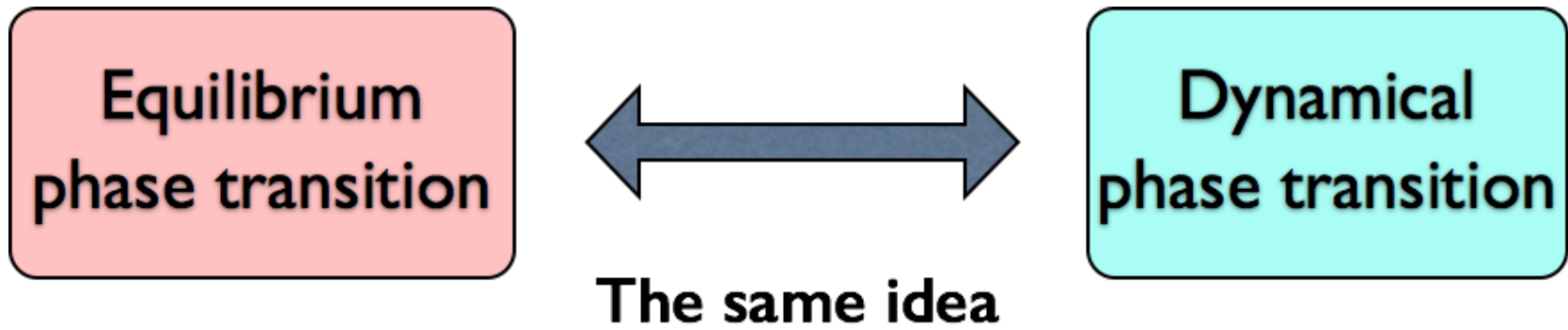


Construction of this talk

1. Preliminary: Introduction of mean-field FA
2. Problems and how to overcome it
3. Discussions

3. Discussions

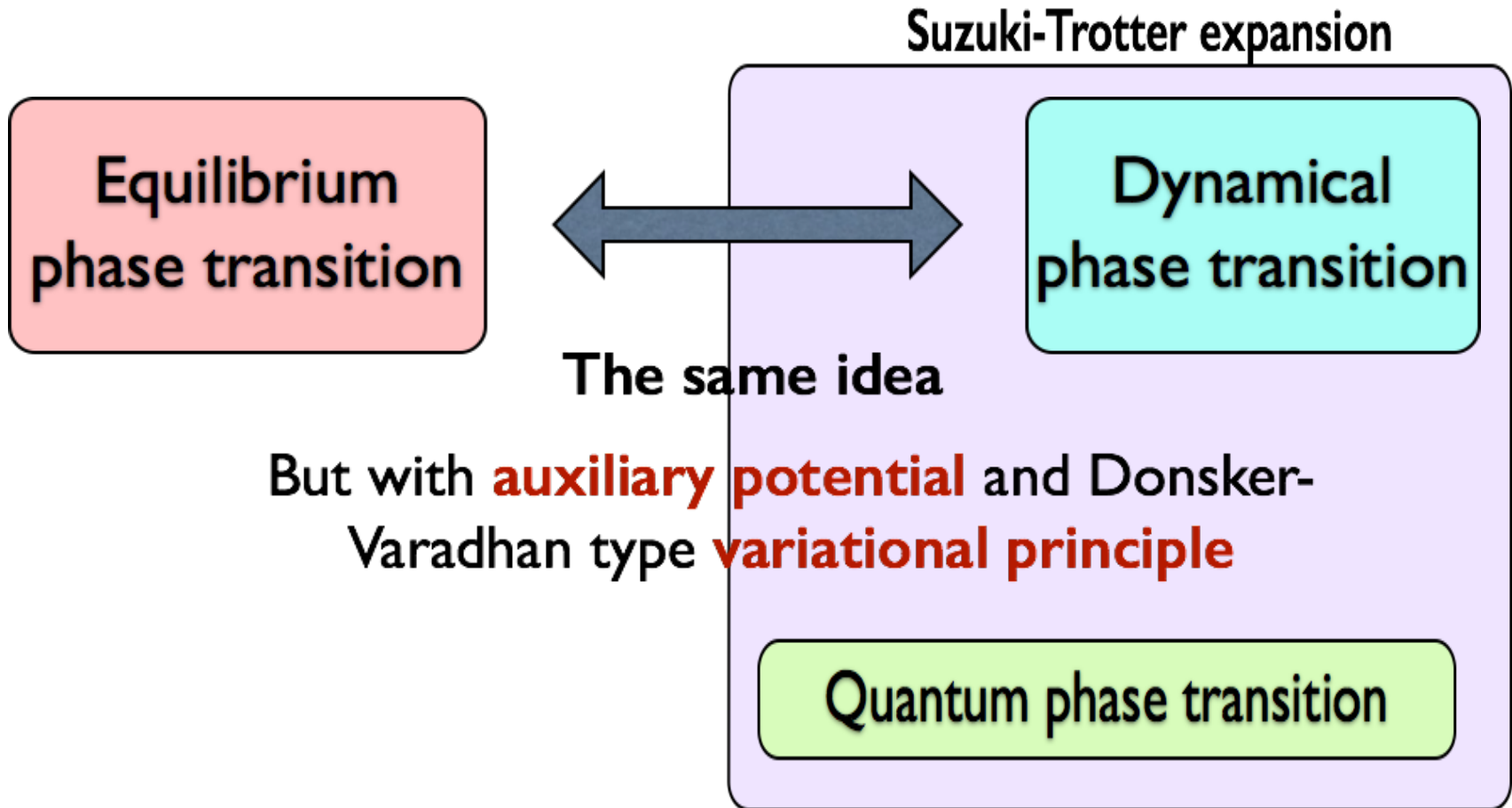
Quantum phase transitions



But with **auxiliary potential** and Donsker-Varadhan type **variational principle**

3. Discussions

Quantum phase transitions



3. Discussions

Quantum phase transitions

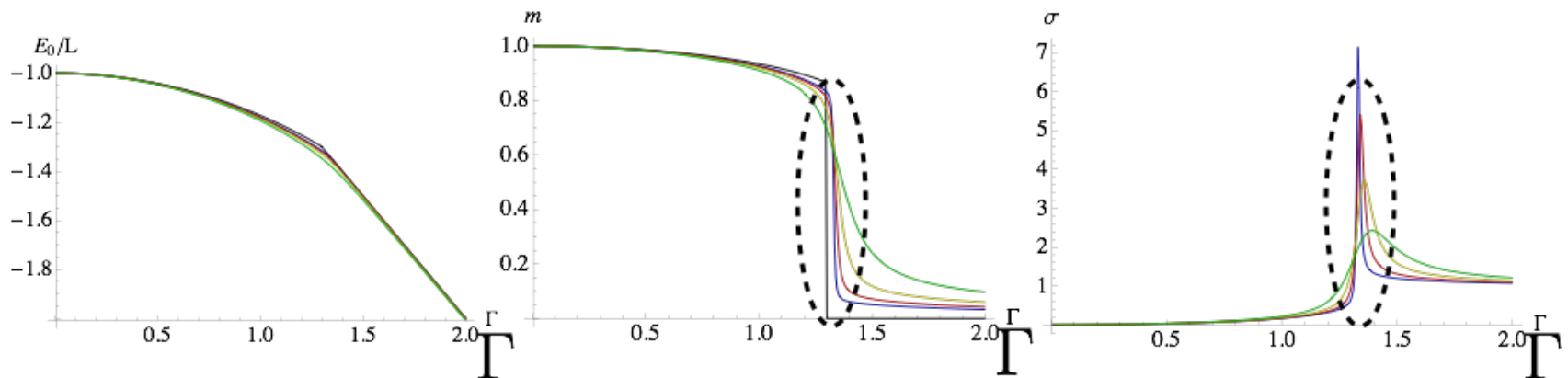
Model: Mean-field quantum ferromagnet with transverse field

Hamiltonian
$$\hat{H} = -L \left[(1/L) \sum_{i=1}^L \hat{\sigma}_i^z \right]^p - \Gamma L \left[(1/L) \sum_{i=1}^L \hat{\sigma}_i^x \right]$$

Victor Bapst and Guilhem Semerjian, *J. Stat. Mech.* **2012**, P06007 (2012).

$p > 2 \rightarrow$ Ground state energy show a (first order) phase transition

Ground state energy Ground state magnetization Ground state susceptibility



3. Discussions

Quantum phase transitions

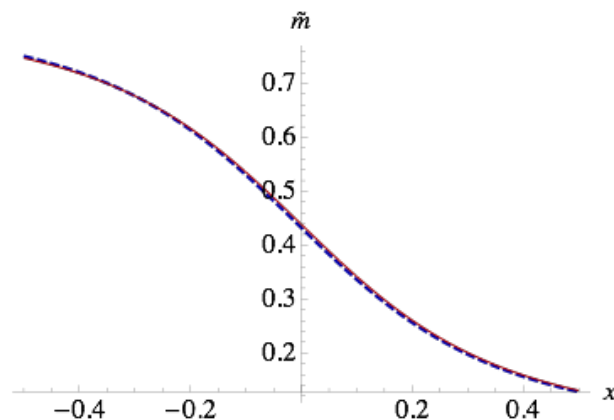
- Scaling function

$$\tilde{m}(x) = \frac{1}{2} \left[\langle m \rangle_p + \langle m \rangle_f - \frac{2x}{\sqrt{1 + 4x^2 [\langle m \rangle_p - \langle m \rangle_f]^{-2}}} \right]$$

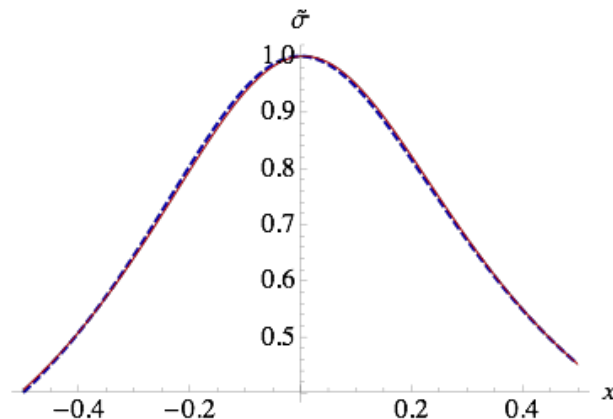
$$\tilde{\sigma}(x) = \frac{1}{C} \left[\langle m^2 \rangle_p + \langle m^2 \rangle_f - \frac{2x [\langle m^2 \rangle_p - \langle m^2 \rangle_f] [\langle m \rangle_p - \langle m \rangle_f]^{-1}}{\sqrt{1 + 4x^2 [\langle m \rangle_p - \langle m \rangle_f]^{-2}}} - 2\tilde{m}(x)^2 \right]$$

Ex.) p=3, L=70

Ground state magnetization



Ground state susceptibility



3. Discussions

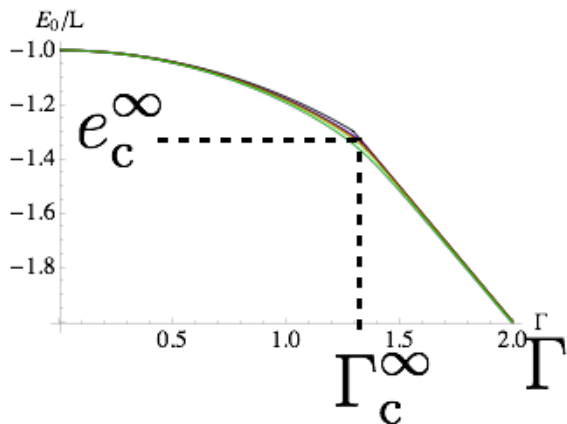
Quantum phase transitions

- Scaling factor

Victor Bapst and Guilhem Semerjian, *J. Stat. Mech.* **2012**, P06007 (2012).

Energy gap between the ground state and first excited state

$$a = \int_0^{m_{fe}^\infty} dm \log \left[-\frac{m^p + e_c^\infty}{\sqrt{1 - m^2 \Gamma_c^\infty}} + \sqrt{\left(\frac{m^p + e_c^\infty}{\sqrt{1 - m^2 \Gamma_c^\infty}} \right)^2 - 1} \right]$$




$$\kappa \simeq e^{aL}$$

Conclusion

- For mean field FA, we performed finite size scaling around 1st order phase transition.
- Idea is similar to classical one, but we used auxiliary potential and variational principle
- The dynamical phase transition is close to quantum phase transition: mean field quantum ferromagnet