Title: Quantum mechanical and information theoretic view on classical glass transitions

Date: May 25, 2010 04:00 PM

URL: http://pirsa.org/10050067

Abstract: Using the mapping of the Fokker-Planck description of classical stochastic dynamics onto a quantum Hamiltonian, we argue that a dynamical glass transition in the former must have a precise definition in terms of a quantum phase transition in the latter. At the dynamical level, the transition corresponds to a collapse of the excitation spectrum at a critical point. At the static level, the transition affects the ground state wavefunction: while in some cases it could be picked up by the expectation value of a local operator, in others the order may be non-local, and impossible to be determined with any local probe. Here we propose instead to use concepts from quantum information theory that are not centered around local order parameters, such as fidelity and entanglement measures. We show that for systems derived from the mapping of classical stochastic dynamics, singularities in the fidelity susceptibility translate directly into singularities in the heat capacity of the classical system. In classical glassy systems with an extensive number of metastable states, we find that the prefactor of the area law term in the entanglement entropy jumps across the transition. We also discuss how entanglement measures can be used to detect a growing correlation length that diverges at the transition. Finally, we illustrate how static order can be hidden in systems with a macroscopically large number of degenerate equilibrium states by constructing a three dimensional lattice gauge model with only short-range interactions but with a finite temperature continuous phase transition into a massively degenerate phase.

Quantum mechanical and information theoretic view on classical glass transitions

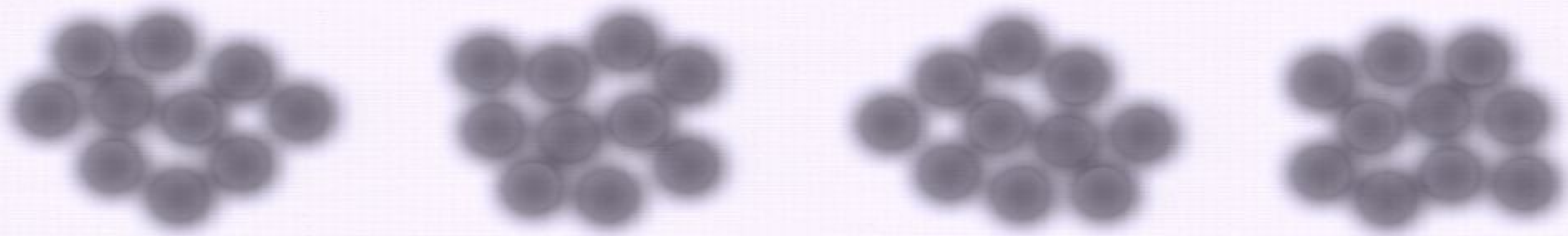
Claudio Chamon

with Claudio Castelnovo and David Sherrington (Oxford)

arXiv:1003.3832, to appear in PRB

BOSTON UNIVERSITY

What is a glass?



α_1 α_2 α_3 α_4

"Liquid"-like state of matter, with no local order parameter

Super slow dynamics

How slow is slow?

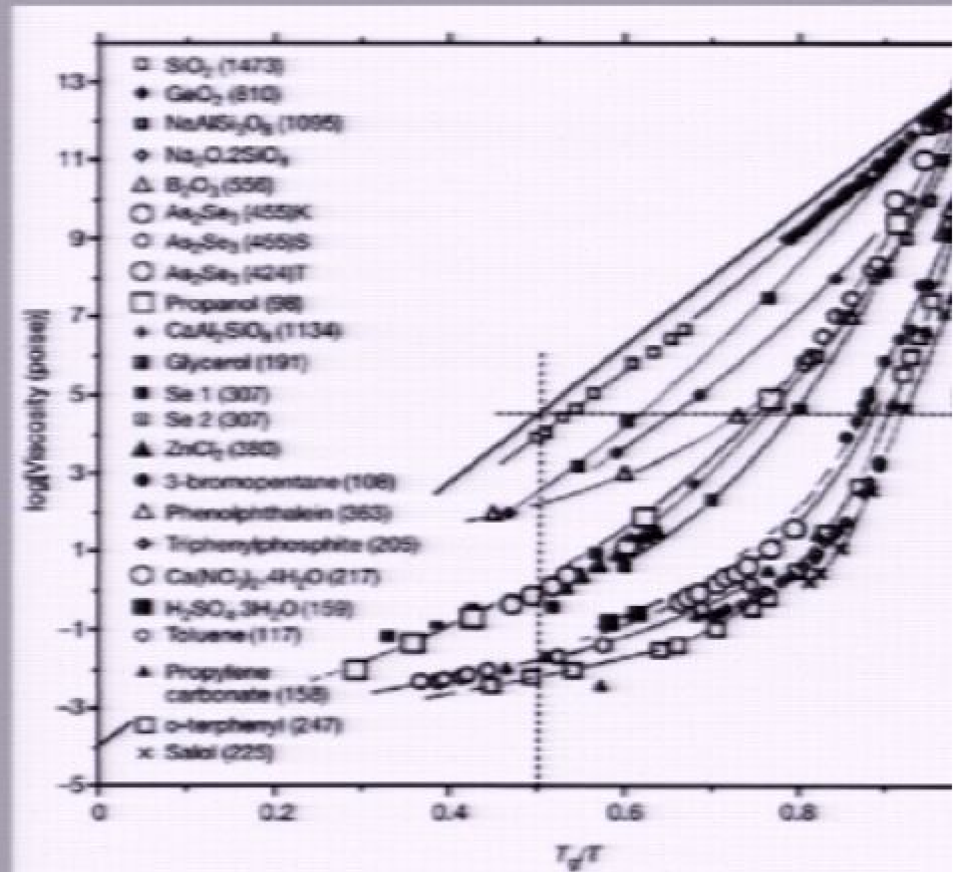
Dynamical glass transition

experimentally (operationally)

$$T < T_g$$
$$\Updownarrow$$
$$\eta > 10^{13}\ \text{Poise}$$

e scales

$$\tau \sim \tau_0\, e^{\frac{C}{T_g - T}}$$ (Vogel-Fulcher law)



L.-M. Martinez and C. A. Angell, Nature

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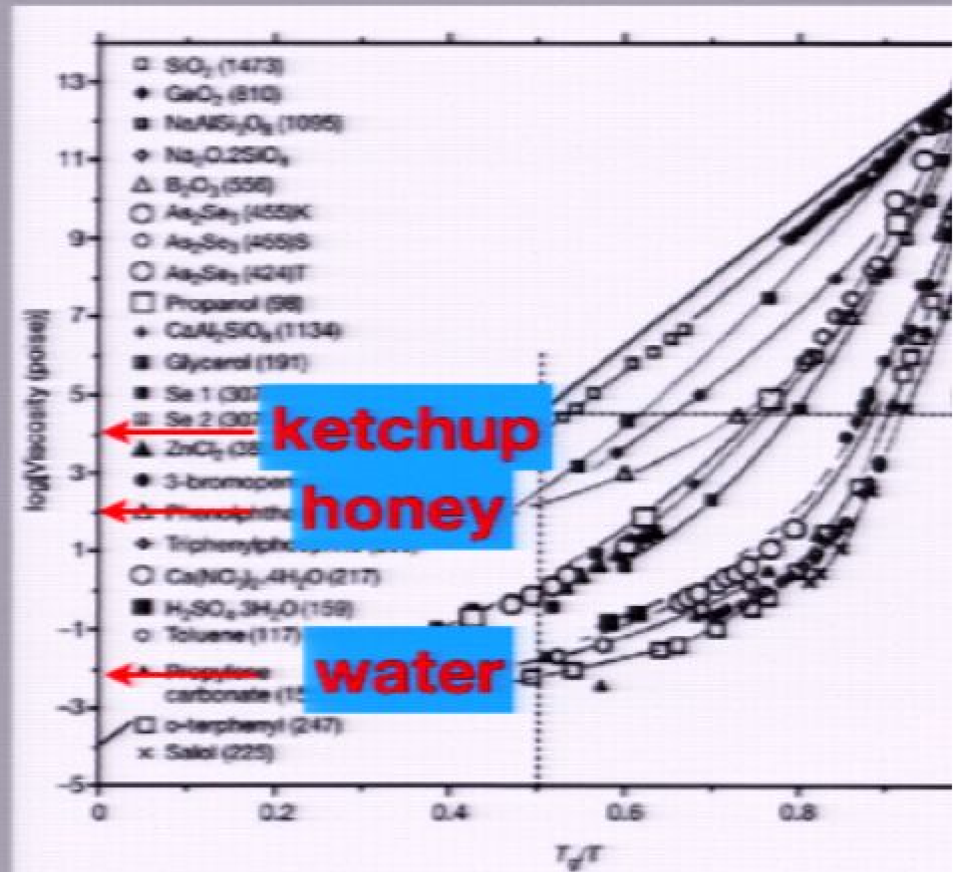

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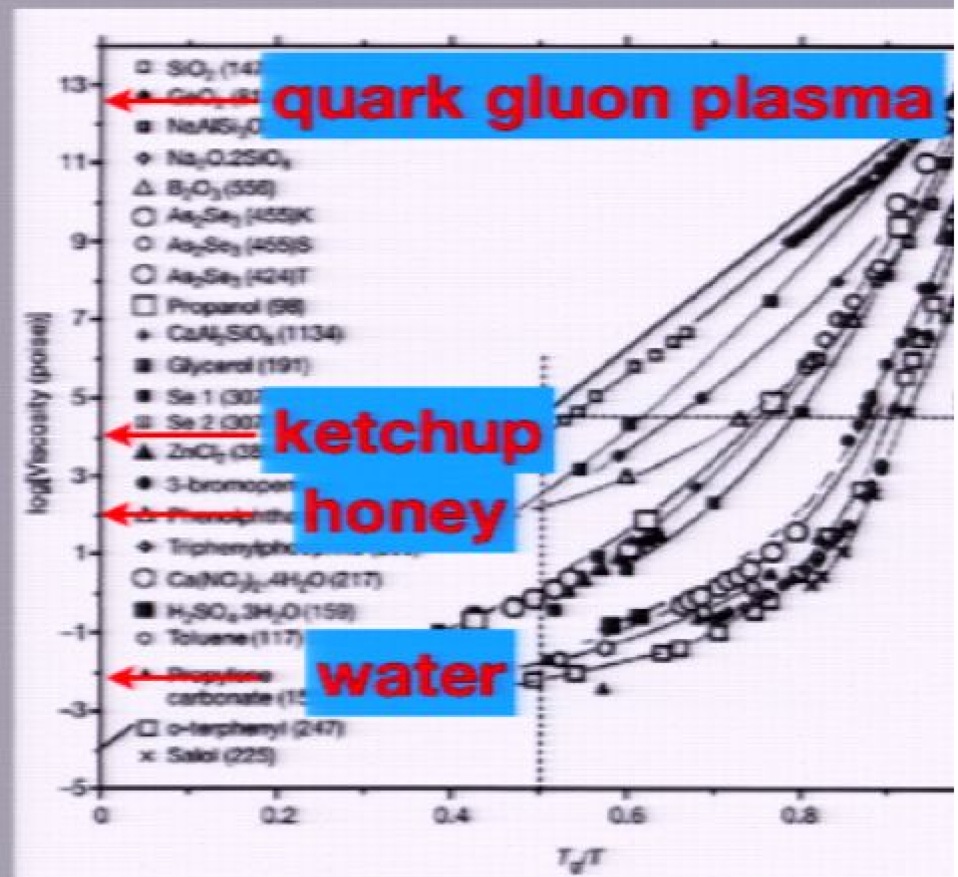

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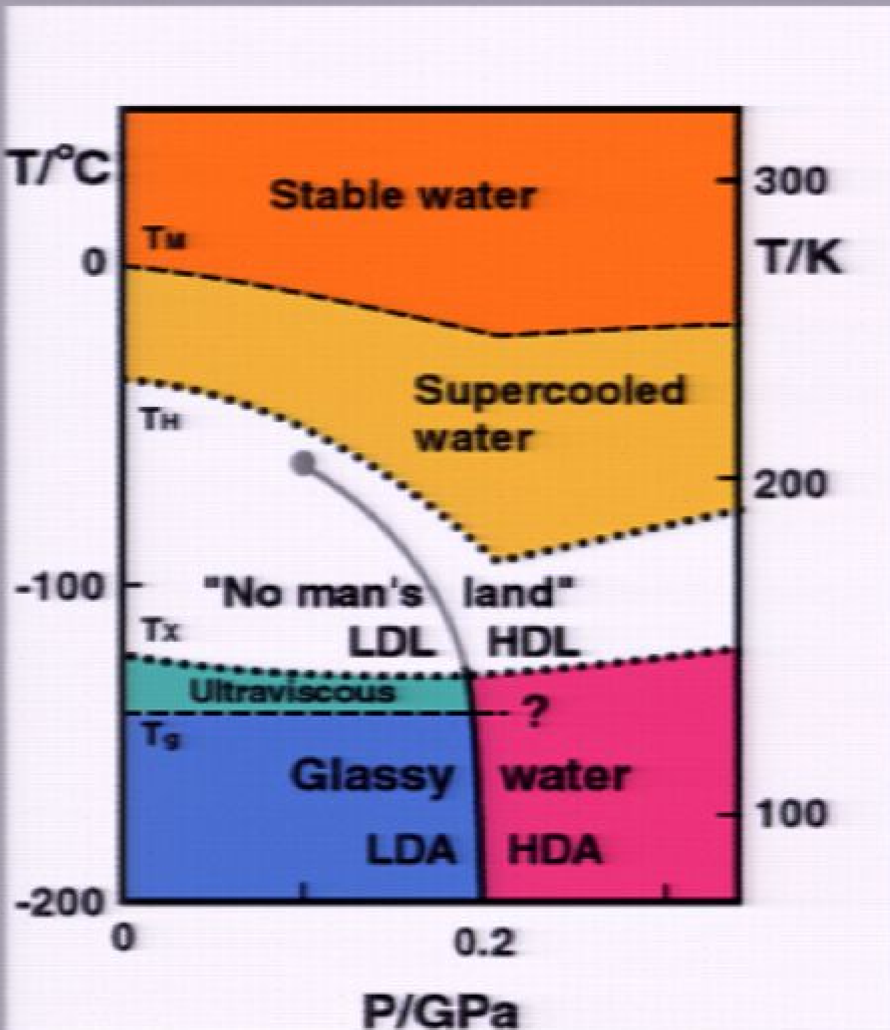
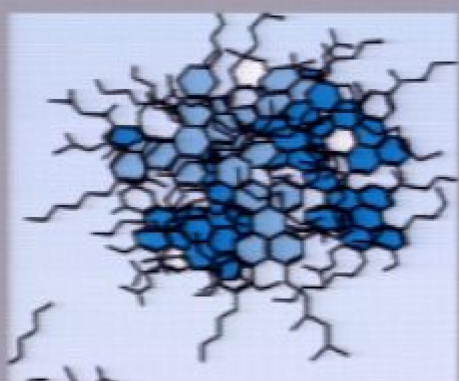
Two examples: water and oil

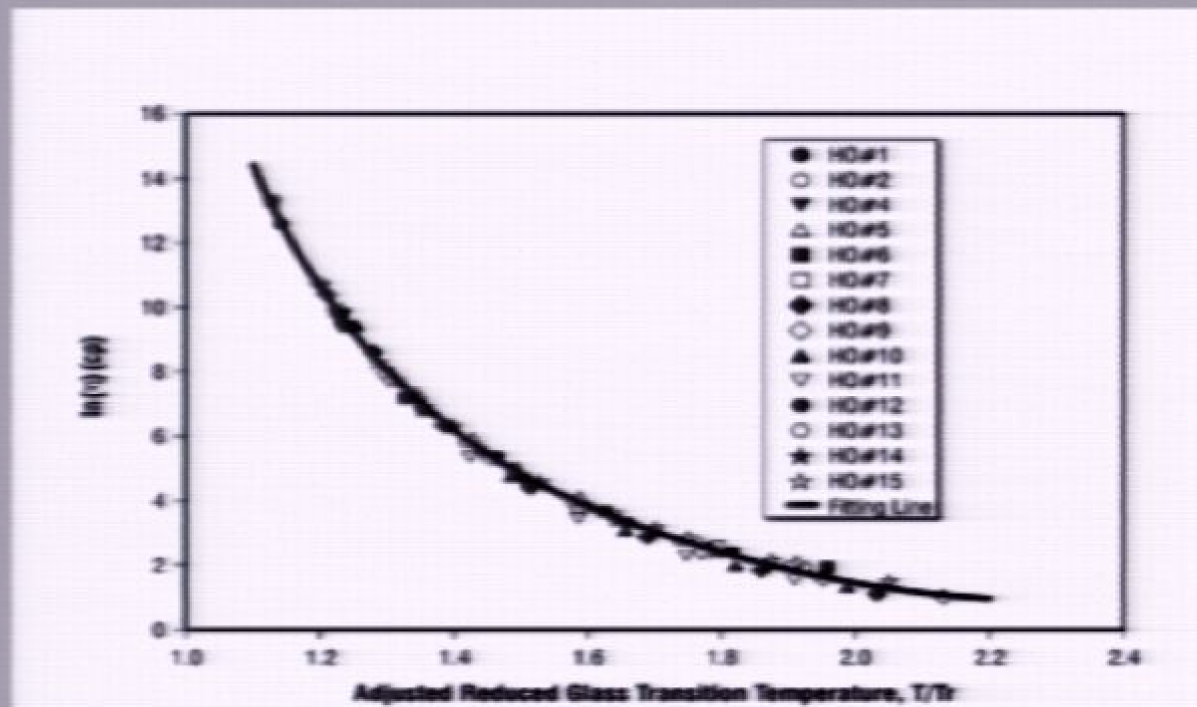


glassy H_2O

O. Mishima and H. E. Stanley; Nature (199

Heavy oils





eld Review (Schlumberger), summer 2007

Cheng and Kharrat, patent app. #20100043538

Universal properties of asphaltene viscocity (w/ D. Freed, Schlumberger Research)

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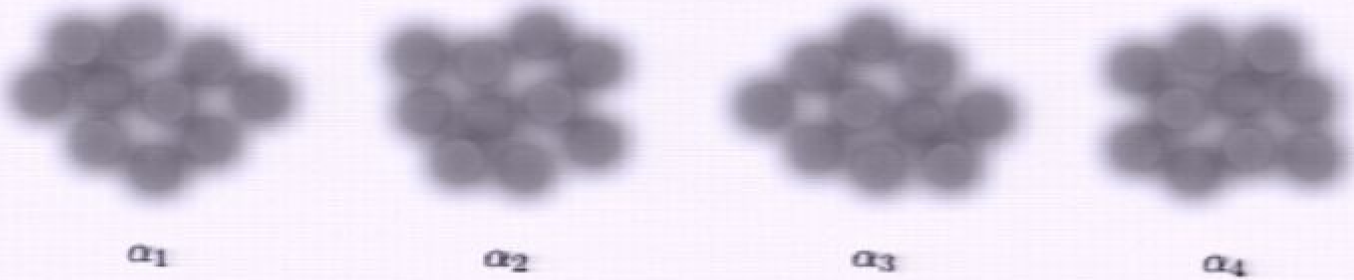

"Liquid"-like state of matter, with no local order parameter

Dynamic transition without an "apparent" thermodynamic transition

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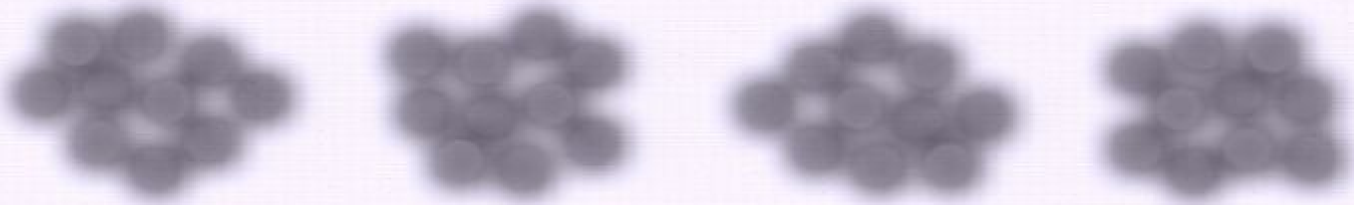

"Liquid"-like state of matter, with no local order parameter

Dynamic transition without an "apparent" thermodynamic transition

What does this mean??????

Markov processes

configurations $\{\mathcal{C}\}$ with energy $E_\mathcal{C}$ have probability $P_\mathcal{C}(t)$

$$\frac{d}{dt}P_\mathcal{C}(t) = \sum_{\mathcal{C}'} W_{\mathcal{C},\mathcal{C}'}\, P_{\mathcal{C}'}(t)$$

↑ transition matrix

prob. conservation: $W_{\mathcal{C},\mathcal{C}} = -\sum_{\mathcal{C}'\neq\mathcal{C}} W_{\mathcal{C},\mathcal{C}'}$

detailed balance: $W_{\mathcal{C},\mathcal{C}'}\, e^{-E_\mathcal{C}/T} = W_{\mathcal{C}',\mathcal{C}}\, e^{-E_{\mathcal{C}'}/T}$

⇨ $P_\mathcal{C}^{\text{eq}}(t) = \frac{1}{Z}\, e^{-\frac{E_\mathcal{C}}{T}}$ is a null right eigenvector of W: $\sum_{\mathcal{C}'} W_{\mathcal{C},\mathcal{C}'}\, P_{\mathcal{C}'}^{\text{eq}}(t) = 0$

⇨ (in a finite system) all other eigenvalues $-\epsilon_n$ are negative

$$\epsilon_0 = 0 < \epsilon_1 < \epsilon_2 < \ldots \qquad \Rightarrow \quad \text{equilibration} \quad e^{-\epsilon_{n\neq 0} t} \to 0$$

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/iewed as a quantum mechanical problem

- symmetrize W by a similarity transformation

Felderhof, Reports Math. Phys. **1**, 215 (1970)

$$H_{\mathcal{C},\mathcal{C}'} \equiv -e^{\beta E_{\mathcal{C}}/2}\, W_{\mathcal{C},\mathcal{C}'}\, e^{-\beta E_{\mathcal{C}'}/2}$$

- quantum mechanical interpretation $H_{\mathcal{C},\mathcal{C}'} \equiv \langle \mathcal{C}|\hat{H}|\mathcal{C}'\rangle$

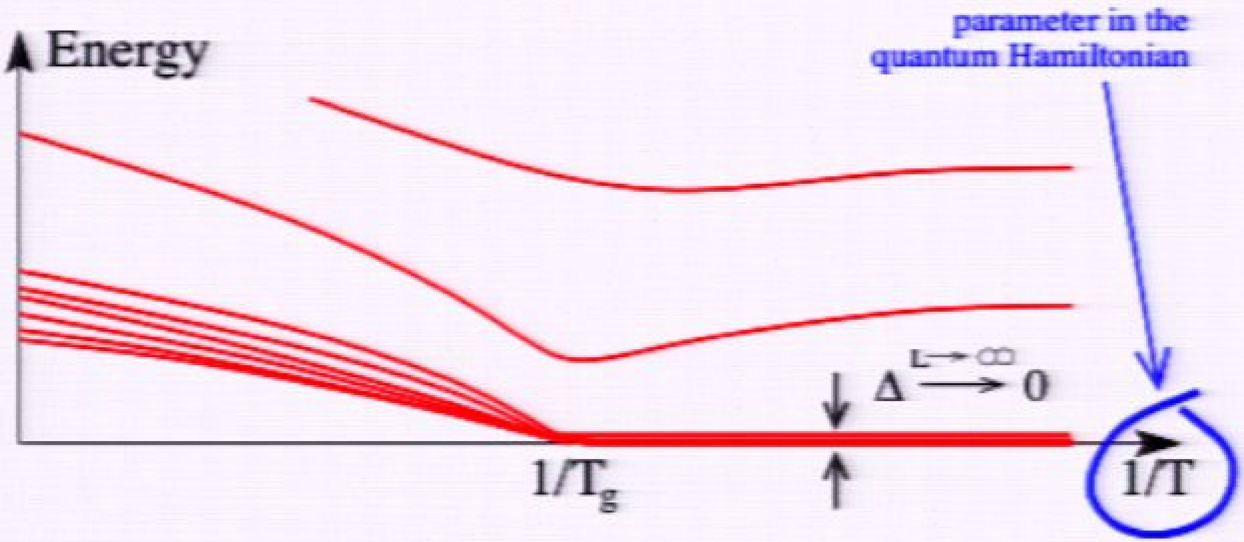
Kivelson, Rokhsar, Sethna, Phys. Rev. B **35**, 8865 (1987);
Henley, J. Phys. C **16**, S891 (2004);
Ardonne, Fendley, Fradkin, Ann. Phys. (NY) **310**, 493 (2004);
Castelnovo, Chamon, Mudry, and Pujol, Ann. Phys. (N.Y.) **318**, 316 (2005)

$$\hat{H} = \sum_{\mathcal{C},\mathcal{C}'} H_{\mathcal{C},\mathcal{C}'} \left[e^{\beta(E_{\mathcal{C}}-E_{\mathcal{C}'})/2}\, |\mathcal{C}\rangle\langle\mathcal{C}| - |\mathcal{C}\rangle\langle\mathcal{C}'| \right]$$

$$\hat{H}\,|\psi_n\rangle = \epsilon_n\,|\psi_n\rangle \qquad \epsilon_0 = 0 < \epsilon_1 < \epsilon_2 < \dots$$

$$|\psi_0\rangle = \frac{1}{\sqrt{Z}} \sum_{\mathcal{C}} e^{-\beta E_{\mathcal{C}}/2}\, |\mathcal{C}\rangle$$

Quantum mechanical perspective - transition



- local energy E_C + local dynamics ⇒ local Hamiltonian
- the dynamical classical problem reduces to a static zero-temperature quantum system
- at some 'critical' coupling Tg , a spectral collapse occurs
- understanding glassiness ⇔ understanding the collapse

Dynamical transition ⇔ quantum phase transition

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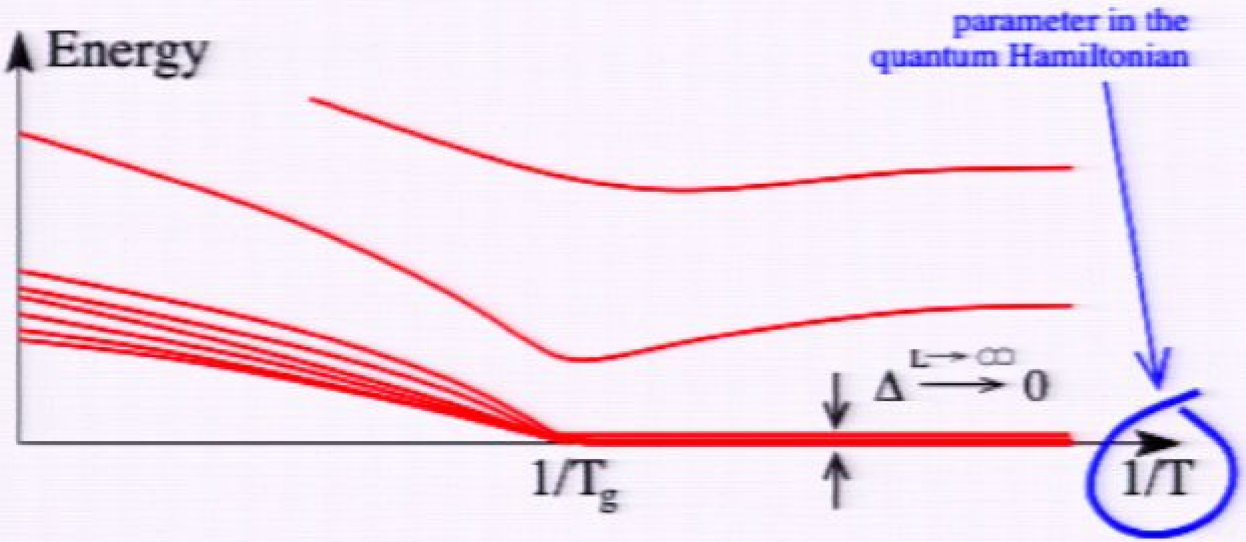

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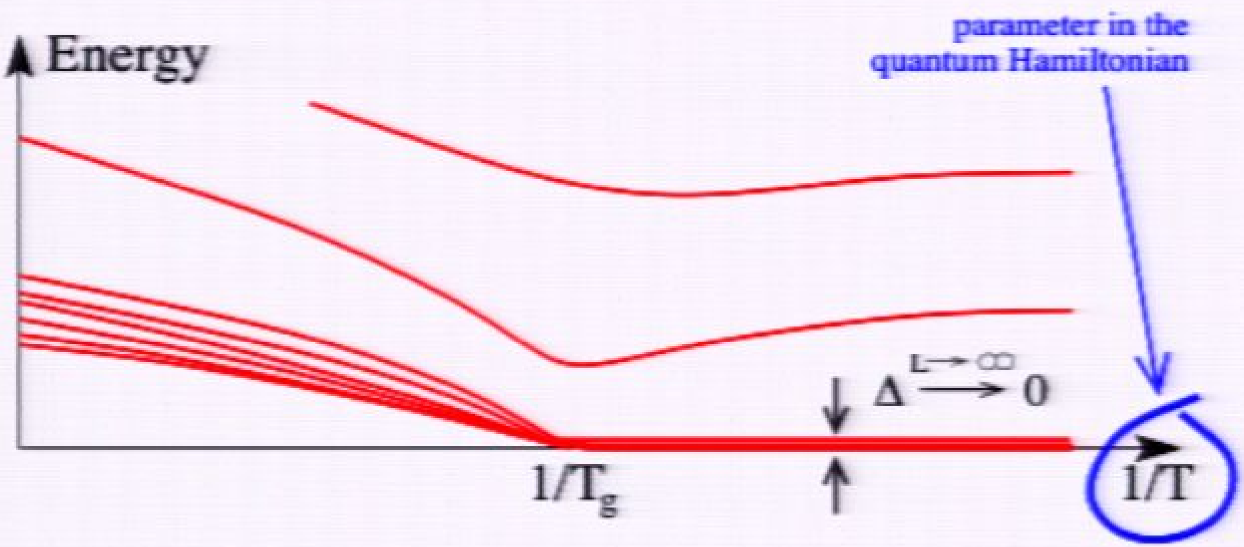

$\Delta \sim \mathcal{O}(L^a)$

vs.

$\Delta \sim \mathcal{O}(e^{L^b})$

Nature is a computer!

Nature's algorithms for glasses fail to converge in observable times

- local energy E_C + local dynamics ⇒ local Hamiltonian
- the dynamical classical problem reduces to a static zero-temperature quantum system
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- understanding glassiness ⇔ understanding the collapse

Dynamical transition ⇔ quantum phase transition

Quantum mechanical perspective - transition (cont.)

Edwards-Anderson order parameter

$$C_c(\tau) \equiv \langle \mathcal{O}(t+\tau)\,\mathcal{O}(t)\rangle_{\text{th}} - \langle \mathcal{O}\rangle_{\text{th}}^2$$
$$= \sum_{n\neq 0} e^{-\varepsilon_n \tau} \left|\langle n|\hat{\mathcal{O}}|0\rangle\right|^2$$
$$\equiv C_c^{\text{quant}}(\tau).$$

$$q_{\text{EA}}(\mathcal{O}) = \sum_{n\in\mathcal{D}, n\neq 0} \left|\langle n|\hat{\mathcal{O}}|0\rangle\right|^2$$

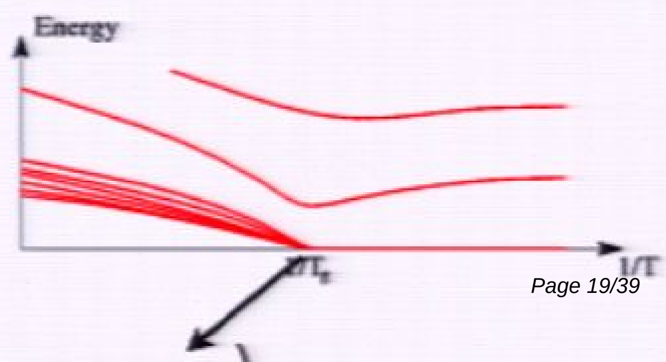
degenerate manifold

$$\chi^{\text{loc}}(\omega = 0) \equiv \int_0^\infty d\tau\, C_c^{\text{quant}}(\tau) = \sum_{n\neq 0} \frac{\left|\langle n|\hat{\mathcal{O}}|0\rangle\right|^2}{\varepsilon_n}.$$

local static (zero-frequency) susceptibility of the quantum system at zero temperature

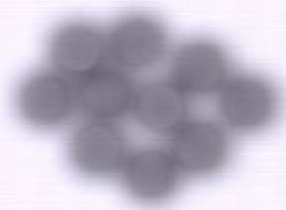
$$\hat{H}(\beta,\lambda) = \hat{H}(\beta)\ +\lambda\hat{O}$$

not classical field
(local change in H is not local in E)



Fidelity

absence of local order parameter



fidelity susceptibility $\chi_{\mathcal{F}}(\beta) \equiv \lim_{\delta\beta\to 0}\left[-2\frac{\ln \mathcal{F}(\beta,\delta\beta)}{\delta\beta^2}\right].$

ardi and Paunkovic
E (2006)

where $\mathcal{F}(\beta,\delta\beta) \equiv \langle\psi_0(\beta-\delta\beta/2)\,|\,\psi_0(\beta+\delta\beta/2)\rangle,$

he particular case when $|\psi_0(\beta)\rangle = \frac{1}{\sqrt{Z}}\sum_{C} e^{-\beta E_C/2}\,|C\rangle$

$$\Rightarrow \quad \begin{aligned} \chi_{\mathcal{F}}(\beta) &= \frac{1}{4}\frac{d^2}{d\beta^2}\ln Z(\beta) \\ &= \frac{1}{4\beta^2}C_V(\beta), \end{aligned}$$

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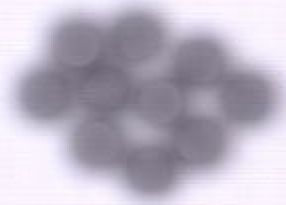

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C A A

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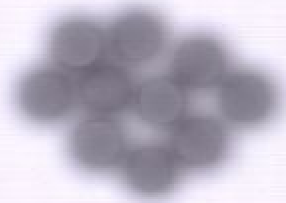

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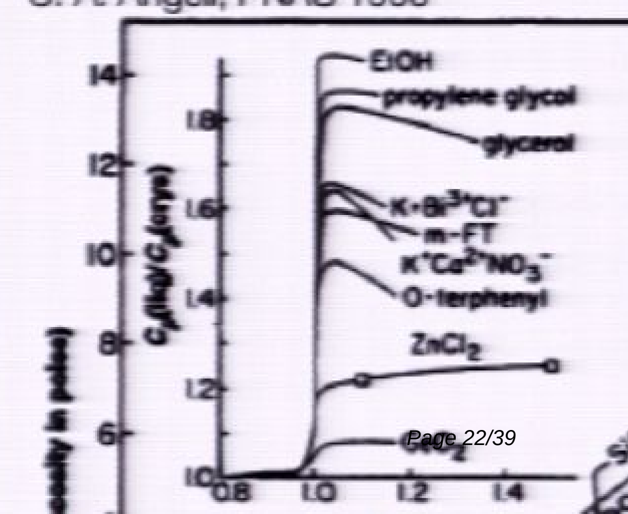
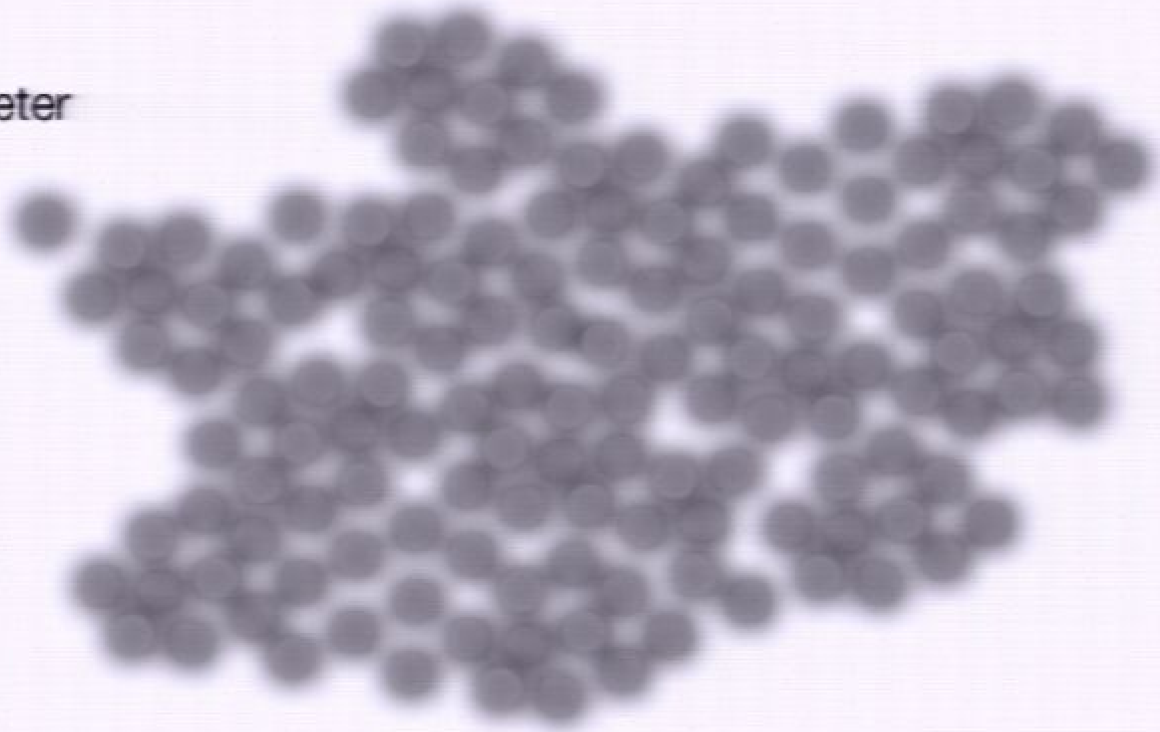
C. A. Angell, PNAS 1995



Entanglement

absence of local order parameter



entanglement entropy

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absence of local order parameter

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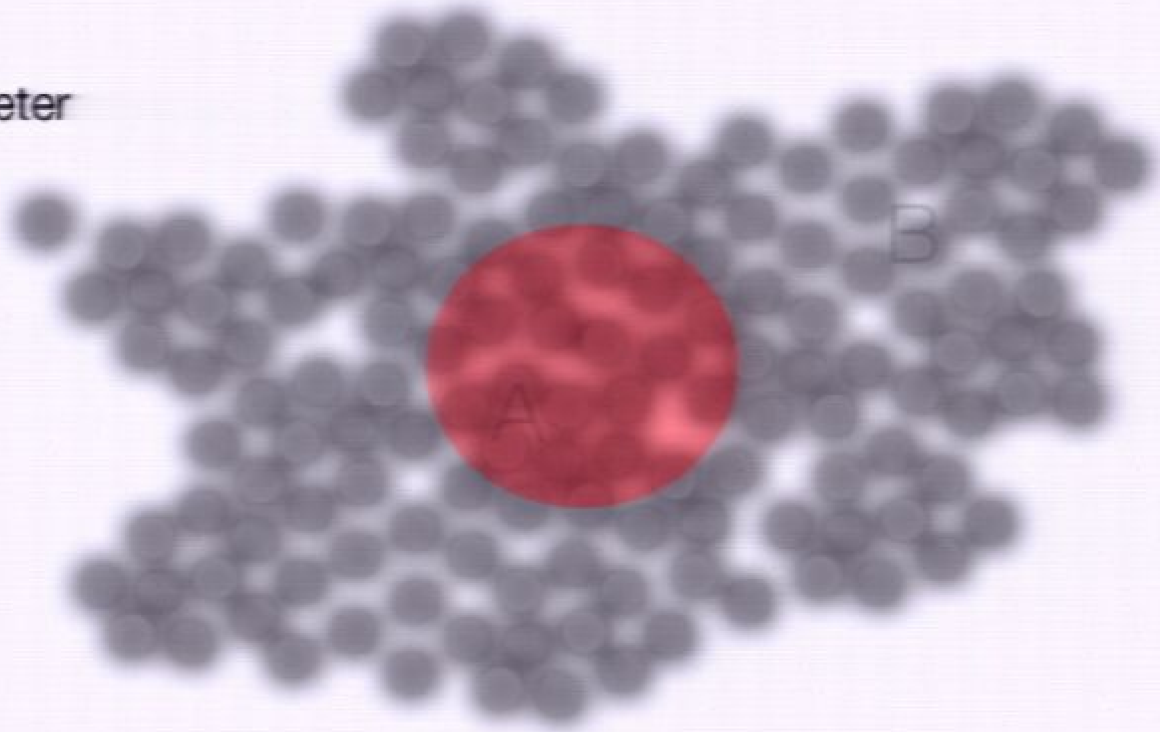

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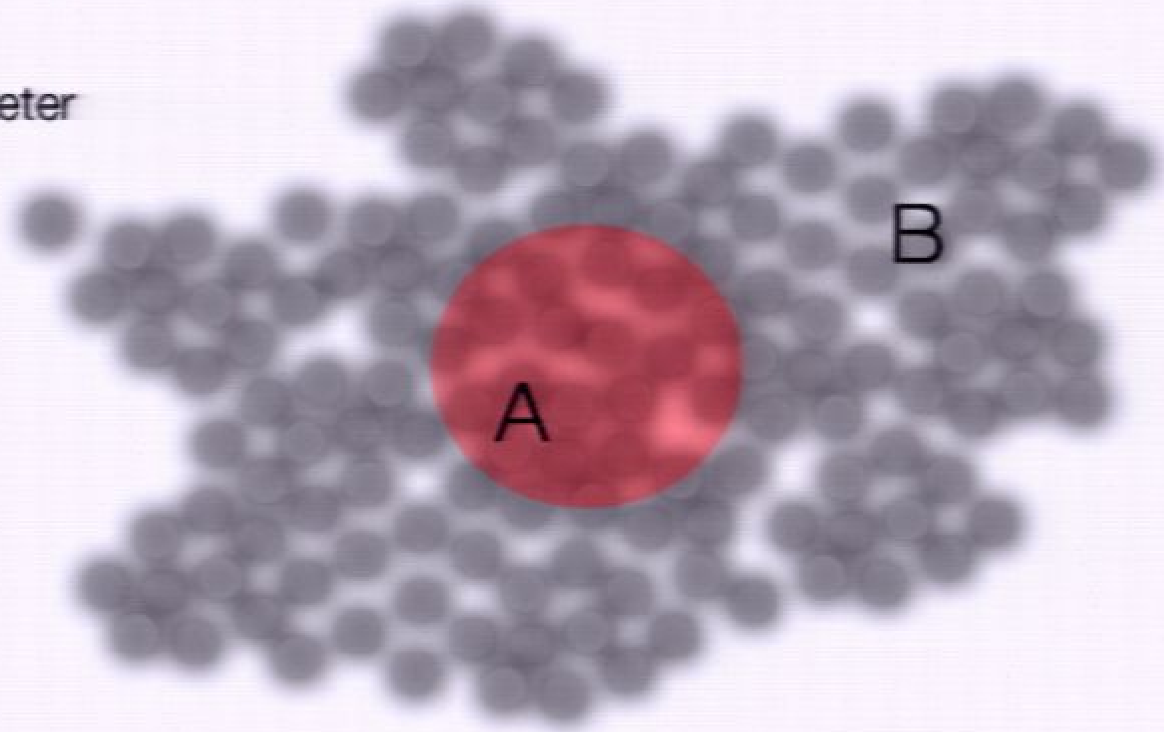

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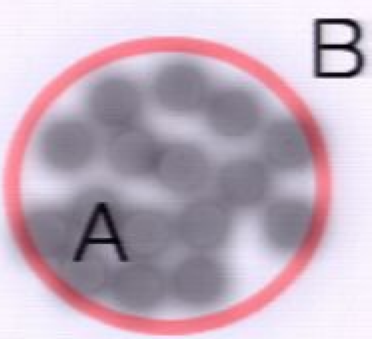

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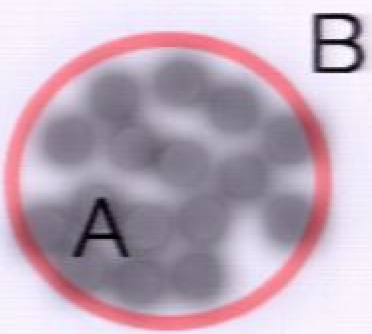
Entanglement II



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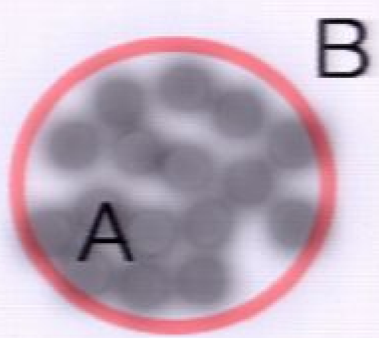
$$\beta F_{A,B} = -\ln Z_D^{A,B} \quad \text{and} \quad \beta F_{A\cup B} = -\ln Z$$

Fradkin and Moore, Phys. Rev. Lett. **97**, 050404 (2006)
Castelnovo and Chamon, Phys. Rev. B **76**, 174416 (2007)

Entanglement III



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boundary energy cumulants measure of heat capacity

$$\begin{aligned}
\Delta F_A &= -\frac{1}{\beta}\ln\frac{Z_D^A}{Z_F^A} \\
&\approx -\frac{1}{\beta}\ln\left[\frac{\sum_{i=1}^{\mathcal{N}} e^{-\beta E_{\alpha_i}}}{\mathcal{N}}\right] \\
&\approx E^*_{\partial} - \frac{1}{\beta}\ln\left[\frac{(\mathcal{N}-1) + e^{\beta\Delta E}}{\mathcal{N}}\right] \\
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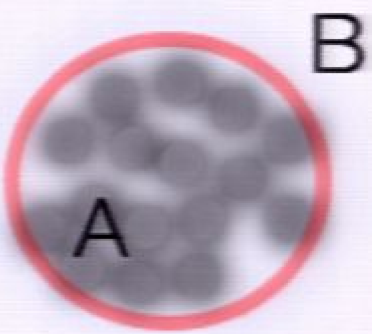
Bouchaud and Biroli, J. Chem. Phys. **121**, 7347 (2004)

if there are $\mathcal{N}$ metastable states in A, one is favored by the boundary condition and has ΔE less energy

Entanglement II



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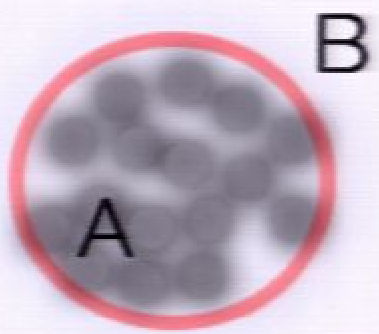

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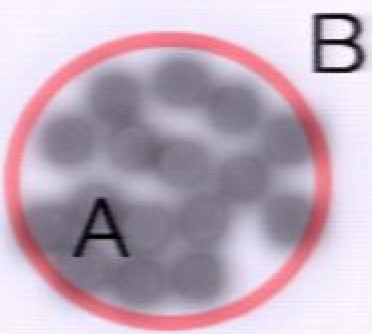

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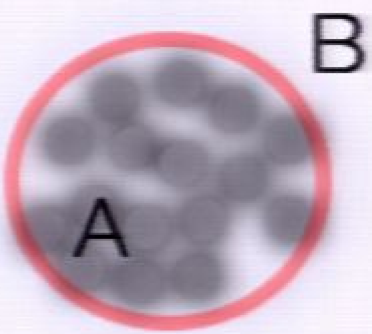


$$S_{AB}(\beta) = \beta\left(\Delta F_A + \Delta F_B\right) + S^F_{AB}(\beta)$$

$$\Delta F_{A,B} \equiv -\frac{1}{\beta}\ln\frac{Z_D^{A,B}}{Z_F^{A,B}}$$

$$S^F_{AB}(\beta) = \ln\langle e^{\beta\left(E^\partial - \langle E^\partial\rangle_{\mathrm{th}}\right)}\rangle_{\mathrm{th}}$$

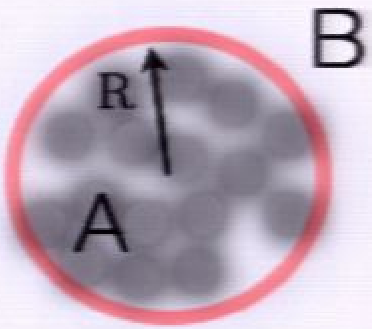
boundary energy cumulants
measure of heat capacity

$$\begin{aligned}
\Delta F_A &= -\frac{1}{\beta}\ln\frac{Z_D^A}{Z_F^A} \\
&\approx -\frac{1}{\beta}\ln\left[\frac{\sum_{i=1}^{\mathcal{N}} e^{-\beta E_{\alpha_i}}}{\mathcal{N}}\right] \\
&\approx E^*_\partial - \frac{1}{\beta}\ln\left[\frac{(\mathcal{N}-1) + e^{\beta\Delta E}}{\mathcal{N}}\right] \\
&\approx E^*_\partial - \frac{1}{\beta}\ln\left[1 + e^{\beta\Delta E - S^*}\right]
\end{aligned}$$

Bouchaud and Biroli, J. Chem. Phys. **121**, 7347 (2004)

if there are $\mathcal{N}$ metastable states in A, one is favored by the boundary condition and has ΔE less energy

Entanglement IV



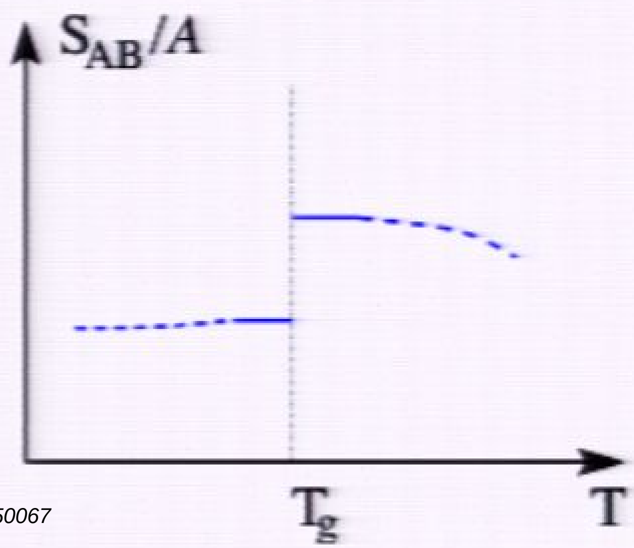
$$\Delta F_A \approx E^*_\partial - \frac{1}{\beta}\ln\left[1 + e^{\beta\Delta E - S^*}\right]$$

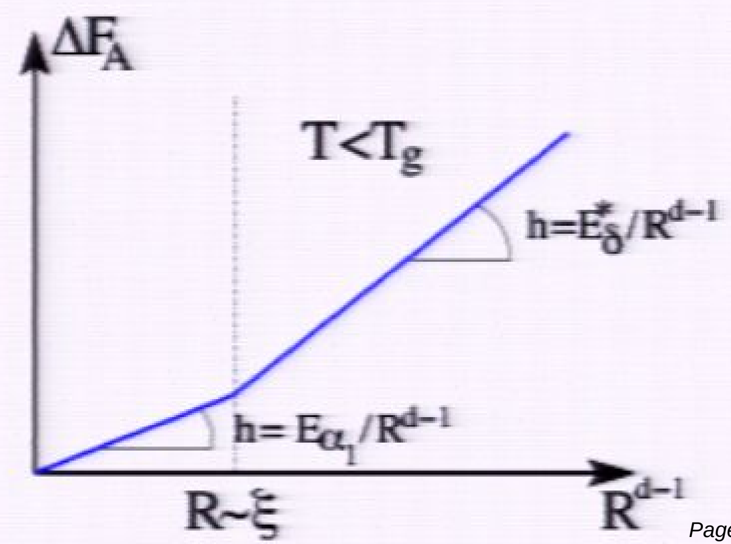
liquid $S^* \sim 1$

$$\Delta F_A \approx E^*_\partial - \Delta E$$

glass $S^* \sim R^d$

$$\Delta F_A \approx E^*_\partial$$



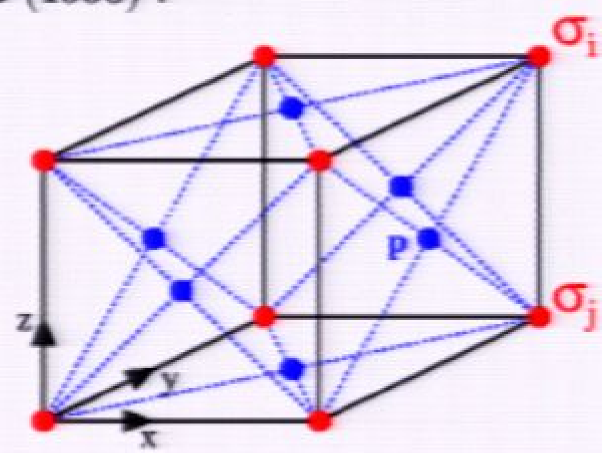


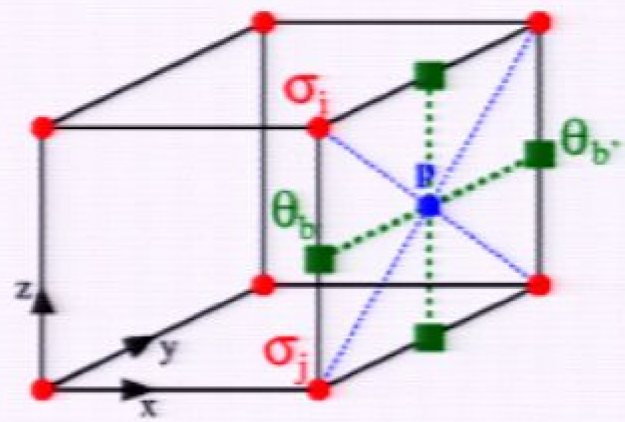
Exactly solvable model with hidden order with massive degeneracy

generalization of

Ambartzumian, Sukiasian, Savvidy and Savvidy, Phys. Lett. B (1992);
G. K. Savvidy and F.J. Wegner, NPB (1994);
Johnston and Malmini, Phys. Lett. B (1996) .

$$
\begin{aligned}
E &= -J_{xy} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}} \\
&\quad -J_{yz} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}} \\
&\quad -J_{zx} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}+\hat{\mathbf{x}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}} \,.
\end{aligned}
$$





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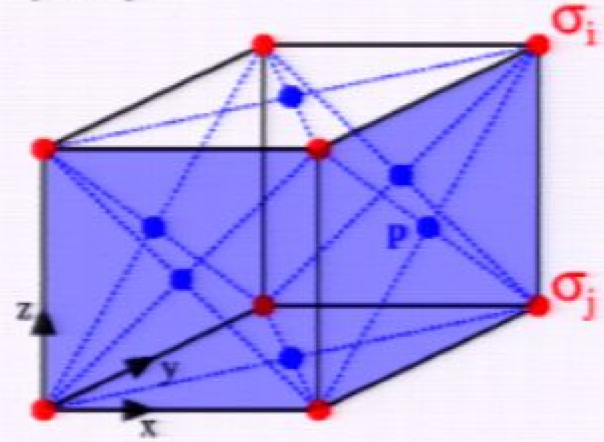
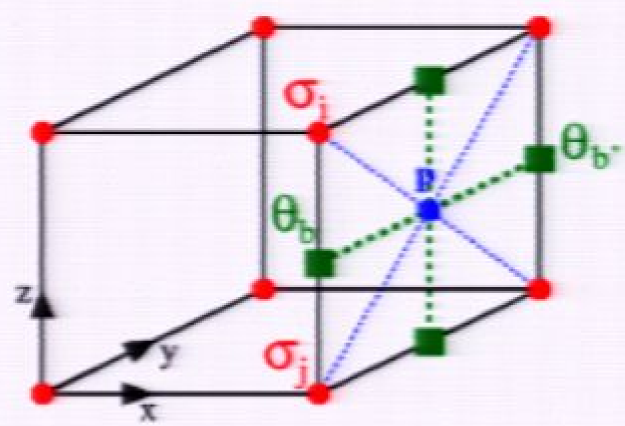
$$
\begin{aligned}
E \;=\; & -J_{xy}\sum_{\mathbf{i}} \sigma_{\mathbf{i}}\,\sigma_{\mathbf{i}+\hat{\mathbf{x}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{y}}} \\
& -J_{yz}\sum_{\mathbf{i}} \sigma_{\mathbf{i}}\,\sigma_{\mathbf{i}+\hat{\mathbf{y}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{z}}} \\
& -J_{zx}\sum_{\mathbf{i}} \sigma_{\mathbf{i}}\,\sigma_{\mathbf{i}+\hat{\mathbf{z}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{z}}+\hat{\mathbf{x}}}\,\sigma_{\mathbf{i}+\hat{\mathbf{x}}}\,.
\end{aligned}
$$



$$J_{yz} = J_{zx} = J \quad \text{and} \quad J_{xy} = 0$$



Exactly solvable model with hidden order with massive degeneracy

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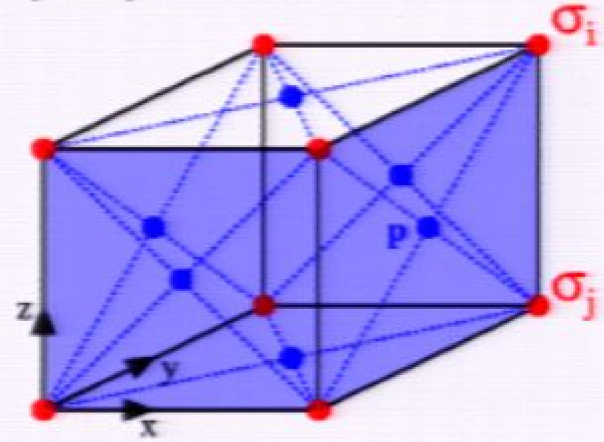
$$E = -J_{xy} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}}$$

$$-J_{yz} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}}$$

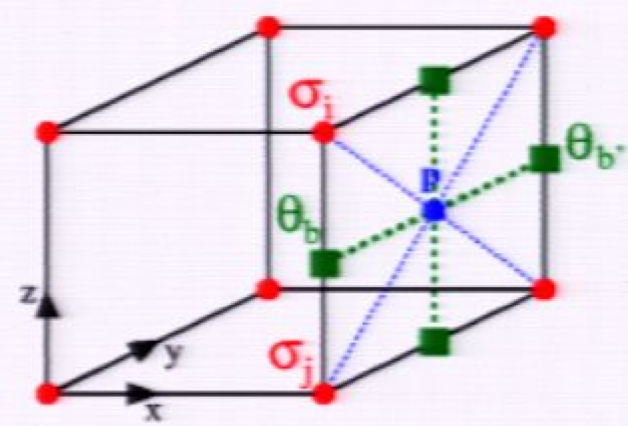
$$-J_{zx} \sum_{\mathbf{i}} \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}+\hat{\mathbf{x}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}} \,.$$



$$J_{yz} = J_{zx} = J \quad \text{and} \quad J_{xy} = 0$$

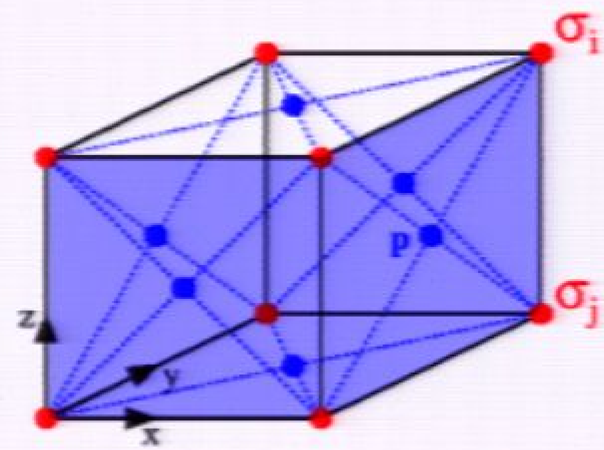
$$E = -J \sum_{\mathbf{b}} [\theta_{\mathbf{b}}\, \theta_{\mathbf{b}+\hat{\mathbf{x}}} + \theta_{\mathbf{b}}\, \theta_{\mathbf{b}+\hat{\mathbf{y}}}]$$

$$T_c = 2J/\log(1+\sqrt{2})$$



Exactly solvable model with hidden order with massive degeneracy II

$$
\begin{aligned}
E = \quad & -\sum_{\mathbf{i}} J^{\mathbf{i}}_{yz}\, \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{y}}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}} \\
& -\sum_{\mathbf{i}} J^{\mathbf{i}}_{zx}\, \sigma_{\mathbf{i}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{z}}+\hat{\mathbf{x}}}\, \sigma_{\mathbf{i}+\hat{\mathbf{x}}} \\
= \quad & -\sum_{\mathbf{b}} \left(J^{\mathbf{b}-\hat{\mathbf{z}}/2}_{zx}\, \theta_{\mathbf{b}}\, \theta_{\mathbf{b}+\hat{\mathbf{x}}} + J^{\mathbf{b}-\hat{\mathbf{z}}/2}_{yz}\, \theta_{\mathbf{b}}\, \theta_{\mathbf{b}+\hat{\mathbf{y}}} \right)
\end{aligned}
$$



$J^{\mathbf{i}}_{zx}$ and $J^{\mathbf{i}}_{yz}$ dynamical

$J^{\mathbf{i}}_{zx} = \pm J$ and $J^{\mathbf{i}}_{yz} = \pm J$, "gaugeable": $J^{\mathbf{i}}_{zx}\, J^{\mathbf{i}+\hat{\mathbf{x}}}_{yz}\, J^{\mathbf{i}+\hat{\mathbf{y}}}_{zx}\, J^{\mathbf{i}}_{yz} = J^4$

nonlocal order: string operator of J's and 2 σ's

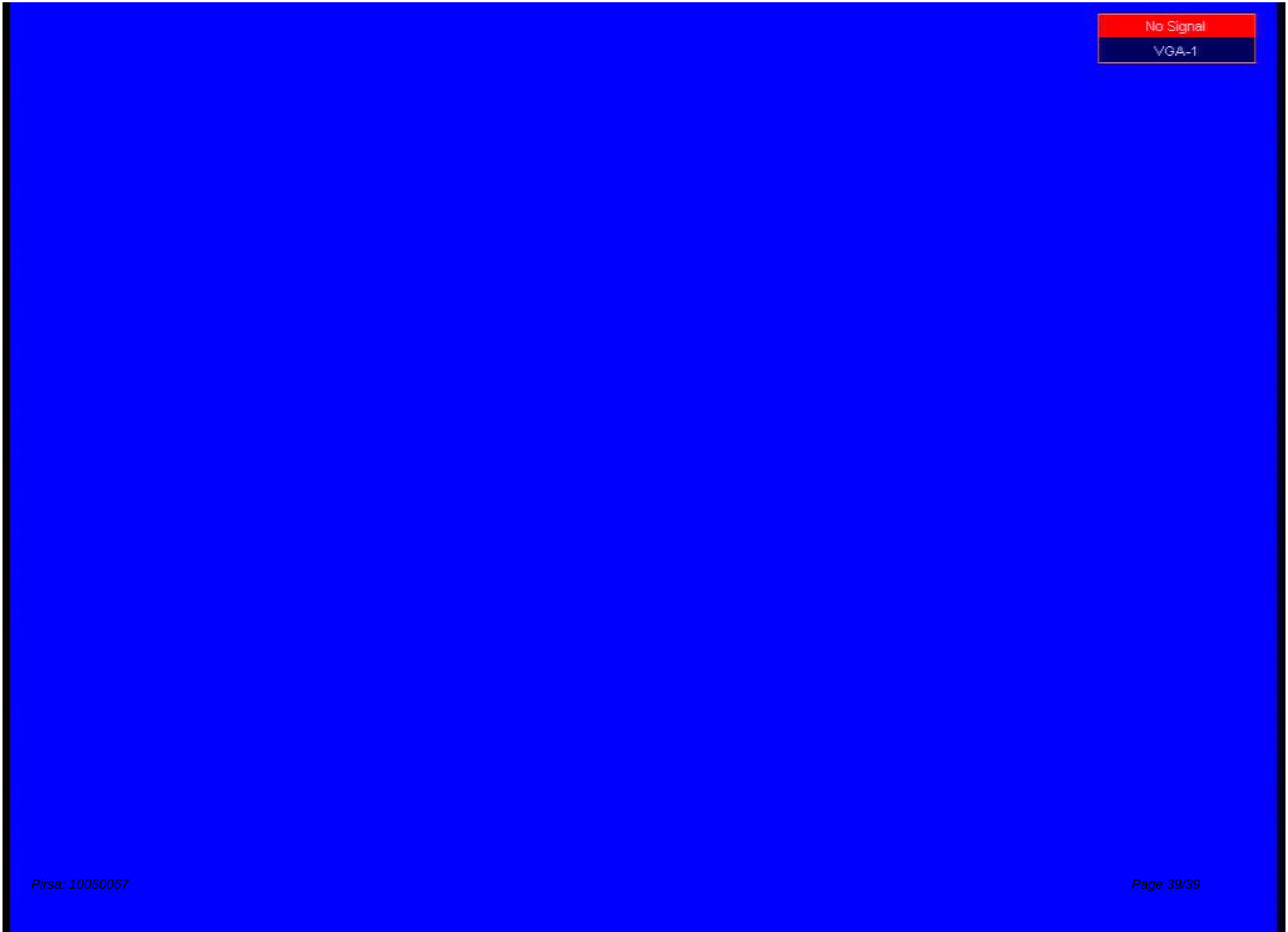
$$\langle J \;\; J\, J \ldots J\, J\, J\, J\, \sigma\, \sigma \rangle$$

Summary: a quantum mechanical and information viewpoint of the glass transition

- A "dynamical" transition has a precise meaning as a quantum phase transition of the mapped system, with a spectral collapse at a critical coupling (temperature)
- A static transition accompanies the dynamical one: we claim there is a true thermodynamical glass transition.
- "Absence" of local order parameter (glasses are spatially liquid like) does not imply lack of static signatures: fidelity is related to heat capacity singularity, and the area law coefficient of the entanglement entropy signals thermodynamic transition.
- Presented a solvable example with macroscopic number of minima, no disorder, and no local order parameter.

W. Anderson , in Science 17 March 1995

The deepest and most interesting unsolved problem in solid tate theory is probably the theory of the nature of glass and the lass transition. This could be the next breakthrough in the oming decade. The solution of the problem of spin glass in the te 1970s had broad implications in unexpected fields like neural etworks, computer algorithms, evolution, and computational omplexity. The solution of the more important and puzzling glass roblem may also have a substantial intellectual spin-off. Whether will help make better glass is questionable."


No Signal
VGA-1