Granular Mode-Coupling Theory

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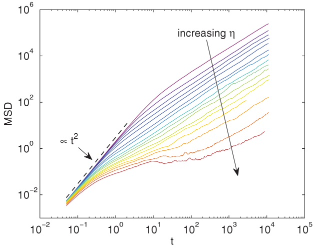
Reminder: What we have

Mean Square Displacement shows a plateau for increasing density

Plateaus are a signature of caging

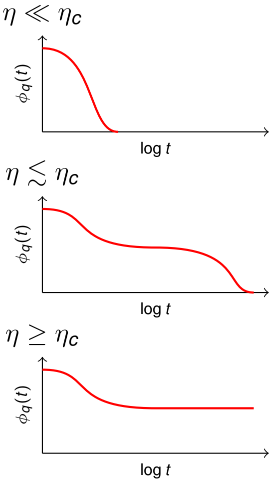
Caging is seen as either the cause or a signature of a glass transition

- No Static Order Parameter is known



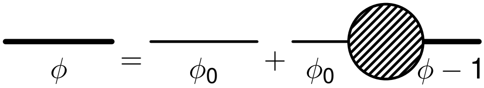
Reminder: What we want

- A theory for the Coherent Scattering Function
  - Edwards-Anderson Order Parameter $f_q = \phi(q, t \to \infty)$
  - Bifurcation from $f_q = 0$ to $f_q > 0$
- Hydrodynamics works well for the fluid but is linear
  - Interactions of Modes give Nonlinearities



Interacting Sound Waves

Dyson Equation for Coherent Scattering Function $\phi(q, t)$



Hydrodynamic (Free) Solution $\phi_0(q, t) = \cos(cqt)\exp(-\Gamma q^2 t)$

Equation of Motion

Density Field $\rho(\boldsymbol{r}, t) = \sum_i \delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$

Coherent Scattering Function $\phi(q, t) = \langle\langle \rho_{\boldsymbol{q}} | \rho_{\boldsymbol{q}}(t) \rangle\rangle$

$$0 = (\partial_t^2 + \nu_q \partial_t + \Omega_q^2)\phi(q, t)$$

Speed of Sound Ω_q / q

Sound Damping ν_q

Memory Kernels $M(q, t)$ and $L(q, t)$

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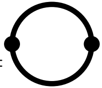
Mode-Coupling Approximation

- Take into account Splitting/Merging of sound waves

$M_{\mathrm{MCT}}[\phi] =$ 

$$M(q,t) \approx \sum_{\boldsymbol{q}=\boldsymbol{k}+\boldsymbol{p}} \mathcal{V}_{\boldsymbol{qkp}} \mathcal{W}_{\boldsymbol{qkp}} \phi(k,t)\phi(p,t)$$

Momentum Conservation demands $\boldsymbol{q} = \boldsymbol{k} + \boldsymbol{p}$

Transition Rates $\mathcal{V}_{\boldsymbol{qkp}}, \mathcal{W}_{\boldsymbol{qkp}}$ will be expressed as expectation values

$$L(q,t) \approx 0$$

- or at least short-lived

Why it helps: A schematic Model

$$\partial_t^2 \phi(t) + \phi(t) + 4\lambda \int_0^t d\tau \phi^2(t-\tau)\partial_\tau \phi(\tau)$$

EA Order Parameter $f = \phi(t \to \infty)$ follows from

$$\frac{f}{1-f} = 4\lambda f^2$$

- Bifurcation at critical $\lambda_c = 1$

Microscopic Dynamics

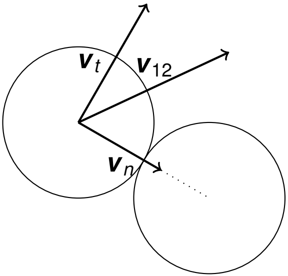
Inelastic Hard Spheres

Hard Spheres completely characterized by

- Mass m
- Radius a
- Coefficient of restitution $\epsilon \in [0, 1]$

Collision law

$$\boldsymbol{v}'_n = -\epsilon\, \boldsymbol{v}_n,$$
$$\boldsymbol{v}'_t = \boldsymbol{v}_t$$



Energy Loss on average per collision $\Delta E \propto 1 - \epsilon^2$

Random Driving Force

Random Force $\xi_i(t)$, gaussian distributed

- Average $\langle \xi_i \rangle = 0$
- Driving power $P_D = \langle \xi_i^2 \rangle$

Stationary State as a balance between driving & dissipation

The Liouville Operator

Observables $A(\Gamma(t))$ are functions of phase space $\Gamma = (\boldsymbol{x}, \boldsymbol{p})$

Liouville Operator $\mathcal{L} = \frac{\partial \Gamma}{\partial t} \frac{\partial}{\partial \Gamma}$ controls rate of change, $\partial_t A = \mathcal{L} A$.

Propagator $\mathrm{U}(t) = \exp(t\mathcal{L})$, i.e., $A(t) = \mathrm{U}(t)A(0)$

Fun Fact $\mathcal{L}_+ \rho_{\boldsymbol{q}} = iqj^L_{\boldsymbol{q}}$

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Our Liouville Operator

Free Streaming $i\mathcal{L}_0 = \sum_j \boldsymbol{v}_j \cdot \frac{\partial}{\partial \boldsymbol{r}_j}$

Collisions $i\mathcal{T}_+ = \sum_{j<k} (\hat{\boldsymbol{r}}_{jk} \cdot \boldsymbol{v}_{jk}) \Theta(-\hat{\boldsymbol{r}}_{jk} \cdot \boldsymbol{v}_{jk}) \delta(r_{jk} - 2a)(b^+_{jk} - 1)$

- Operator b^+_{jk} implements inelastic collision rule

Driving $i\check{\mathcal{L}}^D_+(t) = \sum_j \boldsymbol{\xi}_j(t) \cdot \frac{\partial}{\partial \boldsymbol{v}_j}$

Propagator $\check{\mathrm{U}}(t) = \exp_+(t\check{\mathcal{L}}_+(t))$

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Averages & Averaged Quantities

Averages

$$\langle\!\langle A \rangle\!\rangle = \langle \langle A \rangle_{\Xi} \rangle_{\Gamma} = \int d\Gamma f(\Gamma) \int \mathcal{D}[\Xi] A(\Gamma, \Xi)$$

- Average over all Trajectories of the Driving Force (for a specific initial condition)
- Average over initial conditions

Effective Dynamics

- For two-point correlation functions

$$\langle\!\langle A\check{\mathrm{U}}(t)B\rangle\!\rangle = \left\langle A \left\langle \check{\mathrm{U}}(t)\right\rangle_{\Xi} B\right\rangle_{\Gamma} = \langle A\mathrm{U}(t)B\rangle_{\Gamma}$$

Averaged Dynamics

$$\mathcal{L}_{+}^{D} := \left\langle \check{\mathcal{L}}_{+}^{D}(t)\right\rangle_{\Xi} = P_D \sum_i \frac{\partial^2}{\partial \mathbf{v}_i^2}$$

$$\check{\mathrm{U}}(t) = \exp_{+}(t\check{\mathcal{L}}_{+}(t))$$
$$\mathrm{U}(t) = \exp(t\mathcal{L}_{+})$$

More Adjoints than you'd like

Direction of Time $\mathcal{L}_+, \mathcal{L}_-$

Quantum Scalar Product $(A, B) = \int d\Gamma A(\Gamma) B^*(\Gamma)$

Statistical Scalar Product $\langle A | B \rangle = \int d\Gamma f(\Gamma) A(\Gamma) B^*(\Gamma)$

The f-Liouvillian $(\overline{\mathcal{L}}_\pm A, B) = (A, \mathcal{L}_\pm B)$

The adjoint Liouvillian $\left\langle \mathcal{L}_\pm^\dagger A | B \right\rangle = \langle A | \mathcal{L}_\pm B \rangle$

Detailed Balance $\langle \mathrm{U}(-t) A | B \rangle = \langle A, \mathrm{U}(t) B \rangle$

In Equilibrium $\overline{\mathcal{L}}_\pm = \mathcal{L}_\pm^\dagger = \mathcal{L}_\mp$

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Slow Variables

Conserved Quantities are

Density $\rho_{\boldsymbol{q}}$ and

Current Density $\boldsymbol{j}_{\boldsymbol{q}} = \sum_k \boldsymbol{v}_k \delta(\boldsymbol{r} - \boldsymbol{r}_k) = \hat{\boldsymbol{q}} j^L_{\boldsymbol{q}} + \boldsymbol{j}^T_{\boldsymbol{q}}$

State Vector $\left|\rho_{\boldsymbol{q}}, j^L_{\boldsymbol{q}}\right\rangle$

The Mori-Zwanzig Decomposition

Mori-Projectors $\mathcal{P} = \sum_{\boldsymbol{q}} \left| \rho_{\boldsymbol{q}}, j^L_{\boldsymbol{q}} \right\rangle \left\langle \rho_{\boldsymbol{q}}, j^L_{\boldsymbol{q}} \right|$ and $\mathcal{Q} = 1 - \mathcal{P}$

Laplace Transform $\hat{g}(s) = \mathrm{LT}[g(t)] = i \int_0^\infty e^{-ist} g(t) dt$

Propagator $\hat{\mathrm{U}}(s) = (s - \mathcal{L}_+)^{-1}$

$$\mathcal{P}(s - \mathcal{L}_+)^{-1}\mathcal{P} = [s - \mathcal{P}\mathcal{L}_+\mathcal{P} - \mathcal{P}\mathcal{L}_+\mathcal{Q}(s - \mathcal{Q}\mathcal{L}_+\mathcal{Q})^{-1}\mathcal{Q}\mathcal{L}_+\mathcal{P}]^{-1}$$

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Equations of Motion

$$0 = (\partial_t^2 + \nu_q \partial_t + \Omega_q^2)\phi(q,t) + \int_0^t d\tau M(q, t - t\tau)\partial_\tau \phi(q,\tau) + \int_0^t d\tau L(q, t-\tau)\phi(q,\tau)$$

- $\Omega_q^2 \propto \langle \rho_{\boldsymbol{q}} | \mathcal{L}_+ j_{\boldsymbol{q}}^L \rangle \langle j_{\boldsymbol{q}}^L | \mathcal{L}_+ \rho_{\boldsymbol{q}} \rangle$
- $\nu_q = \langle j_{\boldsymbol{q}}^L | \mathcal{L}_+ j_{\boldsymbol{q}}^L \rangle$
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The Mode Coupling Approximation

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$$\approx |\rho_{\mathbf{k}}\rho_{\mathbf{p}}\rangle \phi(k,t)\phi(p,t) \langle\rho_{\mathbf{k}}\rho_{\mathbf{p}}|$$

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Simplifying Assumptions

- Positions and (precollisional) Velocities are uncorrelated (Molecular Chaos)
- The velocity distribution factorizes
- The second moment of the one particle velocity pdf exists

Result

- $\nu_q = \frac{1+\epsilon}{3}\omega_E[1 + 3j_0''(qd)]$
- $\Omega_{j\rho} = qT$
- $\Omega_{\rho j} = qT\left(\frac{1+\epsilon}{2} + \frac{1-\epsilon}{2}S_q\right)$
- $V_q^2 = \frac{T}{S_q}\left(\frac{1+\epsilon}{2} + \frac{1-\epsilon}{2}S_q\right)$

$$M(q,t) = \frac{1+\epsilon}{2}\int_0^\infty d^3k S_k S_{|\boldsymbol{q}-\boldsymbol{k}|} \times \{[\hat{\boldsymbol{q}}\cdot\boldsymbol{k}]c_k + [\hat{\boldsymbol{q}}\cdot(\boldsymbol{q}-\boldsymbol{k})]c_{|\boldsymbol{q}-\boldsymbol{k}|}\}^2\phi(k,t)\phi(|\boldsymbol{q}-\boldsymbol{k}|,t)$$

Direct Correlation Function $c_k := 1 - S_k^{-1}$

Open Problems

Better Distribution Function

- Avoid Factorization of velocities
- Avoid Factorization between Positions and Velocities
- Non Gaussian Velocity PDF not so important

Integration through Transients

- Start from Elastic Hard Spheres
- Switch on Inelasticity & Driving
- Treat as Pertubation in ITT formalism
- Does not work

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Easy (I think)

- Other Interactions
- (Additional) overall viscous damping

Hard (I am afraid)

- Nonrandom Driving Force
- Boundary Driving

Shearing via ITT

- What reference state to use?
- Include more Correlation Functions?
- Interpretation of nonlinear equations

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Summary

- MCT can be generlized to NESS
- Predicts a Glass Transition for a values of ε
- Loss of Detailed Balance is clearly visible
- There is room for improvement

Thank you for your attention

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