メニュー

1. イントロダクション・ガラス転移とは

2. 流体力学から分子運動論まで:
   モード結合理論超入門

3. ランダム一次転移理論(RFOT):
   ガラスの平均場描像

4. ガラス理論の検証

5. 最近の研究から

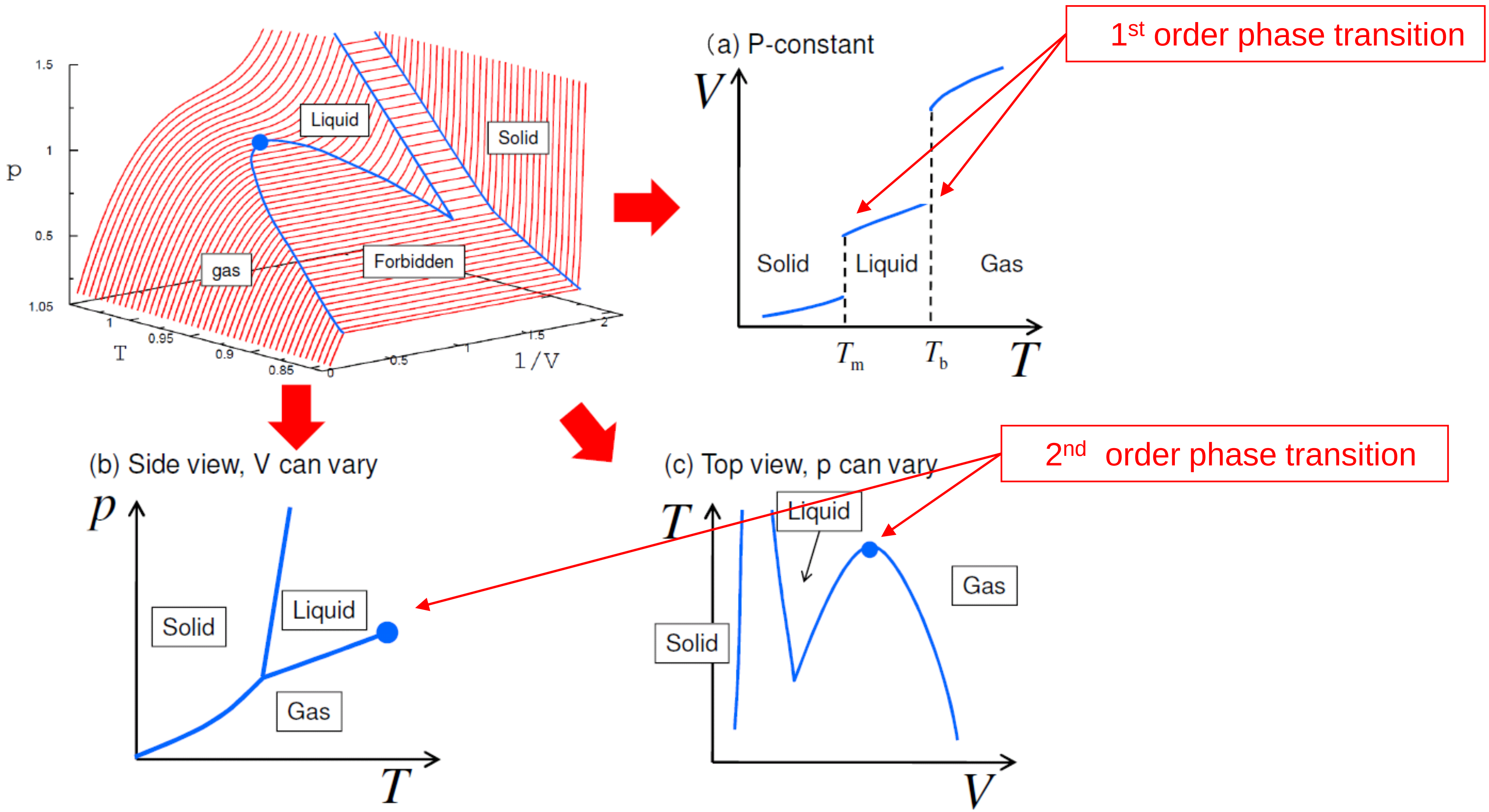
ランダム一次転移理論(RFOT):ガラスの平均場描像

- Introduction
- Thermodynamic theory of p3 spin glass
- Dynamic theory of p3 spin glass
- Translate to Glasses
- Finite Dimensional Systems

ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Introduction*

Phase diagram of atomic systems and Phase transition



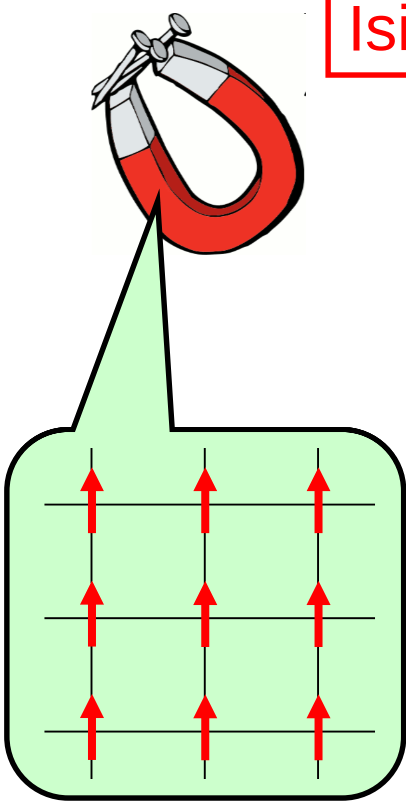
ランダム一次転移理論(RFOT):ガラスの平均場描像

● Introduction

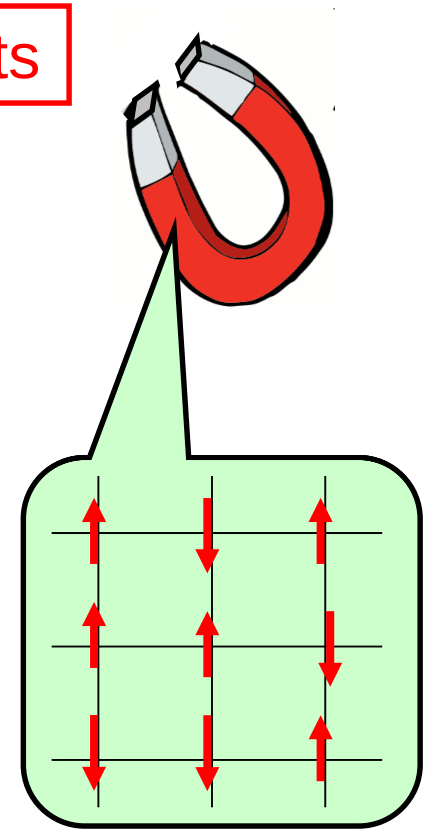
Mean Field Theory of 2nd order phase transition

Ising spin model of ferromagnets

$$H = -J \sum_{i,j} S_i S_j$$



Low temperature

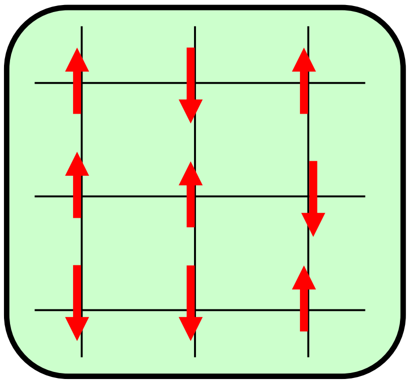


High temperature

ランダム一次転移理論(RFOT):ガラスの平均場描像

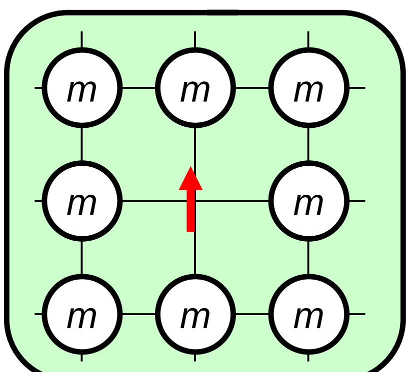
● *Introduction*

Mean Field Theory of 2nd order phase transition



$$H = -J\sum_{i,j} S_i S_j$$

mean field approximation



$$H = -J\sum_{i,j} S_i \langle S_j \rangle = -Jmz\sum_{i} S_i$$

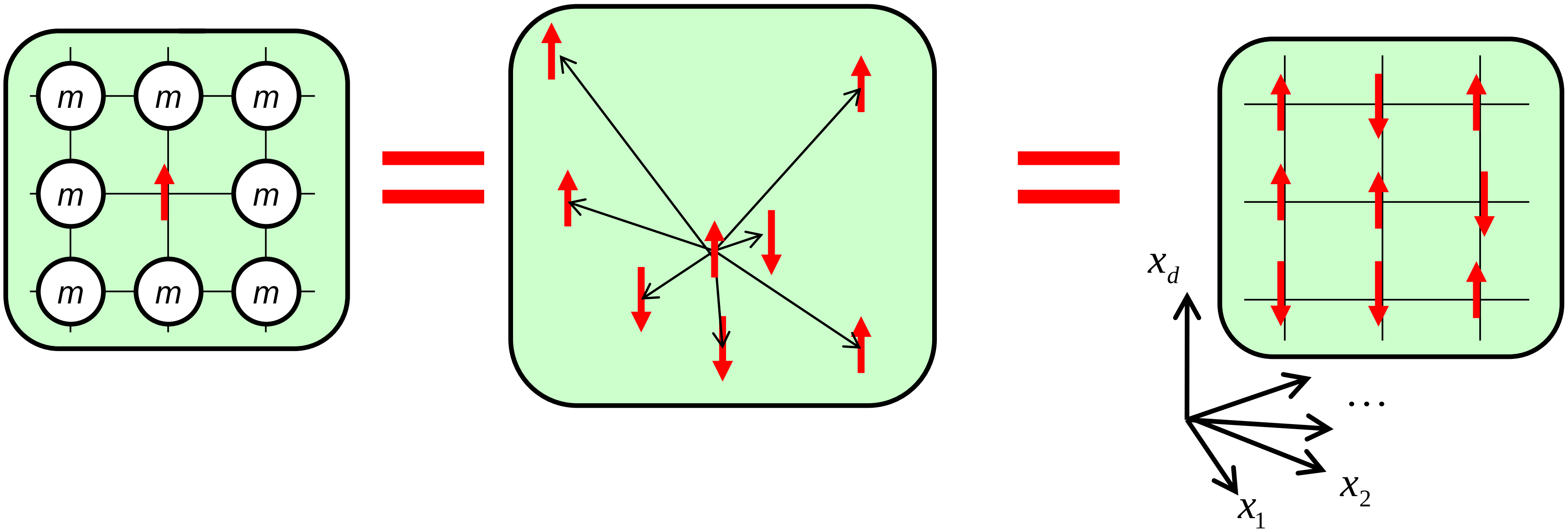
$$\langle S_j \rangle = m$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

● Introduction

Mean Field Theory of 2nd order phase transition

Mean field theory becomes exact if



The range of the interaction is infinitely long.

The spatial dimension is sufficiently large.

ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Introduction*

Mean Field Theory of 2nd order phase transition

Free energy functional as a function of “*m*” can be computed as

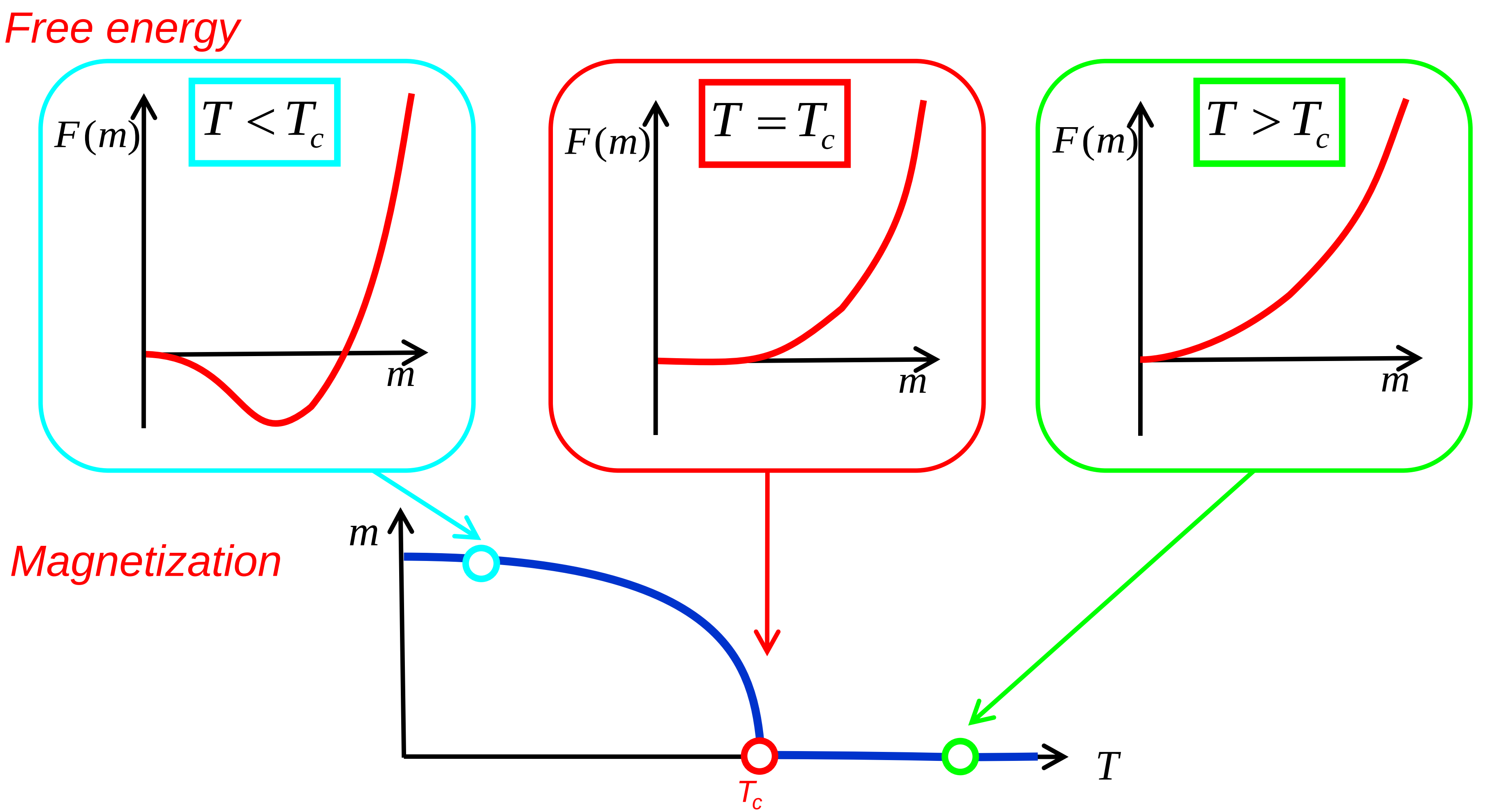
$$Z(m,T) = \mathrm{Tr}\,\delta\left(m - \frac{1}{N}\sum S_i\right)\exp[-\beta H]$$

$$F(m,T) = -kT\log Z(m,T) = \frac{J}{2}m^2 - \log\left[2\cosh\left(\beta Jm\right)\right]$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

● Introduction

Mean Field Theory of 2nd order phase transition



ランダム一次転移理論(RFOT):ガラスの平均場描像

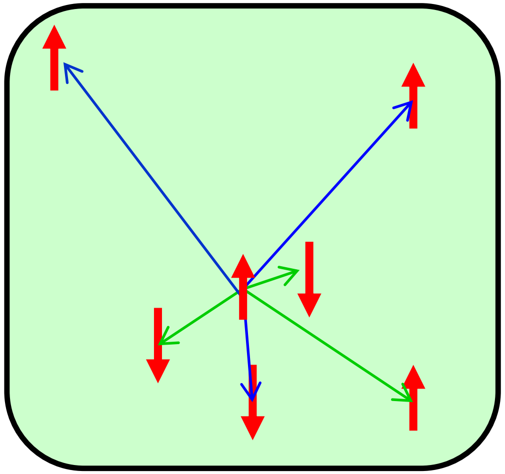
● Introduction

Mean Field Theory of 1st order phase transition

p=3 Ising spin model of ferromagnets

$$H = -J \sum_{i,j,k} S_i S_j S_k$$

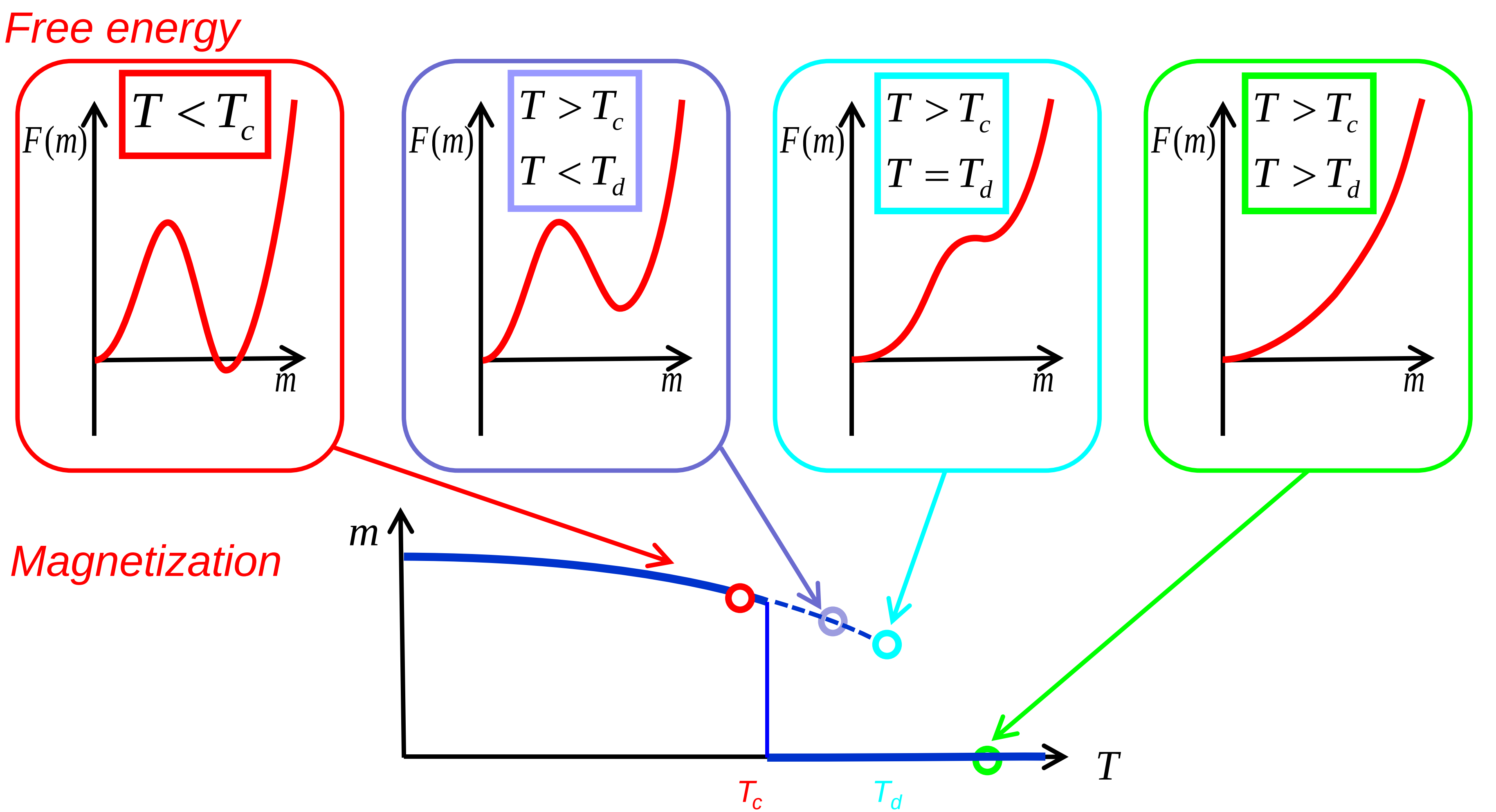
$$F(m,T) = \frac{J}{3} m^3 - \log\left[2\cosh\left(\beta J m^2 / 2\right)\right]$$



ランダム一次転移理論(RFOT):ガラスの平均場描像

● Introduction

Mean Field Theory of 1st order phase transition



ランダム一次転移理論(RFOT):ガラスの平均場描像

● Thermodynamic theory of p3 spin glass

Spin-Glass transition

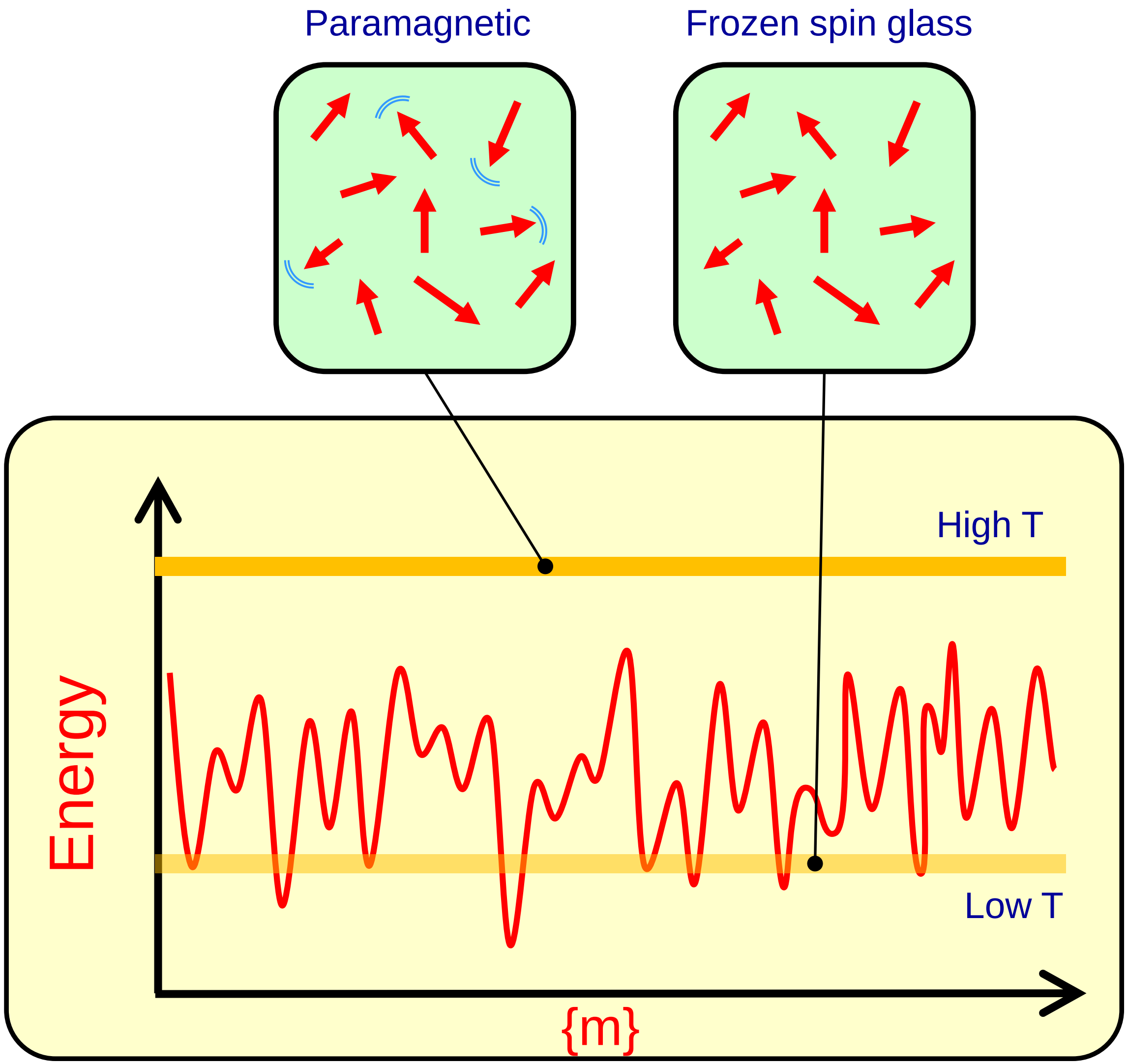
$$H = -\sum_{i,j,k} J_{ijk} S_i S_j S_k$$

$$P(J_{ijk}) \propto \exp[-AJ_{ijk}^2]$$

Order parameter: Overlap

$$\bar{q} = \frac{1}{N}\overline{\sum_{i=1}^{N} \langle S_i \rangle^2}$$

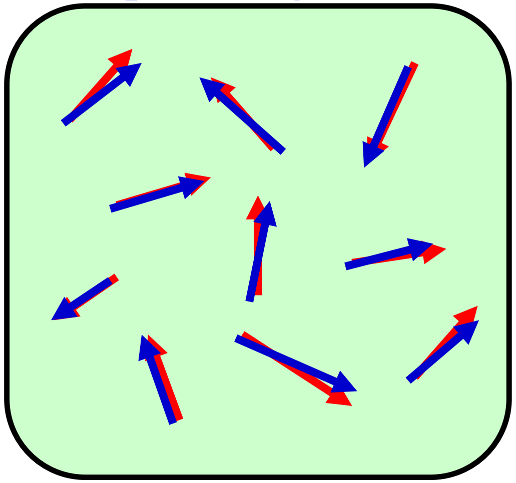
$$m = \frac{1}{N}\overline{\sum_{i=1}^{N} \langle S_i \rangle} = 0$$ is no good.



ランダム一次転移理論(RFOT):ガラスの平均場描像

● Thermodynamic theory of p3 spin glass

Overlap quantifies how much their configuration is similar if they fall into the same stable basin

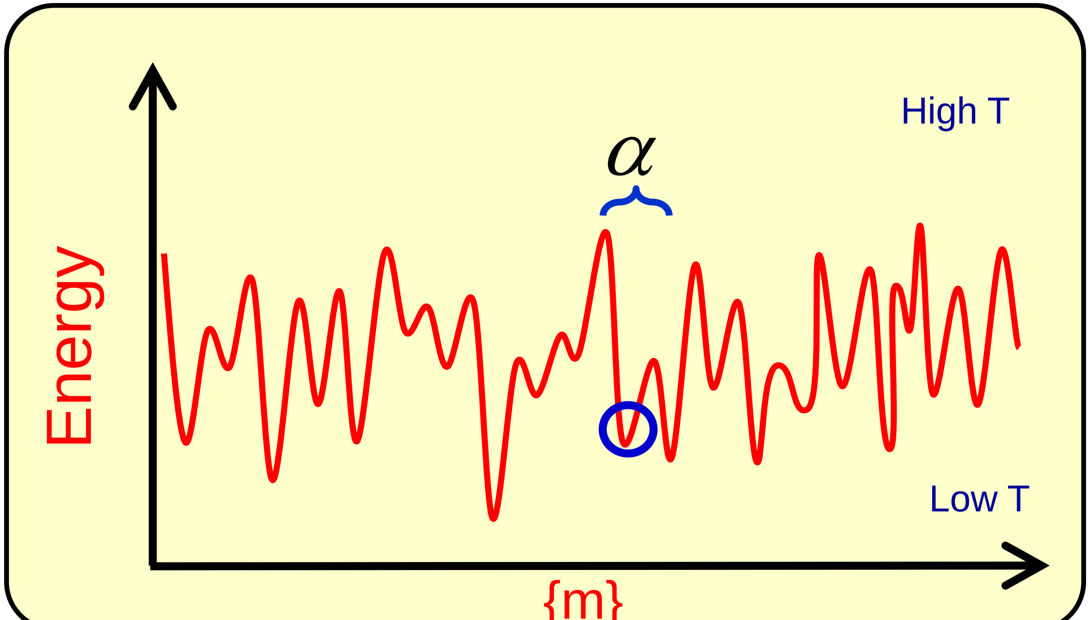


Order parameter: Overlap

$$\bar{q} = \frac{1}{N}\overline{\sum_{i=1}^{N} \left\langle S_i \right\rangle^2}$$

$$= \frac{1}{N}\overline{\sum_{i=1}^{N} Tr S_i^a S_i^b \exp[-\beta(H^a + H^b)]}$$

$$= \frac{1}{N}\overline{\sum_{i=1}^{N} \left\langle S_i^a S_i^b \right\rangle}$$



ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Thermodynamic theory of p3 spin glass*

A good introduction for beginners
T. Castellani and A. Cavagna, *"Spin-glass theory for pedestrians"*
J. Stat. Mech. Theory and Experiment, P05012 (2005)

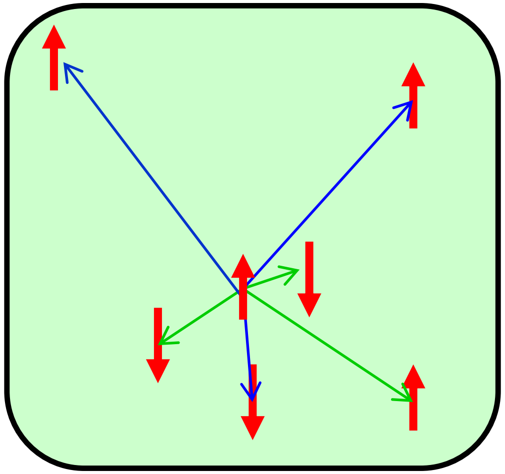
p=3 Spherical Spin Glass model

$$H = -\sum_{i,j,k} J_{ijk} S_i S_j S_k$$

with spherical constraint

$$\sum_{i=1}^{N} S_i^2 = N$$

$$P(J_{ijk}) \propto \exp[-A J_{ijk}^2]$$



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- ***Thermodynamic theory of p3 spin glass***

Free energy can be computed using *the* replica method

$$F = -kT\overline{\log Z} = -kT\lim_{n\to 0}\frac{\overline{Z^n}-1}{n}$$

"The Equation of State of the overlap q"

$$\Rightarrow \begin{cases} \overline{q} = 0 & T > T_K \\ \overline{q} \neq 0 & T < T_K \end{cases}$$

Spin Glass Transition

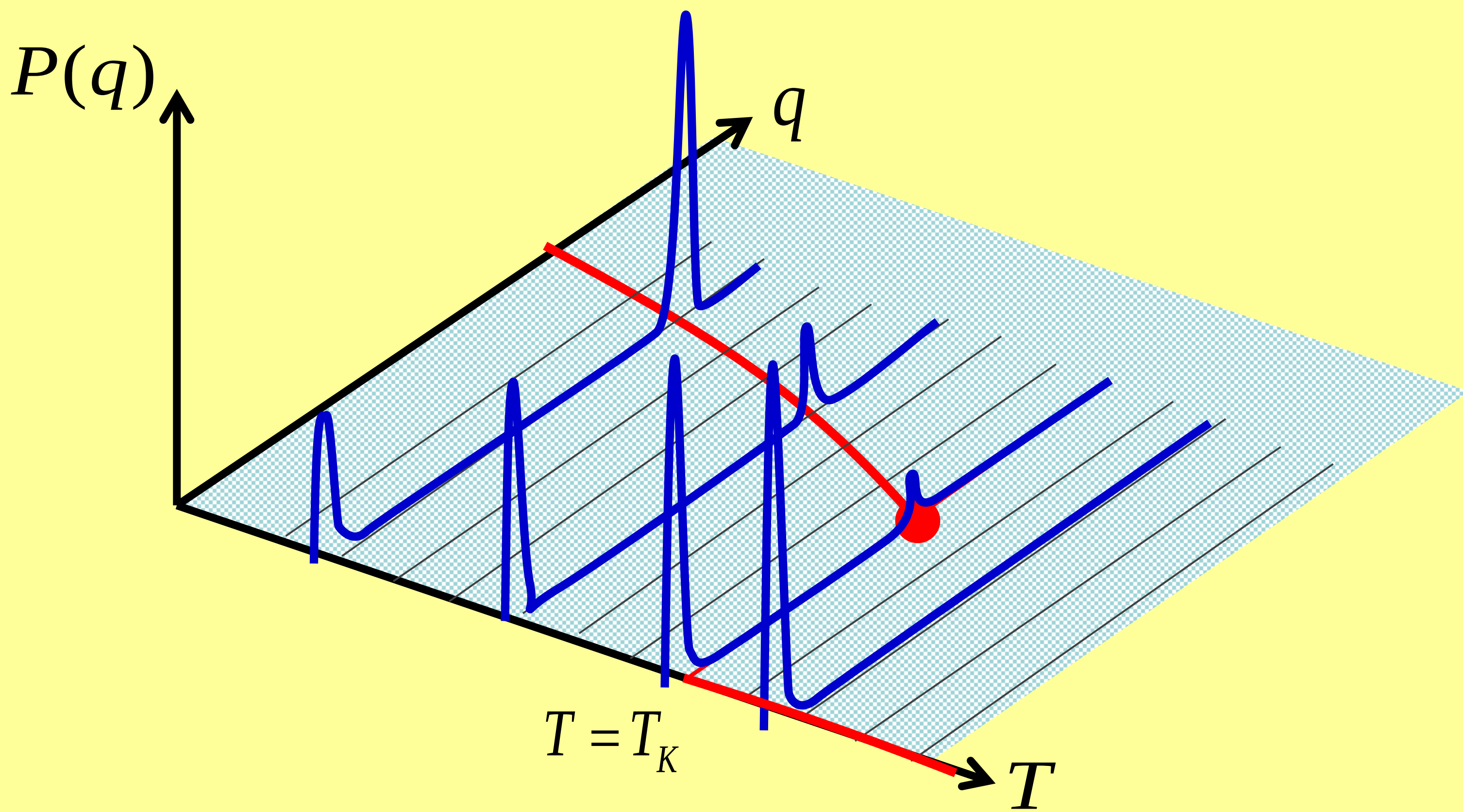
One-Step Replica Symmetry Breaking Transition (1RSB)

ランダム一次転移理論(RFOT):ガラスの平均場描像

- ***Thermodynamic theory of p3 spin glass***

One-Step Replica Symmetry Breaking Transition (1RSB)

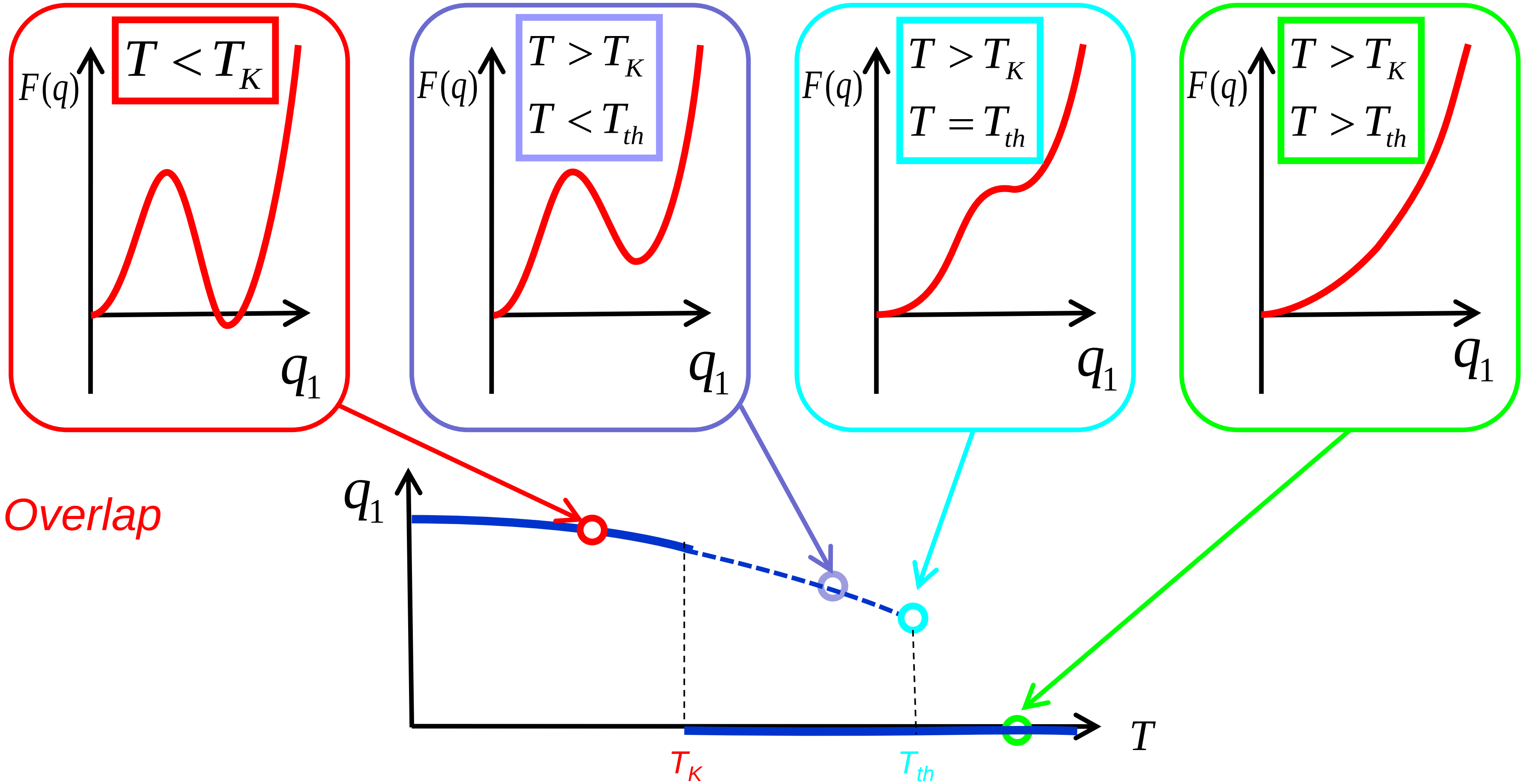
Distribution of the overlap



ランダム一次転移理論(RFOT)：ガラスの平均場描像

● Thermodynamic theory of p3 spin glass

Free energy as a function of Overlap



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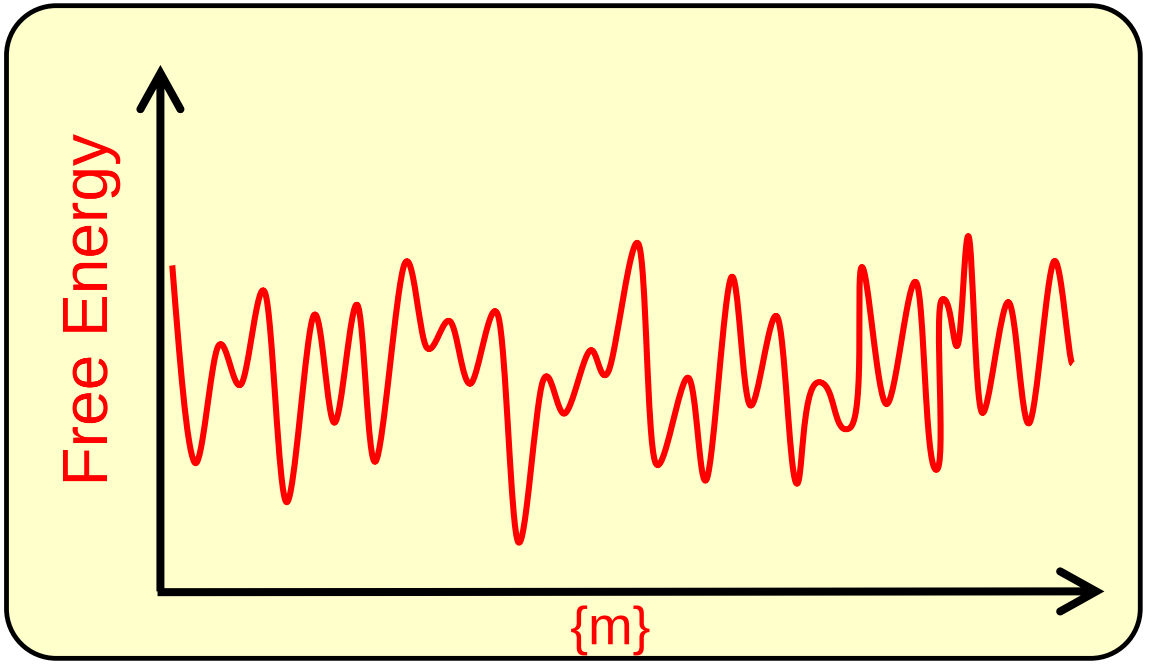
● Thermodynamic theory of p3 spin glass

A Free energy as a functional of the magnetization for a given random potential: TAP free energy

$$f_{TAP}(\{m\},T) = -\frac{1}{N}F_{TAP}(m_1, m_2, \cdots, m_N, T)$$

$$= -\frac{1}{N}\sum_{i,j,k} J_{ijk} m_i m_j m_k - \frac{T}{2}\ln(1-q_1) - \frac{4}{T}\left(2q_1^{\,3} - 3q_1^{\,2} + 1\right)$$



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● *Thermodynamic theory of p3 spin glass*

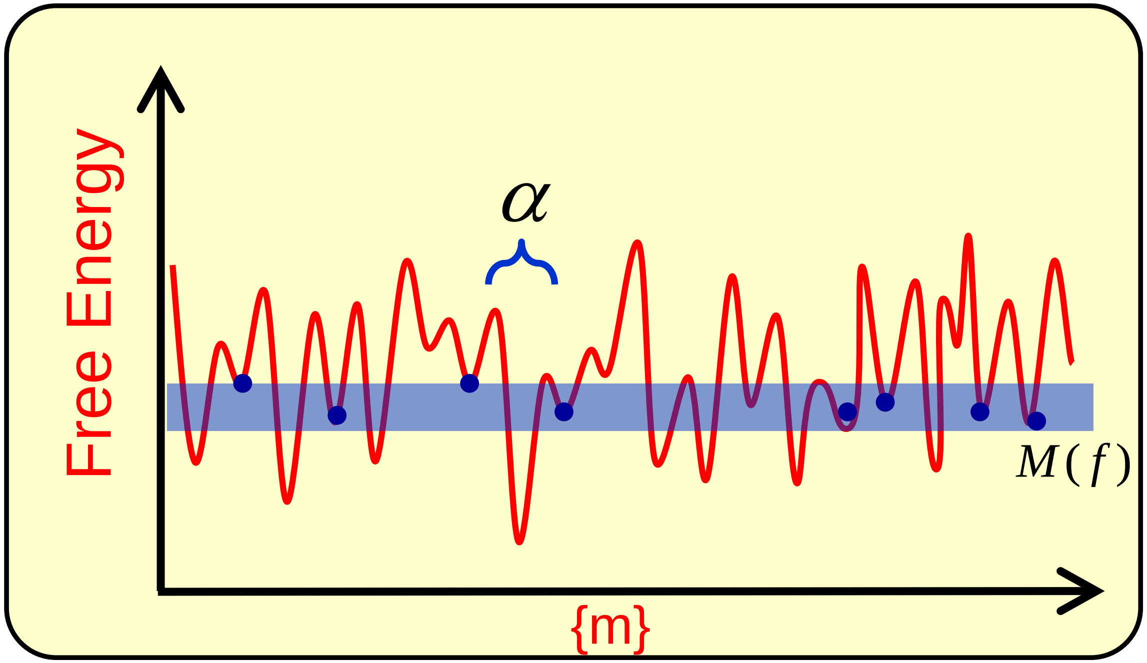
Alternative way to express the free energy in terms of its free energy landscape

$$Z = \sum_{\{S\}} \exp[-\beta H] = \sum_{\alpha} Z_{\alpha} = \sum_{\alpha} \exp[-\beta N f_{\alpha}]$$

$$= \int df \, M(f) e^{-\beta N f}$$

α : Each state (basin) separated by the maxima

$M(f)$: Number of minima



ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Thermodynamic theory of p3 spin glass*

Alternative way to express the free energy in terms of its free energy landscape

$$\overline{Z} = \overline{\int df \; M(f) e^{-\beta N f}} = \exp\left[N(-\beta f^* + S_c(f^*))\right]$$

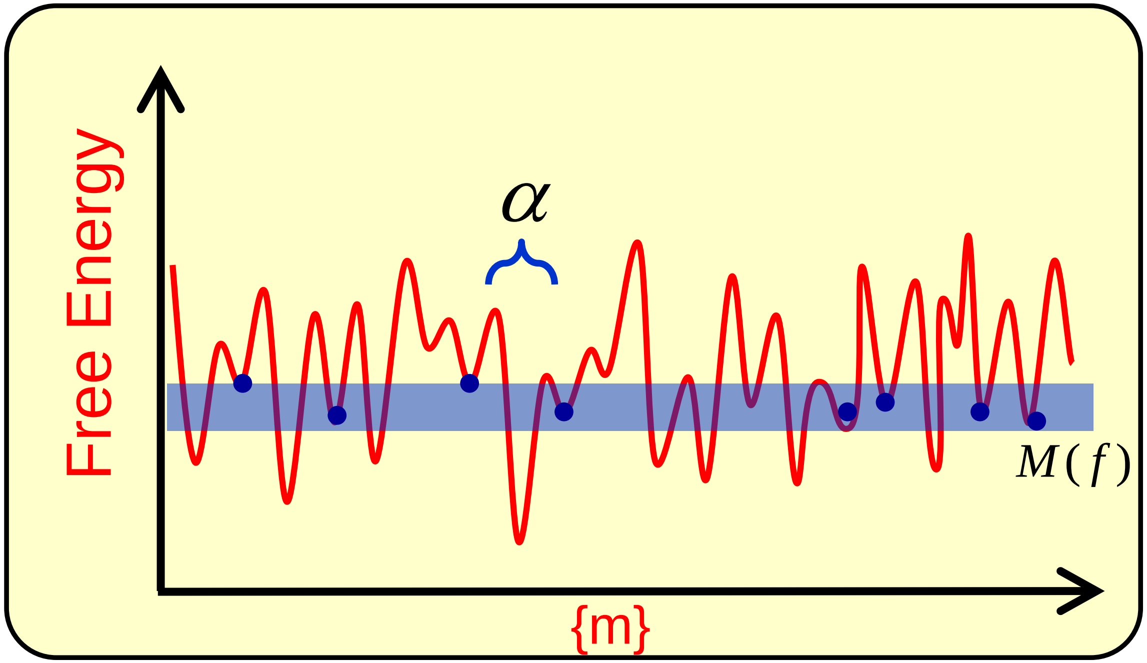
After taking the saddle points

or

$$\frac{F}{N} = -\frac{kT}{N}\ln \overline{Z} = f^* - TS_c(f^*)$$

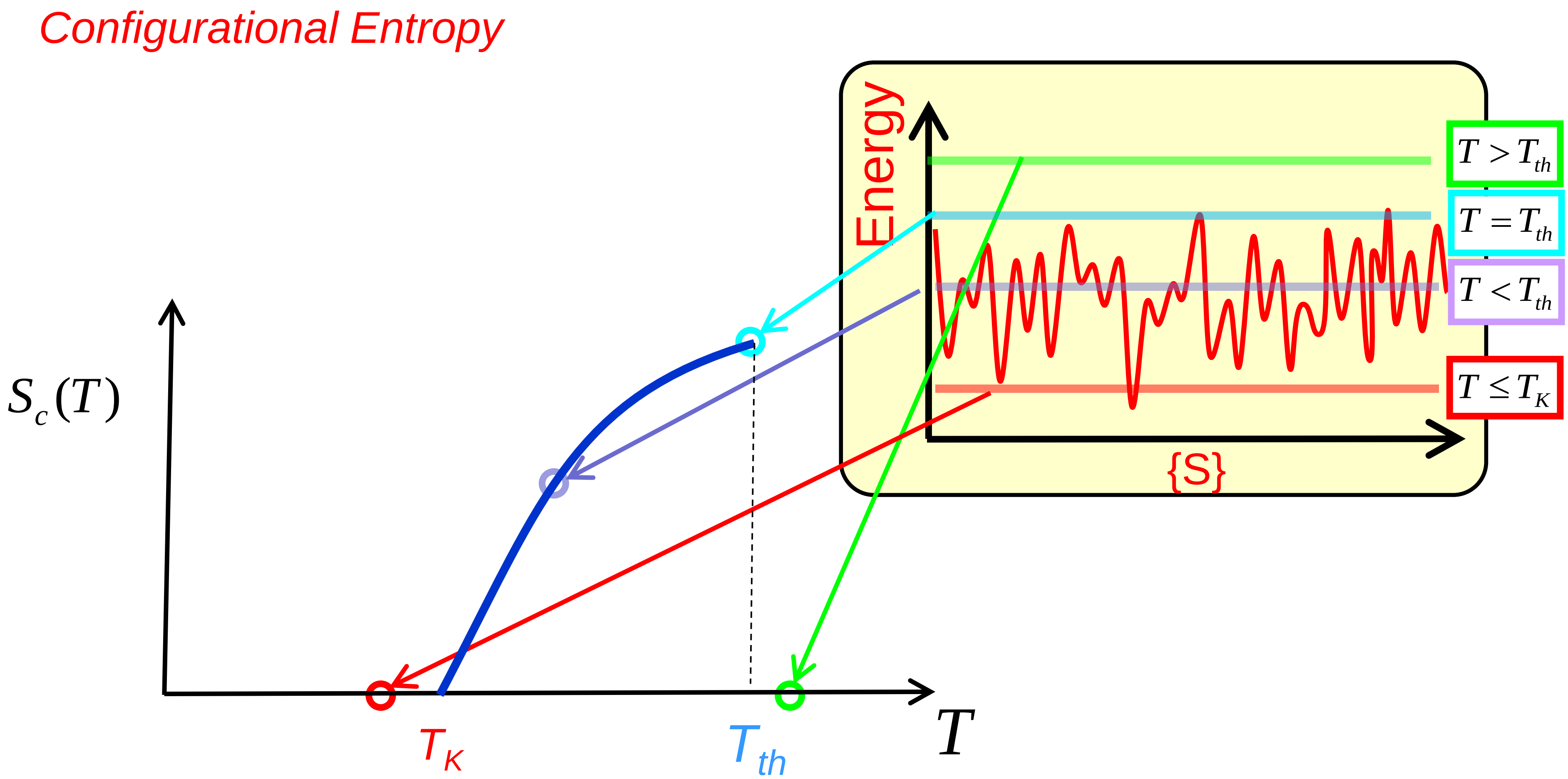
$$S_c(f) = \ln M(f)$$

Configurational Entropy



ランダム一次転移理論(RFOT):ガラスの平均場描像

● Thermodynamic theory of p3 spin glass



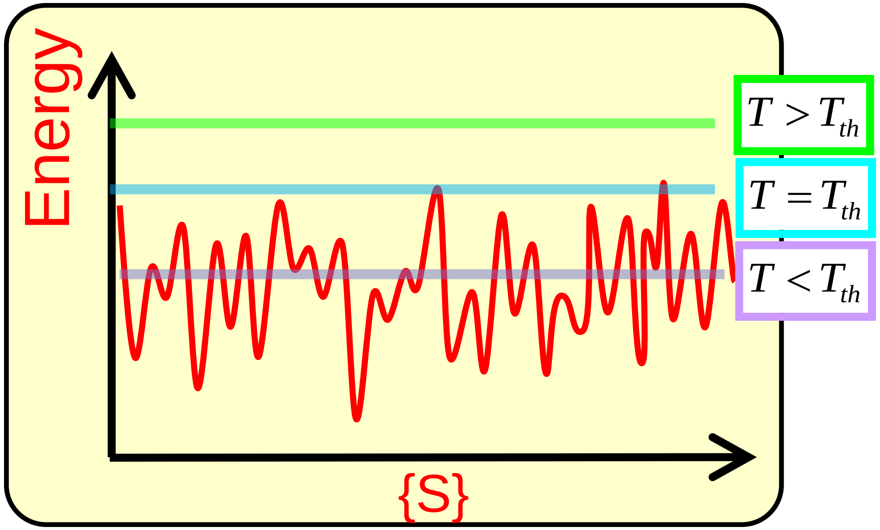
ランダム一次転移理論(RFOT):ガラスの平均場描像

● Thermodynamic theory of p3 spin glass

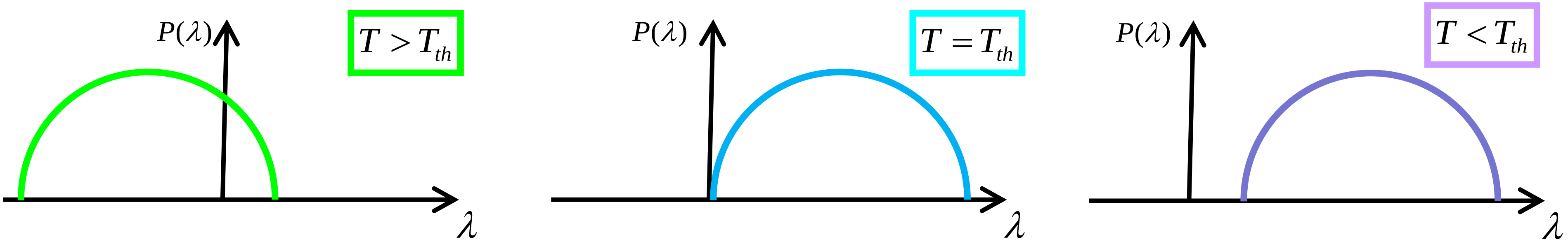
Distribution of Hessians of Energy

$$P(\lambda) = \overline{\left\langle \sum_{\nu} \delta(\lambda - \lambda_{\nu}) \right\rangle}$$

λ_{ν} : Eigenvalue of Hessian $\dfrac{\partial^2 H}{\partial S_i \partial S_j}$



Unstable to Saddles to Minima



ランダム一次転移理論(RFOT)：ガラスの平均場描像

● Dynamic theory of p3 spin glass

Langevin equation for the p3 spherical spin model

$$\dot{S}_i = -\mu S_i - \frac{\partial H}{\partial S_i} + \eta_i \qquad H = -\sum_{i,j,k} J_{ijk} S_i S_j S_k$$

Lagrange multiplier (μ)

Random force (η_i)

$$\left\langle \eta_i(t)\eta_j(t')\right\rangle = kT\delta_{ij}\delta(t-t')$$

$$\dot{S}_i = -\mu S_i - \sum_{i,j,k} J_{ijk} S_j S_k + \eta_i$$

We want to evaluate dynamics for

$$C(t) = \frac{1}{N}\overline{\left\langle \sum_i S_i(t) S_i(0) \right\rangle}$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

- **Dynamic theory of p3 spin glass**

Deriving the correlation function for nonlinier Langevin equation

$$\dot{S}_i = -\mu S_i - \sum_{i,j,k} J_{ijk} S_j S_k + \eta_i$$

Mathematical structure is exactly the same as the liquid!

$$\frac{dC(t)}{dt} = -TC(t) - \frac{3J^2}{2T}\int_0^t dt' \, C^2(t-t') \frac{dC(t')}{dt'}$$

cf: MCT

$$\frac{\partial F(k,t)}{\partial t} = -\frac{Dk^2}{S(k)} F(k,t) - \int_0^t dt' \, M(k,t-t') \frac{\partial F(k,t')}{\partial t'}$$

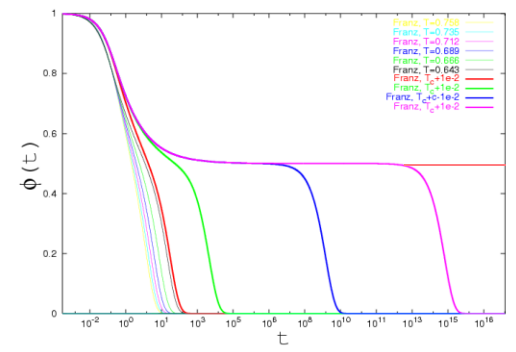
$$M(k,t) = \int dq \, V(q,k-q) F(q,t) F(k-q,t)$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Dynamic theory of p3 spin glass*

● *Critical behavior is also identical with MCT!*

$$\frac{dC(t)}{dt} = -TC(t) - \frac{3J^2}{2T}\int_0^t dt'\, C^2(t-t')\frac{dC(t')}{dt'}$$



● *Nonergodic transition point matches with Threshold Temperature of the free energy!*

$$T_{mct} = T_{th}$$

● *Nonergodic parameter also matches with the overlap!*

$$C(t=\infty) = q_1 \quad \text{at } T < T_{mct}$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

● Thermodynamic theory of p3 spin glass

Distribution of Hessians of Energy

$$P(\lambda) = \overline{\left\langle \sum_{\nu} \delta(\lambda - \lambda_{\nu}) \right\rangle}$$

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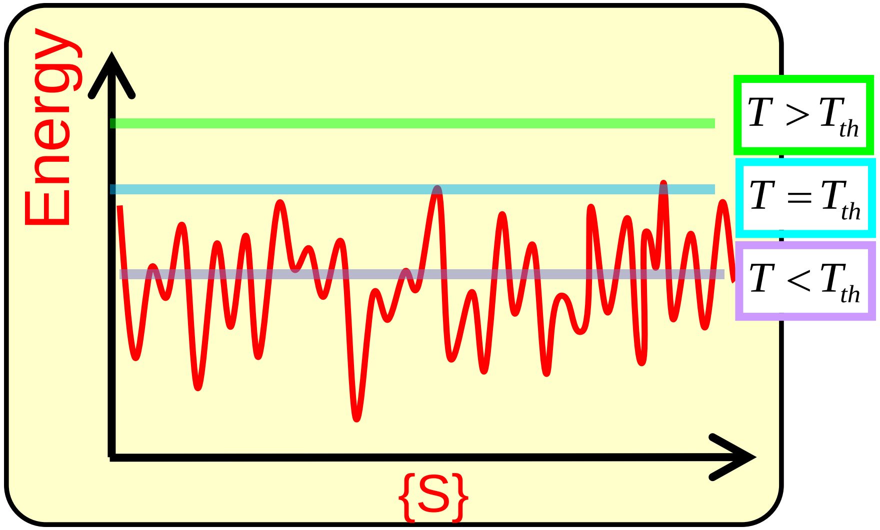
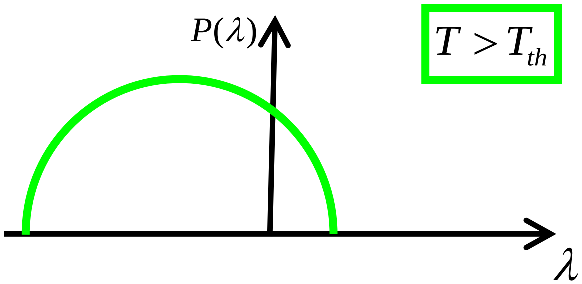
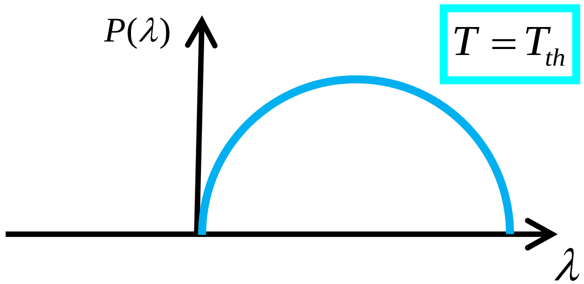
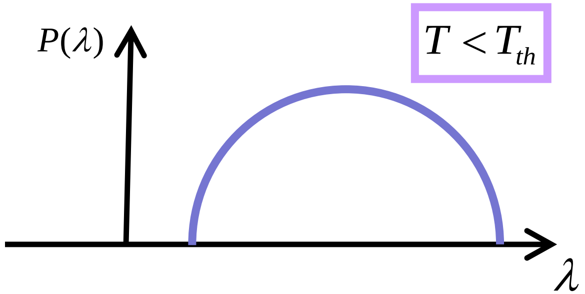


Unstable to Saddles to Minima







ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Dynamic theory of p3 spin glass*

- *At least for this model, Thermodynamic threshold T and Dynamic T are identical.*

- *Slow Dynamics is escorted by the qualitative change of the landscape!   Dynamics arrest can be understood as the extinction of the soft-mode in the landscape.*

- $T_{mct} = T_{th}$ *is the meeting point of Dynamics and Thermodynamics*

ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Translate the story to Glasses*

Spin Glass

Replica and TAP Theory

$$F = N(-\beta f^* + S_c(f^*))$$

Dynamic equation

$$\frac{dC(t)}{dt} = -TC(t) - \frac{3J^2}{2T}\int_0^t dt' C^2(t-t')\frac{dC(t')}{dt'}$$

MCT temperature T_{mct}

Spin glass transition temperature T_K

Glass

Replica Liquid Theory

Mezard, Parisi

$$\begin{cases} \ln g(r) = \beta v(r) + \int \frac{d\vec{q}}{(2\pi)^d} e^{i\vec{q}\cdot\vec{r}} \frac{\rho h^2(q)}{1+\rho h(q)}, \\ \ln \tilde{g}(r) = \int \frac{d\vec{q}}{(2\pi)^d} e^{i\vec{q}\cdot\vec{r}} \left\{ \frac{\rho h^2(q)}{1+\rho h(q)} - \frac{\rho[h(q)-\tilde{h}(q)]^2}{1+\rho[h(q)-\tilde{h}(q)]} \right\} \end{cases}$$

Mode-Coupling Theory (MCT)

$$\frac{\partial F(q,t)}{\partial t} = -\frac{Dq^2}{S(q)}F(q,t) + \int_0^t dt' \ M(q,t-t')\frac{\partial F(q,t')}{\partial t'}$$

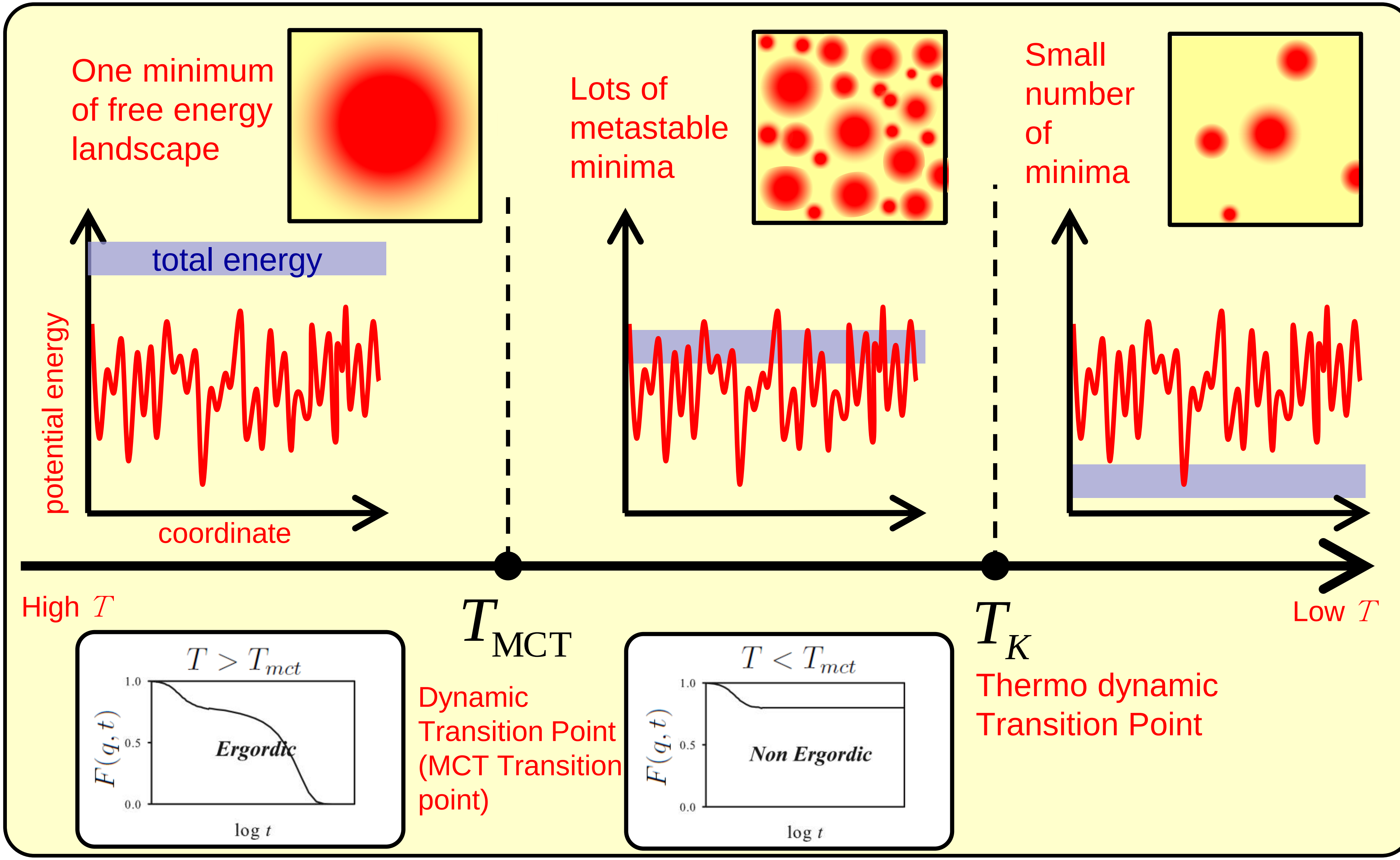
$$M(q,t) = \frac{\rho D}{2}\int \frac{d^d k}{(2\pi)^d}\left[kc(k) + (q-k)c(q-k)\right]^2 F(k,t)F(q-k,t)$$

MCT temperature T_{mct}

Kauzmann temperature T_K

ランダム一次転移理論(RFOT):ガラスの平均場描像

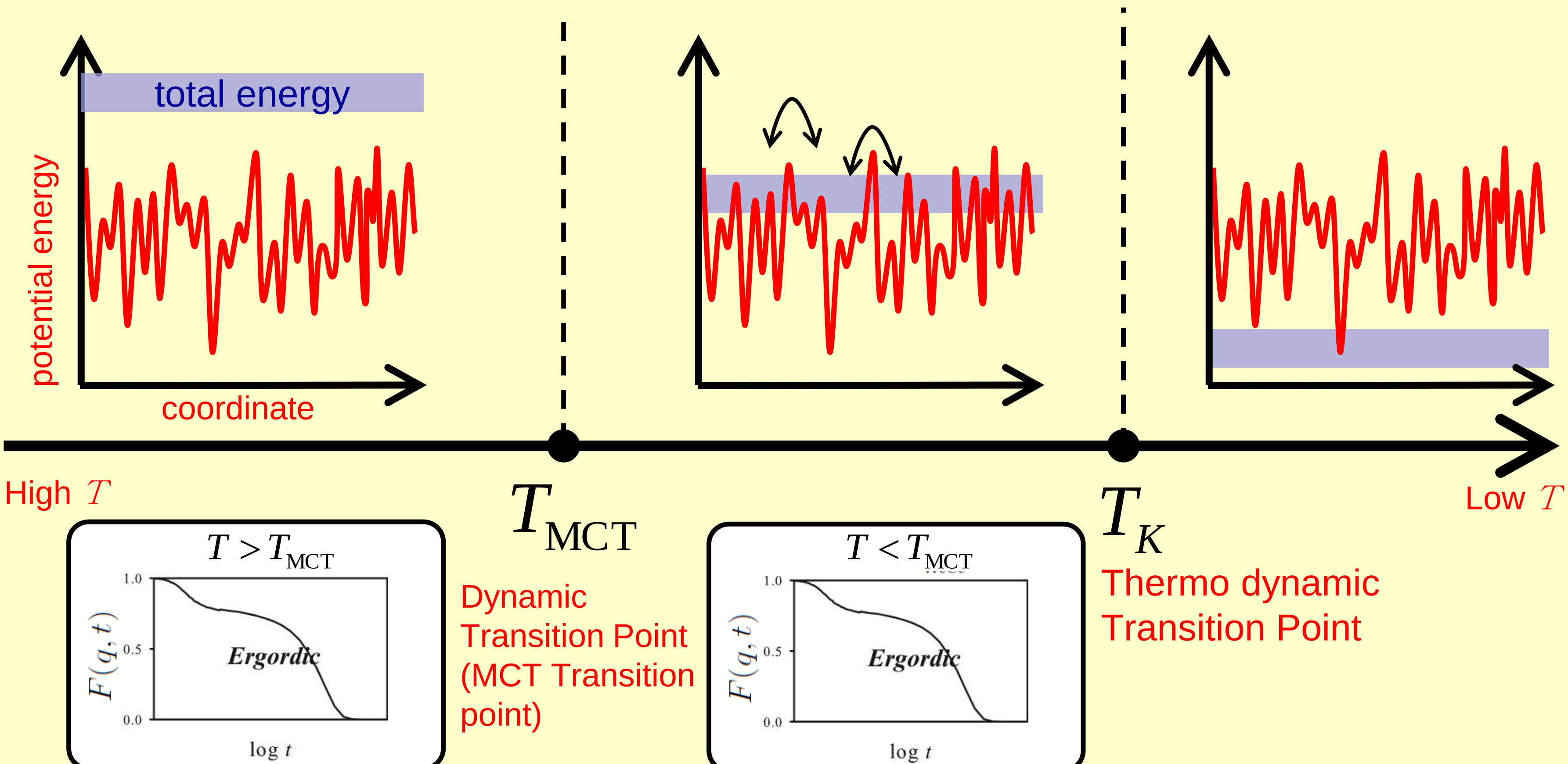
Mean field theory of the glass transition



ランダム一次転移理論(RFOT):ガラスの平均場描像

- ***Random First Order Transition Theory*** (Wolynes et al)

Activation processes will kick in and MCT transition would be washed away and become a cross-over



ランダム一次転移理論(RFOT)：ガラスの平均場描像

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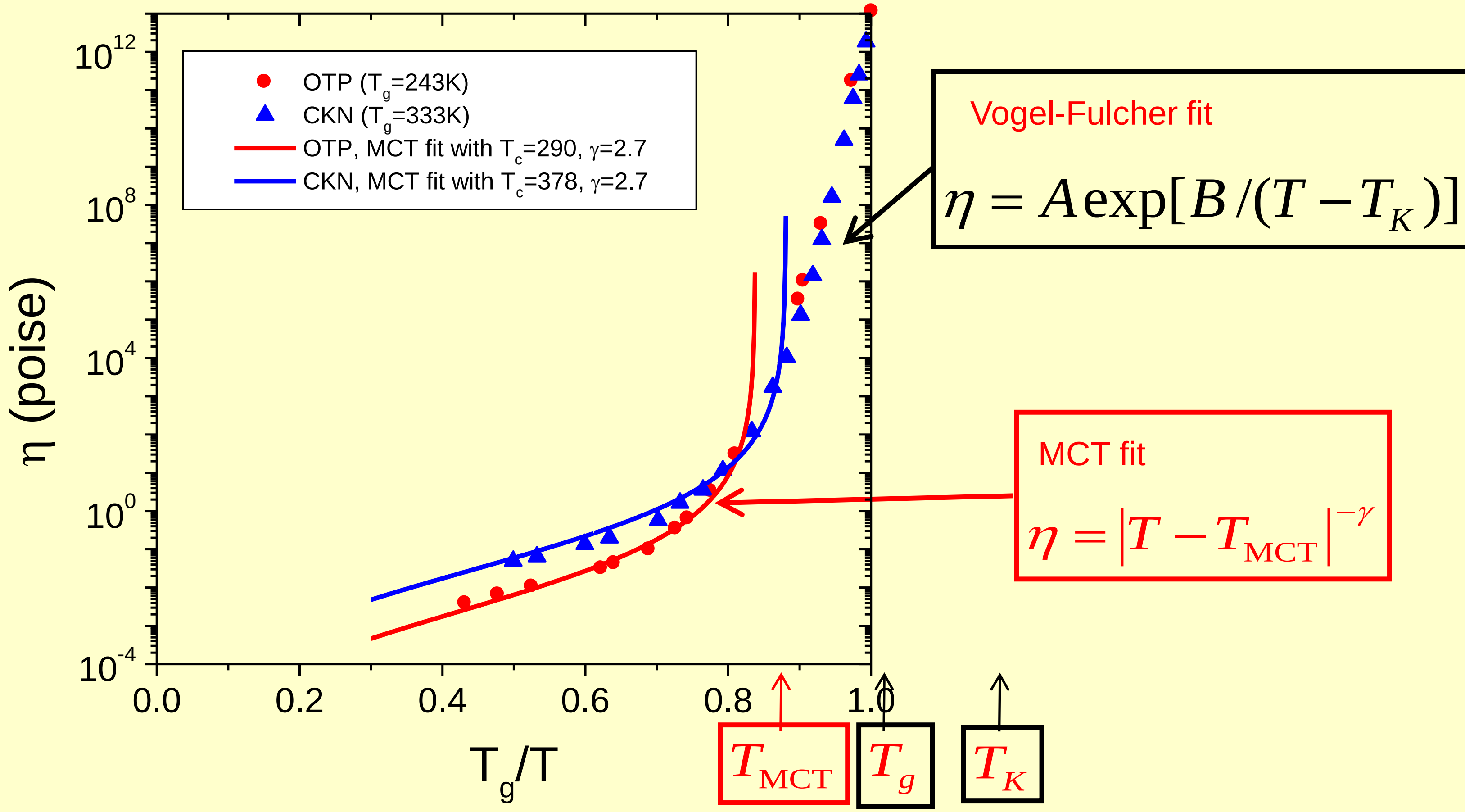
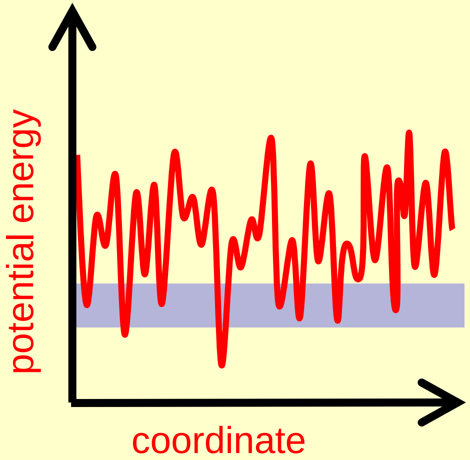
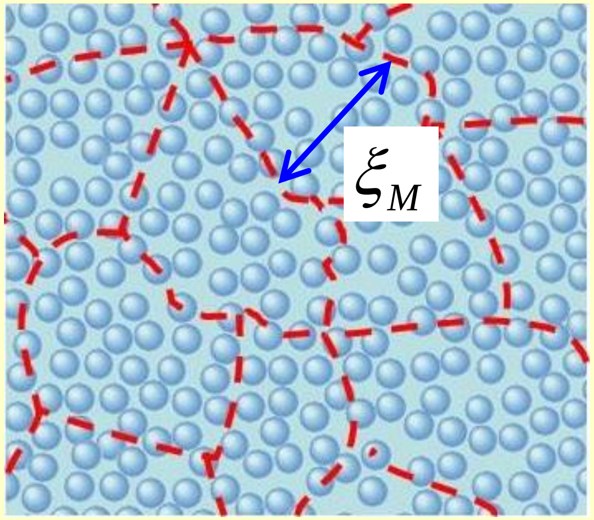


ランダム一次転移理論(RFOT):ガラスの平均場描像

- ***Random First Order Transition Theory*** (Wolynes et al)

Many minima or basin will separate the whole system into small patches of "states" or Mosaic.





Many droplets of "states" tiles the whole space.
And transition from one state to another state takes place due to thermal fluctuations.

Activation processes

ランダム一次転移理論(RFOT):ガラスの平均場描像

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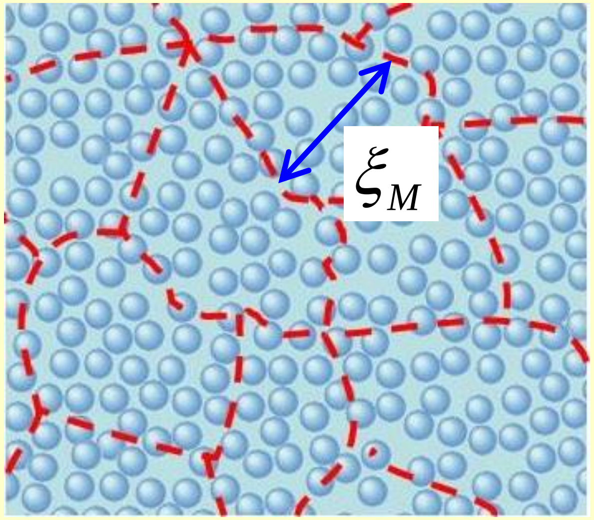

A naïve nucleation argument for the mosaics

$$\Delta F = \sigma \xi_M^{\theta} - S_c \xi_M^{d}$$

Free energy barrier for activation is given by

$$\frac{\partial \Delta F^*}{\partial \xi_M} = 0$$

$$\xi_M \propto \left(\frac{\sigma}{T S_c} \right)^{1/(d-\theta)} \qquad \Delta F^* = \left(\frac{\sigma}{T S_c} \right)^{d/(d-\theta)}$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

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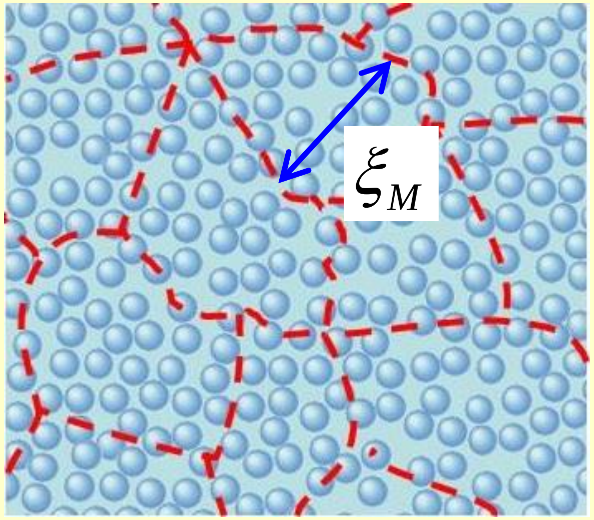

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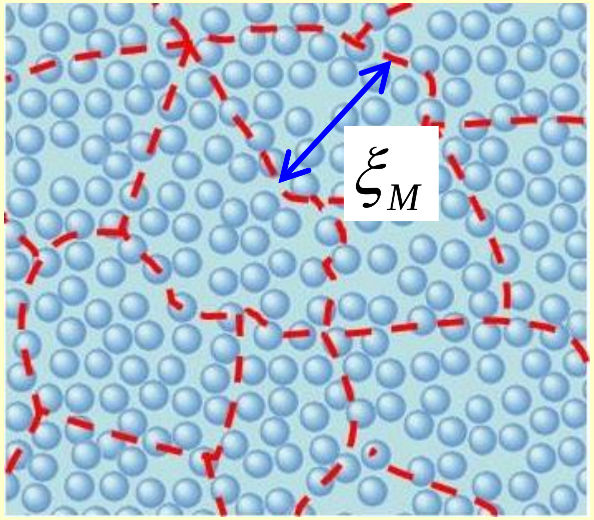
ランダム一次転移理論(RFOT):ガラスの平均場描像

Random First Order Transition Theory (Wolynes et al)

Many minima or basin will separate the whole system into small patches of "states" or Mosaic.



The relaxation time (if simple activation argument is applied)

$$\tau_\alpha \propto \exp\left[\frac{\Delta F^*(\xi_M)}{kT}\right]$$

$$\propto \exp\left[A\left(\frac{\sigma}{TS_c}\right)^{d/(d-\theta)}\right]$$

If $\theta = \dfrac{d}{2}$

$$\tau_\alpha \propto \exp\left[\frac{A}{TS_c}\right]$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

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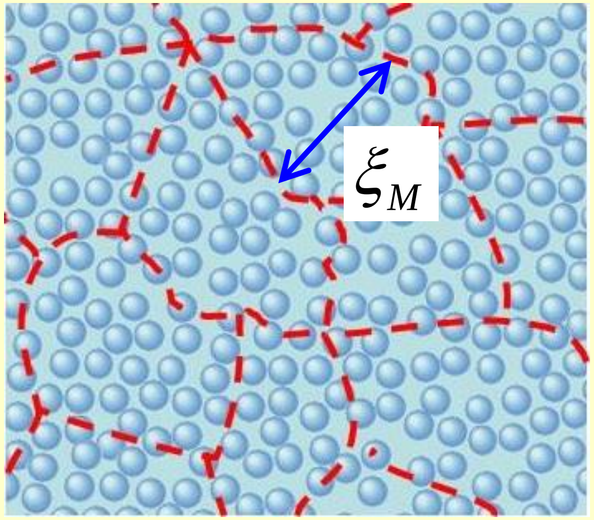


The relaxation time (if simple activation argument is applied)

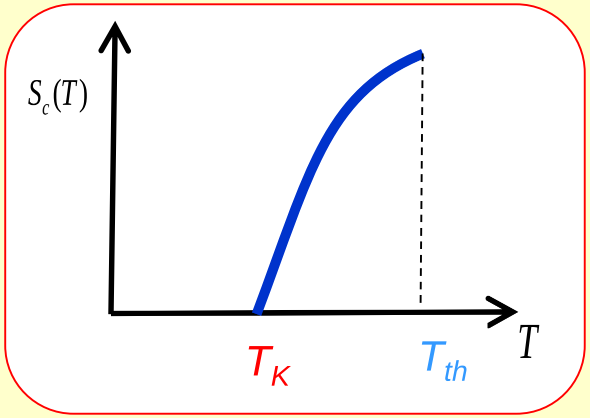
$$\tau_\alpha \propto \exp\left[\frac{A}{TS_c}\right]$$

The Adam-Gibbs equation

Using the fact $S_c \propto T_K - T$

$$\tau_\alpha \propto \exp\left[\frac{A}{T_K - T}\right]$$

The Vogel-Fulcher law



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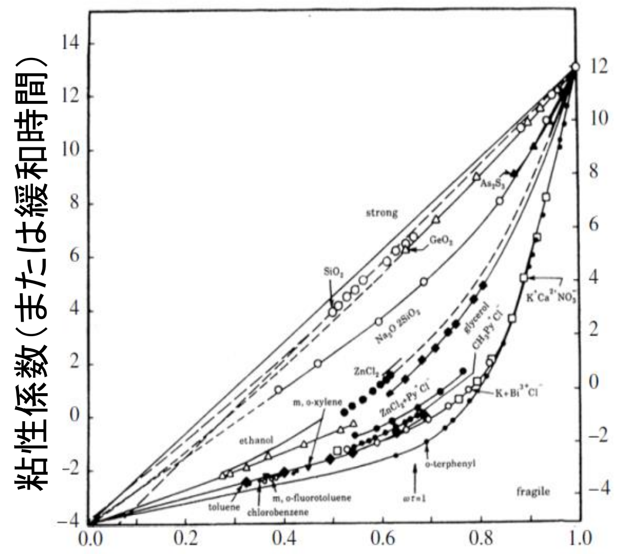
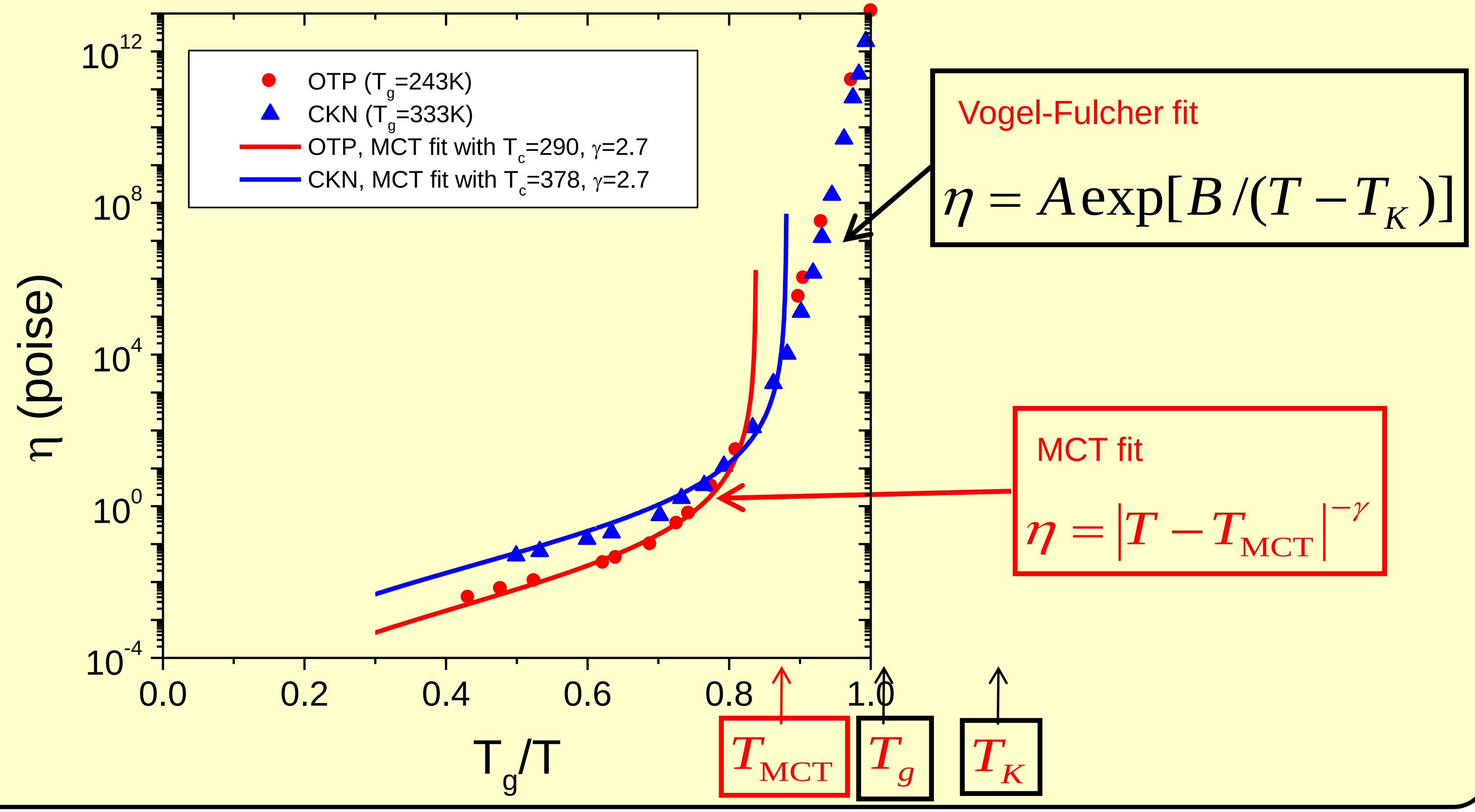


$$\frac{T_g}{T}$$

ランダム一次転移理論(RFOT):ガラスの平均場描像

● *Random First Order Transition Theory* (Wolynes et al)

Activation processes will kick in and MCT transition would be washed away and become a cross-over



ランダム一次転移理論(RFOT):ガラスの平均場描像

- ***Random First Order Transition Theory*** (Wolynes et al)

RFOT is elegant and simple…but

Is this true?

No one has ever spotted or seen the mosaics and RFOT still remains to be more or less a folklore…