FDR-preserving perturbation schemes for the dynamics of interacting Brownian particles: MCT and beyond

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Outline

- Glass transition
- Mode coupling theory
- Dean-Kawasaki equation
- ABL's time-reversal symmetry
- FDR-consistent field theory

  Auxiliary field method

  Weak coupling expansion (ongoing)
- Summary and outlook

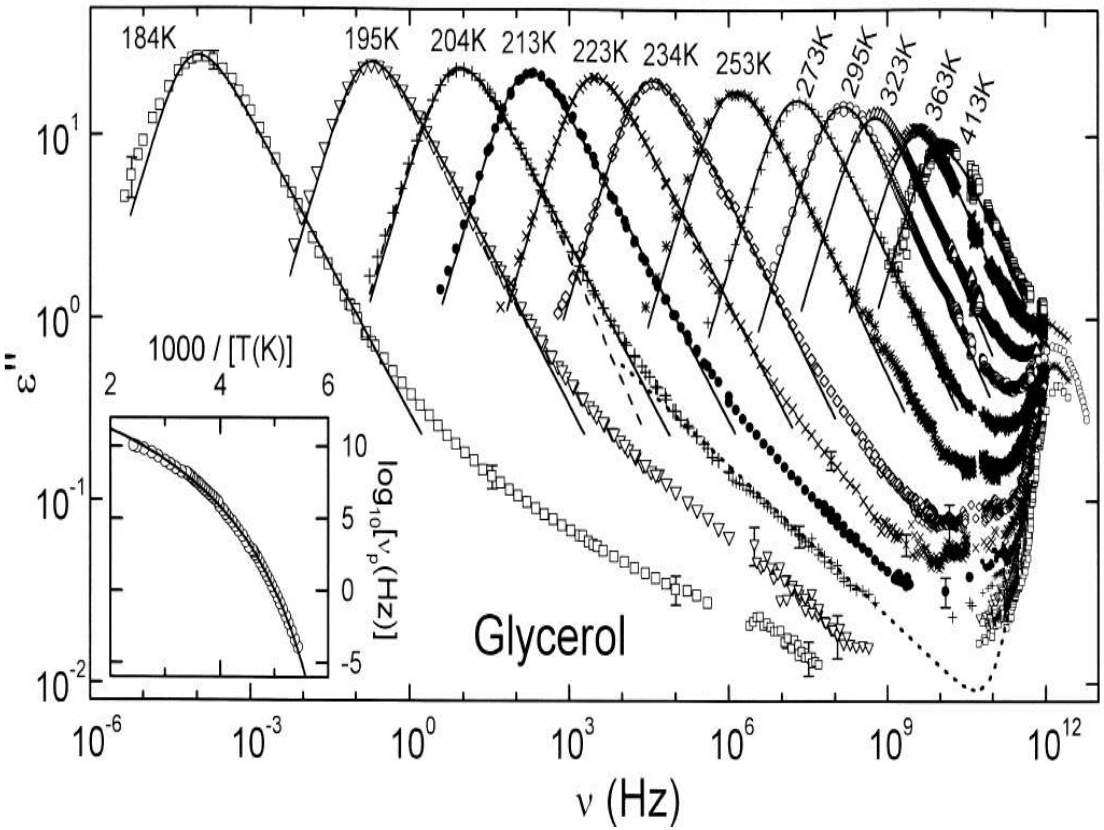
The Liquid-Glass Transition

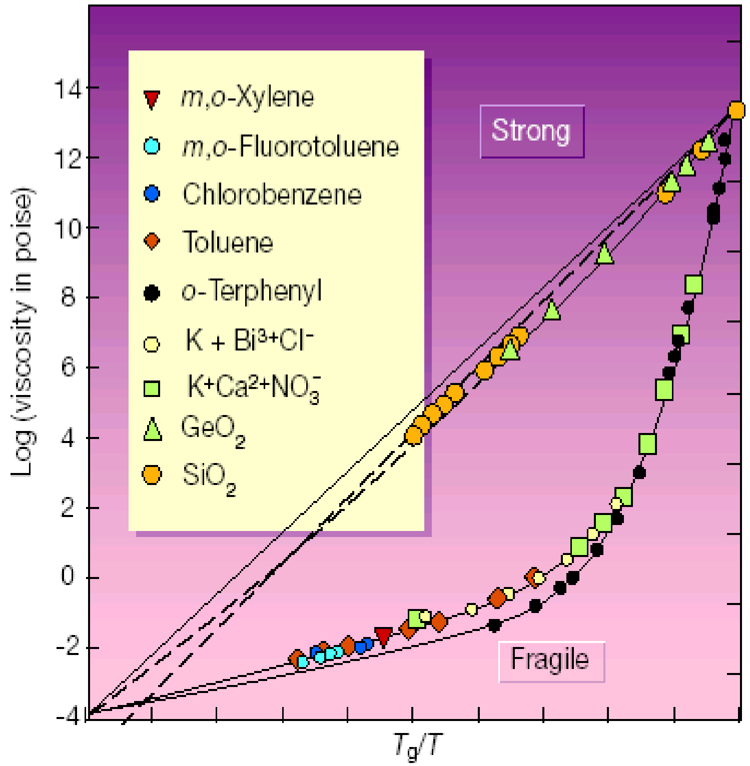
Supercooled liquids exhibit fascinating kinetic features:

- **Dramatic slowing down**:

  Tremendous time-scale change involved

(~15 decades from ps to a few thousand sec)





Angell plot: strong vs fragile liquids

- **Non-exponential response**: $F(t) \sim \exp\left[-(t/\tau)^{\beta}\right], \quad 0 < \beta < 1$

- **Kinetic heterogeneity**:
  - * Broad time-scale distribution over spatial regions.
  - * Heterogeneous regions growing with lowering T.

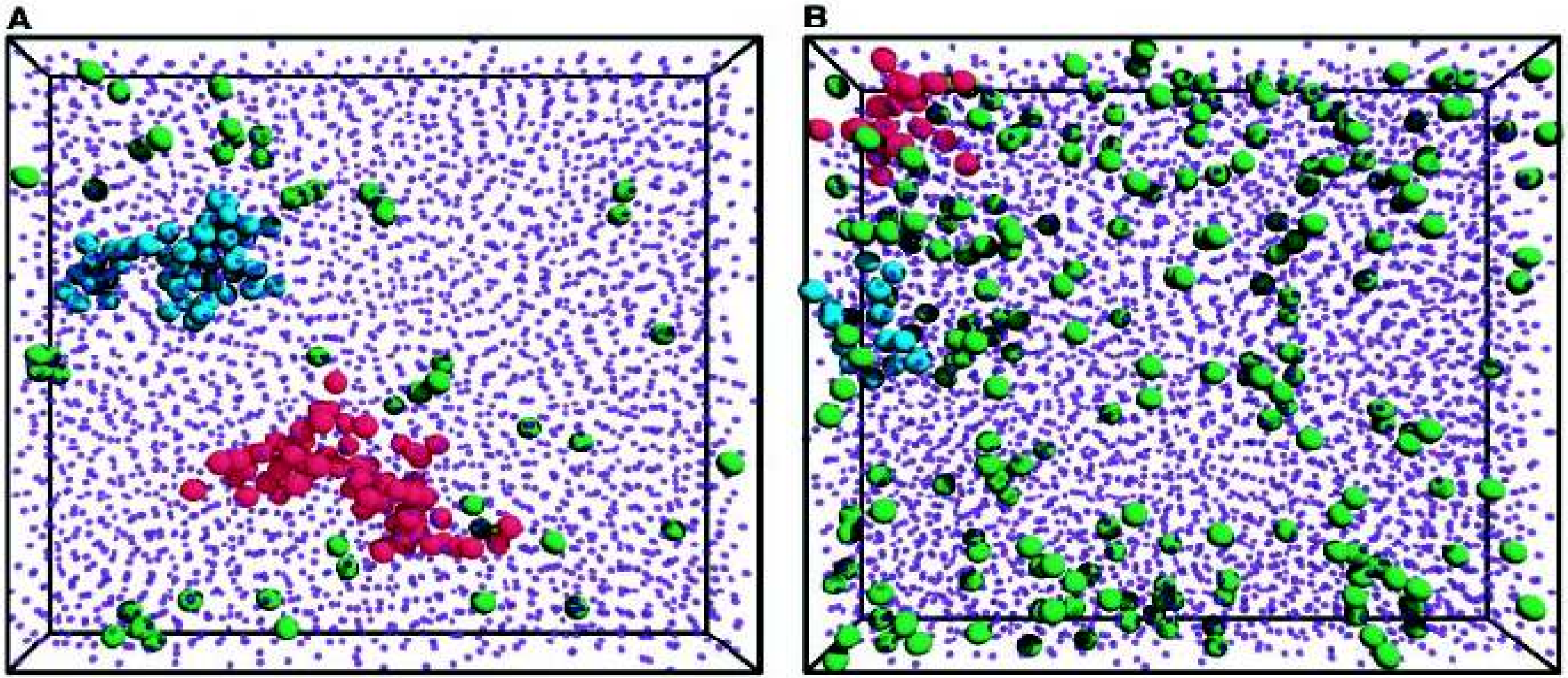


Fig. 4. The locations of the fastest particles (large spheres) and the other particles (smaller spheres). The spheres are drawn smaller for clarity; the particles all have the same physical size, which is the size of the large spheres shown in this figure. (**A**) "Supercooled" sample with $\phi = 0.56$, $\Delta t^* = 1000$ s; the fastest particles had a displacement >0.67 μm. The red cluster contained 69 particles; the light blue cluster contained 50 particles. (**B**) "Glassy" sample with $\phi = 0.61$, $\Delta t^* = 720$ s; the fastest particles had a displacement >0.33 μm. The largest cluster (red) contained 21 particles. The "speed" of a particle was determined over a time Δt^* corresponding to the α-relaxation for (A) and the β-relaxation for (B); see text for details.

First-principle understanding on
these slow dynamics of supercooled liquids,
and
the nature of the liquid-glass transition

➔ **A fundamental challenge for statistical physics**

(e.g., J. Langer's Reference Frame article
The mysterious glass transition,
Physics Today, Feb 2007)

The MCT of supercooled liquids

- **A first-principle approach from liquid side**
(Goetze, Sjoelander, Sjoegren 1984, Leutheusser 1984)

- **Focuses on the correlation of density fluctuations to probe structural relaxations of SL:**

$$F(k,t) = \int dr\, e^{-ik\cdot r} \langle \delta\rho(r,t)\delta\rho(0,0)\rangle$$

- **Exact eq. for the correlation function F(k,t) of density fluctuations via projection operator method:**

$$\ddot{F}(k,t)+\Gamma_k\dot{F}(k,t)+\frac{k_B T k^2}{mS(k)}F(k,t)+\int_0^t ds\, M(k,t-s)\dot{F}(k,s)=0$$

4-pt density correlation

- **A closed eq. for F(k,t) with the factorization approximation:**

$$\ddot{F}(k,t)+\Gamma_k\dot{F}(k,t)+\frac{k_BTk^2}{mS(k)}F(k,t)+\int_0^t ds\, M(k,t-s)\dot{F}(k,s)=0$$

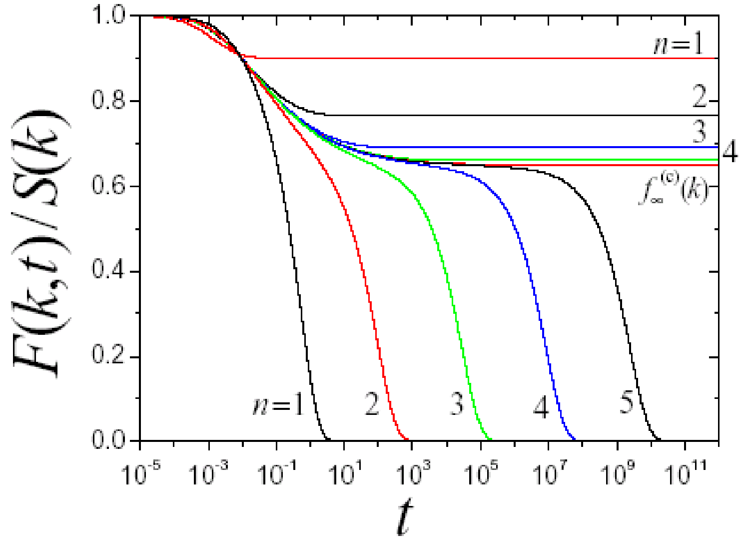
$$M(k,t)\simeq\frac{k_BT}{2m\rho_0}\int_{\mathbf{q}}V_{\mathbf{k}}(\mathbf{q},\mathbf{k}-\mathbf{q})F(q,t)F(|\mathbf{k}-\mathbf{q}|,t)$$

$$V_{\mathbf{k}}(\mathbf{q},\mathbf{k}-\mathbf{q})\equiv\left[\hat{\mathbf{k}}\cdot\mathbf{q}c(q)+\hat{\mathbf{k}}\cdot(\mathbf{k}-\mathbf{q})c(|\mathbf{k}-\mathbf{q}|)\right]^2$$

$$S(q)=F(q,0)=1/(1-\rho_0c(q))$$

- **Input: Static structure factor of liquid, S(q)**

→ **Dynamic information of liquid; No-free parameter**

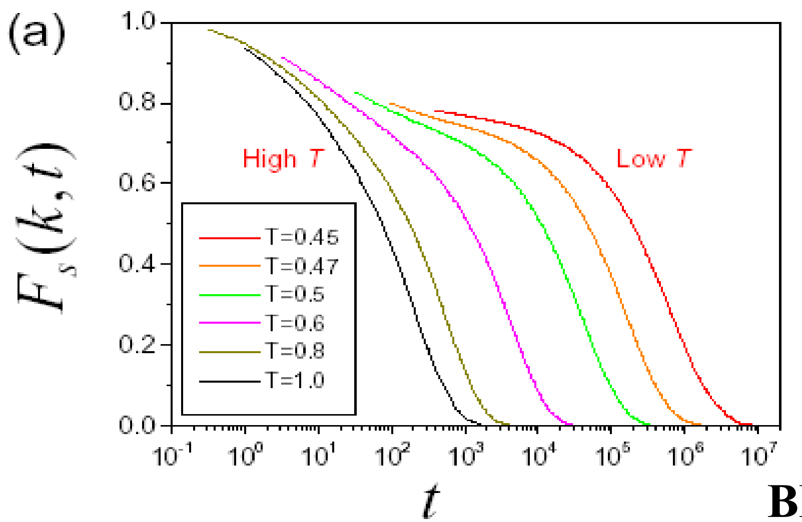


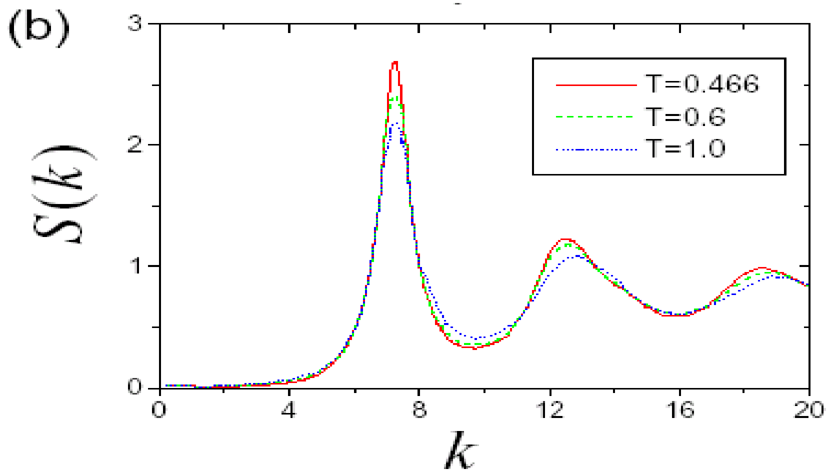
Numerical sol. for HS system with PY solution for S(k), Miyazaki 07

$$k = \frac{2\pi}{\sigma}, \quad \frac{\phi_c - \phi}{\phi_c} = \pm 10^{-n}, \quad \phi_c = 0.51$$

$$\frac{\partial F(k,t)}{\partial t} = -\frac{D_0 k^2}{S(k)} \left\{ F(k,t) + \int_0^t \mathrm{d}t' \; M(k, t-t') \frac{\partial F(k,t')}{\partial t'} \right\}$$

$$M(k,t) = \frac{S(k)}{2\rho_0 k^2} \int \frac{\mathrm{d}\mathbf{q}}{(2\pi)^3} \; V_{\mathbf{k}}^2(\mathbf{q}, \mathbf{k}-\mathbf{q}) F(|\mathbf{k}-\mathbf{q}|, t) F(q,t)$$





BD simulation for LJ binary liquid
Kob et al ('97)

Predictions of MCT

Two-step relaxation

- Relaxation toward the plateau

$$f(k,t) = f(k) + A(t/\tau_\beta)^{-a}$$ **(fast beta)**

- Cage-breaking relaxation

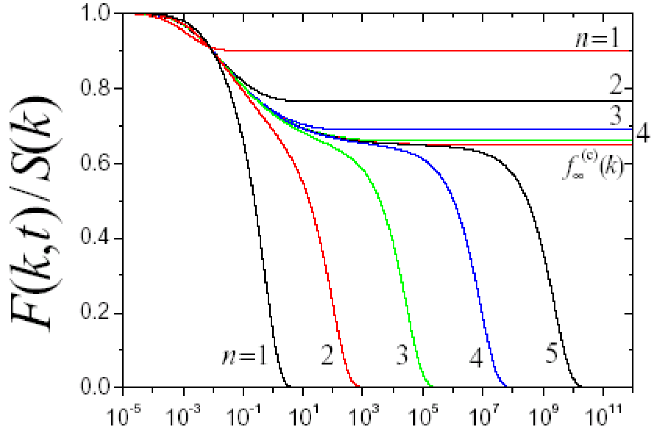
$$f(k,t) = f(k) - B(t/\tau_\alpha)^{b}$$ **(slow-beta)**

$$f(k,t) = f_0 \exp\left[- A_k (t/\tau_\alpha)^{\beta_k}\right]$$ **(alpha)**

- Analytic relations

$$\frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)}$$

$$\tau_\beta \sim |\varepsilon|^{-\frac{1}{2a}}, \quad \tau_\alpha \sim |\varepsilon|^{-\left(\frac{1}{2a}+\frac{1}{2b}\right)}, \quad \varepsilon = \frac{\phi - \phi_c}{\phi_c}$$



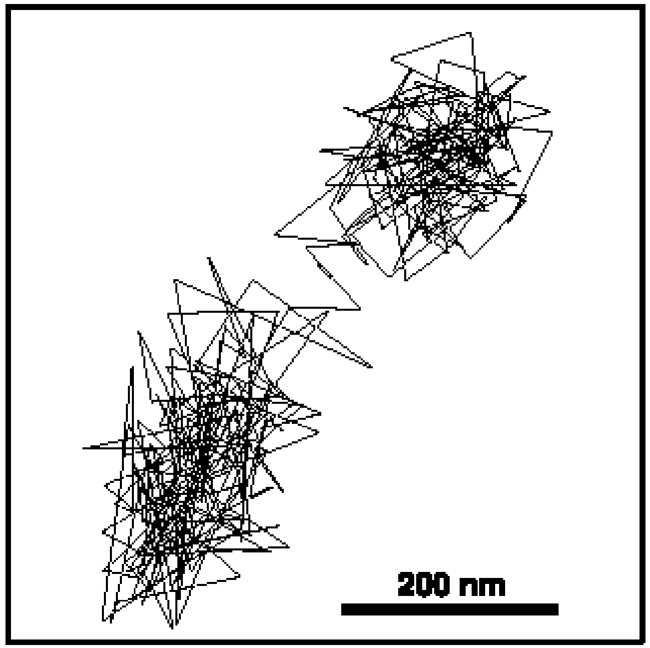


Fig. 2. A typical trajectory for 100 min for ϕ = 0.56. Particles spent most of their time confined in cages formed by their neighbors and moved significant distances only during quick, rare cage rearrangements. The particle shown took ~500 s to shift position. The particle was tracked in 3D; the 2D projection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

Dynamic transition

Relaxing (Ergodic) phase $f(k) = 0$ — **Liquid**

ϕ_c

Frozen (Nonergodic) phase $f(k) > 0$ — **Glass**

ϕ

$$\text{NEP} \quad f(k) \equiv \lim_{t\to\infty} \frac{F(k,t)}{S(k)} = \frac{M(k,t=\infty)}{1+M(k,t=\infty)}$$

- **This transition is NOT observed in experiments: the transition itself is an artifact of the factorization approx. inherent in the present MCT.**

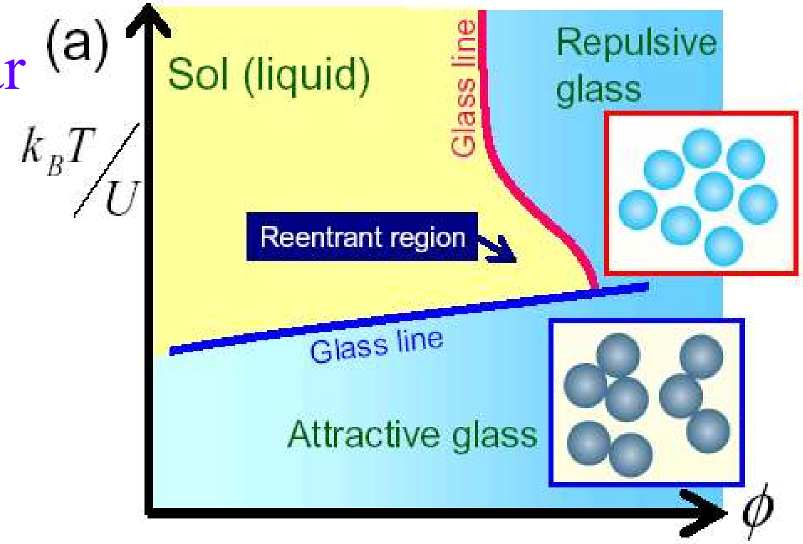
- **MCT misses out the thermal activation process which is believed to be the dominant mechanism at high density, (or low temp) preventing the system from freezing.**

➔ Major defect of MCT

Further developments of MCT

- Molecular MCT (Chong-Hirata Schilling, Goetze…).
- MCT for colloids with short-range attractive tails
- MCT for supercooled liquid under shear
- MCT for 4-point correlation function

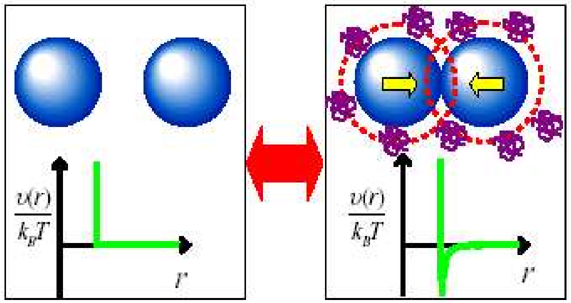
(a)



Recent reviews

S. Das, Rev. Mod. Phys 76, 785 (2004).
D. Reichman and P. Charbonneau,
J. Stat Mech P05013 (2005).

(b)



K. Miyazaki, 物性研究 88, 621 (2007)
Glass Transition and MCT: Recent Development and Fundamental Questions

MCT's fundamental approximation

- Exact eq. for the correlation function of density fluctuations:

$$\ddot{F}(k,t)+\Gamma_k\dot{F}(k,t)+\frac{k_B T k^2}{mS(k)}F(k,t)+\int_0^t ds\, M(k,t-s)\dot{F}(k,s)=0$$

- Factorization approximation (FA):

$$M(k,t)\simeq\frac{k_B T}{2m\rho_0}\int_{\mathbf{q}} V_{\mathbf{k}}(\mathbf{q},\mathbf{k}-\mathbf{q})F(q,t)F(|\mathbf{k}-\mathbf{q}|,t)$$

$$V_{\mathbf{k}}(\mathbf{q},\mathbf{k}-\mathbf{q})\equiv\left[\hat{\mathbf{k}}\cdot\mathbf{q}c(q)+\hat{\mathbf{k}}\cdot(\mathbf{k}-\mathbf{q})c(|\mathbf{k}-\mathbf{q}|)\right]^2$$

$$S(q)=F(q,0)=1/(1-\rho_0 c(q))$$

- **FA is a totally uncontrolled approximation**:
  Very hard to systematically improve the theory within the projection operator method.

Field theoretic approach

- systematic:

  lowest order theory ➔ MCT.

  higher order ➔ corrections to MCT.

- a natural framework for NEQ dynamics.

- hopes to incorporate thermal activation processes.

A pioneering work (Das-Mazenko 1986)

• MSR-renormalized perturbation theory for fluctuating hydrodynamic eqs. for dense liquids:

$$\frac{\partial \rho}{\partial t} + \nabla . \mathrm{g} = 0, \qquad \frac{\partial g_i}{\partial t} = -\sum_j \nabla_j [\frac{g_i g_j}{\rho}] - \rho \nabla_i \frac{\delta F_U}{\delta \rho} - \sum_j L^o_{ij} \frac{g_j}{\rho} + \theta_i \ .$$

• Kinetic slowing down driven by density nonlinearity.

• Velocity field to remove the $1/\rho$ nonlinearity:

$$\mathrm{g}(\mathrm{x}, t) = \rho(\mathrm{x}, t) \mathrm{V}(\mathrm{x}, t).$$

• Dynamic transition is rounded off (cf. SDD '93):

[Recent debates: Cates-Ramaswamy, Andreanov-Biroli-Lefevre, Das-Mazenko, Nishino-Hayakawa, Yeo]

Dean-Kawasaki equation

- **A Langevin eq. for the density alone:**

$$\partial_t \rho(\mathbf{r},t) = \nabla \cdot \left(\rho(\mathbf{r},t)\nabla \frac{\delta H[\rho]}{\delta \rho(\mathbf{r},t)}\right) + \nabla \cdot (\sqrt{\rho(\mathbf{r},t)}\xi(\mathbf{r},t))$$

$$< \xi_\alpha(\mathbf{r},t)\xi_\beta(\mathbf{r}',t') >= 2T\delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$

$$\begin{aligned} H[\rho] &= H_{id}[\rho] + H_{int}[\rho] \\ H_{id}[\rho] &= T\int d\mathbf{r}\,\rho(\mathbf{r})\left(\ln\frac{\rho(\mathbf{r})}{\rho_0} - 1\right) \\ H_{int}[\rho] &= \frac{g}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\delta\rho(\mathbf{r})\,U(\mathbf{r}-\mathbf{r}')\,\delta\rho(\mathbf{r}') \end{aligned}$$

- **Obtained via elimination of the momentum field g in the Das-Mazenko's FH eqs. with**

$U(\mathbf{r}) \to -Tc(\mathbf{r})$ **(Ramakrishnan-Yousouff free energy).**

➔ **A dynamic density functional equation (Kawasaki 1994).**

[momentum fluct. relax much faster than density fluct.]

Dean-Kawasaki equation

- **Exact eq. for the microscopic density** $\rho(r,t)=\sum_{i=1}^{N}\delta(r-X_i(t))$

  of interacting B-ptls. with pair potential U (Dean 1996):

$$\frac{dX_i(t)}{dt}=-\sum_{j=1}^{N}\nabla U(X_i(t)-X_j(t))+\eta_i(t)$$

$$\left\langle \eta_i(t)\eta_j(t)\right\rangle = 2T\delta_{ij}I\delta(t-t')$$

[generalized by Nakamura-Yoshimori, JPA 2009]

- **A model for dynamics of colloidal suspensions (without HI).**

$$\partial_t \rho(\mathbf{r},t) = \nabla \cdot \left(\rho(\mathbf{r},t)\nabla \frac{\delta H[\rho]}{\delta\rho(\mathbf{r},t)}\right) + \nabla \cdot (\sqrt{\rho(\mathbf{r},t)}\xi(\mathbf{r},t))$$

$$= T\nabla^2\rho + g\nabla \cdot \left(\rho\nabla \int d\mathbf{r}' U(\mathbf{r}-\mathbf{r}')\delta\rho(\mathbf{r}',t)\right) + \nabla \cdot (\sqrt{\rho(\mathbf{r},t)}\xi(\mathbf{r},t))$$

- **Non-interaction part:**

Diffusion + Multiplicative noise structure

Brownian gas ➔ A nontrivial but soluble FT

(Velenich, Chamon, Cugliandolo, Kreimer, JPA 2008)

- **Unique features come from non-int. part/mutiplicative noise.**

- **Interaction part: mode coupling nonlinearity → Slowing-down**

DK eq. ➔ MC nonlinearity + thermal activation (FP view)

The MSR-type functional method

Stochastic eq. → Action $S[\rho,\hat{\rho}]$

Equations of motion (Schwinger-Dyson eq.)

$$G_0^{-1}(\mathbf{13})\cdot G(\mathbf{32}) \quad = \quad \delta(\mathbf{12})+\Sigma(\mathbf{13})\cdot G(\mathbf{32})$$

Treats C and G on equal footing

$$C(r-r',t-t') = <\delta\rho(r,t)\delta\rho(r',t')>$$

$$G(r-r',t-t') = i<\delta\rho(r,t)\hat{\rho}(r',t')>$$

RPT for Σ

EQ dynamics: FDR & TTI $\quad -\partial_t C(r-r',t-t') = T\ R(r-r',t-t')$

- FDR should be obeyed in each order of PT.
- EQ info is input to the dynamic eq.

For typical stochastic models (e.g., Model A or B),

- G=R
- FDR is consistent with PT.

None hold for the Dean-Kawasaki eq.!

(Miyazaki-Reichman JPA 2005)

Dynamic action

$H = H_{id} + H_{\text{int}}$

$$\langle A[\rho] \rangle = \int \mathcal{D}\rho\, A[\rho] \Big\langle \delta\Big[\dot\rho - \nabla\cdot\Big(\rho\nabla\frac{\delta F}{\delta\rho}\Big) - \eta\Big]\Big\rangle_\eta$$
$$= \int \mathcal{D}\rho \int \mathcal{D}\hat\rho\, A[\rho] \exp(\mathcal{S}[\rho,\hat\rho])$$

thermal noise

- **Non-interaction part**

$$S_{id}[\rho,\hat\rho] = \int d\mathbf{r} \int dt \Big\{ i\hat\rho\Big[\partial_t\rho - \nabla\cdot\Big(\rho\nabla\frac{\delta H_{id}}{\delta\rho}\Big)\Big] - T\rho(\nabla\hat\rho)^2\Big\}$$
$$= \int d\mathbf{r} \int dt \Big\{ i\hat\rho\Big[\partial_t\rho - T\nabla^2\rho\Big] - T\rho(\nabla\hat\rho)^2\Big\}$$

➔ A cubic FT, but solvable

- **Interaction part**

$$S_{int}[\rho,\hat\rho] = -\int d\mathbf{r} \int dt\, i\hat\rho\nabla\cdot\Big(\rho\nabla\frac{\delta H_{int}}{\delta\rho}\Big),$$
$$= -g\int d\mathbf{r}\int dt\; i\rho_0\,\hat\rho(\mathbf{r},t)\nabla^2 \int d\mathbf{r}' U(\mathbf{r}-\mathbf{r}')\delta\rho(\mathbf{r}',t)$$
$$- \; g\int d\mathbf{r}\int dt\; i\hat\rho(\mathbf{r},t)\nabla\cdot\Big(\delta\rho(\mathbf{r},t)\nabla\int d\mathbf{r}' U(\mathbf{r}-\mathbf{r}')\delta\rho(\mathbf{r}',t)\Big)$$

Dynamic features of the DK equation

(contrasting to the Model A/ B dynamics)

(Miyazaki-Reichman JPA 2005)

- **Physical response (to the ext. force) is a 3-point function**

$$R(\mathbf{r},t;\mathbf{r}'t') = i\left\langle \rho(\mathbf{r},t)\nabla'\cdot\left(\rho(\mathbf{r}',t')\nabla'\hat{\rho}(\mathbf{r}',t')\right)\right\rangle$$

$$= i\rho_0\nabla^2\left\langle \rho(r,t)\hat{\rho}(r',t')\right\rangle + \cdots$$

Noise-response G

FDR: $-\partial_t C(r-r',t-t') = T\,R(r-r',t-t')$

- **Direct loop expansion for** $S[\rho,\hat{\rho}]$ **does NOT respect the FDR at each loop order.**

How would one develop a FDR-consistent PT?

Time-reversal (TR) symmetry

- **Andreanov-Biroli-Lefevre (ABL) (2006)**

discovered the TR symmetry of the action

$$S[\rho,\hat{\rho}] = \int d\mathbf{r} \int dt \left\{ i\hat{\rho}\left[\partial_t \rho - \nabla \cdot \left(\rho \nabla \frac{\delta F}{\delta \rho}\right)\right] - T\rho(\nabla\hat{\rho})^2 \right\}$$

- **The action is invariant under**

U

$$\begin{aligned} \rho(\mathbf{r},-t) &= \rho(\mathbf{r},t) \\ \hat{\rho}(\mathbf{r},-t) &= -\hat{\rho}(\mathbf{r},t) + \frac{i}{T}\frac{\delta F}{\delta \rho(\mathbf{r},t)} \end{aligned}$$

T

$$\hat{\rho}(\mathbf{r},-t) = \hat{\rho}(\mathbf{r},t) + iA(\rho(\mathbf{r},t))$$

$$\nabla \cdot (\rho(\mathbf{r},t)\nabla A(\rho(\mathbf{r},t))) = \frac{1}{T}\partial_t \rho(\mathbf{r},t)$$

- **FDR from both U and T.**
- **Both U and T are nonlinear.**
- **2 paths of preserving the TR sym. in PT.**

I. Auxiliary field method (ABL, KK)

- **U is nonlinear due to** $F_{id}[\rho]$:

$$\hat{\rho}(\mathbf{r},-t) = -\hat{\rho}(\mathbf{r},t) + \frac{i}{T}\frac{\delta F}{\delta\rho(\mathbf{r},t)}$$

$$\frac{1}{T}\frac{\delta F_{id}[\rho]}{\delta\rho(\mathbf{r},t)} = \ln\frac{\rho(\mathbf{r},t)}{\rho_0} \equiv \frac{\delta\rho(\mathbf{r},t)}{\rho_0} \underbrace{-\sum_{n=2}^{\infty}\frac{1}{n}\Big(-\frac{\delta\rho(\mathbf{r},t)}{\rho_0}\Big)^n}_{\equiv\mathcal{F}(\delta\rho(\mathbf{r},t))},$$

- **Linearize U via a new set of conj. fields**

$$\theta(\mathbf{r},t) = \mathcal{F}(\delta\rho(\mathbf{r},t)) \equiv -\sum_{n=2}^{\infty}\frac{1}{n}\Big(-\frac{\delta\rho}{\rho_0}\Big)^n$$

- $S[\rho,\hat{\rho}] \Rightarrow S[\rho,\hat{\rho},\theta,\hat{\theta}]$

$$\delta\Big(\theta - \mathcal{F}(\rho)\Big) \rightarrow \exp\Big[\int d\mathbf{r}\int dt\, i\hat{\theta}\Big(\theta - \mathcal{F}(\rho)\Big)\Big].$$

- **Gaussian truncation does not work:**

$$\mathcal{F}(\delta\rho) = 0 \to F_{id}^{G}[\rho] \simeq \frac{T}{2\rho_0} \int d\mathbf{r} \left(\delta\rho(\mathbf{r})\right)^2$$

➔ **Makes U linear, but**

➔ **Incorrect dynamics in the absence of particle interaction**

$$\nabla \cdot \left(\rho(\mathbf{r},t) \nabla \frac{\delta F_{id}^{G}[\rho]}{\delta\rho(\mathbf{r},t)} \right) = T\nabla^2 \rho(\mathbf{r},t) + \underline{\frac{T}{\rho_0} \nabla \cdot (\delta\rho \nabla \rho)}$$

New action

$$S[\rho,\hat{\rho},\theta,\hat{\theta}] = S_g + S_{ng}$$

$$s_g \equiv i\hat{\rho}\Big[\partial_t\rho - T\nabla^2\rho - \underline{\rho_0 T\nabla^2\theta} - \rho_0\nabla^2\hat{U}*\delta\rho\Big] - T\rho_0(\nabla\hat{\rho})^2 + i\hat{\theta}\theta$$

$$s_{ng} \equiv i\hat{\rho}\Big[-\nabla\cdot\Big(\delta\rho\nabla\hat{U}*\delta\rho\Big) - \underline{\frac{T}{\rho_0}\nabla\cdot(\delta\rho\nabla\rho)} - \underline{T\nabla\cdot(\delta\rho\nabla\theta)}\Big]$$

$$- \; T\delta\rho(\nabla\hat{\rho})^2 - \underline{i\hat{\theta}\mathcal{F}(\rho)}$$

non-polynomial

- **Each part is invariant under O** $\quad det(O) = -1.$

O

$$\begin{aligned} \rho(\mathbf{r},-t) &= \rho(\mathbf{r},t), \qquad \theta(\mathbf{r},-t) = \theta(\mathbf{r},t) \\ \hat{\rho}(\mathbf{r},-t) &= -\hat{\rho}(\mathbf{r},t) + i\theta(\mathbf{r},t) + i\hat{K}*\delta\rho(\mathbf{r},t) \\ \hat{\theta}(\mathbf{r},-t) &= \hat{\theta}(\mathbf{r},t) + i\partial_t\rho(\mathbf{r},t) \end{aligned}$$

- **The physical response function:** $R(\mathbf{r},t;\mathbf{r}',t') = \frac{i}{T}\Big\langle \delta\rho(\mathbf{r},t)\,\hat{\theta}(\mathbf{r}',t')\Big\rangle$

- **The linear FDRs from O.**

Loop expansion for $S[\rho,\hat{\rho},\theta,\hat{\theta}] = S_g + S_{ng}$

- **Now preserves the FDR at each order.**

- **Linear FDRs for G and Σ via the TR symmetry.**

$$G_0^{-1}(13)\cdot G(32) = \delta(12) + \Sigma(13)\cdot G(32)$$

- **Static info is input into the dynamics.**

- **Thermal noise nonlinearity is treated perturbatively.**

$$-T\,\delta\rho\,(\nabla\hat{\rho})^2$$

Dynamic eq. for $G_{\rho\rho}(k,t)$

$$\dot{G}_{\rho\rho}(\mathbf{k},t) = -\frac{\rho_0 T k^2}{S(\mathbf{k})} G_{\rho\rho}(\mathbf{k},t) - \int_0^t ds\, \mathcal{M}(\mathbf{k},t-s)\dot{G}_{\rho\rho}(\mathbf{k},s)$$

$$\begin{aligned}\mathcal{M}(\mathbf{k},t) &= \frac{1}{\rho_0 T k^2}\left(\Sigma_{\hat{\rho}\hat{\rho}} - \rho_0 T k^2 \Sigma_{\hat{\theta}\hat{\rho}}\right)(\mathbf{k},t) + \left(\Sigma_{\hat{\rho}\hat{\theta}} - \rho_0 T k^2 \Sigma_{\hat{\theta}\hat{\theta}}\right)(\mathbf{k},t) \\ &+ \left(\Sigma_{\hat{\rho}\hat{\rho}} \otimes \Sigma_{\hat{\theta}\hat{\theta}}\right)(\mathbf{k},t) - \left(\Sigma_{\hat{\theta}\hat{\rho}} \otimes \Sigma_{\hat{\rho}\hat{\theta}}\right)(\mathbf{k},t) + \frac{1}{\rho_0 T k^2}\left(\Sigma_{\hat{\rho}\hat{\rho}} \otimes \mathcal{M}\right)(\mathbf{k},t)\end{aligned}$$

One loop approx.: MCT equation

$$\dot{G}_{\rho\rho}(\mathbf{k},t) = -\frac{\rho_0 T k^2}{S(\mathbf{k})} G_{\rho\rho}(\mathbf{k},t) - \int_0^t ds\, \Sigma_{mc}(\mathbf{k},t-s)\dot{G}_{\rho\rho}(\mathbf{k},s)$$

$$\begin{aligned}\Sigma_{mc}(\mathbf{k},t) &= \frac{1}{\rho_0 T k^2}\left(\Sigma_{\hat{\rho}\hat{\rho}}(\mathbf{k},t) - \rho_0 T k^2 \Sigma_{\hat{\theta}\hat{\rho}}(\mathbf{k},t)\right) + \left(\Sigma_{\hat{\rho}\hat{\theta}}(\mathbf{k},t) - \rho_0 T k^2 \Sigma_{\hat{\theta}\hat{\theta}}(\mathbf{k},t)\right) \\ &= \frac{T}{2\rho_0 k^2}\int_{\mathbf{q}} \left[(\mathbf{k}\cdot\mathbf{q})c(\mathbf{q}) + (\mathbf{k}\cdot(\mathbf{k}-\mathbf{q}))c(\mathbf{k}-\mathbf{q})\right]^2 G_{\rho\rho}(\mathbf{q},t) G_{\rho\rho}(\mathbf{k}-\mathbf{q},t)\end{aligned}$$

- **DCF c(q) naturally emerges from the bare potential U(q) due to the correct static input.**

Summary: Auxiliary field method

- **New set of conj. variables enter:**

$$S[\rho,\hat{\rho}] \Rightarrow S[\rho,\hat{\rho},\theta,\hat{\theta}] = S_g + S_{ng}$$

- **Loop expansion for the new action preserves the FDR: each part of the action is invariant under O.**

- **Linear FDRs /Non-polynomial nonlinearity.**

- **Thermal noise nonlinearity is treated perturbatively.**

- **One loop theory recovers the standard MCT eq.**

- **Needs to work out the corrections to MCT.**

II. Weak coupling expansion

- **Decompose the original action into:**

$$S[\rho,\hat\rho] = S_{id}[\rho,\hat\rho] + S_{int}[\rho,\hat\rho],$$

$$\begin{aligned} S_{id}[\rho,\hat\rho] &= \int d\mathbf{r} \int dt \left\{ i\hat\rho \Big[\partial_t\rho - \nabla\cdot\Big(\rho\nabla\frac{\delta H_{id}}{\delta\rho}\Big)\Big] - T\rho(\nabla\hat\rho)^2 \right\} \\ &= \int d\mathbf{r} \int dt \left\{ i\hat\rho \Big[\partial_t\rho - T\nabla^2\rho\Big] - T\rho(\nabla\hat\rho)^2 \right\} \end{aligned}$$

$$\begin{aligned} S_{int}[\rho,\hat\rho] &= -\int d\mathbf{r} \int dt\, i\hat\rho\nabla\cdot\Big(\rho\nabla\frac{\delta H_{int}}{\delta\rho}\Big), \\ &= -g\int d\mathbf{r}\int dt\; i\rho_0\,\hat\rho(\mathbf{r},t)\nabla^2\int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')\delta\rho(\mathbf{r}',t) \\ &- \; g\int d\mathbf{r}\int dt\; i\hat\rho(\mathbf{r},t)\nabla\cdot\Big(\delta\rho(\mathbf{r},t)\nabla\int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')\delta\rho(\mathbf{r}',t)\Big) \end{aligned}$$

- $S_{id}[\rho,\hat\rho]$ **and** $S_{int}[\rho,\hat\rho]$ **are invariant under T.**

- **Expand** $e^{S_{\text{int}}[\rho,\hat{\rho}]}$ **:**

$$\langle B[\rho,\hat{\rho}]\rangle = \left\langle B[\rho,\hat{\rho}]\, e^{S_{int}[\rho,\hat{\rho}]}\right\rangle_{id} = \left\langle B[\rho,\hat{\rho}] \sum_{n=0}^{\infty} \frac{1}{n!}\Big(S_{int}[\rho,\hat{\rho}]\Big)^n\right\rangle_{id}$$

- **To preserve the FDR, the thermal noise in** $S_{id}[\rho,\hat{\rho}]$ **should (and can) be treated non-perturbatively:**

$$\langle\tilde{B}[\rho,\hat{\rho}]\rangle_{id} = \left\langle\tilde{B}[\rho,\hat{\rho}]\,\exp\left[-T\int d\mathbf{r}\int dt\,\delta\rho(\nabla\hat{\rho})^2\right]\right\rangle_0 = \left\langle\tilde{B}[\rho,\hat{\rho}]\sum_{n=0}^{\infty}\frac{(-T)^n}{n!}\Big(\int d\mathbf{r}\int dt\,\delta\rho(\nabla\hat{\rho})^2\Big)^n\right\rangle_0$$

$\langle\cdots\rangle_0$ **: average over the Gaussian action**

$$S_G[\rho,\hat{\rho}] = \int d\mathbf{r}\int dt\left\{i\hat{\rho}\left[\partial_t\rho - T\nabla^2\rho\right] - T\rho_0(\nabla\hat{\rho})^2\right\}$$

• **Gaussian decomposition makes the expansion rapidly terminate due to**

$$\rho\hat{\rho}^2 - \textbf{nonlinearity}$$

and

$$\left\langle \hat{\rho}(1)\,\hat{\rho}(2) \right\rangle_0 = 0 \qquad \textbf{causality}$$

$1 \equiv (\mathbf{r}_1, t_1)$, etc

e.g., $\left\langle \rho(1)\rho(2)\rho(3)\hat{\rho}(1)\,\hat{\rho}(2)\hat{\rho}(3) \right\rangle_0 \neq 0.$

$$\left\langle \rho(1)\rho(2)\rho(3)\hat{\rho}(1)\,\hat{\rho}(2)\hat{\rho}(3)\hat{\rho}(4)\hat{\rho}(5) \right\rangle_0 = 0.$$

➔ **Thermal noise is treated exactly in each order!**

Self-consistent eqs. of motion for C and G

$$\phi \equiv \delta\rho$$

$$\hat{\phi} \equiv \hat{\rho}$$

- $\left\langle \frac{\delta S}{\delta \hat{\phi}(1)} \phi(2) \right\rangle = 0$
- $\left\langle \frac{\delta S}{\delta \hat{\phi}(1)} \hat{\phi}(2) \right\rangle = -\delta(1-2)$

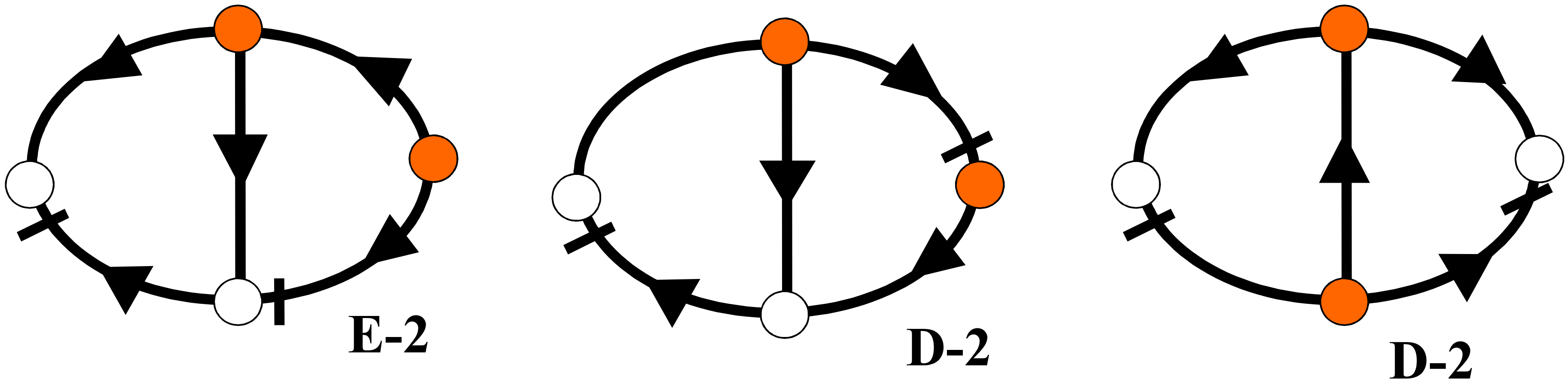
- **Self-consistent replacements of bare** C_0, G_0 **with C, G.**

- **Resulting set of equations:**

$$\dot{C}(\mathbf{k},t) = -\frac{\rho_0 T k^2}{S(\mathbf{k})} C(\mathbf{k},t) + \int_{-\infty}^{t} ds\, E(\mathbf{k},t-s) C(\mathbf{k},s) - \int_{-\infty}^{0} ds\, D(\mathbf{k},t-s) G(\mathbf{k},-s)$$

$$\dot{G}(\mathbf{k},t) = -\frac{\rho_0 T k^2}{S(\mathbf{k})} G(\mathbf{k},t) + \int_{0}^{t} ds\, E(\mathbf{k},t-s) G(\mathbf{k},s)$$

$$
\begin{aligned}
E(\mathbf{k},t) &= (-T)\int_{\mathbf{q}} \mathbf{q}\cdot(\mathbf{k}-\mathbf{q})\ \mathbf{k}\cdot\Big[\mathbf{q}U_{\mathbf{q}}+(\mathbf{k}-\mathbf{q})U_{\mathbf{k}-\mathbf{q}}\Big]G(\mathbf{q},t)G(\mathbf{k}-\mathbf{q},t)\\
&+\ i\int_{\mathbf{q}} \mathbf{k}\cdot\Big[\mathbf{q}U_{\mathbf{q}}+(\mathbf{k}-\mathbf{q})U_{\mathbf{k}-\mathbf{q}}\Big]\ (\mathbf{k}-\mathbf{q})\cdot\Big[\mathbf{q}U_{\mathbf{q}}-\mathbf{k}U_{\mathbf{k}}\Big]\ C(\mathbf{q},t)G(\mathbf{k}-\mathbf{q},t)\\
&+\ (\text{2-loop contributions})
\end{aligned}
$$



$$
\begin{aligned}
D(\mathbf{k},t) &= 2T\int_{\mathbf{q}} \mathbf{k}\cdot(\mathbf{k}-\mathbf{q})\ \mathbf{k}\cdot\Big[\mathbf{q}U_{\mathbf{q}}+(\mathbf{k}-\mathbf{q})U_{\mathbf{k}-\mathbf{q}}\Big]C(\mathbf{q},t)G(\mathbf{k}-\mathbf{q},t)\\
&+\ (-i/2)\int_{\mathbf{q}} \Big[\mathbf{k}\cdot\Big(\mathbf{q}U_{\mathbf{q}}+(\mathbf{k}-\mathbf{q})U_{\mathbf{k}-\mathbf{q}}\Big)\Big]^2\ C(\mathbf{q},t)C(\mathbf{k}-\mathbf{q},t)\\
&+\ (\text{2-loop contributions})
\end{aligned}
$$

- **The 1-loop contributions are just the ones obtained from the direct loop expansion applied for the full action.**

  Miyazaki-Reichman (2005)

- **FDR-preservation generates new, 2-loop, contributions.**

- **Interesting to analyze the simultaneous set of eqs. for C and G:**

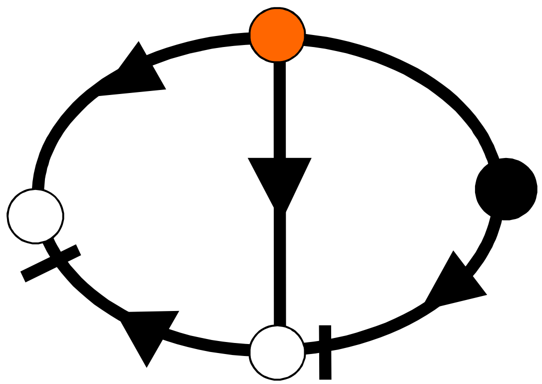
  ← Not possible to obtain a closed eq. for C alone

  due to the nonlinear FDR between C and G.

Nonlinear FDR between C and G

$$R(\mathbf{r},t;\mathbf{r}'t') = i\left\langle \rho(\mathbf{r},t)\nabla'\cdot\left(\rho(\mathbf{r}',t')\nabla'\hat{\rho}(\mathbf{r}',t')\right)\right\rangle$$
$$= i\rho_0\nabla^2\left\langle \rho(r,t)\hat{\rho}(r',t')\right\rangle + \cdots$$

$$-\frac{1}{T}\dot{C}(\mathbf{k},t) = -i\rho_0 k^2 G(\mathbf{k},t) + \int_0^t ds\, N(\mathbf{k},s)G(\mathbf{k},t-s)$$
$$N(\mathbf{k},s) = \int_{\mathbf{q}} \mathbf{k}\cdot(\mathbf{k}-\mathbf{q})\ \mathbf{k}\cdot\left[\mathbf{q}U_{\mathbf{q}} + (\mathbf{k}-\mathbf{q})U_{\mathbf{k}-\mathbf{q}}\right]C(\mathbf{q},s)G(\mathbf{k}-\mathbf{q},s)$$
$$+ \ (\text{2-loop contributions})$$



Summary and Outlook

- **A weak coupling theory uses invariance under T**

  ➔ **preserves the FDR in EQ dynamics**

  ➔ **non-perturbative treatment of thermal noise**

  ➔ **New 2-loop contributions coming in.**

Do these corrections smooth out the dynamic transition?

- **Well suited to be extended to the NEQ situations:**

Aging dynamics **Dynamics under shear flow**

No FDR and No time translation invariance.