Comparing two dynamics with the same energy landscape

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Brownian dynamics: glassy vs trivial

Motivations behind a twisted idea

Langevin dynamics of interacting colloids

Model B version of the dynamics

Unsettled issues

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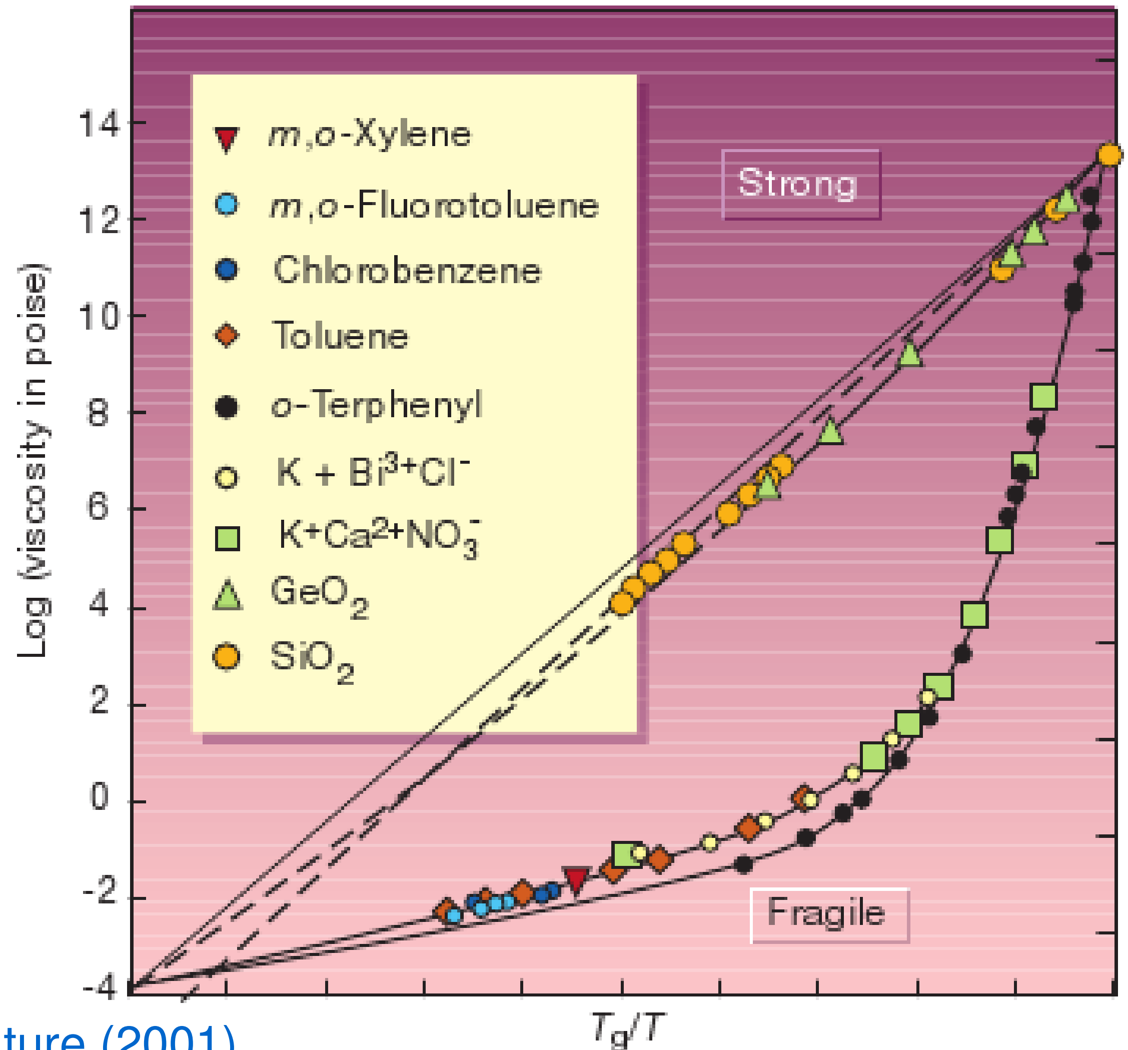
Viscosity shoots up

Angell plot

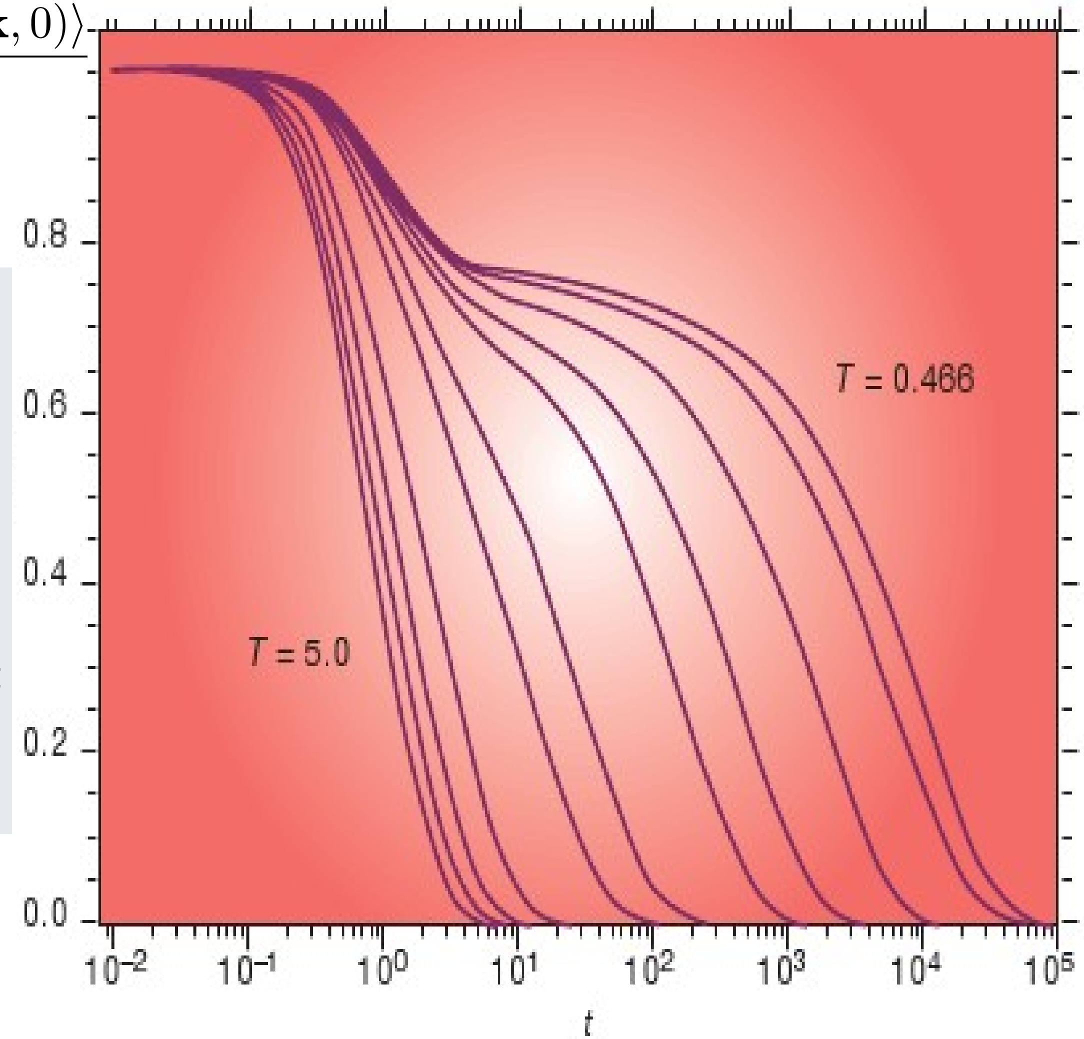


C.A. Angell, Science (1995).
C.A. Debenedetti and F.H. Stillinger, Nature (2001).

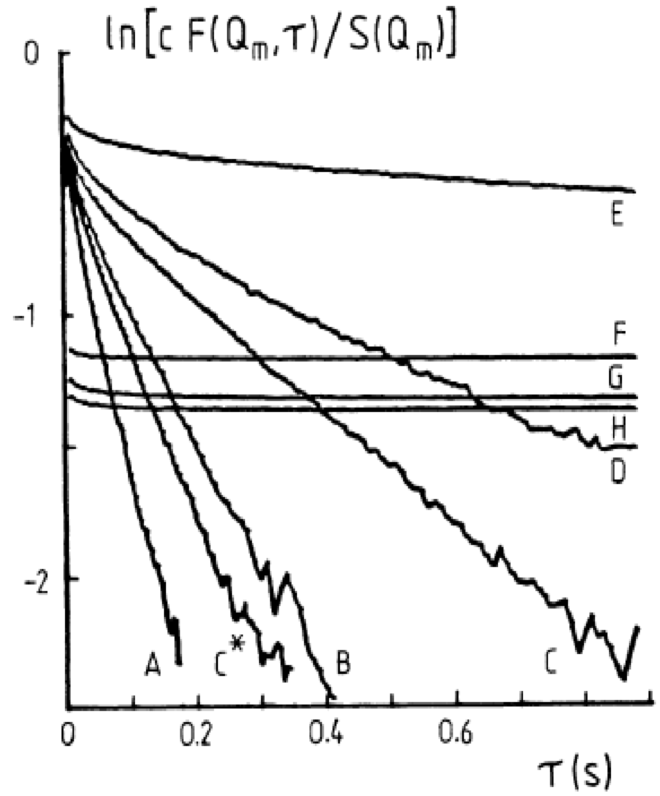
Relaxation can take for ever

$$\frac{\langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle}{\rho_0 S_{\mathbf{k}}}$$

Figure 9 Evolution of the self-intermediate scattering function for A-type atoms for the same supercooled Lennard–Jones mixture as in Fig. 6, at $q\sigma_{AA} = 7.251$, corresponding to the first peak of the static structure factor of species A (ref. 92). Here q is the magnitude of the wave vector. Temperature and time are in units of ε_{AA}/k_B and $\sigma_{AA}(m/48\varepsilon_{AA})^{1/2}$, respectively. Temperatures from left to right are 5, 4, 3, 2, 1, 0.8, 0.6, 0.55, 0.5, 0.475, and 0.466. The self-intermediate scattering function is the space Fourier transform of the van Hove function $G_s(r, t)$, which is proportional to the probability of observing a particle at $r \pm dr$ at time t given that the same particle was at the origin at $t = 0$. Note the two-step relaxation behaviour upon decreasing T. Molecular dynamics simulations of 1,000 atoms. (Adapted from refs 9 and 92.)



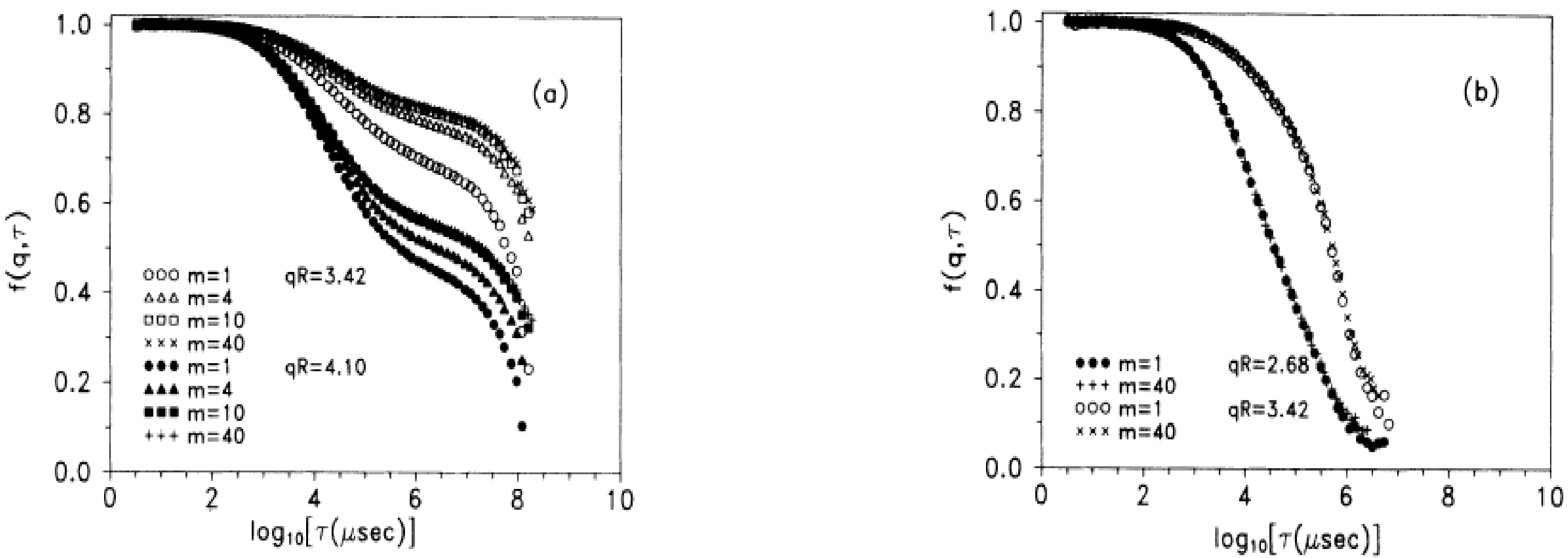
Also in colloidal systems (PMMA)



Pusey & Van Megen, PRL (1987)

FIG. 1. Semilogarithmic plots of the dynamic structure factor $[cF(Q_m,\tau)/S(Q_m)]$, measured at the main peaks of the static structure factor, against delay time τ for suspensions of collodial spheres (samples A to H, see Table I). For the "nonergodic" samples F, G, H an enlarged scattering volume was used, leading to a reduced amplitude c (see text). Note (i) initial rapid and longer-time slow decays and (ii) marked divergence of the slow decay time with increasing concentration (A → H).

More recent experiments (PMMA)



Van Megen & Underwood, PRE (1994)

FIG. 3. Intermediate scattering functions versus the logarithm of the delay time τ for (a) $\phi=0.574$ and (b) $\phi=0.535$ estimated from Eqs. (16) and (22) using different numbers m of independent measurements of time-averaged intensities and intensity autocorrelation functions. See Sec. III B for details. The ISF's shown here and in subsequent figures are normalized so that $f(q,0)=1$.

Local heterogenous picture

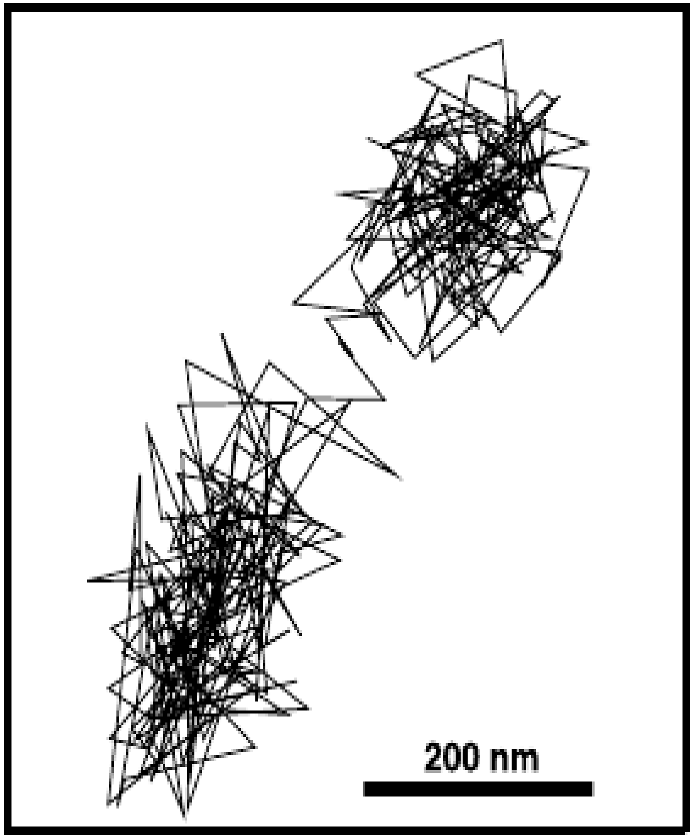
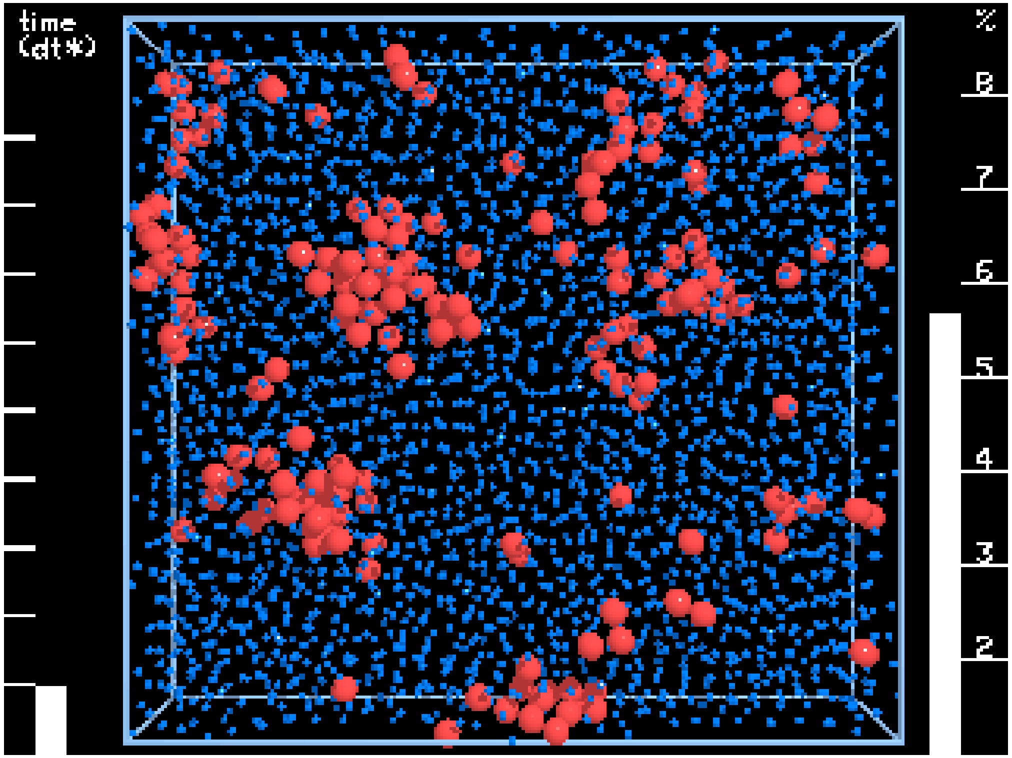


Fig. 2. A typical trajectory for 100 min for $\phi = 0.56$. Particles spent most of their time confined in cages formed by their neighbors and moved significant distances only during quick, rare cage rearrangements. The particle shown took ~500 s to shift position. The particle was tracked in 3D; the 2D projection is shown.

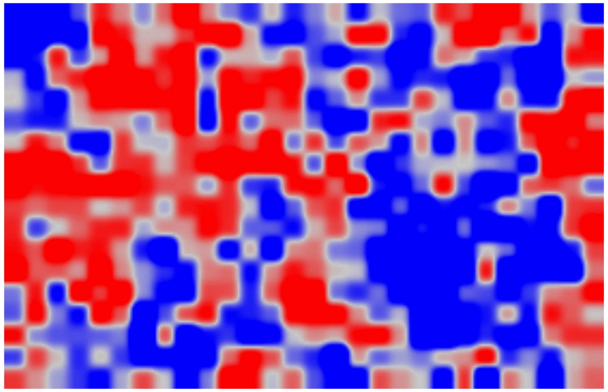
Weeks, Crocker, Levitt,
Schofield & Weitz, Science (2000)

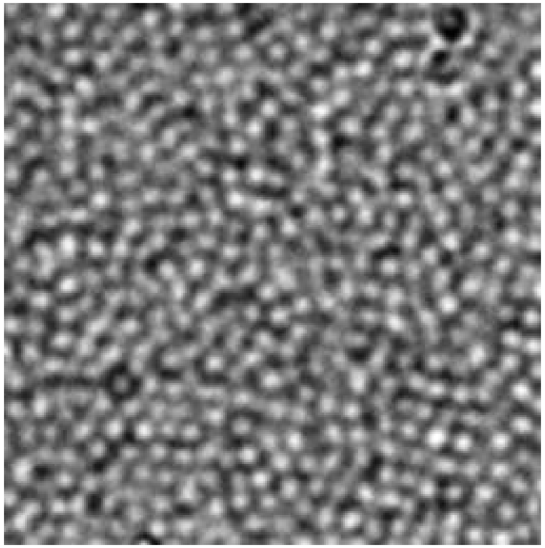
Heterogeneities

Taken from E. Weeks, 3D confocal microscope imaging (at 56% volume fraction)



Heterogeneities



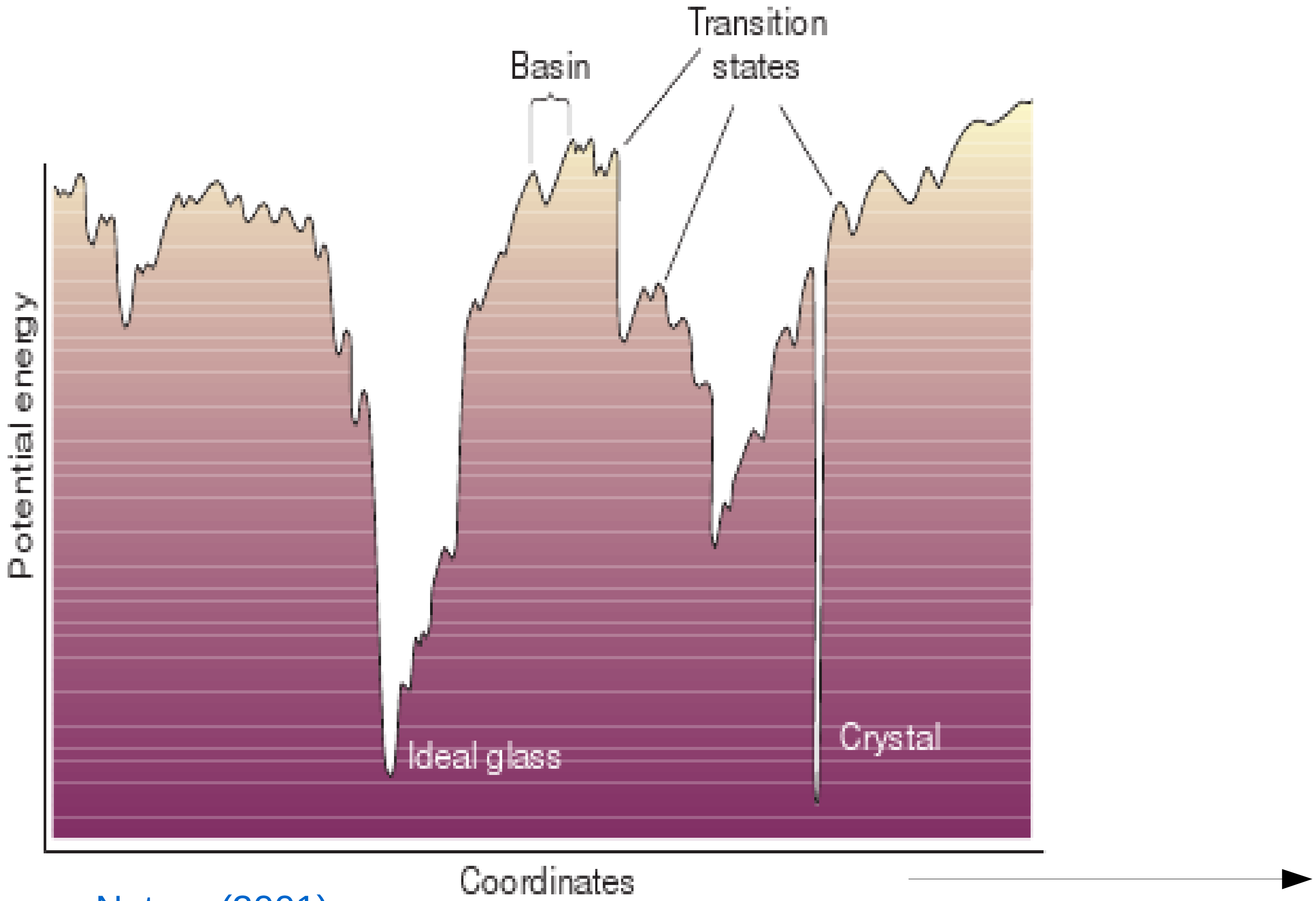


R. Colin & B. Abou (2013), pNIPAM, 32 °C

What is a glass?

- Viscosity increase
- Slow relaxation and dynamical arrest
- Dynamical heterogeneities and intermittency

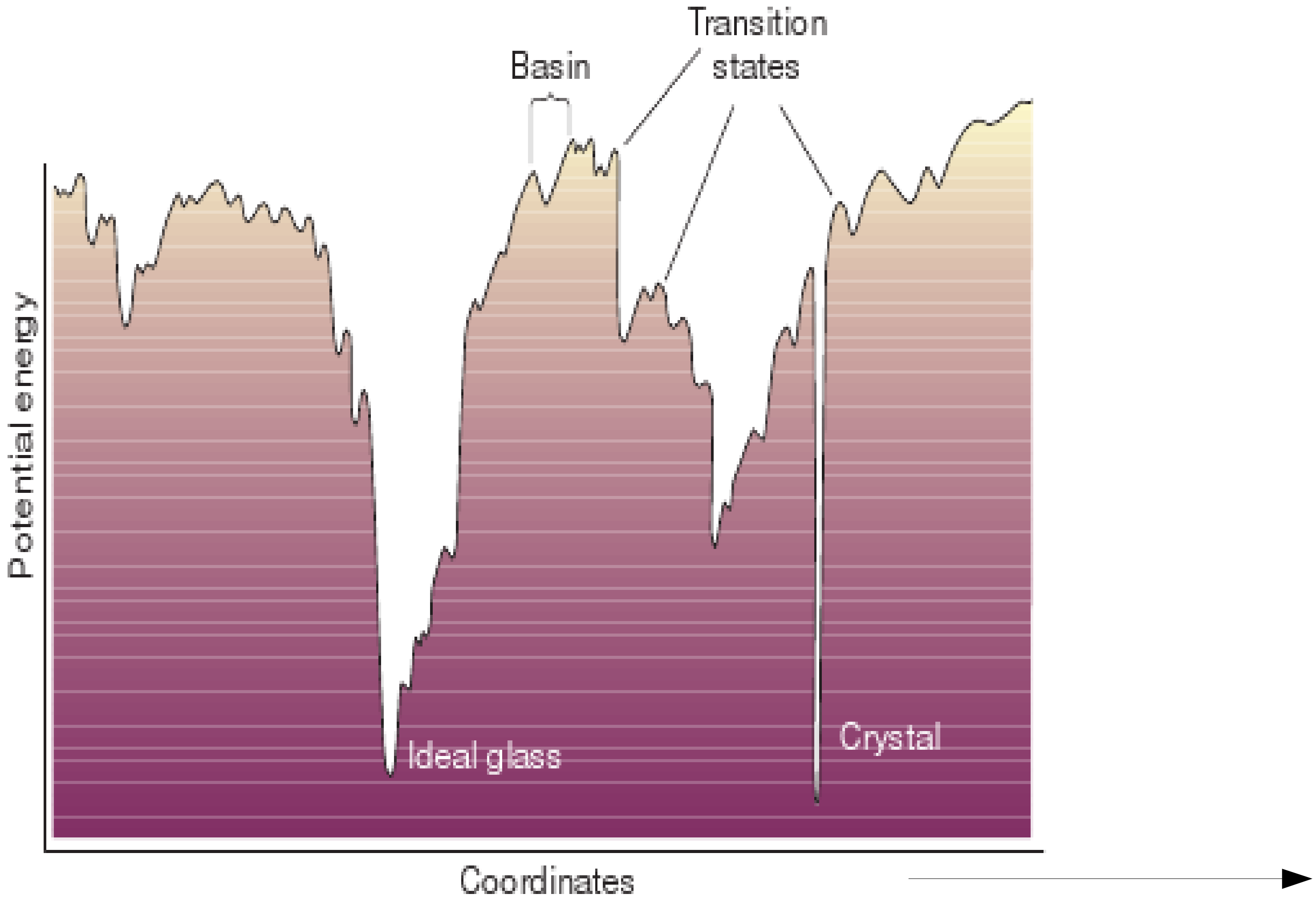
Energy landscape



Debenedetti & Stillinger, Nature (2001)

particle coordinates

Energy landscape



density modes

Statics based theories

- Cooperatively rearranging regions, Adam & Gibbs, 1965
- Free volume, Cohen & Turnbull, 1970
- Energy landscape, Goldstein, 1969
- Random First Order, Kirkpatrick, Thirumalai & Wolynes, 1989
- Replicas, Mézard & Parisi, 1999, based on an idea from Monasson

Landscape

For N interacting particles,

$$Z = \int \mathrm{d}^3 r_1 \ldots \mathrm{d}^3 r_N \mathrm{e}^{-\beta \mathcal{H}}$$

$$\mathcal{H} = \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j)$$

Landscape

Alternatively

$$Z = \int \mathcal{D}\rho \mathrm{e}^{-\beta \mathcal{F}[\rho]}$$

$$\mathcal{F}[\rho] = T \int_{\mathbf{r}} \rho \ln \rho + \frac{1}{2} \int_{\mathbf{r},\mathbf{r}'} \rho(\mathbf{r}) V(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}')$$

Landscape

Alternatively

$$Z = \int \mathcal{D}\rho \mathrm{e}^{-\beta \mathcal{F}[\rho]}$$

$$\mathcal{F}[\rho] = T \int_{\mathbf{r}} \rho \ln \rho + \frac{1}{2} \int_{\mathbf{r},\mathbf{r}'} \rho(\mathbf{r}) V(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}')$$

entropy

energy

Density Functional Theory

Search (and find) the minima of

$$\mathcal{F}[\rho] = T \int_{\mathbf{r}} \rho \ln \rho + \frac{1}{2} \int_{\mathbf{r},\mathbf{r}'} \rho(\mathbf{r}) V(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}')$$

Many local minima. No a priori knowledge.

Kaur & Das, Phys. Rev. Lett. (2001)

Replicas

Use a copy of the system to help the original system polarize into a metastable state.

$$Z(m,\beta) = \int \prod_{a=1}^{m} \mathcal{D}\rho_a \mathrm{e}^{-\beta \sum_a \mathcal{F}_a - \beta\varepsilon \frac{1}{2} \sum_{ab} \rho_a(\mathbf{r}) w(\mathbf{r}-\mathbf{r}')\rho_b(\mathbf{r}')}$$

ε =small

$w(\mathbf{r}_i^a - \mathbf{r}_j^b)$ =attractive potential between replicas

Replicas

Phase transition with

$$\langle(\rho_1(\mathbf{r})-\rho_0)(\rho_2(\mathbf{r}')-\rho_0)\rangle = \langle\delta\rho_1(\mathbf{r})\delta\rho_2(\mathbf{r}')\rangle$$

as the order parameter when temperature is decreased.

Identified as the glass transition.

Replicas

Phase transition with

$$\langle(\rho_1(\mathbf{r}) - \rho_0)(\rho_2(\mathbf{r}') - \rho_0)\rangle = \langle\delta\rho_1(\mathbf{r})\delta\rho_2(\mathbf{r}')\rangle$$

$$\lim_{m\to 1}\lim_{\varepsilon\to 0}\lim_{N\to\infty}\langle\delta\rho^{(a)}(\mathbf{k})\delta\rho^{(b)}(-\mathbf{k})\rangle$$

as the order parameter when temperature is decreased.

Identified as the glass transition.

Dynamics based theories

Colloidal particles dispersed in a solution:

- Positions $\mathbf{r}_j(t),\ j = 1, \ldots, N$
- Density ρ_0 rather than the volume fraction $\phi = \rho_0 \frac{1}{6} \pi \sigma^3$
- Temperature $T = \frac{1}{\beta}$
- Pairwise interactions $V(\mathbf{r}) = \varepsilon \left(1 - r/\sigma\right)^2 \Theta(\sigma - r)$

with $\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$

Dynamics based theories

Overdamped Langevin dynamics

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = -\sum_{j \neq i} \boldsymbol{\nabla} V(\mathbf{r}_i - \mathbf{r}_j) + \sqrt{2T}\boldsymbol{\xi}_i$$

$$\langle \xi_i^\alpha(t) \xi_j^\beta(t') \rangle = \delta^{\alpha\beta}\delta_{ij}\delta(t - t')$$

$$P_{\mathrm{eq}}[\{\mathbf{r}_\ell\}] = Z^{-1}\mathrm{e}^{-\beta \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j)}$$

Fluctuation-Dissipation theorem holds.

Or systems with constrained dynamics

This is a phenomenological description, not a theory.

Lattice models with dynamical evolution rules such that

- The stationary equilibrium distribution is that of an ideal gas (flat energy landscape);
- Dynamics are extremely slow.

Playing with dynamics

Markov process with states $\mathcal{C}$

Transition rates that fulfill the detailed balance condition wrt

$$P_{\mathrm{eq}}(\mathcal{C}) = \frac{\mathrm{e}^{-\beta H(\mathcal{C})}}{Z}$$

$$W(\mathcal{C} \to \mathcal{C}') P_{\mathrm{eq}}(\mathcal{C}) = W(\mathcal{C}' \to \mathcal{C}) P_{\mathrm{eq}}(\mathcal{C}')$$

Choice 1:

De Dominicis, Orland, Lainée, J. Physique Lett. (1985)

Rates

$$W(\mathcal{C} \to \mathcal{C}') = P_{\mathrm{eq}}(\mathcal{C}')$$

Relaxation rate is -1 (highly degenerate).

Choice 2:

Koper & Hilhorst, Physica A (1989)

Rates

$$W(\mathcal{C} \to \mathcal{C}') = B_{\mathcal{C}'} V_{\mathcal{C}} V_{\mathcal{C}'} = \mathrm{e}^{-\frac{\beta}{2}(H(\mathcal{C}')-H(\mathcal{C}))}$$

$$\mathrm{e}^{-\beta H(\mathcal{C}')} \quad \mathrm{e}^{+\beta H(\mathcal{C})} \quad \mathrm{e}^{+\beta H(\mathcal{C}')}$$

Eigenvalues:

$$0 = \lambda_1 < \mathrm{e}^{\beta H_1} Z(-\beta) < \lambda_2 < \mathrm{e}^{\beta H_2} Z(-\beta) < \ldots$$

Beware: mean-field dynamics.

Langevin version

Particle in a potential landscape:

$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\mathrm{d}V}{\mathrm{d}x} + \sqrt{2\gamma T}\eta(t)$$

Langevin version

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Multiplicative noise: $\gamma \to \gamma(x)$

$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} \overset{\text{Itô}}{=} -\frac{\mathrm{d}V}{\mathrm{d}x} + T\frac{\gamma'}{\gamma} + \sqrt{2\gamma T}\eta(t)$$

Langevin version

Particle in a potential landscape:

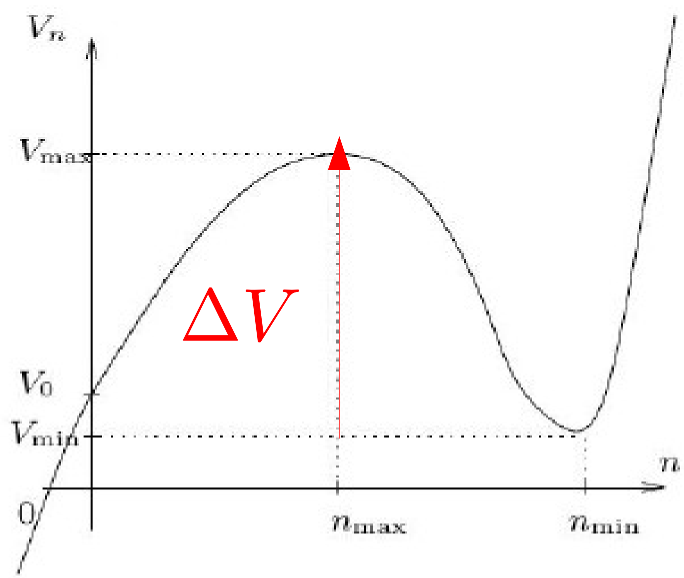
$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\mathrm{d}V}{\mathrm{d}x} + \sqrt{2\gamma T}\eta(t)$$

Multiplicative noise: $\gamma \to \gamma(x) = \mathrm{e}^{+\beta V(x)}$

$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} \overset{\text{Itô}}{=} -\frac{\mathrm{d}V}{\mathrm{d}x} + T\frac{\gamma'}{\gamma} + \sqrt{2\gamma T}\eta(t)$$

Kramers escape problem

Particle in a potential landscape:



$$\tau \sim \mathrm{e}^{-\beta \Delta V} \text{ vs } \tau \sim 1$$

Brownian dynamics: glassy vs trivial

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Model B version of the dynamics

Unsettled issues

Towards the Dean-Kawasaki equation

Individual particle dynamics

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = -\sum_{j \neq i} \boldsymbol{\nabla} V(\mathbf{r}_i - \mathbf{r}_j) + \sqrt{2T}\boldsymbol{\xi}_i$$

Collective dynamics

Particle dynamics is given. Collective density modes

$$\rho(\mathbf{x},t) = \sum_{j=1}^{N} \delta^{(3)}(\mathbf{x} - \mathbf{r}_j(t))$$

must evolve according to

$$\partial_t \rho = -\boldsymbol{\nabla} \cdot \mathbf{j}_L(\mathbf{x},t)$$

Dean, JPA (1995)

Collective dynamics

Physics

$$\mathbf{j}_L = \text{Fick's law} + \text{force density} + \text{noise}$$

Collective dynamics

Physics

$$\mathbf{j}_L = \text{Fick's law} + \text{force density} + \text{noise}$$

$$-T\boldsymbol{\nabla}\rho$$

Collective dynamics

Physics

$$\mathbf{j}_L = \text{Fick's law} + \text{force density} + \text{noise}$$

$$\rho(\mathbf{x},t)\int_{\mathbf{y}}(-\boldsymbol{\nabla}_{\mathbf{x}}V(\mathbf{x}-\mathbf{y}))\rho(\mathbf{y},t)$$

Collective dynamics

Physics

$$\mathbf{j}_L = \text{Fick's law} + \text{force density} + \text{noise}$$

$$\downarrow$$

$$\sqrt{2T\rho}\,\boldsymbol{\xi}(\mathbf{x},t)$$

$$\langle \xi^\alpha(\mathbf{x},t)\xi^\beta(\mathbf{x}',t')\rangle = \delta^{\alpha\beta}\delta^{(3)}(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

Collective dynamics

Summary

$$\mathbf{j}_L = -\rho \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta \rho} + \sqrt{2T\rho}\boldsymbol{\xi}$$

Dean, JPA (1995)

FDT-fulfilling form of the noise ensures that

$$P_{\mathrm{eq}} = \frac{\mathrm{e}^{-\beta \mathcal{F}[\rho]}}{Z}$$

Collective dynamics

Langevin dynamics

$$\mathbf{j}_L = -\rho \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta \rho} + \sqrt{2T\rho}\boldsymbol{\xi}$$

Density evolves in the landscape $\mathcal{F}[\rho]$ with diffusion constant ρ

Think of $\gamma \frac{\mathrm{d}x}{\mathrm{d}t} = -V'(x) + \sqrt{2\gamma T}\xi$

THE dynamics based theory

Mode-coupling theory leading to an approximate evolution equation for

$$C(\mathbf{k},t) = \langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle$$

THE dynamics based theory

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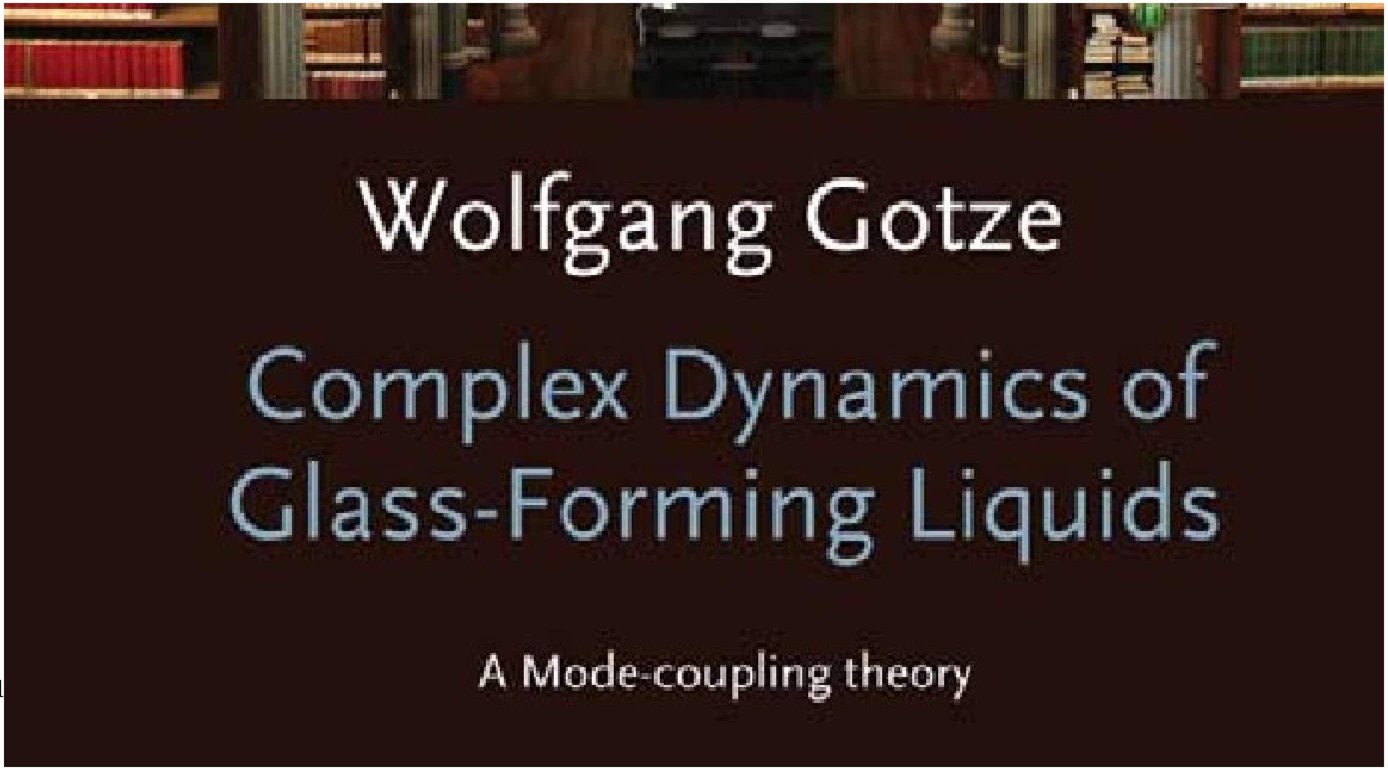

THE dynamics based theory

Mode-coupling theory leading to an approximate evolution equation for

$$C(\mathbf{k},t) = \langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle$$

THE dynamics based theory

Structure factor

$$C(\mathbf{k},t) = \langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle, \quad C(\mathbf{k},0) = \rho_0 S_{\mathbf{k}}$$

$$\partial_t C + Tk^2(1+\beta\rho_0 V(\mathbf{k}))C = -\int_0^t \mathrm{d}\tau M(\mathbf{k},t-\tau)C(\mathbf{k},\tau)$$

Mori-Zwanzig projection techniques

Szamel & Löwen, PRA (1991)

THE dynamics based theory

$$\partial_t C + \frac{Tk^2}{S_{\mathbf{k}}} C = -\frac{\rho_0 T}{2k^2} \int_0^t \mathrm{d}\tau \int_{\mathbf{q}} (\mathbf{k}\cdot\mathbf{q} c_{\mathbf{q}} + \mathbf{k}\cdot(\mathbf{k}-\mathbf{q}) c_{\mathbf{k}-\mathbf{q}})^2$$

$$\times C(\mathbf{q}, t-\tau) C(\mathbf{k}-\mathbf{q}, t-\tau)$$

$$\times \partial_\tau C(\mathbf{k}, \tau)$$

where $S_{\mathbf{k}} = (1 - \rho_0 c_{\mathbf{k}})^{-1}$

Szamel & Löwen, PRA (1991)

MCT's predictions

Introduce the non-ergodicity parameter

$$f_{\mathbf{k}} \equiv \lim_{t\to\infty} \frac{C(\mathbf{k},t)}{\rho_0 S_{\mathbf{k}}}$$

Solve for the long-time limit:

$$\frac{f_{\mathbf{k}}}{1-f_{\mathbf{k}}} = \frac{\rho_0 S_{\mathbf{k}}}{2k^4} \int_{\mathbf{q}} S_{\mathbf{q}} S_{\mathbf{k}-\mathbf{q}} (\mathbf{k}\cdot\mathbf{q} c_{\mathbf{q}} + \mathbf{k}\cdot(\mathbf{k}-\mathbf{q}) c_{\mathbf{k}-\mathbf{q}})^2 f_{\mathbf{q}} f_{\mathbf{k}-\mathbf{q}}$$

Mode-coupling theory (MCT)

Drawbacks

- applies to 2 point functions only;

- not a systematic expansion;

Szamel, Flenner & Hayakawa, EPL (2013)

- no small parameter;

- spurious predictions at low temperature;

- and violates the FDT.

Brownian dynamics: glassy vs trivial

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Model B version of the dynamics

Unsettled issues

Probe the influence of dynamics

Postulate alternative dynamics for the density modes

$$\mathbf{j}_B = -\rho_0 \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta \rho} + \sqrt{2T\rho_0}\boldsymbol{\xi}$$

Density evolves in the landscape $\mathcal{F}[\rho]$ with diffusion constant ρ_0

Alters dynamics, but statics is unchanged:

$$P_{\mathrm{eq}} = Z^{-1} \mathrm{e}^{-\beta \mathcal{F}}$$

Claim: exponential relaxation

Consider again

$$C(\mathbf{k},t) = \langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle$$

Claim: exponential relaxation

Consider again

$$C(\mathbf{k},t) = \langle \delta\rho(\mathbf{k},t)\delta\rho(-\mathbf{k},0)\rangle$$

We will argue that $C(\mathbf{k},t) \sim \mathrm{e}^{-t/\tau_{\mathbf{k}}}$

Entering technicalities

Starting point

$$\mathrm{Prob}[\rho(t'), 0 \leq t' \leq t] = \mathrm{e}^{-\int \mathrm{d}t' \, \frac{1}{2} \boldsymbol{\xi}^2}$$

where $\boldsymbol{\xi}[\rho]$ such that $\partial_t \rho = -\boldsymbol{\nabla} \cdot \mathbf{j}_B$

$$\mathbf{j}_B = -\rho_0 \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta \rho} + \sqrt{2T\rho_0}\boldsymbol{\xi}$$

This is a model B-like dynamics.

Entering technicalities

Martin-Siggia-Rose-Janssen-De Dominicis

$$Z_{\mathrm{dyn}} = \int \mathcal{D}\rho\mathcal{D}\bar{\rho}\mathrm{e}^{-S[\bar{\rho},\rho]}$$

where $$S[\bar{\rho},\rho] = \int_{t,\mathbf{x}} \bar{\rho}\left(\partial_t\rho - \rho_0\boldsymbol{\nabla}^2\frac{\delta\mathcal{F}}{\delta\rho}\right) - T\rho_0(\boldsymbol{\nabla}\bar{\rho})^2$$

FDT is a symmetry

Action $$S[\bar\rho,\rho] = \int_{t,\mathbf{x}} \bar\rho\left(\partial_t\rho - \rho_0\boldsymbol{\nabla}^2\frac{\delta\mathcal{F}}{\delta\rho}\right) - T\rho_0(\boldsymbol{\nabla}\bar\rho)^2$$

is invariant under

$$\begin{cases} t \to -t \\ \rho \to \rho \\ \bar\rho \to -\bar\rho + \beta\frac{\delta\mathcal{F}}{\delta\rho} \end{cases}$$

FDT is a symmetry

Action $$S[\bar{\rho},\rho] = \int_{t,\mathbf{x}} \bar{\rho}\left(\partial_t\rho - \rho_0\boldsymbol{\nabla}^2\frac{\delta\mathcal{F}}{\delta\rho}\right) - T\rho_0(\boldsymbol{\nabla}\bar{\rho})^2$$

is split into

$$\begin{cases} S_0 = \int \bar{\rho}(\partial_t\delta\rho + Tk^2(1+\beta\rho_0 V(\mathbf{k}))\delta\rho - \rho_0 Tk^2\bar{\rho}^2 \\ S_{\mathrm{int}} = \int \rho_0 T(-\boldsymbol{\nabla})^2\bar{\rho}\left[\ln\left(1+\frac{\delta\rho}{\rho_0}\right) - \frac{\delta\rho}{\rho_0}\right] \end{cases}$$

Symmetry not an issue anymore.

FDT is a symmetry

Action $S[\bar\rho,\rho] = \int_{t,\mathbf{x}} \bar\rho \left(\partial_t \rho - \rho_0 \boldsymbol{\nabla}^2 \frac{\delta \mathcal{F}}{\delta \rho} \right) - T\rho_0 (\boldsymbol{\nabla} \bar\rho)^2$

Correlations

$$G = \begin{matrix} \bar\rho \\ \rho \end{matrix} \left\{ \overbrace{\begin{pmatrix} 0 & R(\mathbf{k},t) \\ R(\mathbf{k},-t) & C(\mathbf{k},t) \end{pmatrix}}^{\bar\rho \qquad \rho} \right.$$

$$R(\mathbf{k},t) = \langle \bar\rho(-\mathbf{k},0)\delta\rho(\mathbf{k},t)\rangle = \rho_0 \mathbf{k}^2 \text{true response function}$$

$$R(\mathbf{k},t) = -\frac{1}{\rho_0 T \mathbf{k}^2} \partial_t C(\mathbf{k},t)$$

$$\frac{\langle \delta\rho(\mathbf{x},t)\rangle}{\delta\mu(\mathbf{x}',t')}$$

Luttinger-Ward functional

Work at fixed correlations

$$S \to S + \frac{1}{2}(\bar{\rho} \;\; \rho) G \begin{pmatrix} \bar{\rho} \\ \rho \end{pmatrix}$$

Determine

$$\Gamma[G] = \text{generating functional of 2PI diagrams}$$

such that physics is given by the solution of

$$\left.\frac{\delta \Gamma}{\delta G}\right|_{\text{physical } G} = 0$$

In practice: Shwinger-Dyson

This becomes

$$G_0^{-1}G = \mathbf{1} - \Sigma[G]G$$

$$\Sigma[G] = \text{sum of 2PI two-point vertex functions}$$

And $\Sigma[G]$ can be found from

$$S_{\text{int}} = \int -\rho_0 T \boldsymbol{\nabla}^2 \bar{\rho}\theta[\rho], \quad \theta = \ln\left(1 + \frac{\delta\rho}{\rho_0}\right) - \frac{\delta\rho}{\rho_0}$$

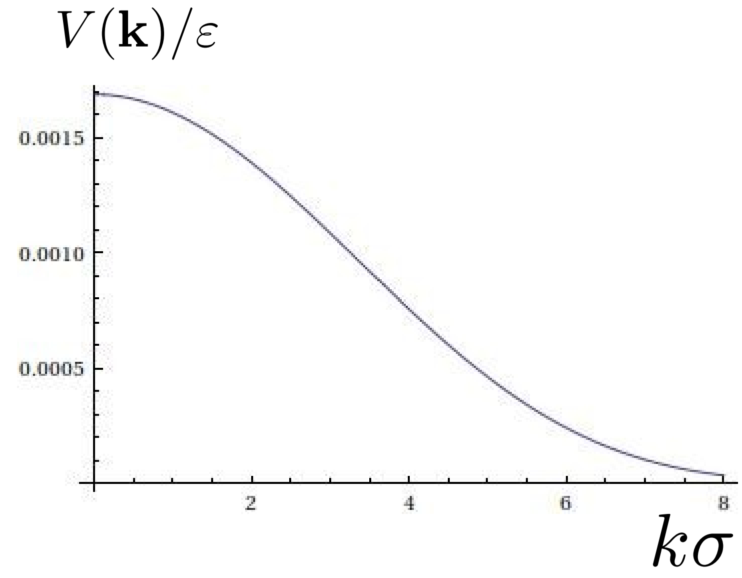
A few remarks

Interaction part independent of the potential.

Up to a constant, same as in a model A.

Potential appears only through

$$T\mathbf{k}^2 \to T\mathbf{k}^2 \left(1 + \beta \rho_0 V(\mathbf{k})\right)$$



An evolution equation

Luttinger-Ward functional

$\Sigma[G] = \Sigma[C]$ by virtue of FDT: $R = -\dot{C}/(\rho_0 T k^2)$

+ relations between the components via the FDT.

Exact relationship (nontrivial):

$$\left(\partial_t + \frac{T\mathbf{k}^2}{S_\mathbf{k}}\right) C(\mathbf{k}, t) = \frac{1}{\rho_0 T k^2} \int_0^t \mathrm{d}\tau \Sigma(\mathbf{k}, t-\tau) \partial_\tau C(\mathbf{k}, \tau)$$

No ergodic/non-ergodic transition

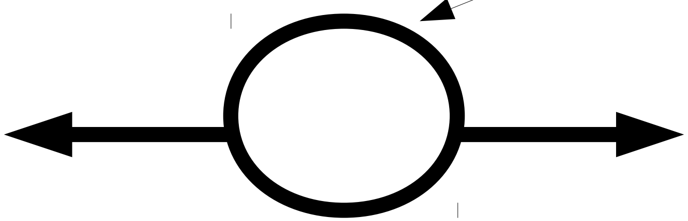
For the non-ergodicity parameter

$$\frac{f_{\mathbf{k}}}{1-f_{\mathbf{k}}} = -\frac{1}{\rho_0 T k^2}\Sigma(\mathbf{k}, t=\infty)$$

Simplest MCT-like truncation

For the simplest truncation

$C(\mathbf{q},\tau) \sim S_{\mathbf{q}} \times f_{\mathbf{q}}$

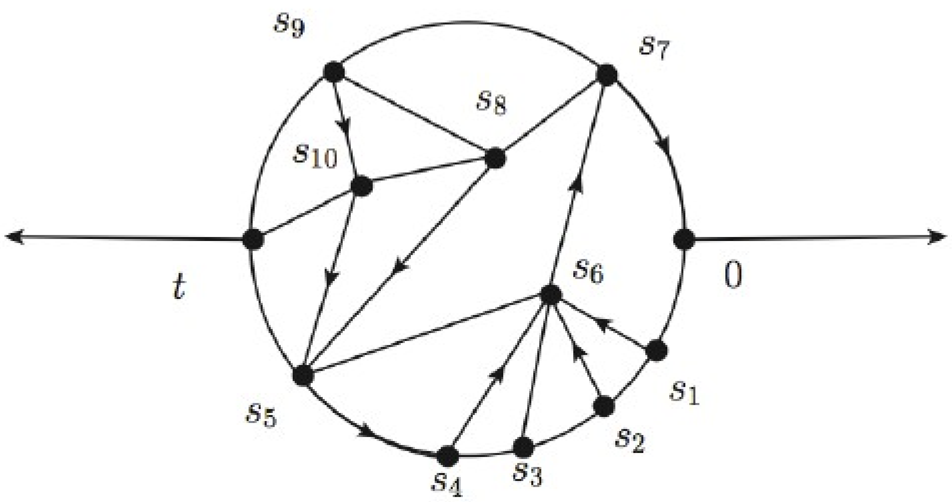


$$\frac{f_{\mathbf{k}}}{1-f_{\mathbf{k}}} = -\frac{1}{\rho_0 T k^2}\Sigma(\mathbf{k}, t=\infty) \quad \Sigma[C] \sim -\int_{\mathbf{q}} S_{\mathbf{q}} S_{\mathbf{k}-\mathbf{q}} f_{\mathbf{q}} f_{\mathbf{k}-\mathbf{q}}$$

No kernel, no convergence, no nontrivial solution.

Improved

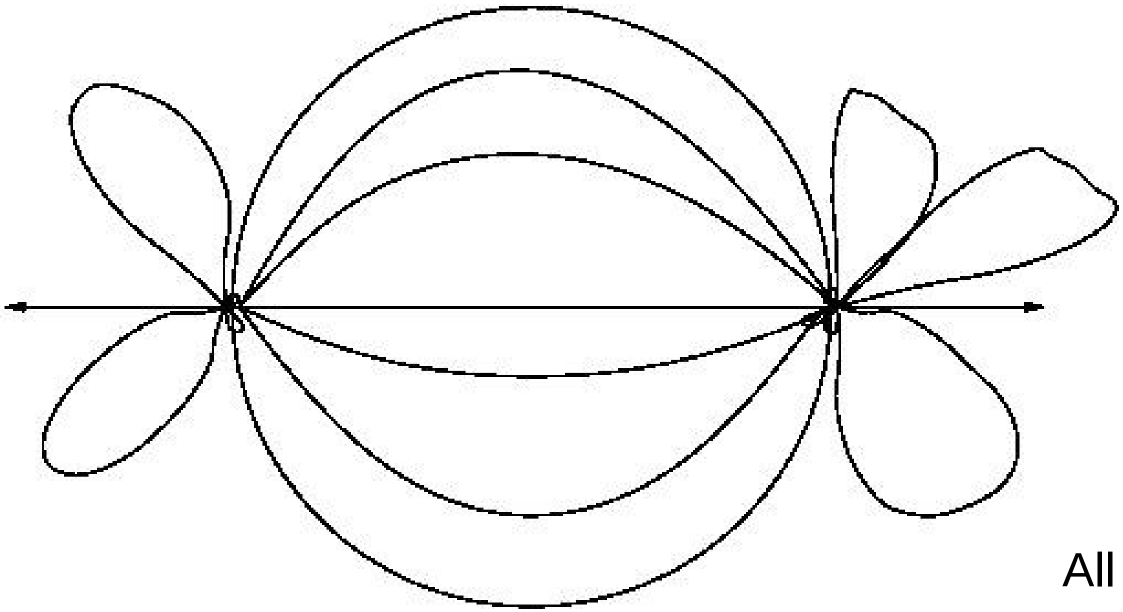
Any order



$$\Sigma[C] \sim \int \prod_{a:\ \text{arrowed}} S_{\mathbf{q}_a}(1 - f_{\mathbf{q}_a}) \prod_{r:\ \text{regular}} S_{\mathbf{q}_r} f_{\mathbf{q}_r}$$

No kernel, no convergence, no nontrivial solution.

Infinite resummation: dynamics

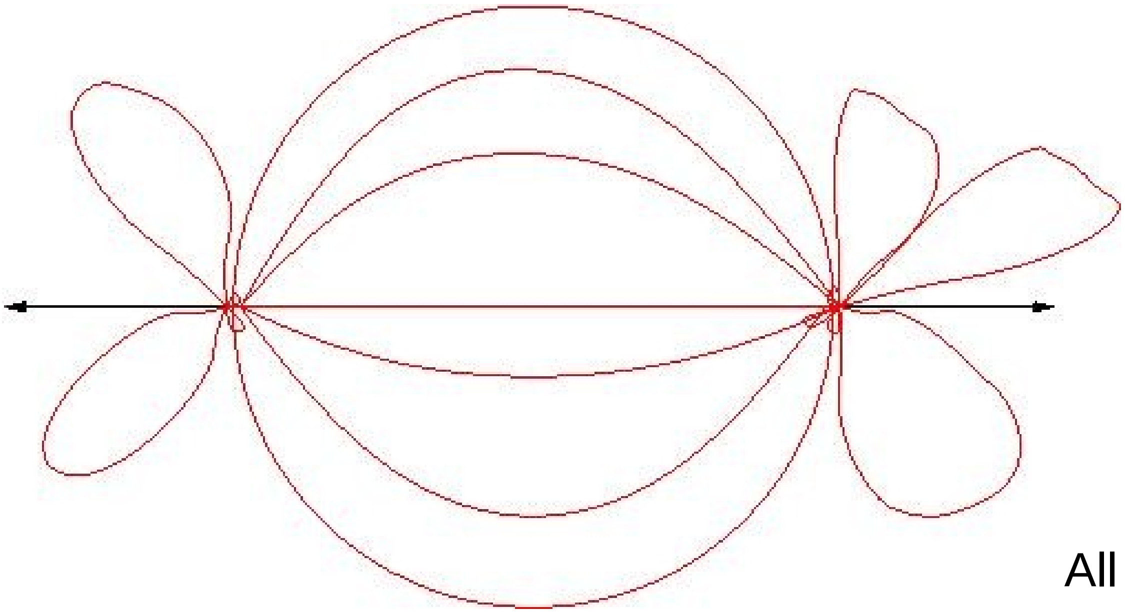


All vertices, up to order 2

$$\Sigma[C] \sim \int \prod_{\mathbf{q} \in \text{inside leg}} C(\mathbf{q}, t-\tau) \times C(\mathbf{0}, 0)^{\#\text{ of petals}}$$

Divergent series (can perhaps be resummed).

Infinite resummation: dynamics



All vertices, up to order 2

pink part is $A(\mathbf{k},t) = \langle \theta(\mathbf{k},t)\theta(-\mathbf{k},0)\rangle$

$$\theta = \ln\left(1+\frac{\delta\rho}{\rho_0}\right) - \frac{\delta\rho}{\rho_0}$$

Renormalized kernel

Resummed kernel is

$$\Sigma[C] \propto A(\mathbf{k}, t)$$

But $A = \langle \theta\theta \rangle$ is unknown. However, if $B = \langle \delta\rho\theta \rangle$

$$\begin{cases} \partial_t C + Tk^2(1 + \beta\rho_0 V(\mathbf{k}))C = -\rho_0 Tk^2 B \\ \partial_t B + Tk^2(1 + \beta\rho_0 V(\mathbf{k}))B = -\rho_0 Tk^2 A \end{cases}$$

Renormalized kernel

Resummed kernel is

$$\Sigma[C] \propto A(\mathbf{k}, t) \qquad (1)$$

But $A = \langle \theta\theta \rangle$ is unknown. However, if $B = \langle \delta\rho\theta \rangle$

$$\begin{cases} \partial_t C + Tk^2(1 + \beta\rho_0 V(\mathbf{k}))C = -\rho_0 Tk^2 B & (2) \\ \partial_t B + Tk^2(1 + \beta\rho_0 V(\mathbf{k}))B = -\rho_0 Tk^2 A & (3) \end{cases}$$

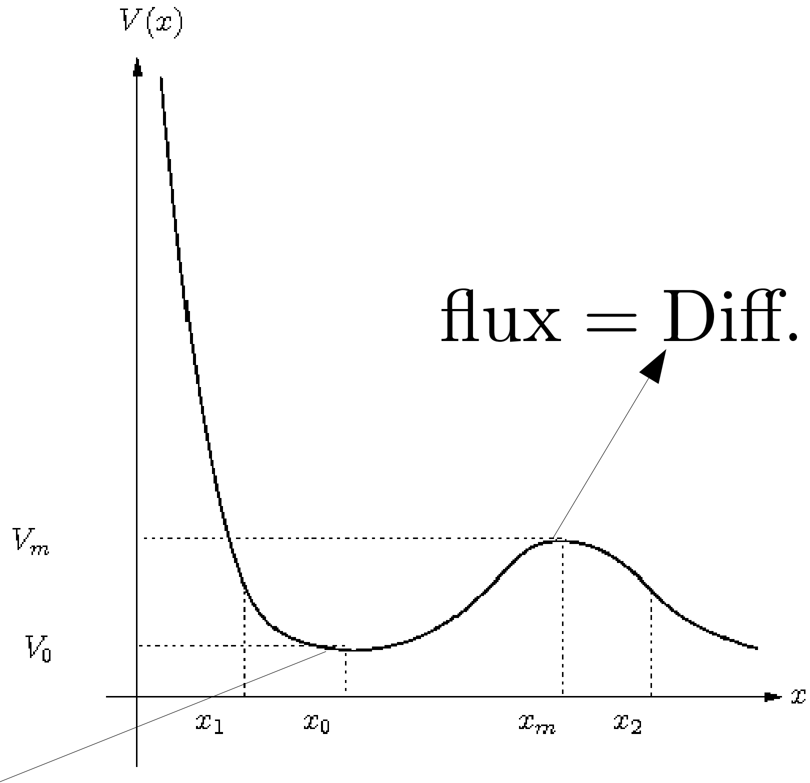
Exponential relaxation

Find

$$C(\mathbf{k},t) \sim \exp(-t/\tau_{\mathbf{k}}),\ \tau_{\mathbf{k}}^{-1} \sim Tk^2(1+\beta\rho_0 V(\mathbf{k}))$$

Physical interpretation

Physical picture: Kramers escape problem

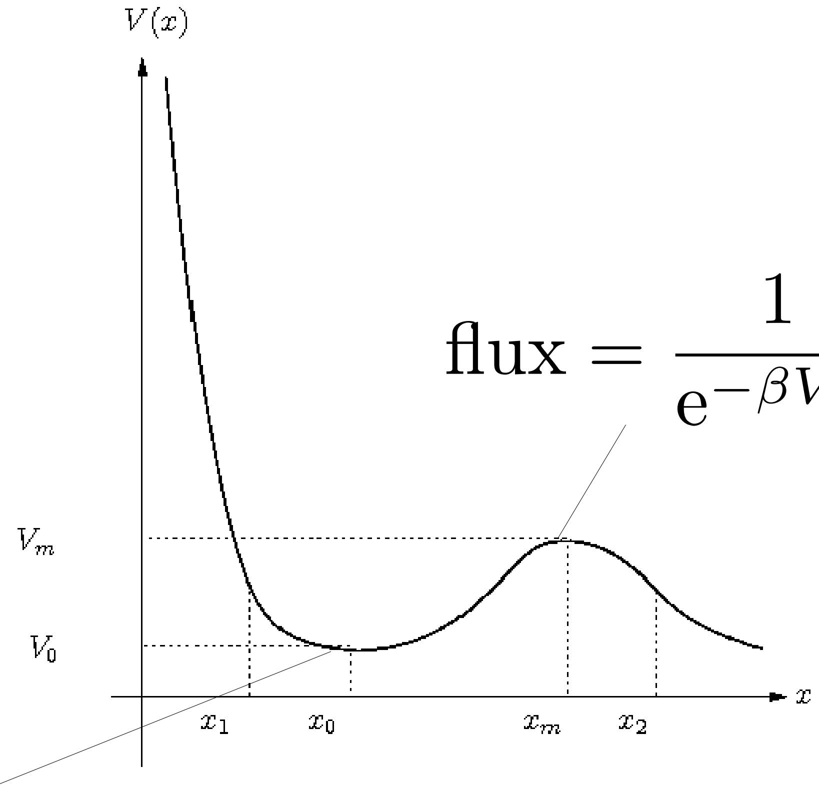


$$\text{flux} = \text{Diff. cst.} \times \mathrm{e}^{-\beta V_m} \sim \mathrm{e}^{-\beta V_m}$$

$$\text{flux} = \text{Diff. cst.} \times \mathrm{e}^{-\beta V_0} \sim \mathrm{e}^{-\beta V_0}$$

Physical interpretation

Diffusion equation: $\mathbf{j}_B = -T\boldsymbol{\nabla}\left(\frac{1}{\rho}\boldsymbol{\nabla}\rho\right)\ldots$



$$\text{flux} = \frac{1}{e^{-\beta V_m}} \times e^{-\beta V_m} \sim \mathcal{O}(1)$$

$$\text{flux} = \mathcal{O}(1)$$

Cates, private com.

Brownian dynamics: glassy vs trivial

Motivations behind a twisted idea

Langevin dynamics of interacting colloids

Model B version of the dynamics

Unsettled issues

What about replicas?

1. Under which dynamics are replica calculations meaningful?

2. Barriers in high-dimensional space are not relevant, but dynamic entropy is. In what sense?

Replicas and Dynamics

Let $$f_{\mathbf{k}} = \frac{\langle \delta\rho^{(1)}(\mathbf{k})\delta\rho^{(2)}(-\mathbf{k})\rangle}{\rho_0 S_{\mathbf{k}}}$$

Crisanti has shown a result that implies that the long-time limit of the dynamic nonergodicity parameter is the same as in replicas (1RSB), if model B dynamics is used (or model A).

Crisanti, Nucl. Phys. B (2008)

Lattice versions

“Langevin dynamics” on a lattice

$$W(n_i, n_j \to n_i - 1, n_j + 1) = D n_i \mathrm{e}^{-\frac{\beta}{2}(E' - E)}$$

Energy of a configuration

$$E = \frac{1}{2} \sum_{k,\ell} n_k V(k - \ell) n_\ell$$

Lefèvre & Biroli, JSTAT (2007)

Lattice versions

"Model B dynamics" on a lattice

$$W(n_i, n_j \to n_i - 1, n_j + 1) = D\sqrt{\frac{n_i}{n_j + 1}}\mathrm{e}^{-\frac{\beta}{2}(E' - E)}$$

$$= D\mathrm{e}^{-\frac{\beta}{2}(F' - F)}$$

$$F = \frac{1}{2}\sum_{k,\ell} n_k V(k - \ell) n_\ell - T \sum_\ell \ln \frac{1}{n_\ell!}$$

Lattice versions

“Model B dynamics” evolution operator

$$\mathbb{W}_{\mathcal{C},\mathcal{C}'} = \mathbf{1}_{\mathcal{C}\leftrightarrow\mathcal{C}'} - \left[\sum_{\mathcal{C}''} \mathrm{e}^{-\frac{\beta}{2}(F(\mathcal{C}'')-F(\mathcal{C}))}\right]\delta_{\mathcal{C},\mathcal{C}'}$$

Laplacian+external potential.