Liquid-glass transition in equilibrium, arXiv:1311.1465

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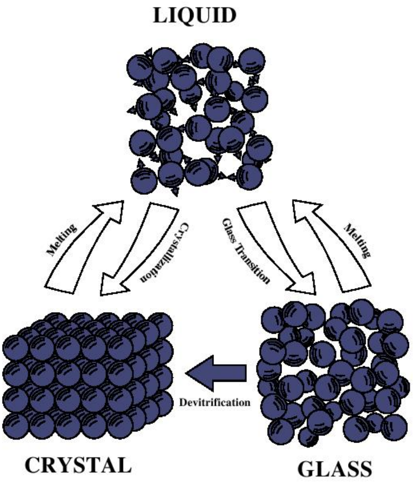
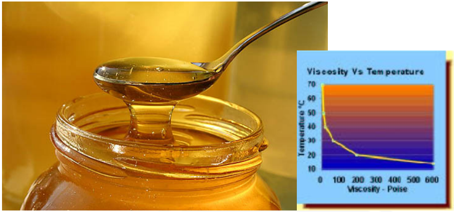
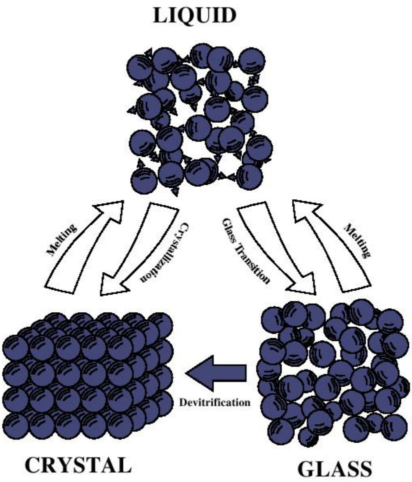
Talk structure

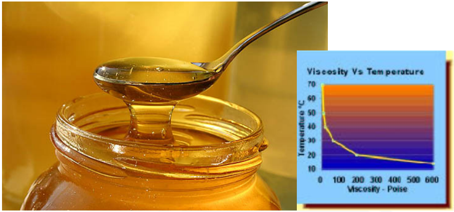
Introduction to glasses





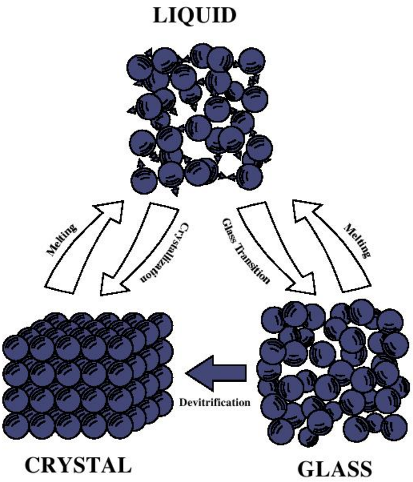
Introduction to glasses

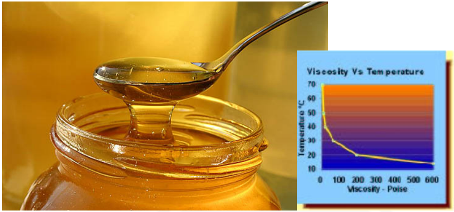




- Dynamic arrest effect?

Introduction to glasses





- Dynamic arrest effect?
- Underlying thermodynamic transition?

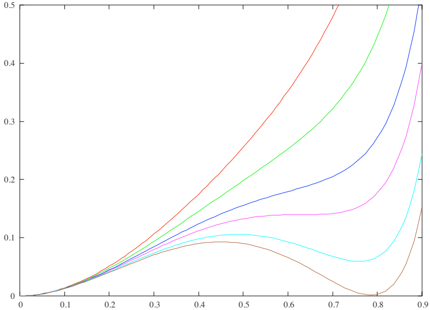
Mean field: Random first order transition (RFOT)

Mean Field

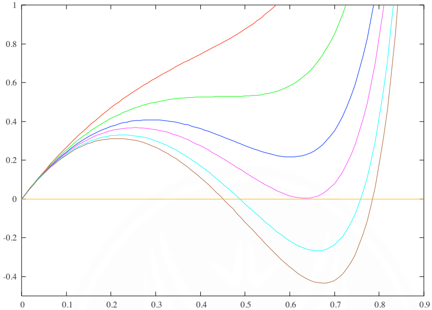
- The structural transition is random first order transition (RFOT)
- For $T < T_{\rm c}$: the ergodicity is lost due to the appearance of an exponentially large number of metastable states
- At $T_{\rm K}(< T_{\rm c})$ ideal glass transition: sharp decrease of available states
- We consider the replica potential $W(q)$ as a function of the degree of similarity between all the possible amorphous configurations
- The glass transition can be detected by the appearance of a second minimum at high q in $W(q)$
- The two minima are related to similar and completely different configurations, not to different phases.

Mean field: Random first order transition (RFOT)

$W(q)$



$W'(q)$



One can observe a precursor of the phase transition in the shape of this potential still deep in the liquid phase!

Two coupled replicas

- External field ϵ: $H_{\mathrm{tot}}(\boldsymbol{R}_1, \boldsymbol{R}_2) = H(\boldsymbol{R}_1) + H(\boldsymbol{R}_2) - \epsilon q(\boldsymbol{R}_1, \boldsymbol{R}_2)$
- The free energy $F(\epsilon) = \min_q W(q) - \epsilon q$
- The glass transition point becomes a coexistence line $\epsilon(T)$ separating the low and high q regions.
- This line extends from T_{K} to higher temperatures, terminating in a critical point at T_{c}.

Universality class of the critical point

- Quenched potential (ϵ acts only on one of the replicas): RFIM.
- Annealed potential (ϵ acts on both replicas): Ising model.

Model and observables

Model

- We study a 50 : 50 mixture of $N = 62,\ 124,\ 250,\ 500$ binary HS
- $d_2 = 1.4\, d_1 \Rightarrow$ Inhibit crystallization
- Constant volume ensemble. Volume fraction $\phi = \frac{\pi N}{12 V}\left(d_A^3 + d_B^3\right)$

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Overlap

- Consider two configurations in equilibrium $\alpha = 1, 2$
- Divide the whole volume in N_c small boxes and compute the occupation: $n_{i,\ T}^{(\alpha)} = 1(0)$ there is (not) particle of type $T(= A, B)$ in the box.
- Overlap $Q_{12} = \frac{1}{N_c}\sum_{i=1}^{N_c} n_{i,\ A}^{(1)} n_{i,\ A}^{(2)} + n_{i,\ B}^{(1)} n_{i,\ B}^{(2)}$.
- Low Q_{12}: completely different confs High Q_{12}: similar conf (glass).

Computing $W(q)$ with the tethered MC method

The free energy cost

$$W(q) = -\frac{1}{N}\log \int\int \mathrm{d}\boldsymbol{R}_1 \mathrm{d}\boldsymbol{R}_2\ \mathrm{e}^{-\beta H(\boldsymbol{R}_1)-\beta H(\boldsymbol{R}_2)}\ \delta\left(q - q_{1,2}\right)$$

Its convolution with a strongly peaked Gaussian

$$\hat{W}(q) = -\frac{1}{N}\log \int\int \mathrm{d}\boldsymbol{R}_1 \mathrm{d}\boldsymbol{R}_2\ \mathrm{e}^{-\beta H(\boldsymbol{R}_1)-\beta H(\boldsymbol{R}_2)}\ \mathrm{e}^{-\frac{kN}{2}(q-q_{1,2})^2}$$

We derivative with respect to q

$$\hat{W}'(q) = \frac{\int\int \mathrm{d}\boldsymbol{R}_1 \mathrm{d}\boldsymbol{R}_2\ k\left[q - q_{1,2}\right]\omega_N(\boldsymbol{R}_1, \boldsymbol{R}_2, V; q)}{\int\int \mathrm{d}\boldsymbol{R}_1 \mathrm{d}\boldsymbol{R}_2\ \omega_N(\boldsymbol{R}_1, \boldsymbol{R}_2, V; q)},$$

with

$$\omega_N(\boldsymbol{R}_1, \boldsymbol{R}_2, \phi; q) = \mathrm{e}^{-\beta H(\boldsymbol{R}_1)-\beta H(\boldsymbol{R}_2)}\ \mathrm{e}^{-\frac{kN}{2}\left[q-q_{1,2}(\boldsymbol{R}_1,\boldsymbol{R}_2)\right]^2}.$$

Computing $W(q)$ with the tethered MC method

That means that the replica field can be understood as the MC thermal average obtained with the tethered measure

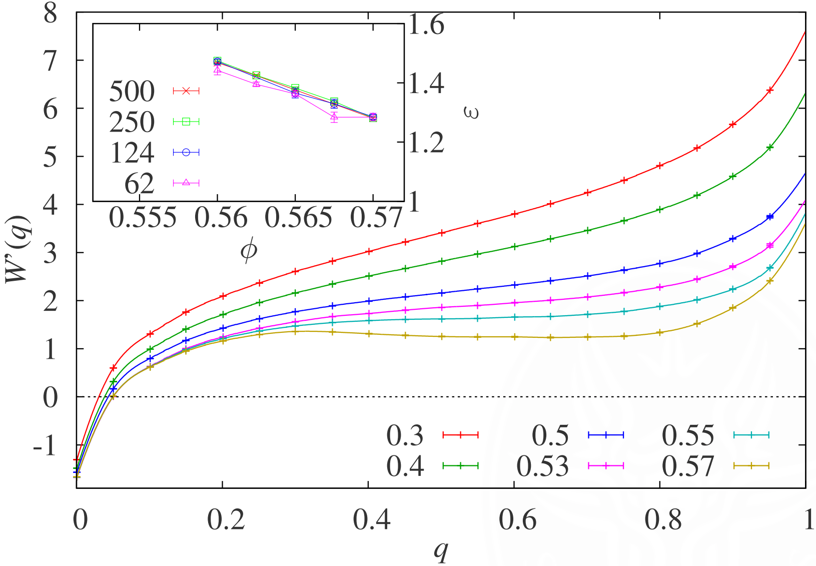
$$\hat{W}'(q) = \langle \hat{\epsilon} \rangle_q , \ \hat{\epsilon} = k\,(q - q_{1,2})$$

The generalization of this formalism to the presence of an external field ϵ: probability distribution density $P_\epsilon(q) \propto \exp\left[-\left(NW(q) - \epsilon q\right)\right]$
Then,

$$\log \hat{P}_\epsilon(q_2) - \log \hat{P}_\epsilon(q_1) = N \int_{q_1}^{q_2} \mathrm{d}q \left[\langle \hat{\epsilon} \rangle_q - \epsilon \right],$$

The coexistence condition $P_{\epsilon_{co}}(q_{\,\mathrm{low}}) = P_{\epsilon_{co}}(q_{\mathrm{high}})$, is equivalent to a Maxwell construction

Maxwell construction



Finding the critical point

- Extend the coexistence line below the critical point: Widow line
- Search ϵ that makes $P_\epsilon(q)$ balanced

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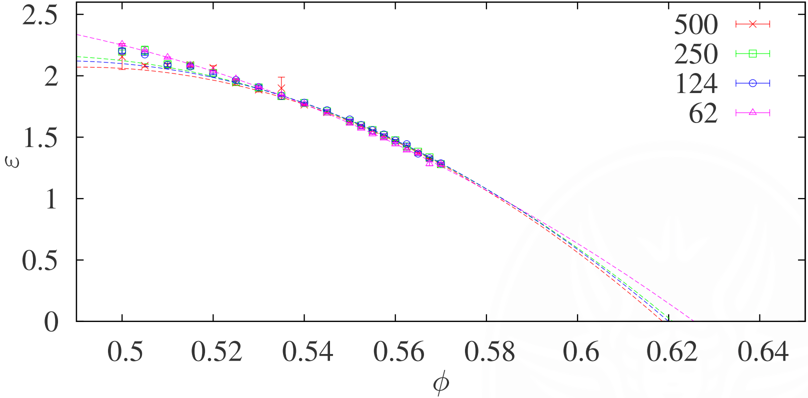

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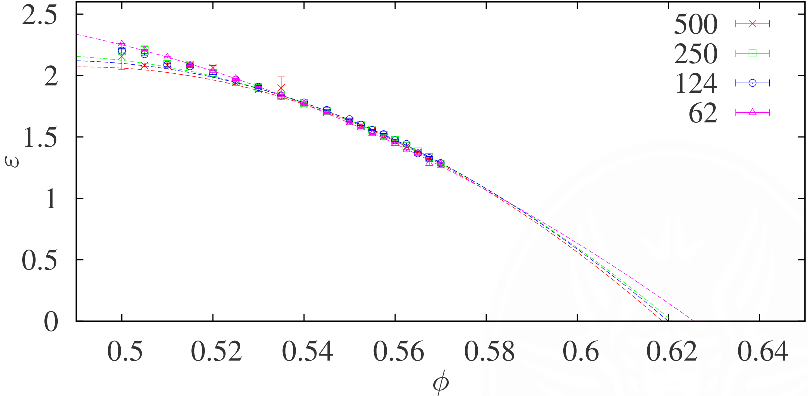
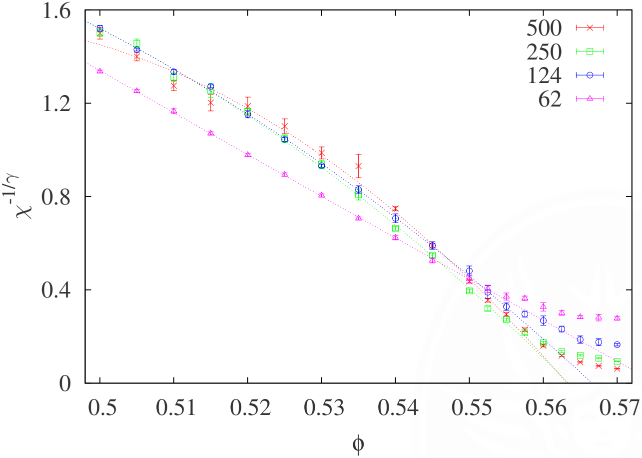


- $S_{\rm conf} \propto q^*\epsilon \Rightarrow \phi_{\rm K}$ from extrapolation to $\epsilon = 0$

Finding the critical point

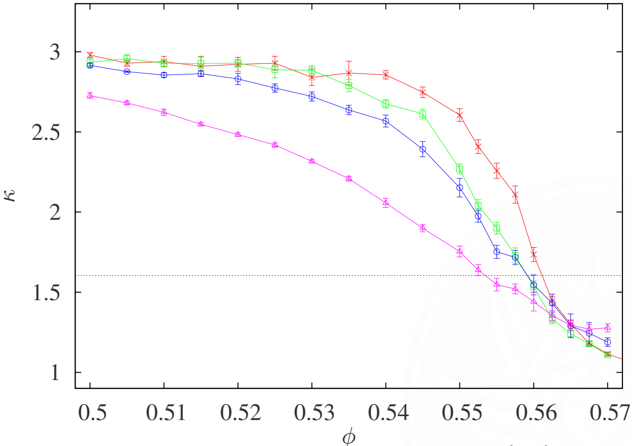
Static susceptibility $\chi = N[\langle q^2 \rangle - \langle q \rangle^2]$



Ising universality class $\Rightarrow \chi \propto |\phi - \phi_c|^{-\gamma}$, with $\gamma = 1.2372$

Finding the critical point

Kurtosis $\kappa = \frac{\langle m \rangle^4}{\langle m^2 \rangle^2}$ with $m = q - \langle q \rangle$ (Binder: $1 - \kappa/3$)



Universal value at ϕ_c: $\kappa = 1.6043(10)$

Conclusions

- We have studied a system of two coupled replicas of a binary mixture of hard spheres
- We compute the replica potential (as in MF) thanks to the tethered algorithm
- We present clear evidences of the existence of a first order line that ends in a critical point (at ϕ's below ϕ_{K})
- This result is in agreement with theories that predict that such transition is a precursor of the standard ideal glass transition
- The critical properties are compatible with those of an Ising system

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THANK YOU VERY MUCH