メニュー

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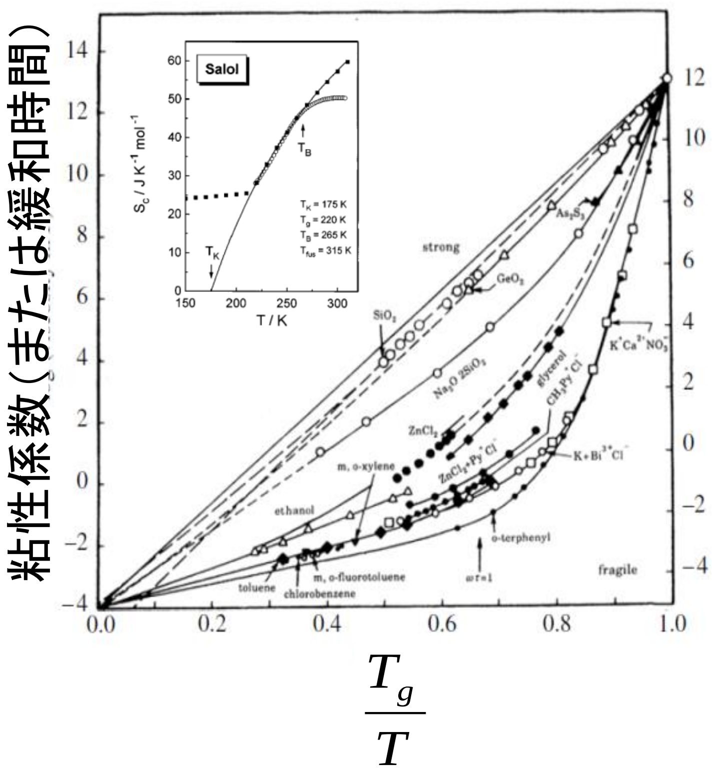
イントロダクション・ガラス転移とは

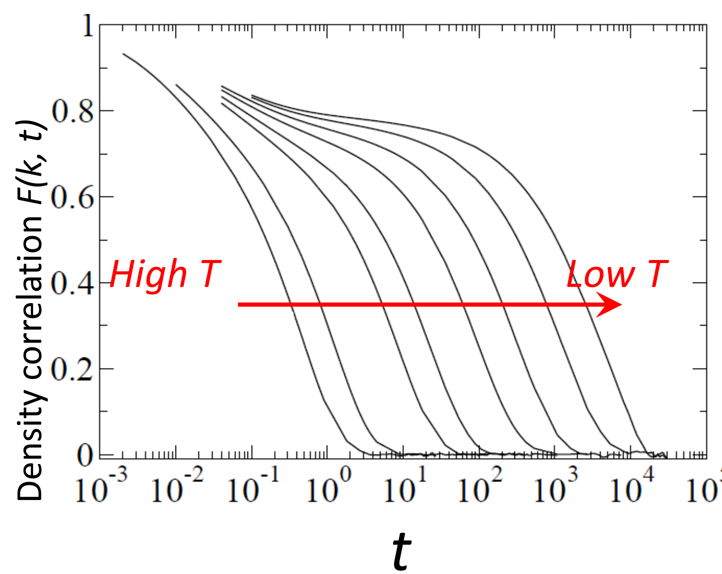
ガラス転移における普遍的なスローダイナミクス

1. *非アレニウス的な粘性係数(緩和時間)の増大*

Macroscopic dynamics



Microscopic dynamics



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

密度の相関関数(原子レベルの揺らぎをモニターする)

流体力学から分子運動論まで:モード結合理論超入門

- *Brief summary of Hydrodynamics and Non-equilibrium stat-phys.*
- *Brief Introduction of MCT*
- *(Fluctuating) Hydrodynamics*
- *Generalized Fluctuating Hydrodynamics*
- *Crush Course of Mode-Coupling Theory*
- *What MCT can and cannot do*

流体力学から分子運動論まで:モード結合理論超入門

● Brief Summary of Hydrodynamics and Non-equilibrium stat-phys.

Macroscopic non-equilibrium phenomena is described by various phenomenological (hydrodynamic) equations

Navier-Stokes equation

$$\begin{cases} \dfrac{\partial \rho_m}{\partial t} = -\nabla \cdot (\rho_m \boldsymbol{v}) \\ \dfrac{\partial \rho_m \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho_m \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \left(\zeta + \dfrac{1}{3}\eta\right) \nabla\nabla \cdot \boldsymbol{v} \end{cases}$$

ρ_m : Mass density p : Pressure η : Shear viscosity ζ : Bulk viscosity

流体力学から分子運動論まで:モード結合理論超入門

● Brief Summary of Hydrodynamics and Non-equilibrium stat-phys.

Diffusion equation

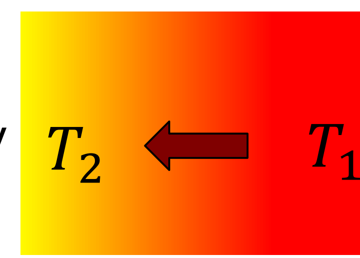
$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho$$

ρ : cocentration D: diffusion constant

Fourier law

$$\frac{\partial T}{\partial t} = \chi\nabla^2 T$$

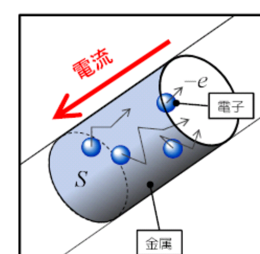
T : Temperature χ: thermal coductivity



Ohm's law

$$j = \sigma E$$

j : electric current σ: conductivity



● Brief Summary of Hydrodynamics and Non-equilibrium stat-phys.

Viscosity, diffusion constant, thermal conductivity, condutivity, etc… are called Transport coefficients

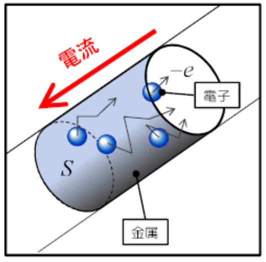
All microscopic information is packed there.

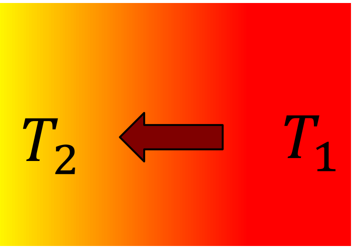
$$\frac{\partial \rho_m v}{\partial t} = -\nabla \cdot \rho_m v v - \nabla p + \eta \nabla^2 v + \left(\varsigma + \frac{2}{3}\eta \right) \nabla \nabla \cdot v$$

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho$$

$$\frac{\partial T}{\partial t} = \chi \nabla^2 T$$

$$j = \sigma E$$





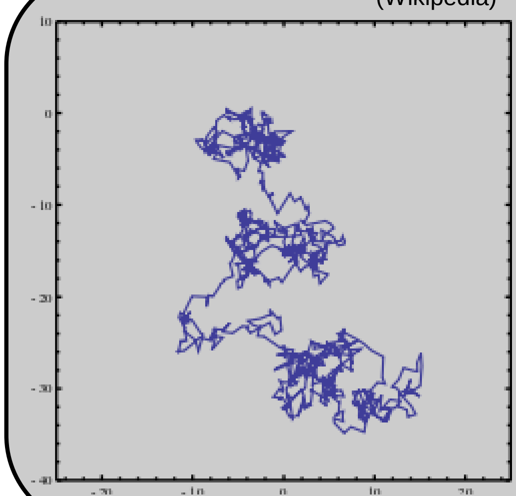
Fluctuation-Dissipation Theorem:

Transport coefficients written by equilibrium fluctuations!

Diffusion equation (Brownian motion)

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho$$

ρ : cocentration D: diffusion constant



(Wikipedia)

Equation of motion for a small diffusing particle

Langevin equation

$$m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -\zeta \boldsymbol{v} + \boldsymbol{f}$$

$\boldsymbol{f}(t)$: Random force

$$\langle \boldsymbol{f}(t) \rangle = 0 \qquad \langle f_i(t) f_j(t') \rangle = A\delta_{ij}\delta(t-t')$$

What is A?

Fluctuation-Dissipation Theorem:

Transport coefficients written by equilibrium fluctuations!

$$\boldsymbol{v}(t) = \frac{1}{m}\int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{-\gamma(t-t')} \boldsymbol{f}(t') \qquad \gamma = \zeta/m$$

$$\langle v_i(t) v_j(0) \rangle = \frac{A}{2m^2\gamma} \mathrm{e}^{-\gamma t} \delta_{ij}$$

$$\langle v_i^2(0) \rangle = \frac{A}{2m^2\gamma} = \frac{k_\mathrm{B}T}{m}$$

$$A = 2m\gamma k_\mathrm{B}T = 2\zeta k_\mathrm{B}T$$

$$\langle f_i(t) f_j(t') \rangle = 2\zeta k_\mathrm{B} T \delta_{ij} \delta(t-t')$$

Fluctuation-Dissipation Theorem

Fluctuation-Dissipation Theorem:

Transport coefficients written by equilibrium fluctuations!

Velocity correlation function

$$C_{ij}(t) \equiv \langle v_i(t) v_j(0) \rangle = \frac{k_{\mathrm{B}}T}{m} \mathrm{e}^{-\gamma t} \delta_{ij}$$

Using $\boldsymbol{R}(t) = \int_0^t \mathrm{d}t' \, \boldsymbol{v}(t')$

$$\langle |\boldsymbol{R}(t)|^2 \rangle = 3 \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \, \langle v_i(t_1) v_i(t_2) \rangle = 3 \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \, C_{ii}(t_1 - t_2)$$

$$\approx 6t \int_0^\infty \mathrm{d}\tau \, C_{ii}(\tau)$$

From the definition of diffusion coefficient $\langle |\boldsymbol{R}(t)|^2 \rangle = 6Dt$

$$D = \int_0^\infty \mathrm{d}t \, \langle v_i(t) v_i(0) \rangle$$

and

$$D = \frac{k_{\mathrm{B}}T}{\zeta}$$

Einstein relation

Fluctuation-Dissipation Theorem:

Transport coefficients written by equilibrium fluctuations!

Diffusion coefficient

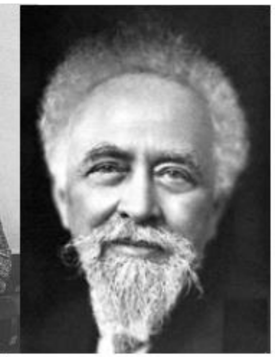
$$D = \int_0^\infty \mathrm{d}t \ \langle v_i(t) v_i(0) \rangle$$

Viscosity

$$\eta = \frac{1}{V k_{\mathrm{B}} T} \int_0^\infty \mathrm{d}t \ \langle \sigma_{xz}(t) \sigma_{xz}(0) \rangle$$

Conductivity

$$\sigma = \frac{1}{k_{\mathrm{B}} T} \int_0^\infty \mathrm{d}t \ \langle J_x(t) J_x(0) \rangle$$



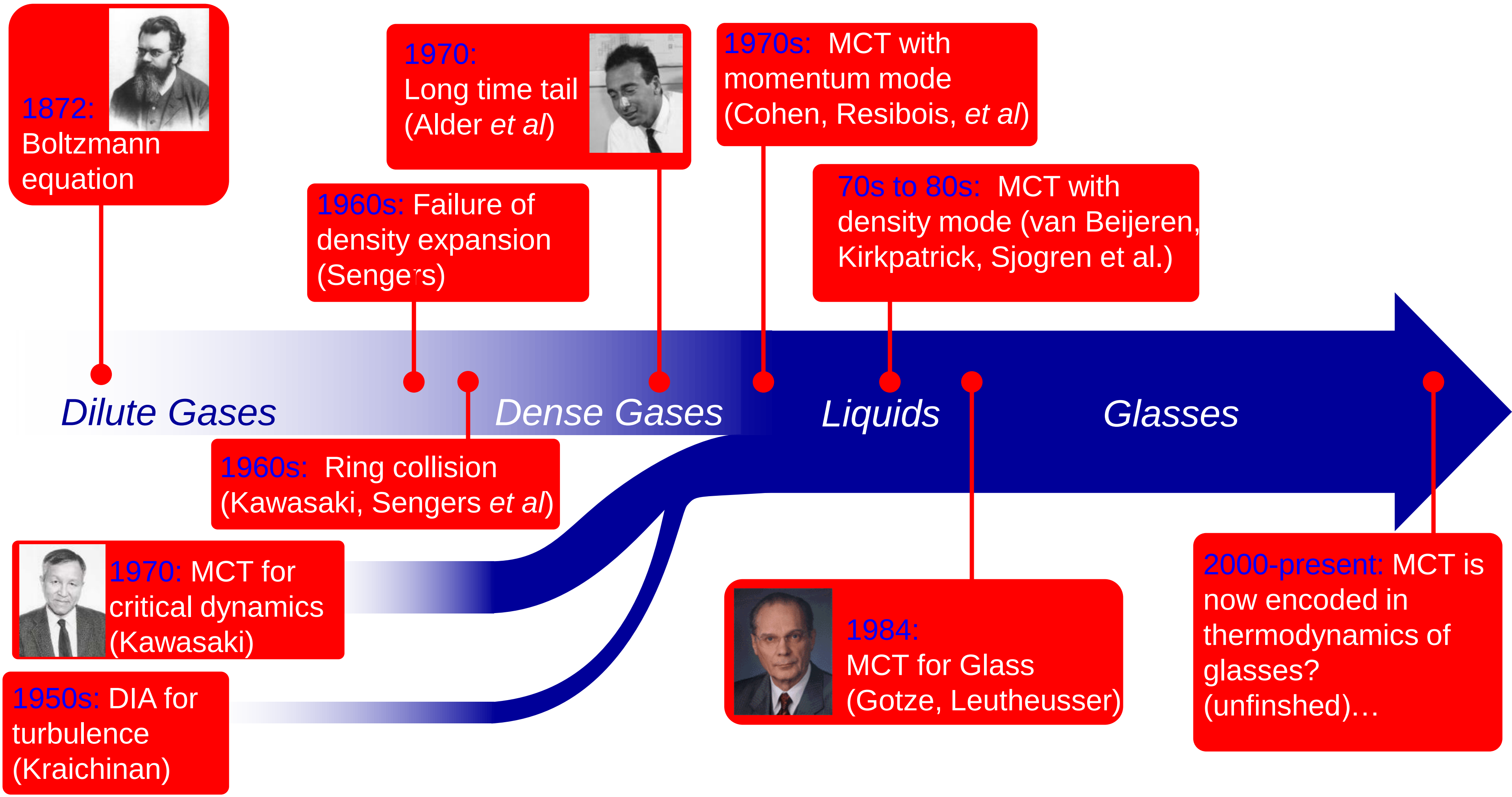
Fluctuation-Dissipation Theorem

Green-Kubo formulae

Linear Response Theory

流体力学から分子運動論まで:モード結合理論超入門

● *History to evaluate transport coefficient*



流体力学から分子運動論まで:モード結合理論超入門

● Brief Introduction of MCT

"Only" first principles theory of the glass transition

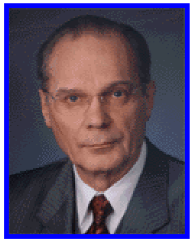
$$\frac{\partial F(k,t)}{\partial t} = -\frac{Dk^2}{S(k)} F(k,t) - \int_0^t dt' M(k,t-t') \frac{\partial F(k,t')}{\partial t'}$$

Structure factor

Memory function (taking care of multibody collisions)

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

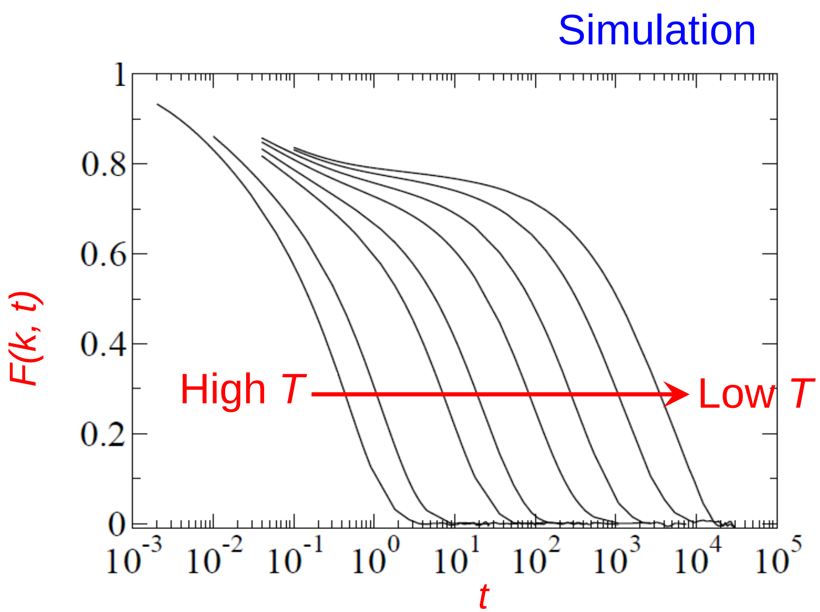
A function of structure factor

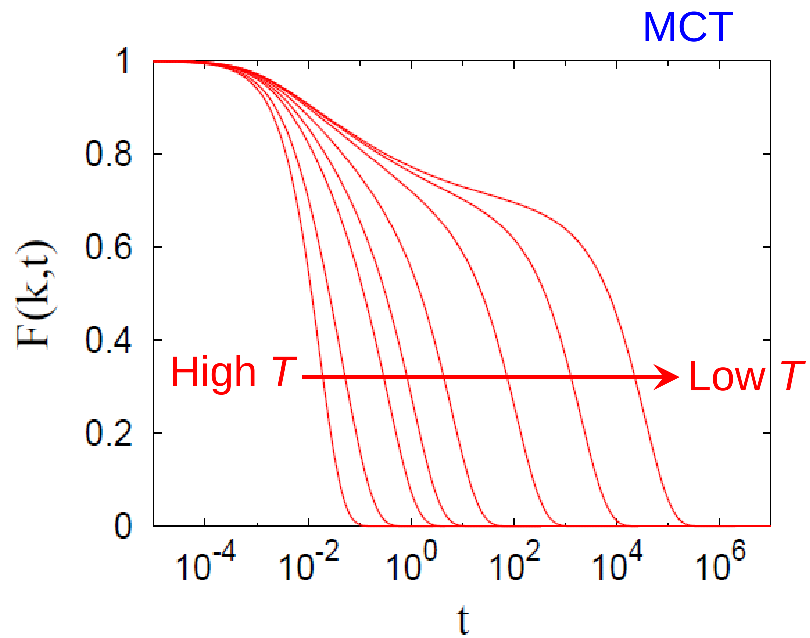


Gotze *et al.* (1984)

● Brief Introduction of MCT

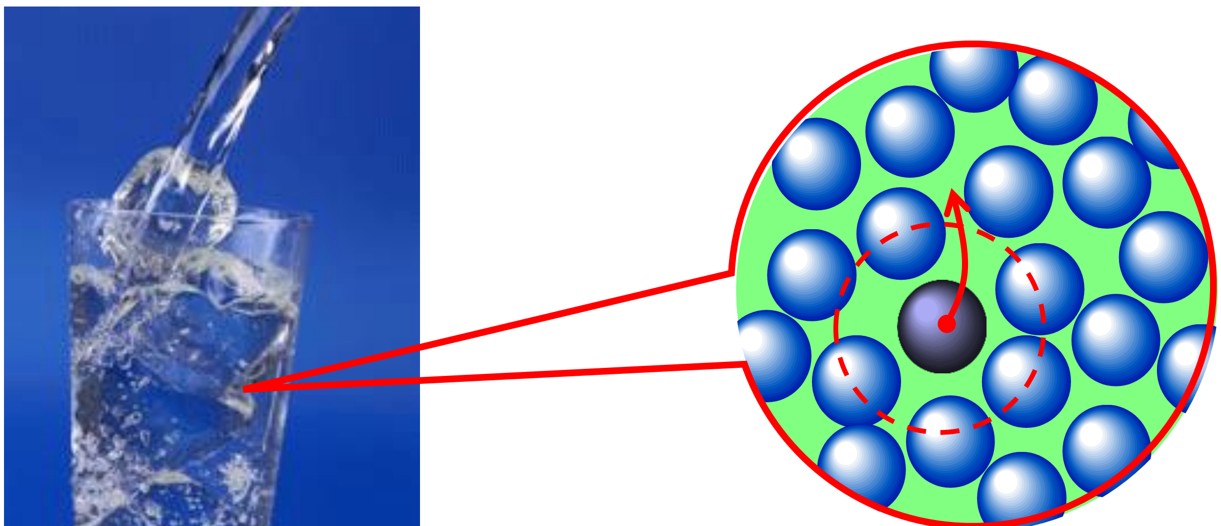
MCT can Predict 2-step relaxation using S(k) as a only input.





流体力学から分子運動論まで:モード結合理論超入門

● Brief Introduction of MCT



Macroscopic Hydrodynamics
Navier-Stokes equation

Diffusive and Congested motion at molecular length scale (Cage effect).
Only relevant length scale is the molecular size (σ)

流体力学から分子運動論まで:モード結合理論超入門

● Brief Introduction of MCT

From macroscopic hydrodynamics to microscopic molecular kinetics

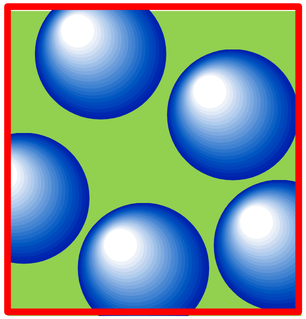
From dense liquid to very dense glassy liquid

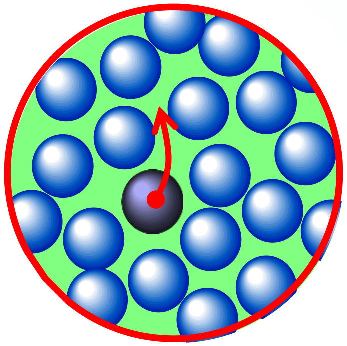
Newton equation

Our approach

Langevin equation

Navier-Stokes equation





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(Fluctuating) Hydrodynamics

Navier-Stokes equation with fluctuations

$$\begin{cases} \dfrac{\partial \rho_m}{\partial t} = -\nabla \cdot (\rho_m \boldsymbol{v}) \\ \dfrac{\partial \rho_m \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho_m \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \left(\zeta + \dfrac{1}{3}\eta\right) \nabla\nabla \cdot \boldsymbol{v} \underline{+ \boldsymbol{f}} \end{cases}$$

ρ_m : Mass density p : Pressure η : Shear viscosity ζ : Bulk viscosity

$$\begin{cases} \langle \boldsymbol{f}(\boldsymbol{r},t)\rangle = 0 \\ \langle f_i(\boldsymbol{r},t) f_j(\boldsymbol{r}',t')\rangle = k_{\rm B}\partial_\alpha\partial_\beta L_{\alpha i,\beta j}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t') \\ \qquad = \partial_\alpha\partial_\beta k_{\rm B}T\left\{\eta\left(\delta_{\alpha j}\delta_{i\beta} + \delta_{\alpha\beta}\delta_{ij} - \dfrac{2}{3}\delta_{\alpha i}\delta_{\beta j}\right) + \zeta\delta_{\alpha i}\delta_{\beta j}\right\}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t') \end{cases}$$

Landau-Lifshitz fluctuating hydrodynamics (see old edition of "Fluid Mechanics")

流体力学から分子運動論まで:モード結合理論超入門

● (Fluctuating) Hydrodynamics

Linearized Navier-Stokes equation with fluctuations

$$\rho(r,t)=\rho_0+\delta\rho(r,t), \qquad \rho\upsilon(r,t)=\rho_0\upsilon_0+J(r,t)$$

$$\begin{cases} \dfrac{\partial \delta\rho}{\partial t} = -\nabla\cdot\boldsymbol{J} \\ \dfrac{\partial \boldsymbol{J}}{\partial t} = -\dfrac{1}{m}\left(\dfrac{\partial p}{\partial \rho}\right)_T \nabla\delta\rho + \nu\nabla^2\boldsymbol{J} + \Gamma\nabla\nabla\cdot\boldsymbol{J} + \boldsymbol{f}' \\ \qquad = -\dfrac{1}{m\rho_0\chi}\nabla\delta\rho + \nu\nabla^2\boldsymbol{J} + \dfrac{1}{\rho_m}\left(\zeta+\dfrac{1}{3}\eta\right)\nabla\nabla\cdot\boldsymbol{J} + \boldsymbol{f} \end{cases}$$

$\chi = -\dfrac{1}{V}\left(\dfrac{\partial V}{\partial p}\right)_T = \dfrac{1}{\rho_0}\left(\dfrac{\partial \rho}{\partial p}\right)_T$: Compressibility $\qquad \nu = \eta/\rho_m$: Kinematic viscosity

In the reciprocal space

$$\begin{cases} \dfrac{\partial \delta\rho_{\mathbf{k}}}{\partial t} = -ikJ_{\mathbf{k}}^{(l)} \\ \dfrac{\partial J_{\mathbf{k}}^{(l)}}{\partial t} = -\dfrac{1}{m\rho_0\chi} ik\delta\rho_{\mathbf{k}} - \Gamma k^2 J_{\mathbf{k}}^{(l)} + f_{\mathbf{k}}^{(l)\prime} \\ \dfrac{\partial J_{\mathbf{k}}^{(1t)}}{\partial t} = -\nu k^2 J_{\mathbf{k}}^{(1t)} + f_{\mathbf{k}}^{(1t)\prime} \end{cases}$$

$\Gamma = (\zeta + 4\eta/3)/\rho_m$

: Sound attenuation coefficient

流体力学から分子運動論まで:モード結合理論超入門

● (Fluctuating) Hydrodynamics

Equation for the density correlation function

$$\frac{\partial^2 F(k,t)}{\partial t^2} = -c^2k^2F(k,t) - \Gamma k^2 \frac{\partial F(k,t)}{\partial t}$$

Equation of damping oscillator

$$c = \frac{1}{\sqrt{\rho_0 \chi}}$$

: Sound velocity

Eigen-modes

$$z = \pm\sqrt{-c^2k^2 + \frac{1}{4}\Gamma^2 k^4} - \frac{1}{2}\Gamma k^2$$

In the hydrodynamic limit; k <<1

$$z \approx \pm ick - \frac{1}{2}\Gamma k^2$$

In the overdamped limit; k >>1

$$z \approx -c^2k^2/\Gamma k^2$$

$$\frac{\partial^2 F(k,t)}{\partial t^2} = -c^2k^2F(k,t) - \Gamma k^2 \frac{\partial F(k,t)}{\partial t}$$

Crossover takes place when $ck \approx \Gamma k^2$ → $\lambda = \Gamma / c \approx 10^{-9}\,\mathrm{m}$

Molecular size!

Generalized Fluctuating Hydrodynamics

We need to extend hydrodynamics to the molecular length scales.

Mori-Zwanzig projection operator method, Generalized Enskog Theory, etc…

$$c^2k^2 \rightarrow c^2(k)k^2$$

$$\Gamma k^2 \rightarrow \Gamma(k)k^2$$

$$\frac{\partial^2 F(k,t)}{\partial t^2} = -c^2k^2F(k,t) - \Gamma k^2\frac{\partial F(k,t)}{\partial t}$$

$$\Rightarrow \quad \frac{\partial^2 F(k,t)}{\partial t^2} = -c^2(k)k^2F(k,t) - \Gamma(k)k^2\frac{\partial F(k,t)}{\partial t}$$

Generalized Fluctuating Hydrodynamics

$$c^2k^2 \to c^2(k)k^2$$

Compressibility in $c^2 = 1/\rho_0\chi$ *can be written in terms of the macroscopic Number fluctuations as (see Landau-Lifshitz. SP Sec12)*

$$\frac{1}{N}\langle \Delta N^2 \rangle = \rho_0 k_{\mathrm{B}} T \chi$$

Using the local density; $\Delta N = \int \mathrm{d}\boldsymbol{r}\ \delta\rho(\boldsymbol{r})$

$$\rho_0 k_{\mathrm{B}} T \chi = \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}' \ \frac{1}{N}\langle \delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}') \rangle$$

Or in its reciprocal space representation

$$\rho_0 k_{\mathrm{B}} T \chi = \lim_{\mathbf{k}\to 0} \frac{1}{N}\langle \delta\rho_{\mathbf{k}}\delta\rho_{-\mathbf{k}} \rangle = \lim_{\mathbf{k}\to 0} S(k)$$

Static structure factor (equal time density correlator)

Thus,

$$c^2 \longrightarrow c^2(k) = \frac{1}{\rho_0\chi(k)} = \frac{k_{\mathrm{B}}T}{S(k)}$$

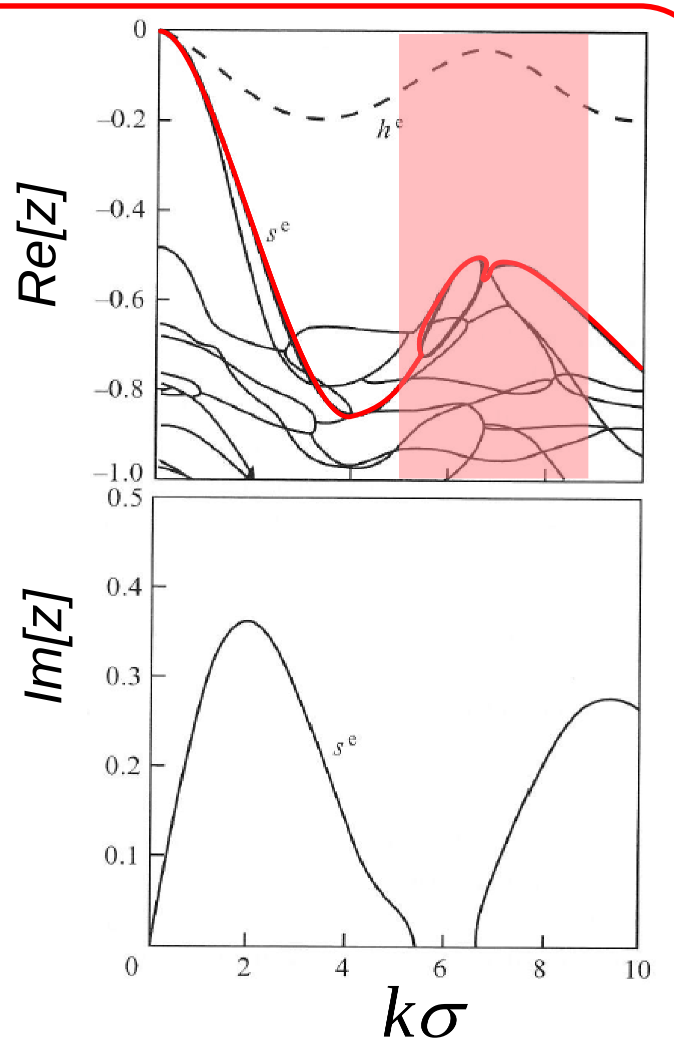
Generalized Fluctuating Hydrodynamics

$$\Gamma k^2 \rightarrow \Gamma(k)k^2$$

Guess from the generalized Boltzman-Enskog Theory (Cohen, Kirkpatrick, etc. 1980s).

This takes the effect of the size of the particle σ, *the change of the phase* exp(ikσ), *and the collision* frequency g(σ) into account in the Boltzmann equation.

$\Gamma(k)k^2$ is almost constant around $k \approx 1/\sigma$



Generalized modes evaluated for dense hard sphere using the generalized B-E equation (from de Montfrooij (2008))

流体力学から分子運動論まで:モード結合理論超入門

● Generalized Fluctuating Hydrodynamics

At large k's, we have

$$\frac{\partial^2 F(k,t)}{\partial t^2} = -c^2(k)k^2F(k,t) - \Gamma(k)k^2\frac{\partial F(k,t)}{\partial t}$$

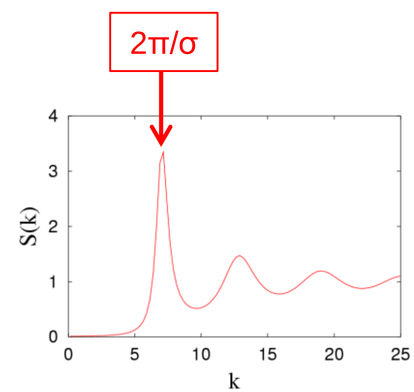
$$c^2(k) = \frac{k_{\mathrm{B}}T}{S(k)} \qquad \Gamma(k)k^2 \equiv \zeta$$

$$\frac{\partial F(k,t)}{\partial t} = -\frac{k_{\mathrm{B}}Tk^2}{\zeta S(k)}F(k,t) = -\frac{Dk^2}{S(k)}F(k,t)$$

Diffusion Equation

Drastic slow down at molecular length scale (de Genne narrowing).

But not slow enough to explain the decades of increase of the relaxation time near the glass transition point.



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● Crush Course of Mode-Coupling Theory

$$\frac{\partial F(k,t)}{\partial t} = -\frac{k_{\mathrm{B}}Tk^2}{\zeta S(k)}F(k,t) = -\frac{Dk^2}{S(k)}F(k,t)$$

What is missing is the non-linear feedback mechanism of the cage diffusion. “The tight cages would decelerate the diffusion, which in turn would make the cage tighter.”

$$\frac{\partial \boldsymbol{J}}{\partial t} = -\frac{1}{m}\rho\nabla\frac{\delta F}{\delta\rho} + \nu\nabla^2\boldsymbol{J} + \Gamma\nabla\nabla\cdot\boldsymbol{J}$$

Gibbs-Duhem $V\mathrm{d}p = N\mathrm{d}\mu$

$+$

$$\mu = \frac{\delta F}{\delta\rho}$$

Free energy (as a functional of density

$$F[\rho] \approx k_{\mathrm{B}}T\left\{\int \mathrm{d}\boldsymbol{r}\ \rho(\boldsymbol{r})\left\{\ln\rho(\boldsymbol{r}) - 1\right\} - \frac{1}{2}\int \mathrm{d}\boldsymbol{r}_1\int \mathrm{d}\boldsymbol{r}_2 c(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta\rho(\boldsymbol{r}_1)\delta\rho(\boldsymbol{r}_2)\right\}$$

$c(\boldsymbol{r})$: Direct correlation function (a function of S(k))

Crush Course of Mode-Coupling Theory

Thus, the pressure term is

$$-\frac{1}{m}\rho\nabla\frac{\delta F}{\delta\rho} \simeq -\frac{k_{\mathrm{B}}T}{m}\left\{\nabla\delta\rho(\boldsymbol{r}) - \rho\nabla\int \mathrm{d}\boldsymbol{r}' c(\boldsymbol{r}-\boldsymbol{r}')\delta\rho(\boldsymbol{r}') - \delta\rho(\boldsymbol{r})\nabla\int \mathrm{d}\boldsymbol{r}' c(\boldsymbol{r}-\boldsymbol{r}')\delta\rho(\boldsymbol{r}')\right\}$$

$$\begin{cases} \dfrac{\partial\delta\rho_{\mathbf{k}}}{\partial t} = -ikJ_{\mathbf{k}}^{(l)} \\ \dfrac{\partial J_{\mathbf{k}}^{(l)}}{\partial t} = -\dfrac{ikk_{\mathrm{B}}T}{mS(k)}\delta\rho_{\mathbf{k}} - \underline{\dfrac{k_{\mathrm{B}}T}{m}\displaystyle\int \mathrm{d}\boldsymbol{q}\; i\hat{\boldsymbol{k}}\cdot\boldsymbol{q}c(\boldsymbol{k}-\boldsymbol{q})\delta\rho_{\mathbf{k}-\mathbf{q}}\delta\rho_{\mathbf{q}}} - \Gamma_k k^2 J_{\mathbf{k}}^{(l)} \end{cases}$$

The nonlinear term in the density fluctuations

Crush Course of Mode-Coupling Theory

9 easy steps to renormalize the nonlinear dynamic equation (MSR field theory)

$$\begin{cases} \dfrac{\partial \delta\rho_{\mathbf{k}}}{\partial t} = -ikJ_{\mathbf{k}}^{(l)} \\ \dfrac{\partial J_{\mathbf{k}}^{(l)}}{\partial t} = -\dfrac{ikk_{\mathrm{B}}T}{mS(k)}\delta\rho_{\mathbf{k}} - \underline{\underline{\dfrac{k_{\mathrm{B}}T}{m}\int \mathrm{d}\boldsymbol{q}\; i\hat{\boldsymbol{k}}\cdot\boldsymbol{q}c(\boldsymbol{k}-\boldsymbol{q})\delta\rho_{\mathbf{k}-\mathbf{q}}\delta\rho_{\mathbf{q}}}} - \Gamma_k k^2 J_{\mathbf{k}}^{(l)} \end{cases}$$

The nonlinear term in the density fluctuations

Step 0: Let's simplify the equation

$$\dot{x}(t) = -\gamma\, x(t) + \lambda\, x^2(t) + \eta(t)$$

with

$$\langle \eta(t)\eta(t')\rangle = 2k_B\gamma\delta(t-t')$$

Crush Course of Mode-Coupling Theory

Step 1: Multiply x(0) from the right, and then take the average over ensemble

For $C_2(t) = \langle x(t)x(0) \rangle$

$$\frac{\partial C_2(t)}{\partial t} = -\gamma\, C_2(t) + \lambda C_{2,1}(t)$$

where $C_{2,1}(t) = \langle x^2(t)x(0) \rangle$

Step 2: From the reversibility of time

$$C_{2,1}(t) = C_{1,2}(t) \equiv \langle x(t)x^2(0) \rangle$$

Step 3: Take the time derivative of $C_{1,2}(t) \equiv \langle x(t)x^2(0) \rangle$

$$\frac{\partial C_{1,2}(t)}{\partial t} = -\gamma\, C_{1,2}(t) + \lambda C_{2,2}(t)$$

where $C_{2,2}(t) = \langle x^2(t)x^2(0) \rangle$

流体力学から分子運動論まで:モード結合理論超入門

● Crush Course of Mode-Coupling Theory

Step 4: Solving the equation formally for $C_{1,2}(t)$

$$C_{1,2}(t) \approx \lambda \int_0^t dt' \exp\left[-\gamma(t-t')\right] C_{2,2}(t')$$

Step 5: Plug this back to equation for $C_2(t)$

$$\frac{\partial C_2(t)}{\partial t} = -\gamma\, C_2(t) + \lambda^2 \int_0^t dt' \exp\left[-\gamma(t-t')\right] C_{2,2}(t')$$

Step 6: Gaussian approximation for $C_{2,2}(t)$

$$C_{2,2}(t) = \left\langle x^2(t) x^2(0) \right\rangle \approx 2\left\langle x(t) x(0) \right\rangle^2 = 2C_2^2(t)$$

● Crush Course of Mode-Coupling Theory

Step 7: Also the simple relaxation can be approximated as

$$\exp[-\gamma\, t] \approx C_2(t)$$

Step 8: Now arrived at equation closed in terms of $C_2(t)$!

$$\frac{\partial C_2(t)}{\partial t} = -\gamma\, C_2(t) - 2\lambda^2 \int_0^t dt'\, C_2^2(t-t')\, \frac{\partial C_2(t')}{\partial t'}$$

Step 9: Translate back to the original variables. Voila!!

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

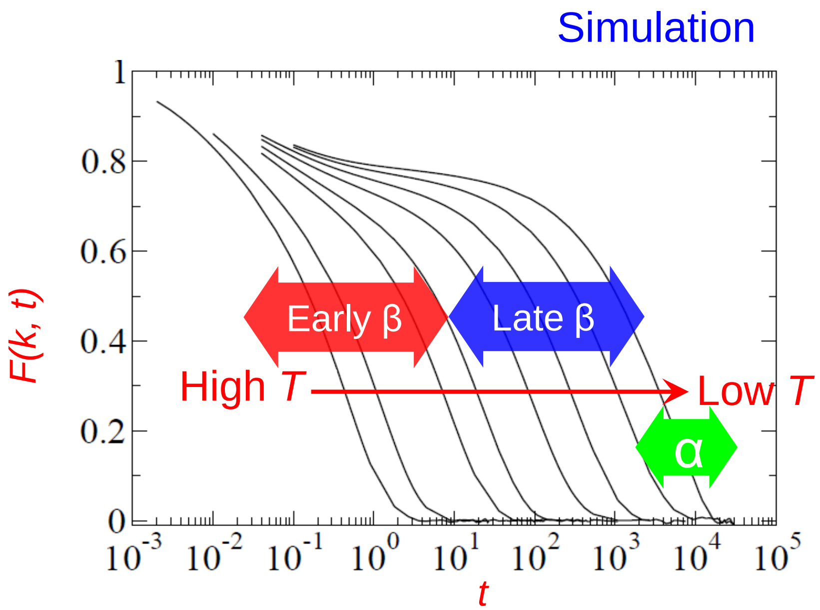
What MCT can and cannot do

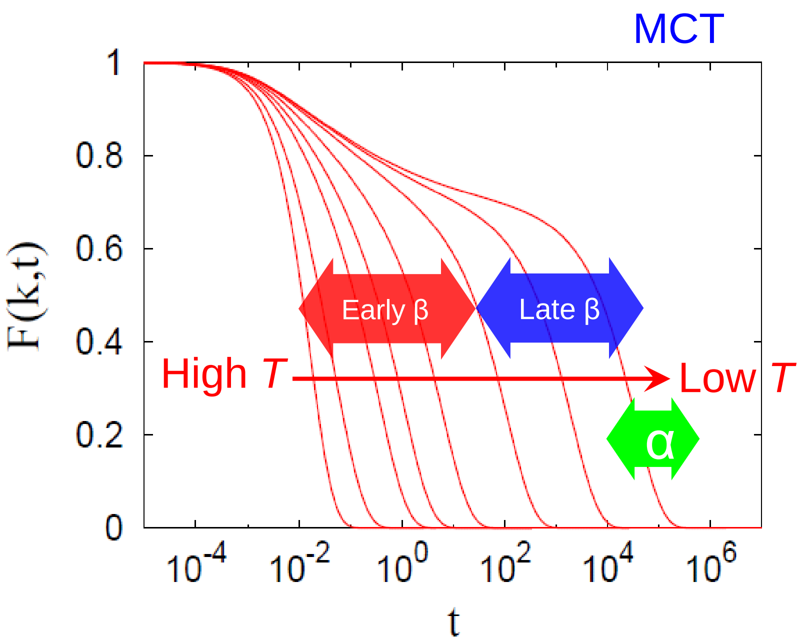
Check List

1. 2段階緩和
2. 非アレニウス的な粘性係数(緩和時間)の増大
3. 引き延ばされた指数関数減衰
4. Stokes-Einstein 則の破れ
5. ダイナミクスのスケーリング
6. 動的不均一性
7. ・・・

● What MCT can and cannot do

MCT can Predict 2-step relaxation





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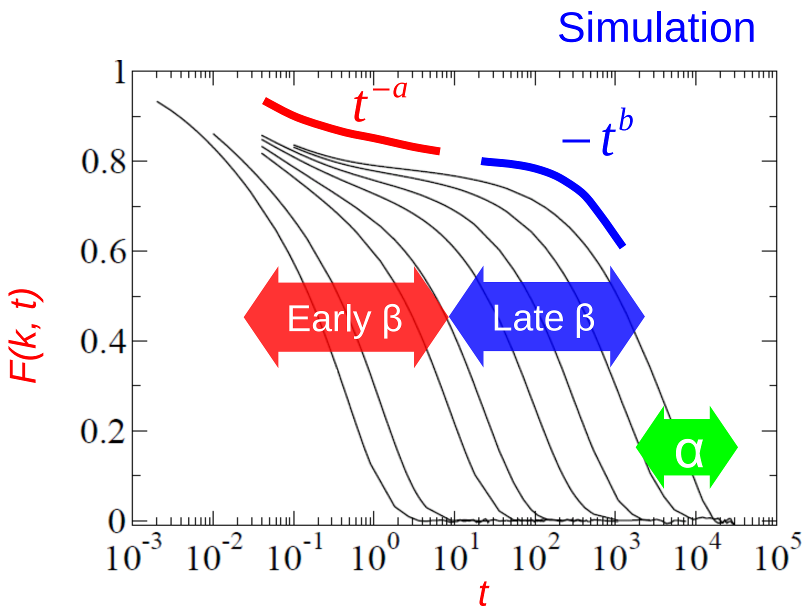
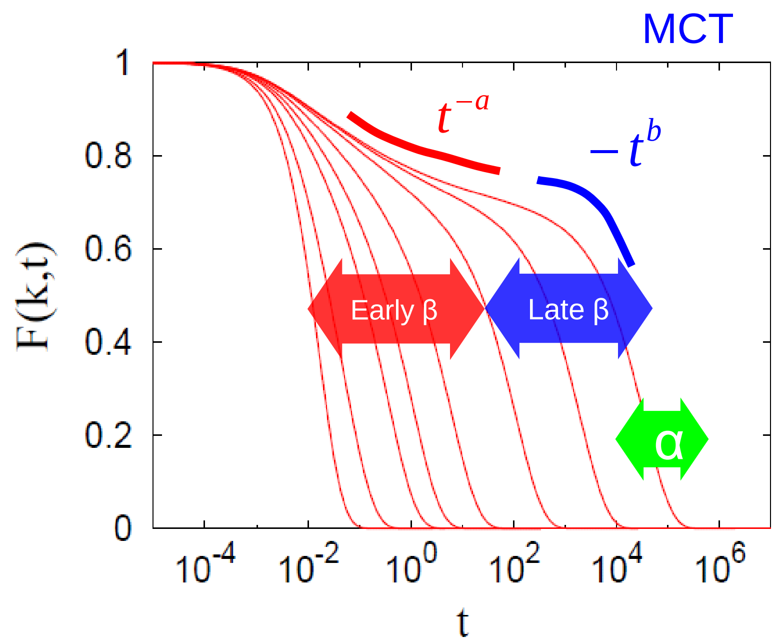




Algebraic β relaxation (von Schweidler law)

For a hard sphere colloidal glass

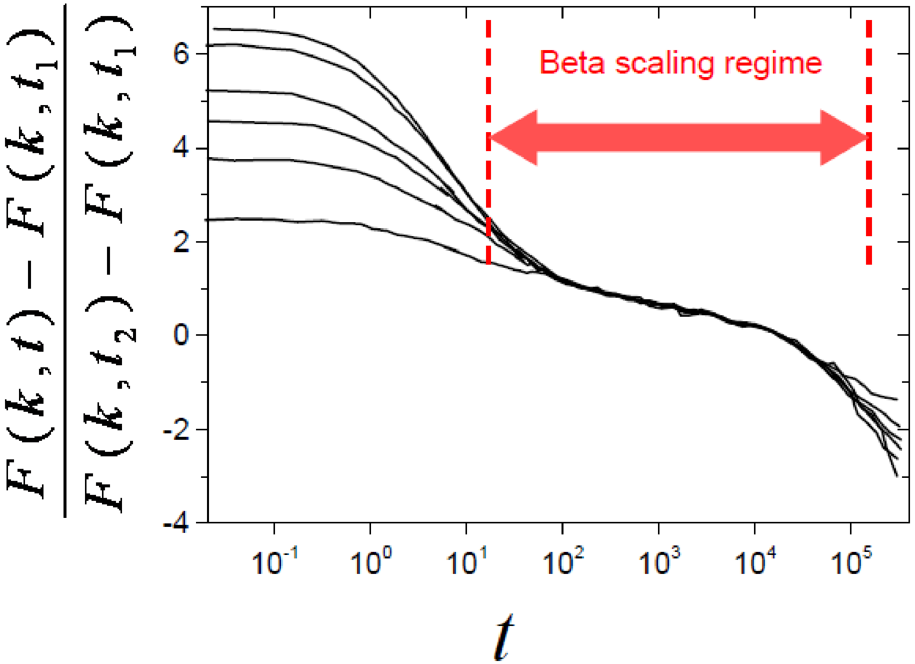
Experiment: $a = 0.328, \quad b = 0.646$

MCT: $a = 0.312, \quad b = 0.583$

流体力学から分子運動論まで:モード結合理論超入門

● What MCT can and cannot do

MCT can Predict 2-step relaxation



(Gleim and Kob '00)

Algebraic β relaxation (von Schweidler law)

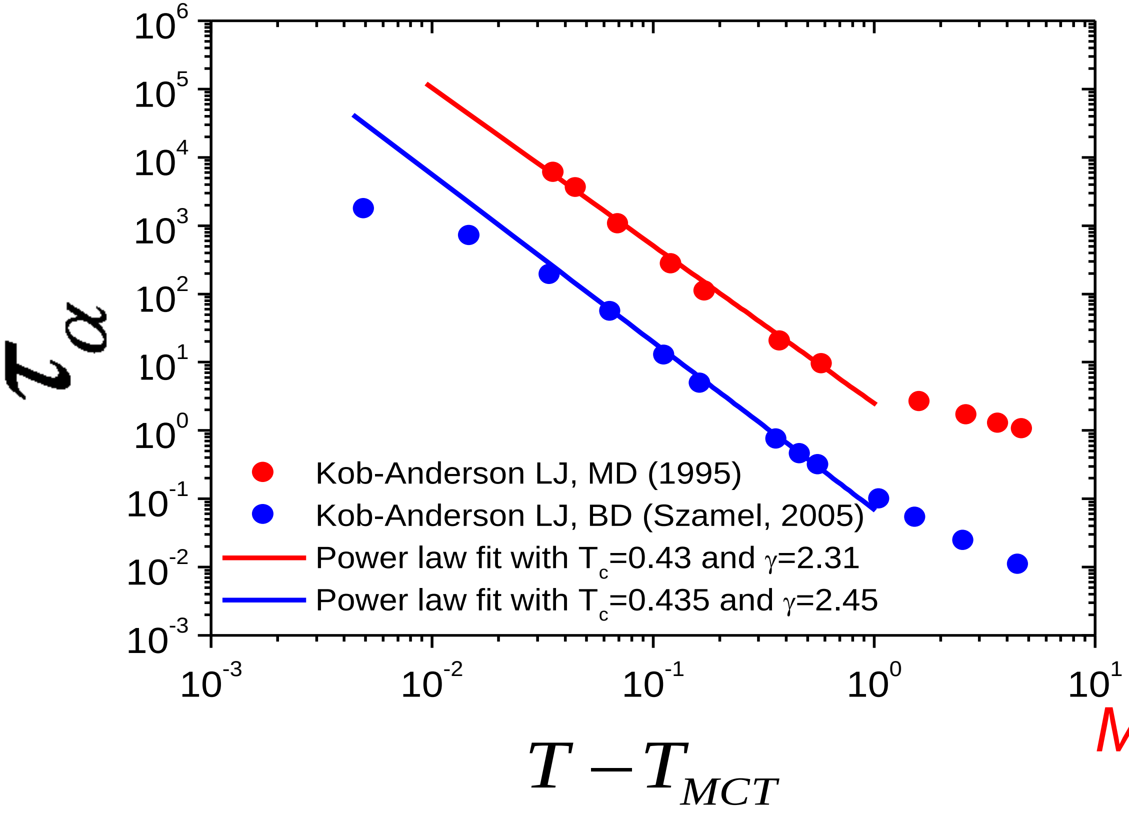
For a hard sphere colloidal glass
(van Megen 1995)

Experiment: $a = 0.328, \quad b = 0.646$

MCT: $a = 0.312, \quad b = 0.583$

● What MCT can and cannot do

MCT can predict power law of α relaxation time and viscosity



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

$$\eta \propto \left| T - T_{\rm MCT} \right|^{-\gamma}$$

with $\gamma = \frac{1}{2a} + \frac{1}{2b}$

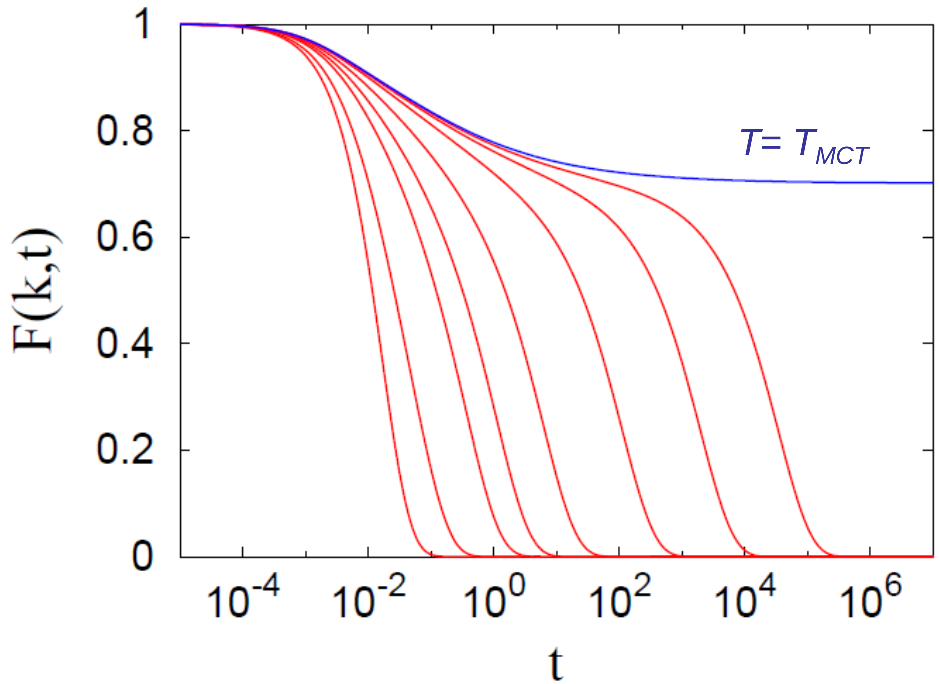
MCT predicts $\gamma = 2.46$

(for LJ binary system)

What MCT can and cannot do

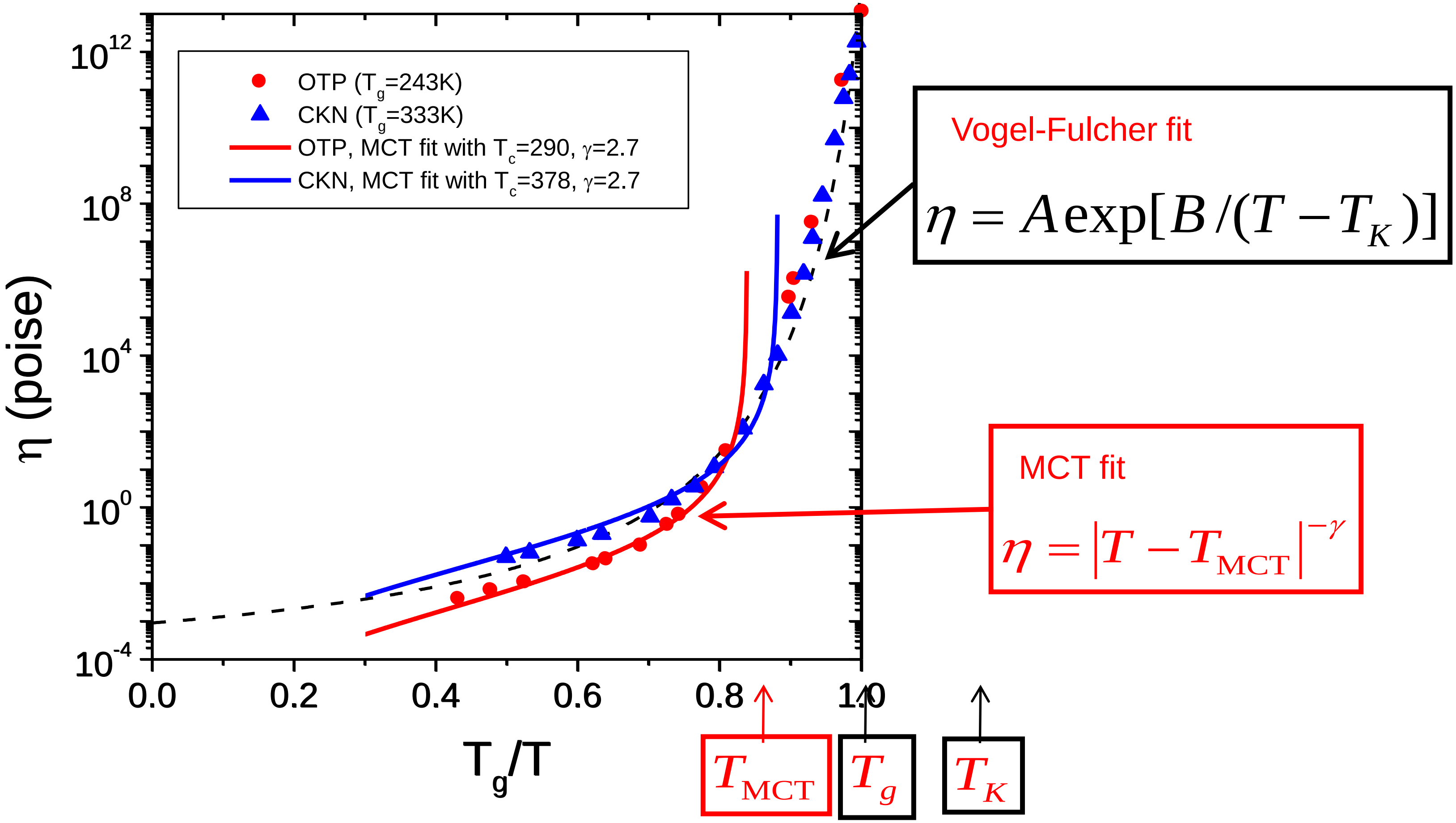
MCT can't go beyond T_{MCT} (> T_g)

Predict a spurious non-Ergodic transition at T_{MCT}.



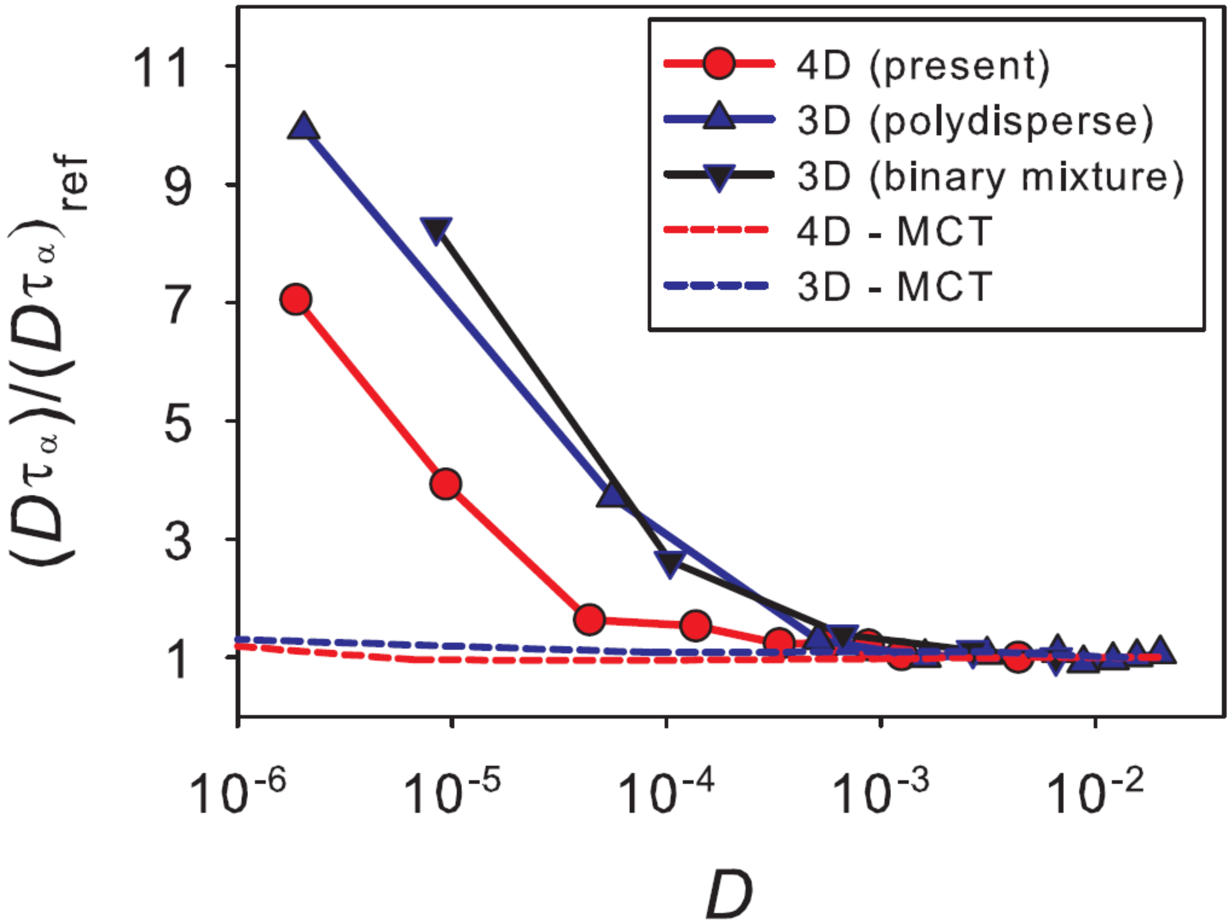
● What MCT can and cannot do

MCT can't go beyond T_{MCT} (> T_g)



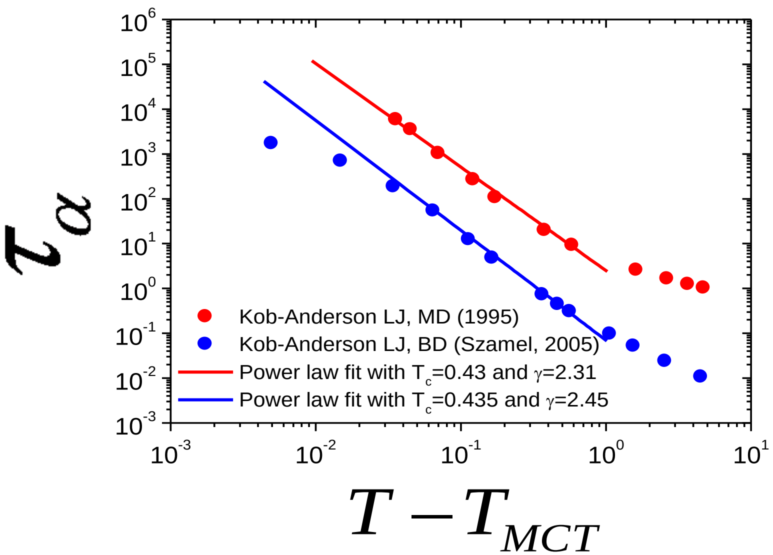
What MCT can and cannot do

MCT can't explain Stokes-Einstein Law $D \propto 1/\tau_\alpha$



What MCT can and cannot do

MCT can't give a quantitatve prediction for T_{mct}



$$\tau_\alpha \propto \left| T - T_{mct}^{(fit)} \right|^{-\gamma}$$

For binary Lennard-Jones system

$$T_{mct}^{(fit)} = 0.435 \qquad T_{mct}^{(theory)} = 0.9515$$

For binary hard-sphere system

$$\varphi_{mct}^{(fit)} = 0.58 \qquad \varphi_{mct}^{(theory)} = 0.52$$

Discuss about it later

● What MCT can and cannot do

Check List

☑ 1. 2段階緩和

2. 非アレニウス的な粘性係数（緩和時間）の増大

3. 引き延ばされた指数関数減衰

4. Stokes-Einstein 則の破れ

☑ 5. ダイナミクスのスケーリング

6. 動的不均一性

7. ・・・