

Summary of lecture 1

- ⊗ In supercooled liquids and granular systems, the approach to jamming is signaled by a dramatic increase of timescales
- ⊗ The best description is in terms of the Vogel-Fulcher-Tamann law which implies activated scaling
- ⊗ Activated scaling implies a logarithmic dependence of length scales on time scales
- ⊗ Measurements indicate a growing dynamical length scale
- * Glassy systems (easy to supercool) are “frustrated” and have complicated energy surfaces
- * There has to be some connection between this property and the anomalous behavior of length and timescales

Blocked states and inherent structures: A promising approach to a unified framework

Stillinger's construction of inherent structures[13]

Edwards' idea of blocked states [14]

Simulations

- Properties of inherent structures (LJ systems)[15]
- Properties of inherent structures of purely repulsive systems[16]

Statistical description in terms of Ensemble of Blocked states (inherent structures)

Basics of statistical mechanics; fundamental postulates and the ensembles of equilibrium statistical mechanics

Write configurational partition function of a liquid in terms of inherent structures, explore consequences

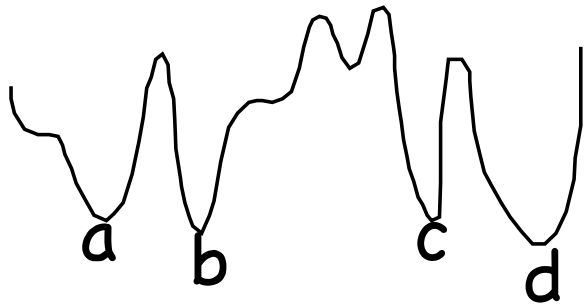
Observations in simulations of Lennard-Jones systems

Introduce a toy model where we can work things out explicitly

Partition function and inherent structures

$$Z_{conf} = \int \prod_i d\vec{r}_i e^{-\beta V(\{r_i\})}$$

Divide the 3N dimensional configuration space in to basins



$$V(\{r_i\}) = V_\alpha + \Delta V_\alpha(\{r_i\})$$

$$Z_{conf} = \sum_\alpha e^{-\beta V_\alpha} \sum' e^{-\beta \Delta V_\alpha(\{r_i\})}$$

$$Z_{conf} = \int dv e^{-\beta N v} \sum_\alpha \delta(v - v_\alpha) \sum' e^{-\beta \Delta V_\alpha(\{r_i\})}$$

$$Z_{conf} = \int dv e^{-\beta N v} e^{N s(v)} \langle \sum' e^{-\beta \Delta V_\alpha(\{r_i\})} \rangle$$

$$Z_{conf} = \int dv e^{-\beta N v} e^{N s(v)} e^{-\beta N f(\beta, v)}$$

Partition function and inherent structures

$$Z_{conf} = \int dv e^{-\beta N v} e^{N s(v)} e^{-\beta N f(\beta, v)}$$

$$Z_{conf} = e^{-\beta N F(v_m)}$$

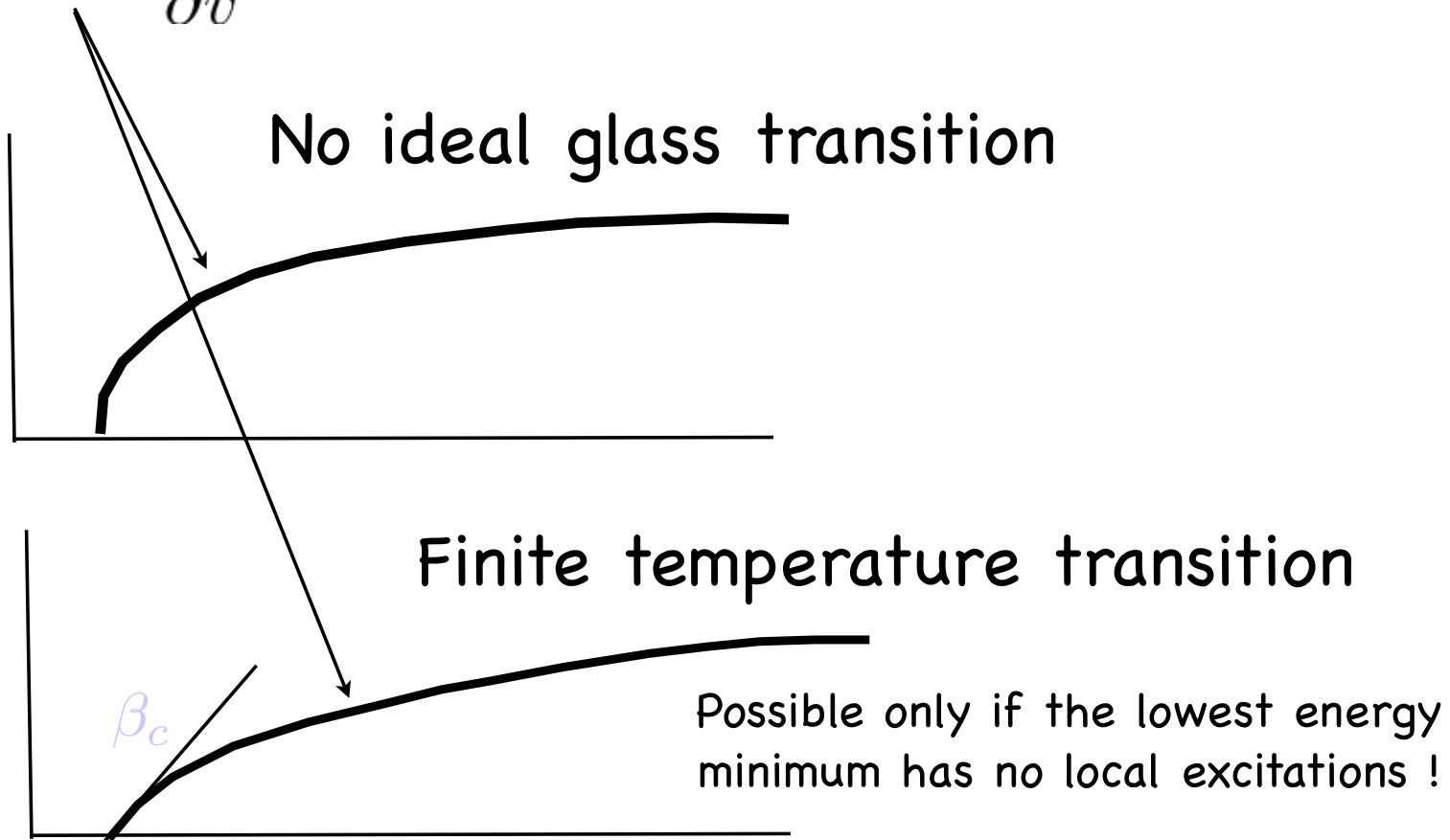
$$\frac{\partial}{\partial v} [s(v) - \beta v - \beta f(\beta, v)] = 0$$

$\exp(s(v))$ is a measure of the # of non-crystalline minima with energy between v and $v + dv$

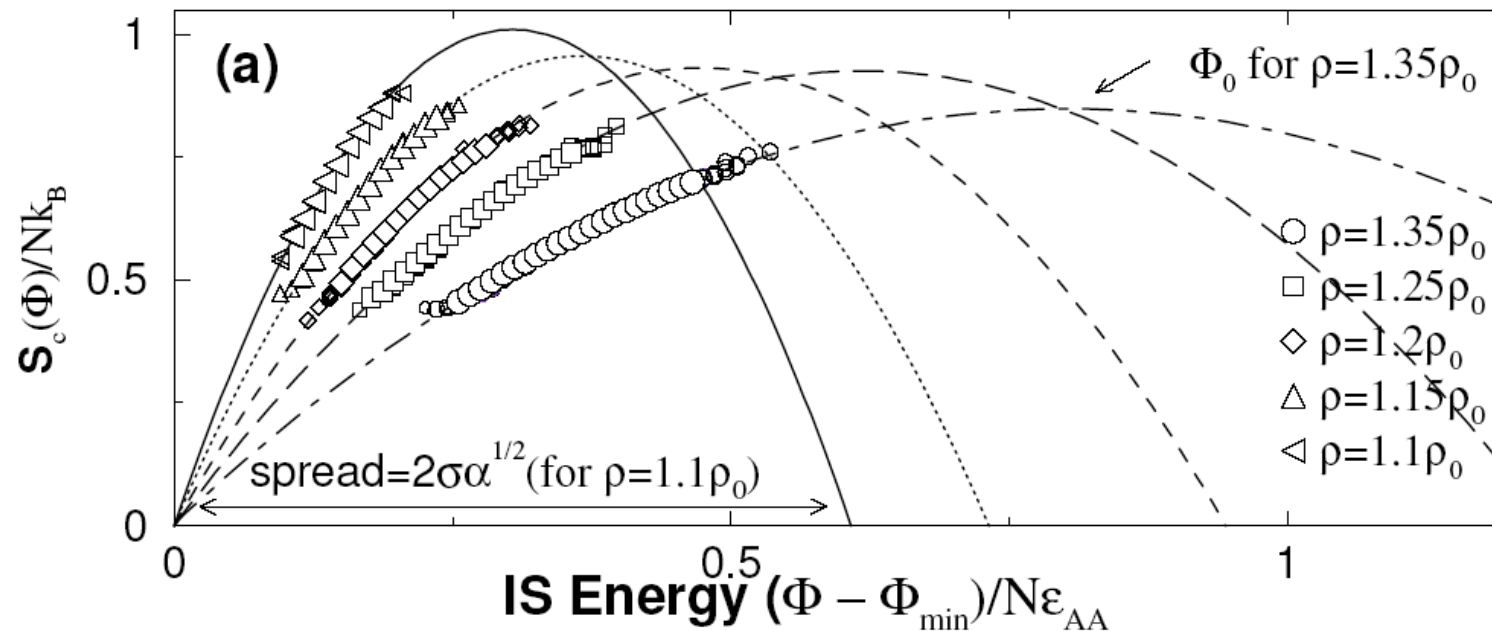
Shape of $s(v)$ is crucial: Does it go to zero with a finite or an infinite slope?

Partition function and inherent structures

$$\frac{\partial}{\partial v} [s(v) - \beta v - \beta f(\beta, v)] = 0$$



Observations in binary Lennard-Jones mixtures



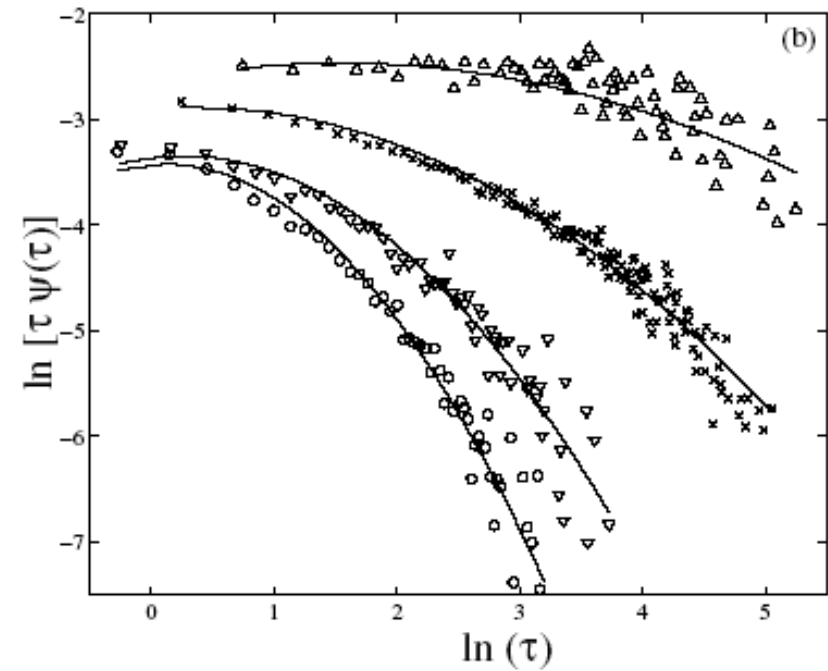
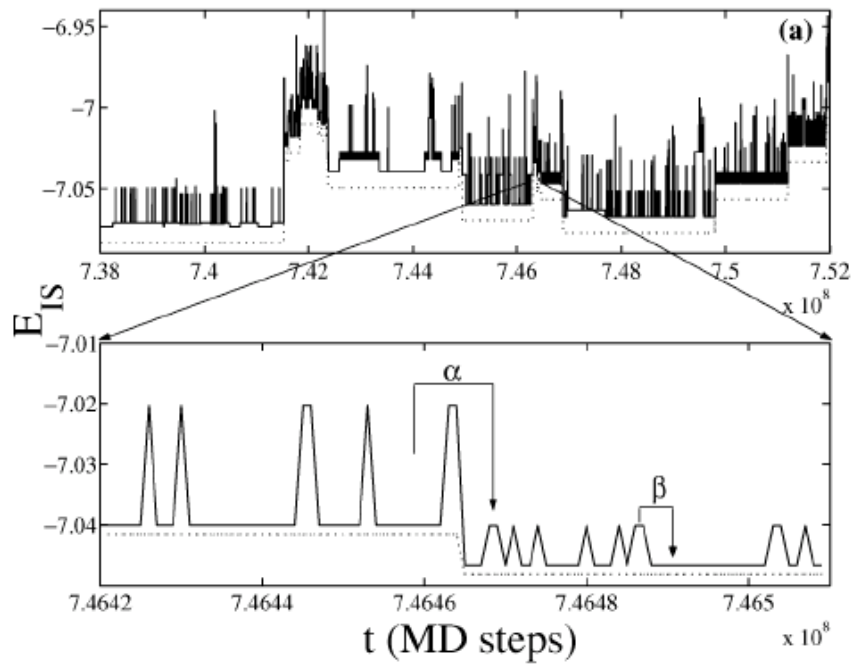
Slope decreases as density increases

Critical density at which infinite slope gives away to finite slope?

Are there models where entropy goes to zero with finite slope?

If so, what are dynamics near such critical points?

Projected Dynamics in inherent structure space



Distribution of hopping times

Review articles:

Bouchaud, Les Houches lectures, cond-mat/0211196 v2 (Granular)

C. A. Angell, *J. Phys. Chem.* **49**, 863 (1988); M. D. Ediger, C. A. Angell, and S. R. Nagel, *ibid.* **100**, 13 200 (1996); W. Götze and L. Sjogren, *Rep. Prog. Phys.* **55**, 241 (1992).

Glasses

- [1] V. Trappe, V. Prasad, Luca Cipelletti, P. N. Segre and D. A. Weitz, *Nature*, 411, 772 (2001).
- [2] Liu, A. J. and Nagel, S. R., *Nature* 396, (1998)
- [3] D. S. Fisher, *Phys. Rev. Lett.* 56, 416 (1986).
- [4] Walter Kob, Lecture notes for LES HOUCHEs 2002 SUMMER SCHOOL - SESSION LXXVII; SLOW RELAXATIONS AND NONEQUILIBRIUM DYNAMICS IN CONDENSED MATTER
- [5] C. Donati, J. F. Douglas, W. Kob, S. J. Plimpton, P. H. Poole, and S. C. Glotzer, *Phys. Rev. Lett.* 80, 2338 (1998); W. Kob, C. Donati, S. J. Plimpton, P. H. Poole, and S. C. Glotzer, *ibid.* 79, 2827 (1997); C. Donati, S. C. Glotzer, P. H. Poole, W. Kob, and S. J. Plimpton, *Phys. Rev. E* 60, 3107 (1999).
- [6] L. Berthier, G. Biroli, J.-P. Bouchaud,, 4 L. Cipelletti, D. El Masri, D. LHote F. Ladieu, and M. Pierno, cond-mat/0512379
- [7] Jean-Philippe Bouchaud and Giulio Biroli, cond-mat/051668
- [8] David Reichman, K. Minazaki and J.-P. Bouchaud, very recent cond-mat
- [9] J. P. Garrahan and D. Chandler, *Proc. Natl. Acad. Sci. U.S.A.* 100, 9710 (2003).
- [10] F. Stillinger, *J. Chem. Phys.*, 88, 7188(1988)
- [11] S. Sastry, P. G. Debenedetti, and F. H. Stillinger, *Nature London!* 393, 554 (1998).
- [12] B. Doliwa and A. Heuer, *Phys. Rev. E* 67, 030501 (2003).
- [13] R. A. Denny, D. R. Reichman, and J. P. Bouchaud, *Phys. Rev. Lett.* 90, 025503 (2003)
- [14] C.S. O'Hearn, L.E. Silbert, A.J. Liu and S.R. Nagel, *Phys. Rev. E.* 68, 011306, (2003) ;C. S. O'Hern, S. A. Langer, A. J. Liu, and S. R. Nagel, *Phys. Rev. Lett.* 88, 075507 (2002).; L. E. Silbert, A. J. Liu and S. R. Nagel, cond-mat/0501616

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- [1] V. Trappe, V. Prasad, Luca Cipelletti, P. N. Segre and D. A. Weitz, *Nature*, 411, 772 (2001).
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- [7] Jean-Philippe Bouchaud and Giulio Biroli, *cond-mat/051668*
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