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

ガラス理論の検証

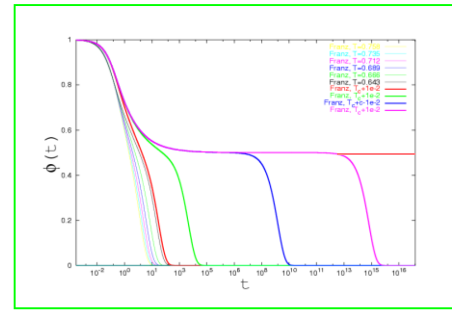
- MCT is encoded in Landscape (RFOT)?
- Adam-Gibbs theory works?
- Vogel-Fulcher works?
- Dyanamic Heterogeneities and

  Correlation Length can be explained?

ガラス理論の検証

- ***MCT is encoded in Landscape (RFOT)?***

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



Mathematical structure is exactly the same as the liquid!

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

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

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

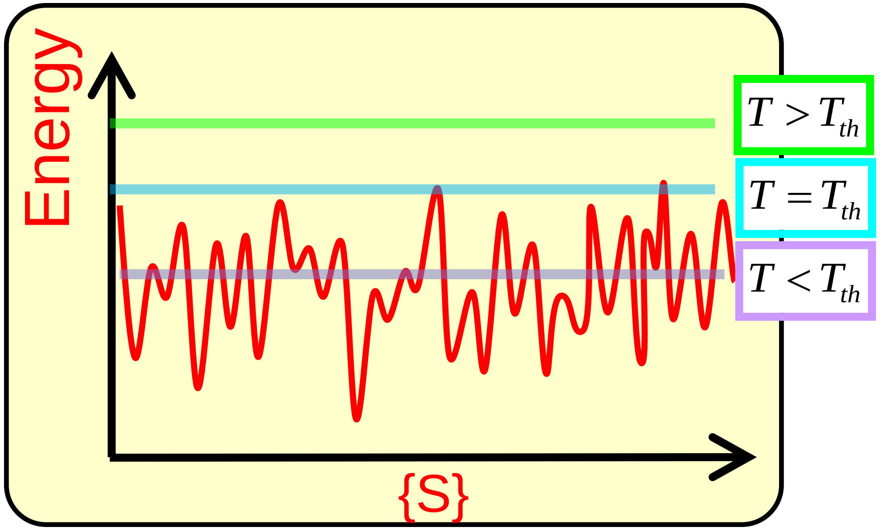
ガラス理論の検証

- **MCT is encoded in Landscape (RFOT)?**

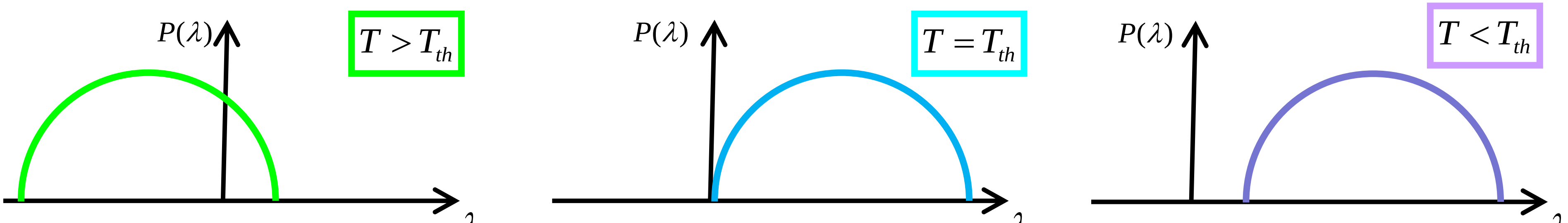
Distribution of Hessians of Energy

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

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



Unstable to Saddles to Minima



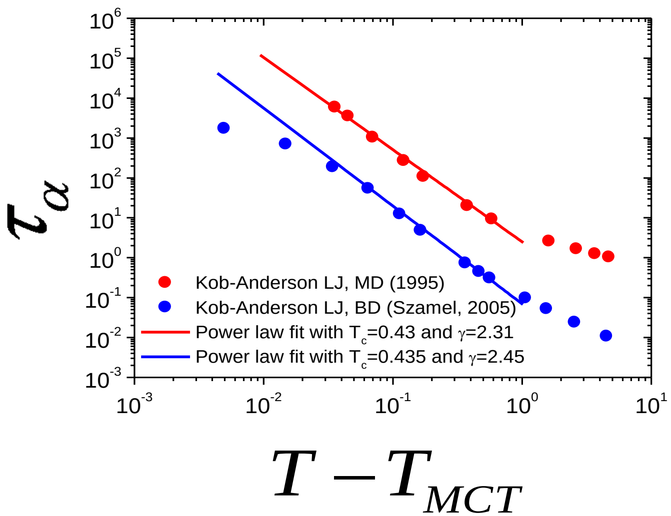
ガラス理論の検証

- ***MCT is encoded in Landscape (RFOT)?***

MCT

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

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



$$\tau_\alpha \propto |T - T_{MCT}|^{-\gamma}$$

$$\gamma = 2.46$$

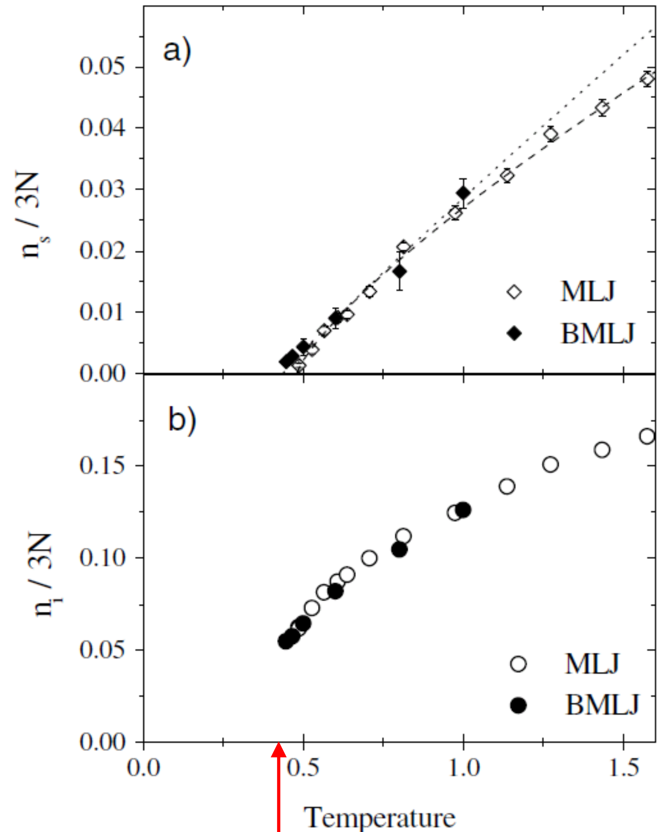
$$T_{MCT} = 0.435$$

ガラス理論の検証

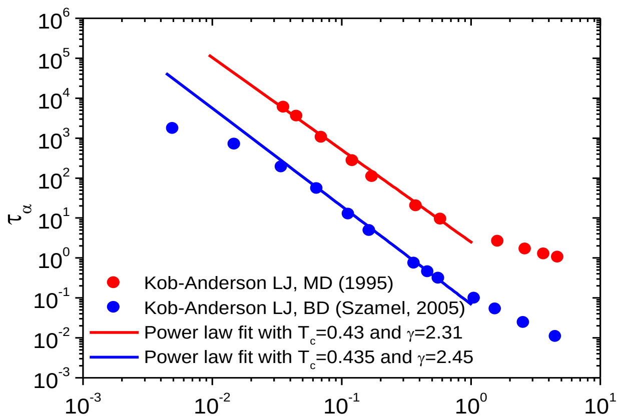
- ***MCT is encoded in Landscape (RFOT)?***

Number of suddles realy vanishes at T_{MCT}!

(Angelini et al. '00)



$$T_{MCT} = 0.435$$



$$T - T_{MCT}$$

ガラス理論の検証

- ***Adam-Gibbs theory works?***

RFOT predicts

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

The Adam-Gibbs equation

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

The Vogel-Fulcher law

ガラス理論の検証

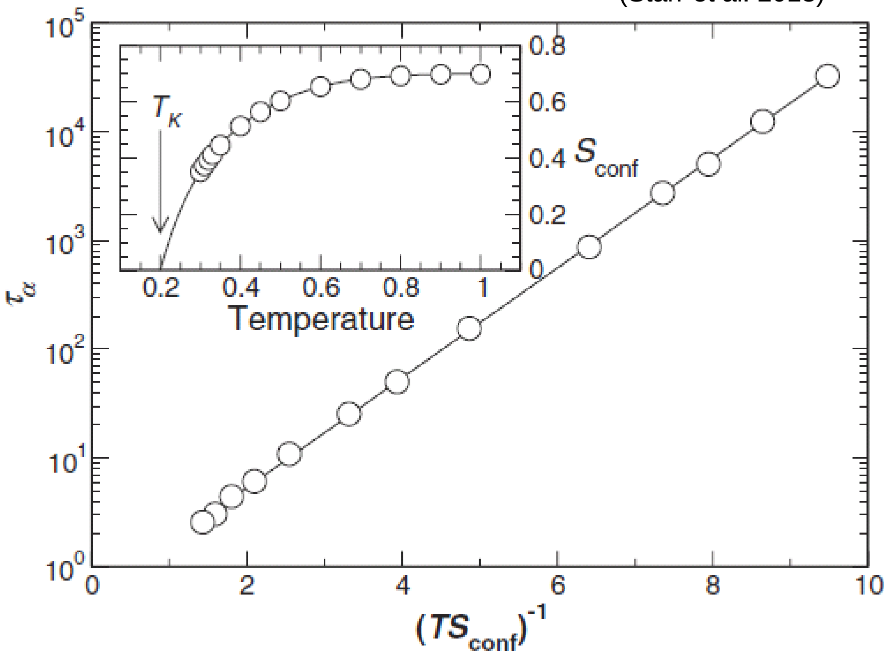
- ***Adam-Gibbs theory works?***

RFOT predicts

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

The Adam-Gibbs equation

(Starr et al. 2013)



ガラス理論の検証

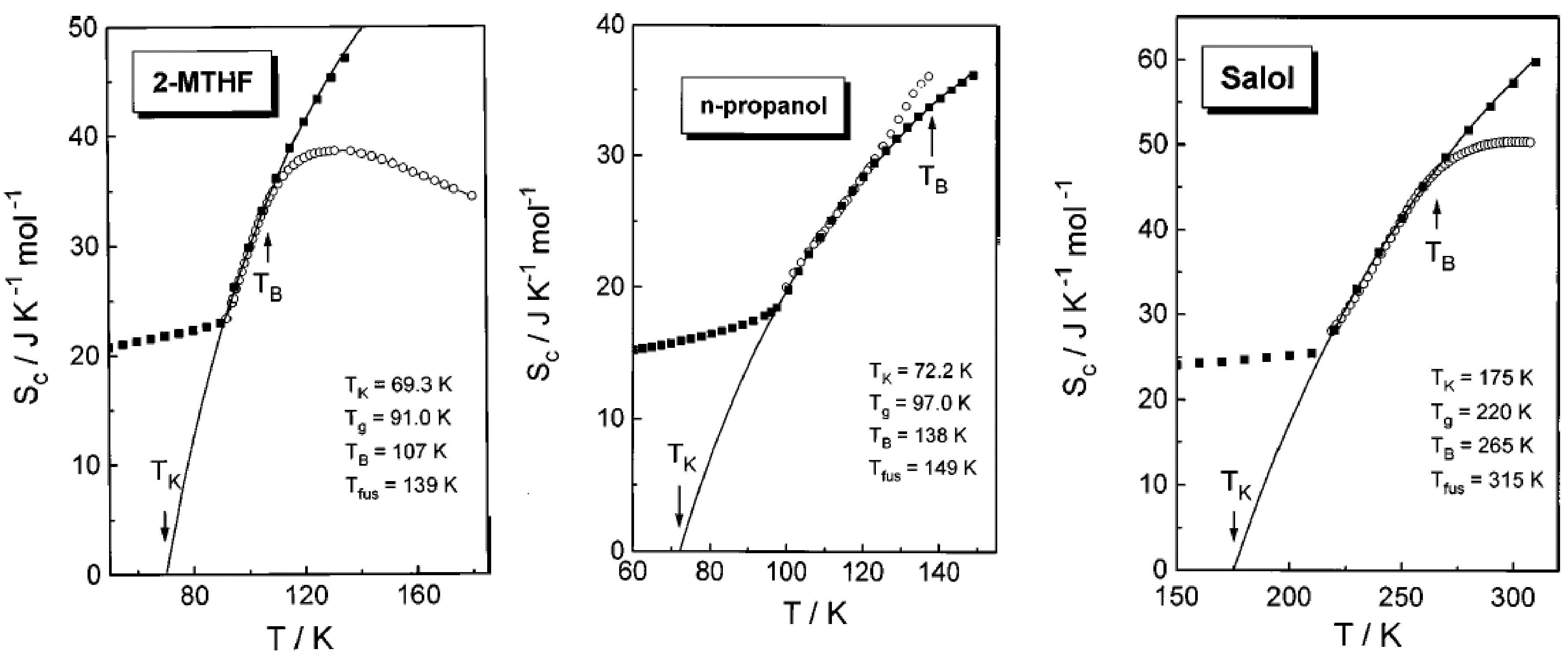
- ***Vogel-Fulcher works?***

RFOT predicts

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

The Vogel-Fulcher law

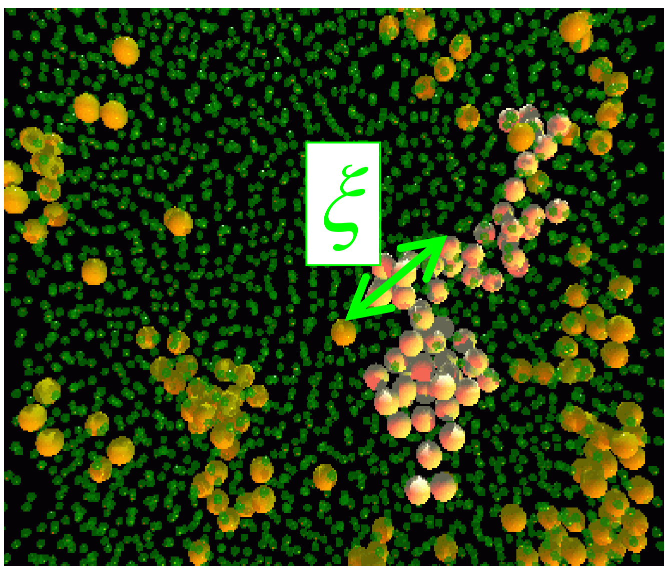
(Richert et al. 1998)



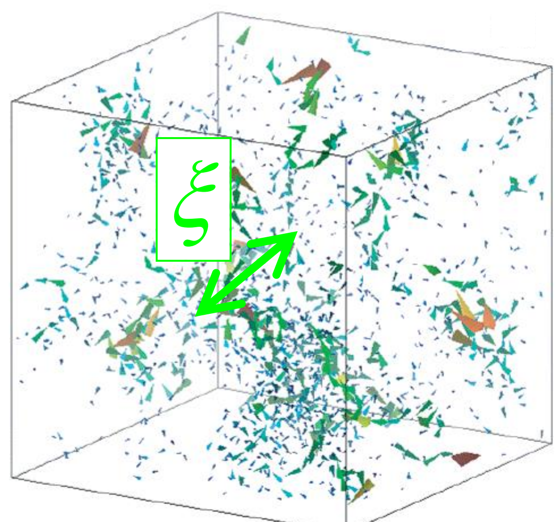
ガラス理論の検証

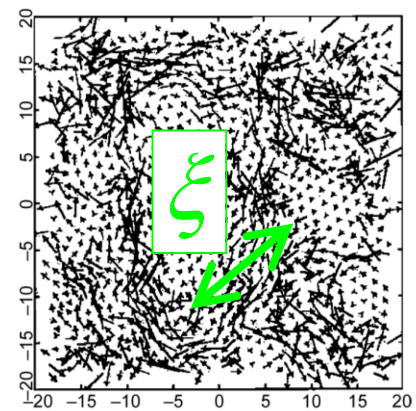
- ***Dyanamic Heterogeneities and Correlation Length can be explained?***

(Week et al. '00)



(Yamamoto et al. '98)

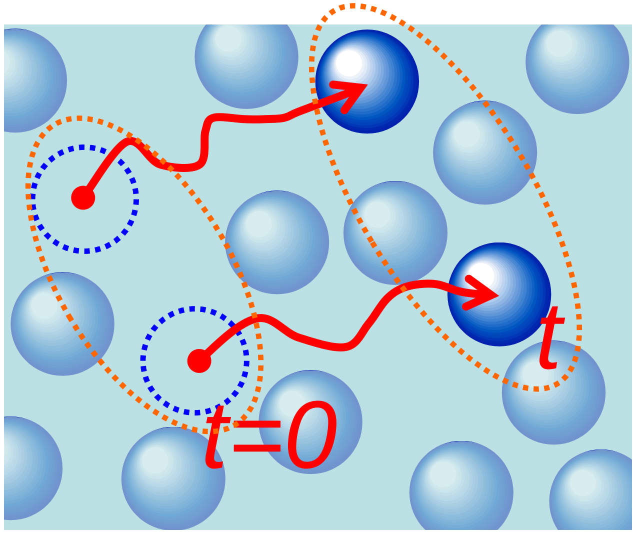




ガラス理論の検証

Quantify the dynamic heterogeneity and correlation length?

Nonlinear susceptibility
or
4 point correlation function



Density-density correlation function (2-point)

$$F(k,t) = \langle \rho_k(t)\, \rho_{-k}(0) \rangle \equiv \langle \hat{F}(k,t) \rangle$$

4-point density correlation function

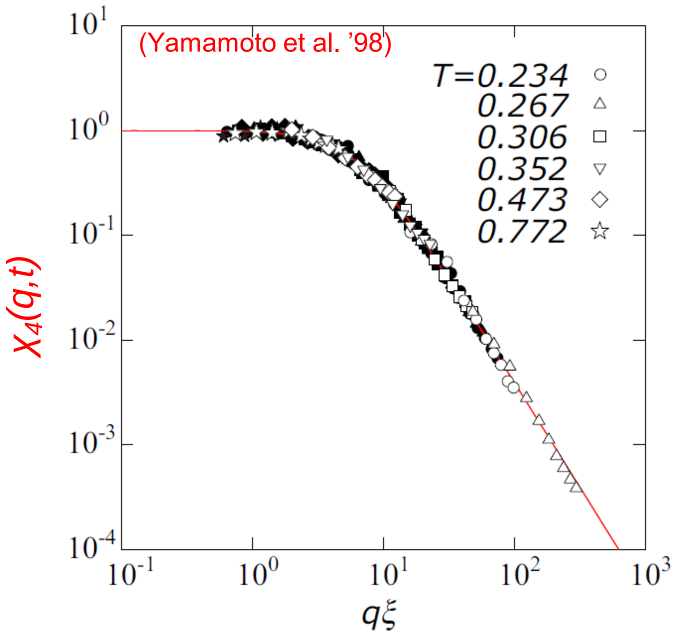
$$G_4(r,t) \approx \langle \rho(r,t)\rho(r,0)\rho(0,0)\rho(0,t) \rangle$$

or

$$\chi_4(t) \approx \int dr\, G_4(r,t) \Leftrightarrow \langle \delta\hat{F}^2(k,t) \rangle$$

ガラス理論の検証

The 4 point correlation function



$\chi_4(q,t)$: Fourier transform of $G_4(r,t)$

Orstein-Zernike like behavior

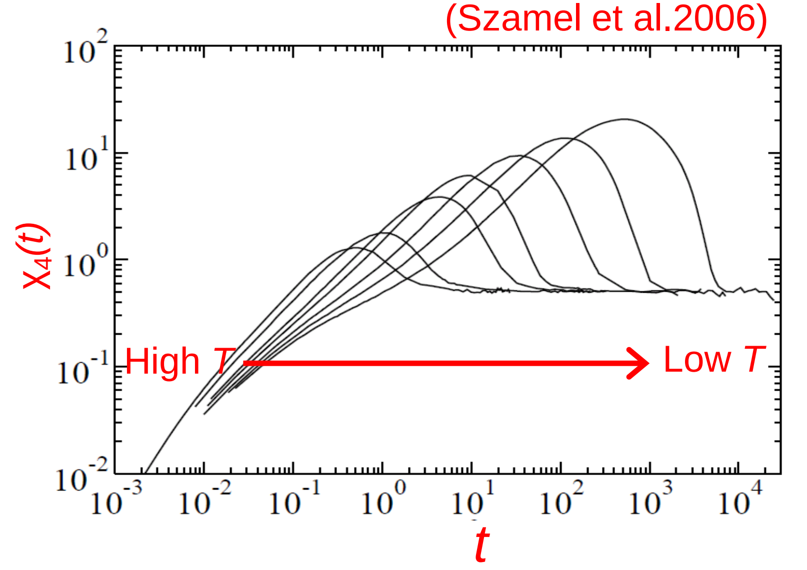
$$\chi_4(q,t) \approx \frac{\xi^2}{1+q^2\xi^2} \quad ?$$

with ξ increasing as T lowered

$$\chi_4(t) = \chi_4(q=0,t)$$

Integral of $G_4(r, t)$ over space

Its amplitude grows as T lowered, reflecting a growing length scales.



ガラス理論の検証

- ***Dyanamic Heterogeneities and Correlation Length can be explained?***

RFOT predicts

$$\xi_M \propto \left(\frac{\sigma}{TS_c}\right)^{1/(d-\theta)} \propto |T - T_K|^{-d/2}$$

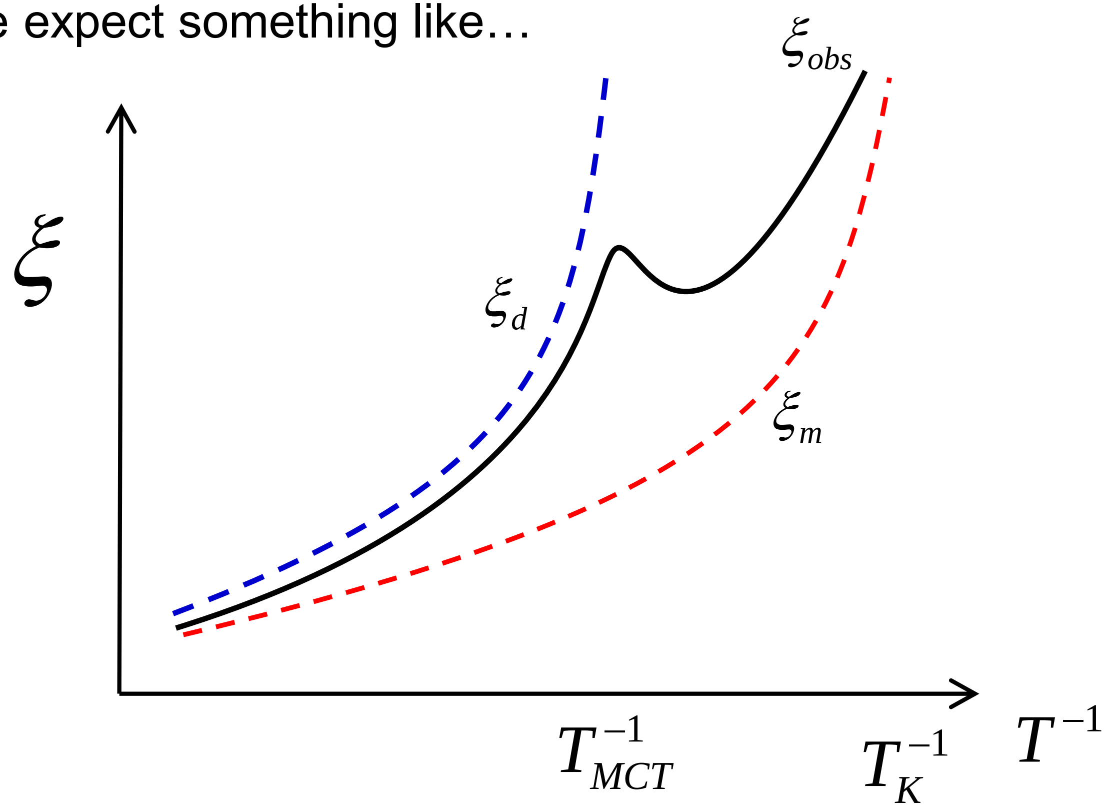
MCT predicts

$$\xi_d \propto |T - T_{MCT}|^{-\nu}$$

ガラス理論の検証

- ***Dyanamic Heterogeneities and Correlation Length can be explained?***

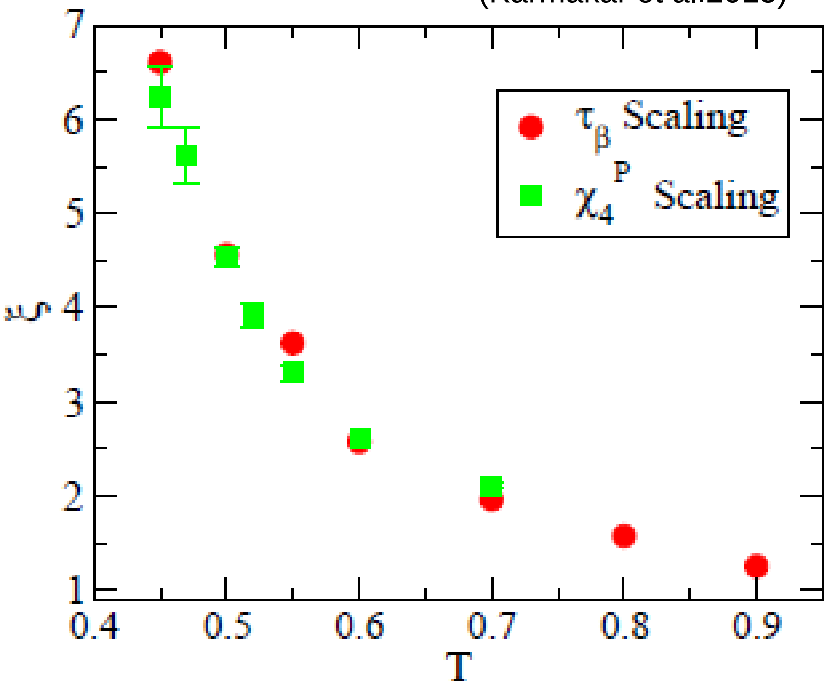
Should we expect something like…



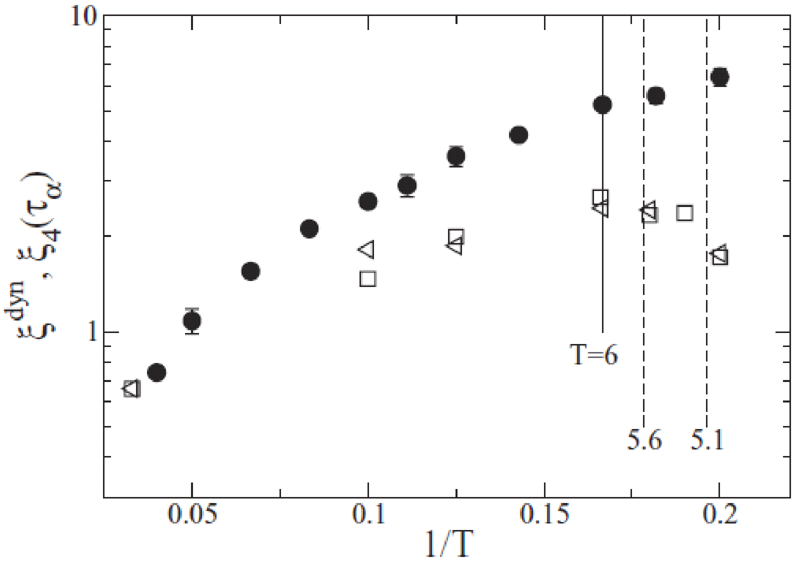
ガラス理論の検証

Typical ovservation of the correlation lenghts

(Karmakar et al.2015)



(Flenner et al.2013)



ガラス理論の検証

● *Inhomogeneous MCT and dynamic correlation length*

Calculate Nonlinear Susceptibility using MCT

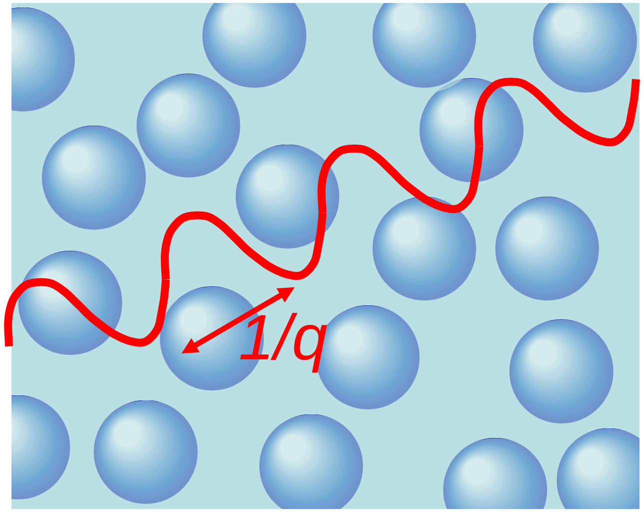
Instead of calculating the 4 point correlation function (it is too complicated),
we shall calculate *the 3 point correlation function*

$$\chi_3(k,q,t) = \langle \rho(k,t)\rho(q,t)\rho(-k-q,0) \rangle$$

Hamiltonian

$$H_{tot} = H + \varepsilon\rho_q$$

Pinning field



$$F(k_1,k_2,t) = \langle \rho(k_1,t)\rho(k_2,0) \rangle$$

Linear response theory says

$$\chi_3(k,q,t) \approx \frac{\partial F(k,k+q,t)}{\partial \varepsilon}$$

Need to construct MCT for $F(k_1,k_2,t)$

ガラス理論の検証

- ***Inhomogeneous MCT and dynamic correlation length***

Basic Idea

Linear Response Theory says

$$H_{tot} = H + xF$$

$$\langle x(t)\rangle_F = \int_{-\infty}^{t} dt' \, \chi(t-t')F(t')$$ with $$\chi(t) = \langle x(t)x(0)\rangle_{eq}$$

Change of *x* due to *F* can be described by correlation function at equilibrium

or

The 1st moment of *x* in the presence of *F* can be written by the 2nd moment of x in the absence of *F*.

or

The 2nd moment of *x* in the absence of *F* can be written by the 1st moment of x in the presence of *F*.

or

The *3rd* moment of *x* in the absence of *F* can be written by the *2nd* moment of x in the presence of *F*.

ガラス理論の検証

- ***Inhomogeneous MCT and dynamic correlation length***

MCT in the presence of the pinning field (thus w/o translational invariance)

$$\frac{\partial^2 F(k_1,k_2,t)}{\partial t^2} + \Omega^2(k_1,q)\,F(q,k_2,t) + \nu\,\frac{\partial F(k_1,k_2,t)}{\partial t} + \int_0^t dt'\,M(k_1,q,t-t')\,\frac{\partial F(q,k_2,t')}{\partial t'} = 0$$

with

$$\Omega^2(k_1,k_2) = \frac{k_B T}{m} k_1 \cdot q_1 \left\langle \sum e^{i(q_1-q_2)R_j} \right\rangle S^{-1}(q_2,k_2)$$

$$M(k_1,k_2,t) = k_1 V(k_1,q_1,q_2) \times \{F(q_1,q_3,t)F(q_2,q_4,t) + F(q_1,q_4,t)F(q_2,q_3,t)\} V(k_2,q_3,q_4)\frac{1}{k_2}$$

ガラス理論の検証

Inhomogeneous MCT and dynamic correlation length

$$\frac{\partial^2 \chi_3(\mathbf{q}_1,\mathbf{q}_2;t)}{\partial t^2} + \Omega_0^2(\mathbf{q}_1)\chi_3(\mathbf{q}_1,\mathbf{q}_2;t) + \Omega_1^2(\mathbf{q}_1,\mathbf{q}_2)F(\mathbf{q}_2,t) + \nu\frac{\partial \chi_3(\mathbf{q}_1,\mathbf{q}_2;t)}{\partial t'}$$
$$+\int_0^t \mathrm{d}t'\ M_0(\mathbf{q}_1,t-t')\frac{\partial \chi_3(\mathbf{q}_1,\mathbf{q}_2;t')}{\partial t'} + \int_0^t \mathrm{d}t'\ M_1(\mathbf{q}_1,\mathbf{q}_2;t-t')\frac{\partial F(\mathbf{q}_2,t')}{\partial t'} = 0$$

with

$$M_0(\mathbf{k},t) = \frac{k_\mathrm{B}T}{2mn}\int\frac{\mathrm{d}\mathbf{q}}{(2\pi)^3}V_{\mathbf{k}}^2(\mathbf{q},\mathbf{k}-\mathbf{q})F(k,t)F(|\mathbf{q}-\mathbf{k}|,t)$$

$$M_1(\mathbf{k}_1,\mathbf{k}_2;t) = \frac{k_\mathrm{B}T}{2mn}\int\frac{\mathrm{d}\mathbf{q}}{(2\pi)^3}\Big[\ V_{\mathbf{k}_1}^2(\mathbf{q},\mathbf{k}_1-\mathbf{q})F(k,t)F(|\mathbf{k}_1-\mathbf{q}|,t)\frac{\mathbf{k}_1\cdot\mathbf{k}_2}{k_2^2}S(q_0)$$
$$+2k_1V_{\mathbf{k}_1}(\mathbf{q},\mathbf{k}_1-\mathbf{q})\chi_3(\mathbf{q},\mathbf{q}_0+\mathbf{q};t)F(|\mathbf{k}_1-\mathbf{q}|,t)V_{\mathbf{k}_2}(\mathbf{k}_1-\mathbf{q},\mathbf{q}_0+\mathbf{q})\frac{1}{k_2}\Big]$$

$$\Omega_0^2(\mathbf{k}) = \frac{k_\mathrm{B}Tk^2}{mS(k)}$$

$$\Omega_1^2(\mathbf{k}_1,\mathbf{k}_2) = \frac{k_\mathrm{B}T}{m}S(q_0)\left\{k_1^2 - \frac{\mathbf{k}_1\cdot\mathbf{k}_2}{S(k_2)}\right\}$$

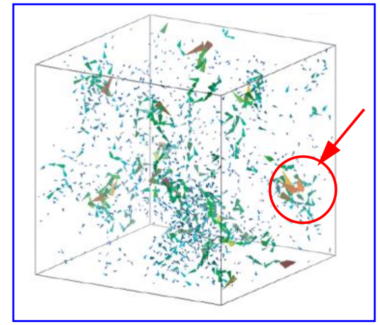
ガラス理論の検証

● *Inhomogeneous MCT and dynamic correlation length*

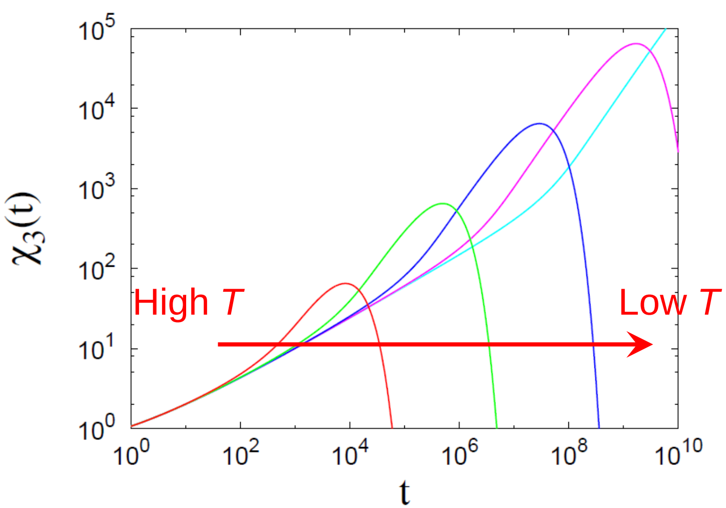
For *q=0:* Integral over space:

$$\chi_3(t) = \chi_3(k, q=0, t)$$

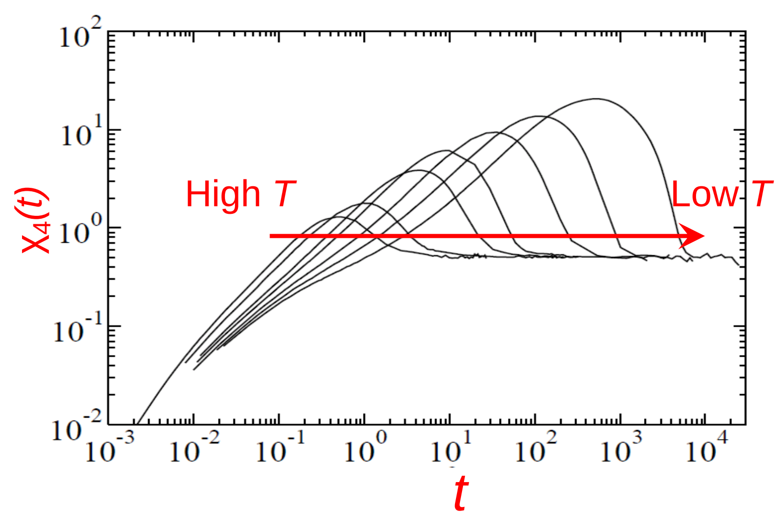
$\propto$ A number of particles in a “cluster”



$\chi_3(t)$ IMCT
(A simplified model calculation)



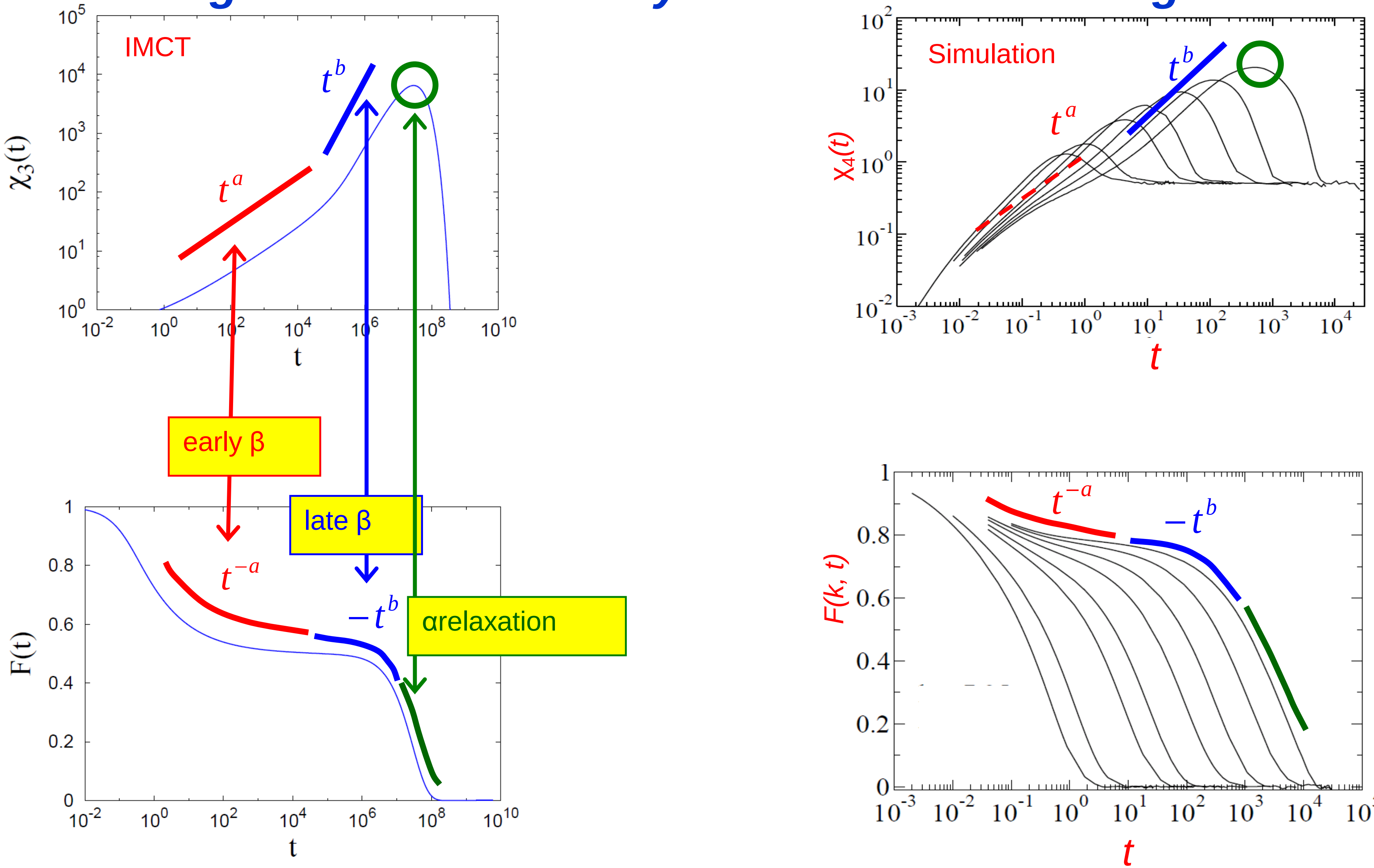
$\chi_4(t)$ Simulation
for a colloid, (Szamel et al.2006)



Cluster size / length scale grow as *T* lowered.

ガラス理論の検証

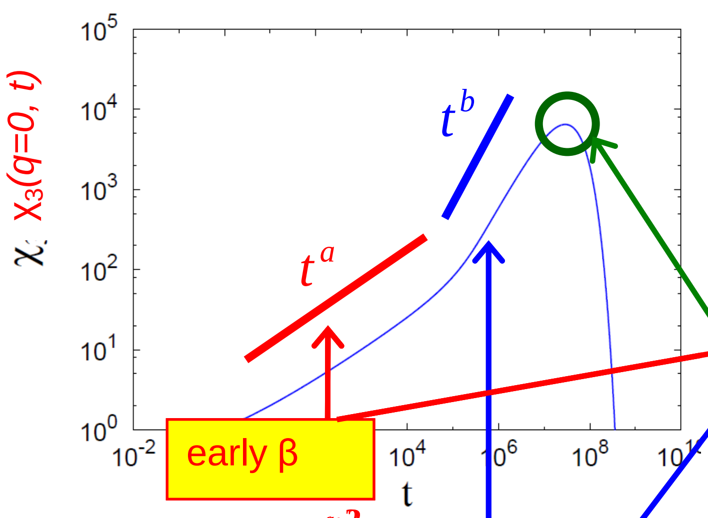
- ***Inhomogeneous MCT and dynamic correlation length***

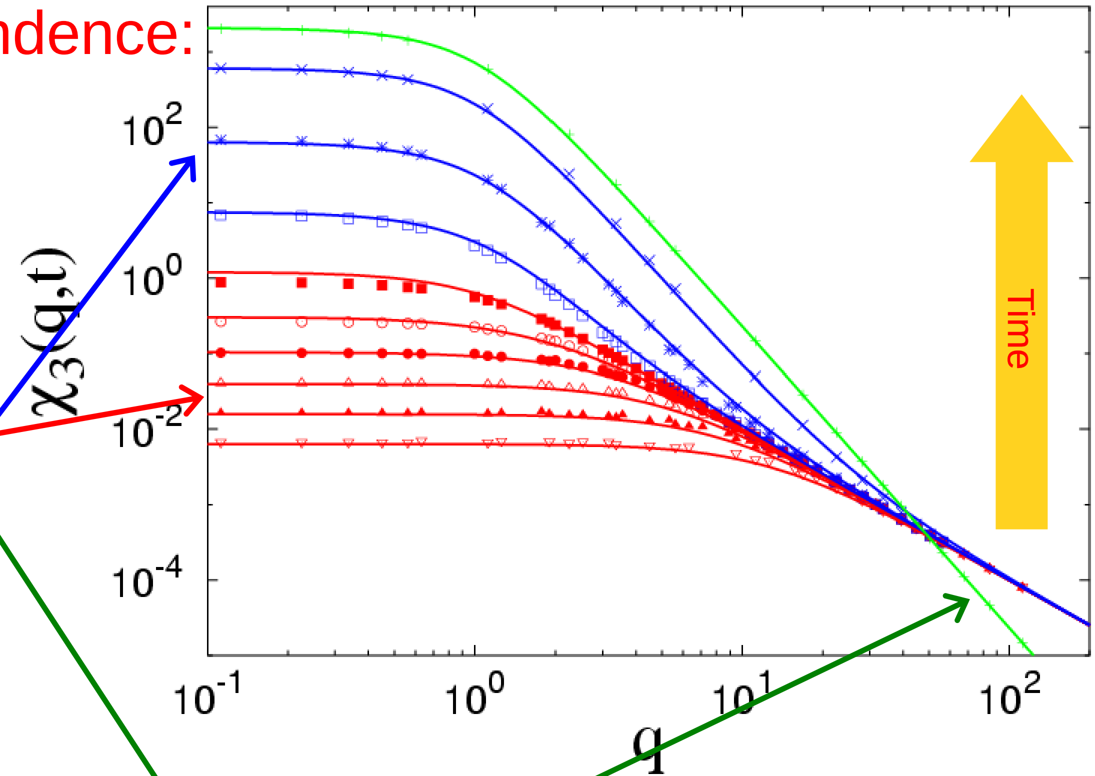


ガラス理論の検証

● *Inhomogeneous MCT and dynamic correlation length*

For *q≠0:* Length scale dependence:





$$\chi_3(q,t) \propto \frac{\xi^2}{1+q^2\xi^2}$$

$$\xi(t) \propto t^{a/2}$$

late β

$$\chi_3(q,t) \propto \frac{B(t)}{1+q^2\xi^2+A(t)q^4\xi^4}$$

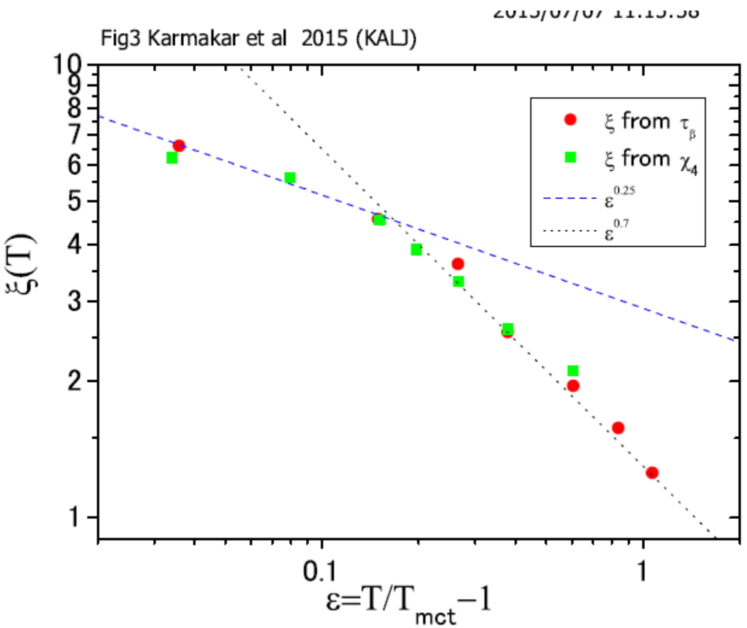
αrelaxation

$$\chi_3(q,t) \propto \frac{\xi^4}{1+q^2\xi^2+Cq^4\xi^4}$$

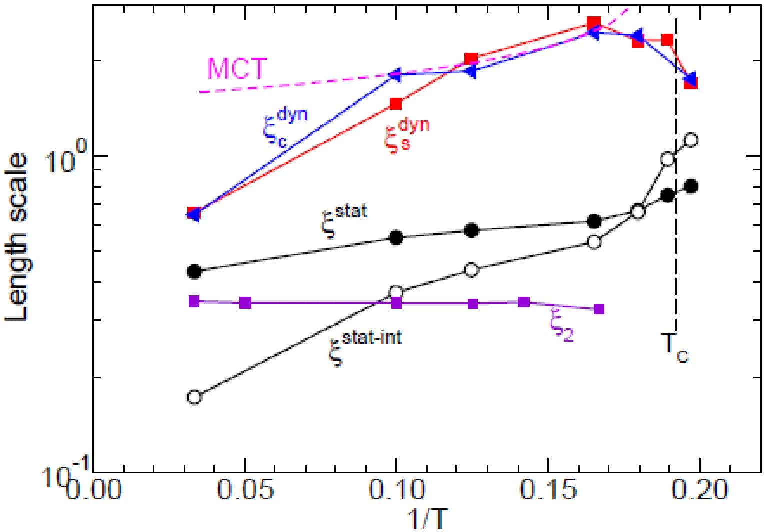
$$\xi(t) \propto |T-T_{\mathrm{MCT}}|^{-1/4}$$

ガラス理論の検証

●Comparison is hardly satisfactory



(Kob et al.2012)



(Flenner et al.2010)