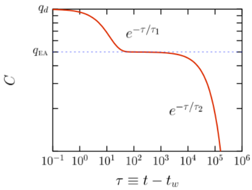
Quantum mechanical view on dynamical glass transitions



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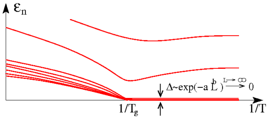
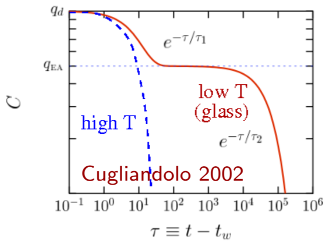


Open Statistical Physics, The Open University, Milton Keynes UK, March 10, 2010

Outline

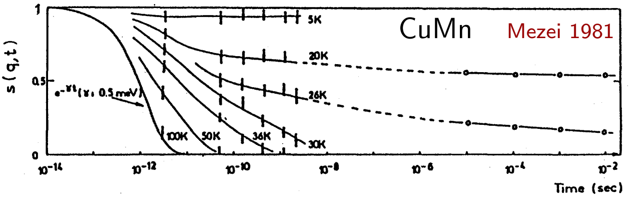
- (very!) brief overview of the salient features in glassy systems
- quantum mechanical perspective: what is it and why is it interesting?
  - classical dynamical transition
    $\Rightarrow$ static (zero-temperature) quantum transition
  - non-vanishing Edwards-Anderson order parameter
    $\Rightarrow$ divergent local susceptibility
  - quantum measures that do not require a priori knowledge of an order parameter (fidelity and entanglement)
- conclusions

Appearance of large relaxation time scales



Two-step decay in correlation functions

$$C_c(t, +\tau, t) \equiv \langle \mathcal{O}(t+\tau)\mathcal{O}(t)\rangle_{\rm th} - \langle \mathcal{O}(t)\rangle^2_{\rm th}$$



The dynamical glass transition (I)

How slow is slow?

- experimentally:

  viscosity larger than 10^{13} Poise

$$T < T_g$$
$$\Updownarrow$$
$$\log[\eta(T)] > 13$$

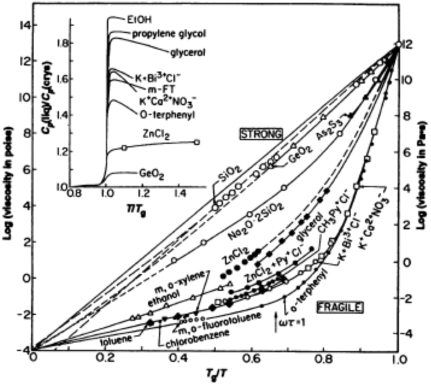
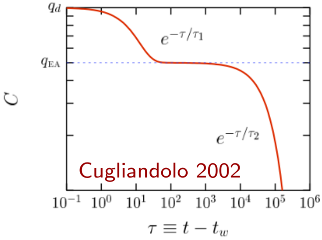


FIG. 3. T_g-scaled Arrhenius plots of viscosity data showing the "strong/fragile" pattern of liquid behavior on which the liquids classification of the same name is based. (*Inset*) The jump in heat capacity at T_g is generally large for the fragile liquids and small for strong liquids, though there are a number of exceptions to this generalization, particularly when hydrogen bonding is present. (Reproduced from ref. 29.)

The dynamical glass transition (II)

How slow is slow?

- theoretically: is there a finite region in parameter space where the time scales actually *diverge*? (e.g., for $T < T_g$, $\exists T_g > 0$)



$$C_c(t, +\tau, t) \equiv \langle \mathcal{O}(t+\tau)\mathcal{O}(t)\rangle_{\mathrm{th}} - \langle \mathcal{O}(t)\rangle_{\mathrm{th}}^2$$

$$q_{\mathrm{EA}}(\mathcal{O}) \equiv \lim_{\tau\to\infty} \lim_{t\to\infty} C_c(t, +\tau, t)$$

Open issues

- how do glass transitions compare to thermodynamic ones? no (local) order parameter
- do concepts like scaling and universality apply?
- there is evidence in support of a divergent dynamical length scale at T_g – what about singularities in the free energy?

quantum mechanical perspective

- ‘unifies’ space and time into a static quantum mechanical system at zero temperature
- provides new angles to investigate dynamical phenomena (e.g., fidelity and entanglement measures not based on an order parameter)

Markov processes with detailed balance (I)

configs: $\{\mathcal{C}\}$, energy $E_\mathcal{C}$

$$P_\mathcal{C}^{(\mathrm{eq})} = \frac{e^{-\beta E_\mathcal{C}}}{Z} \qquad Z = \sum_\mathcal{C} e^{-\beta E_\mathcal{C}} \qquad \left(\beta = \frac{1}{k_B T}\right)$$

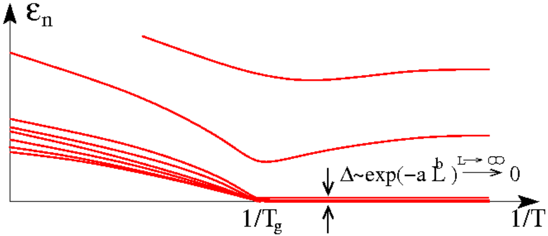
$$\frac{d}{dt} P_\mathcal{C}(t) = \sum_{\mathcal{C}'} W_{\mathcal{C},\mathcal{C}'} P_{\mathcal{C}'}(t) \qquad W_{\mathcal{C},\mathcal{C}'} e^{-\beta E_\mathcal{C}} = W_{\mathcal{C}',\mathcal{C}} e^{-\beta E_{\mathcal{C}'}}$$

- $P^{(\mathrm{eq})}$ is the *null* right eigenvector of W: $\sum_{\mathcal{C}'} W_{\mathcal{C},\mathcal{C}'} P_{\mathcal{C}'}^{(\mathrm{eq})} = 0$
  $\rightarrow$ no decay
- (in a *finite* system) all other eigenvalues $-\varepsilon_n$ are negative, $\varepsilon_0 = 0 < \varepsilon_1 < \varepsilon_2 < \dots$
  $\rightarrow$ exponential decay $\sim e^{-\varepsilon_n t}$

Markov processes with detailed balance (II)

- fixed system size $\Rightarrow$ possibly slow ($\varepsilon_n \ll 1$), but ultimately exponential decay
- glass transition $\Rightarrow$ $\lim_{L\to\infty} \varepsilon_n = 0, \quad \exists\, n$

(*not sufficient*: 2D Ising model)



discrete systems without conserved quantities

understanding a glass transition $\Longleftrightarrow$ understanding the nature of the collapsing relaxation rates

QM perspective: what and why (I)

- symmetrise W by similarity transformation Felderhof 1970

$$H_{\mathcal{C},\mathcal{C}'} \equiv -\exp\left(\beta E_{\mathcal{C}}/2\right) W_{\mathcal{C},\mathcal{C}'} \exp\left(-\beta E_{\mathcal{C}'}/2\right)$$

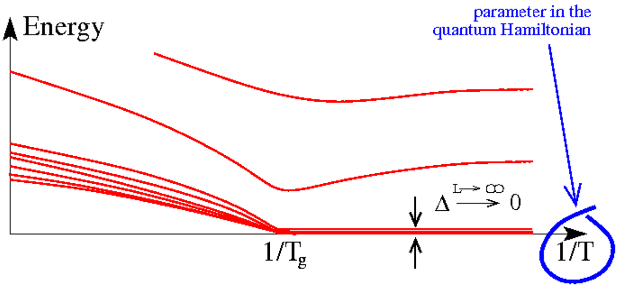
- quantum mechanical interpretation $\langle \mathcal{C}|\hat{H}|\mathcal{C}'\rangle \equiv H_{\mathcal{C},\mathcal{C}'}$:

  Rokhsar + Kivelson 1998; Henley 2004; Castelnovo *et al.* 2005-2006

$$\hat{H}\,|\psi_n\rangle = \varepsilon_n|\psi_n\rangle \qquad \varepsilon_0 = 0 < \varepsilon_1 < \varepsilon_2 < \ldots$$

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

QM perspective: what and why (II)



- *local* energy $E_{\mathcal{C}}$ + *local* dynamics $\Rightarrow$ *local* Hamiltonian
- the dynamical classical problem reduces to a static zero-temperature quantum system
- at some 'critical' coupling T_g, a spectral collapse occurs
- understanding glassiness $\Leftrightarrow$ understanding the collapse

What happens at T_g? (I)

the gap closes: is it a quantum phase transition?

- take $\mathcal{O}$ such that $q_{\mathrm{EA}}(\mathcal{O}) \neq 0$ for $T < T_g$
- classical $\mathcal{O} \to$ quantum operator $\hat{\mathcal{O}} \equiv \sum_{\mathcal{C}} |\mathcal{C}\rangle \mathcal{O}_{\mathcal{C}} \langle \mathcal{C}|$
- we can write correlators $C(t+\tau, t)$ and $q_{\mathrm{EA}}(\mathcal{O})$ in the quantum mechanical language

$$C(t+\tau, t) = \sum_n e^{-\varepsilon_n \tau} \langle \psi_0 | \hat{S}^{-1} \hat{\mathcal{O}} \hat{S} | \psi_n \rangle \langle \psi_n | \hat{S}^{-1} \hat{\mathcal{O}} | P(t) \rangle$$

$$C_c(\tau) = \lim_{t \to \infty} C(t+\tau, t) = \sum_{n \neq 0} e^{-\varepsilon_n \tau} \left| \langle \psi_n | \hat{\mathcal{O}} | \psi_0 \rangle \right|^2$$

$$q_{\mathrm{EA}}(\mathcal{O}) = \lim_{\tau \to \infty} C_c(\tau) = \sum_{n \in \mathcal{D}, n \neq 0} \left| \langle \psi_n | \hat{\mathcal{O}} | \psi_0 \rangle \right|^2$$

What happens at T_g? (II)

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

$$\hat{H}'(\beta,\lambda) = \hat{H}(\beta) + \lambda\hat{\mathcal{O}} \qquad (\neq \text{classical field})$$

$$\chi^{\text{loc}}(\omega=0) \equiv \int_0^\infty d\tau\, C_c(\tau) = \sum_{n\neq 0} \frac{\left|\langle\psi_n|\hat{\mathcal{O}}|\psi_0\rangle\right|^2}{\varepsilon_n}$$

At $T = T_g$, $q_{\text{EA}} = \lim_{\tau\to\infty} C_c(\tau)$ becomes finite, and $\chi^{\text{loc}}(\omega=0)$ diverges

Fidelity susceptibility

quantum measure <u>not</u> based on an order parameter!

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

new tools to study the dynamical transitions as QPTs:

fidelity — Zanardi *et al.* 2007

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

fidelity susceptibility — Zanardi *et al.* 2007, You *et al.* 2007

$$\chi_{\mathcal{F}}(\beta) \equiv \lim_{\delta\beta \to 0} \left[-2 \frac{\ln \mathcal{F}(\beta, \delta\beta)}{\delta\beta^2} \right] = \frac{1}{4\beta^2} C_V(\beta)$$

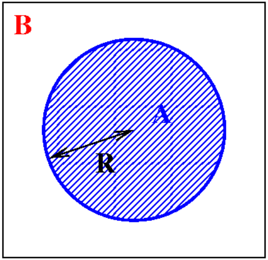
Castelnovo, Chamon, Sherrington

local Hamiltonian + closing of a gap $\longrightarrow$ singularity in $\chi_{\mathcal{F}}(\beta)$

specific heat singularity expected at a (local) glass transition!

Von Neumann entanglement entropy (I)

given the ground state density matrix $\rho = |\psi_0\rangle\langle\psi_0|$, and a bipartition (A, B)



$$\rho_A = \mathrm{Tr}_B\, \rho$$

$$S_{AB} = -\mathrm{Tr}\left[\rho_A \log \rho_A\right] = \alpha L^d + \ldots$$

$$\Longrightarrow \qquad S_{AB}(T) = \Delta F_A(T) + \Delta F_B(T) + S^F_{AB}(T)$$

$$\Delta F_A(T) = -T \ln\left(\frac{Z^D_A}{Z^F_A}\right)$$

$$S^F_{AB}(T) = \ln\left\langle \exp(E^\delta/T)\right\rangle_{\mathrm{th}} - \left\langle E^\delta\right\rangle_{\mathrm{th}}/T$$

Von Neumann entanglement entropy (II)

focus on $\Delta F_A(T) \sim \ln[Z_A^D / Z_A^F]$

- above T_g: the system adapts to the fixed B.C. $\rightarrow \Delta F_A \sim E_\delta^*$
- below T_g: $\mathcal{N} > 1$ distinct free en. minima
  • one minimum preferred by the fixed B.C. ($E_\delta \simeq E_\delta^*$)
  • all others equally disfavoured ($E_\delta \simeq E_\delta^* + \Delta E$)

$$\Delta F_A \sim \ln\left(\frac{Z_A^D}{Z_A^F}\right) \sim \frac{E_\delta^*}{T} - \ln\left(e^{-\Delta E/T} + e^{-S^*}\right)$$

$$\Delta E \sim R^{d-1} \qquad S^* = \ln \mathcal{N} \sim R^d$$

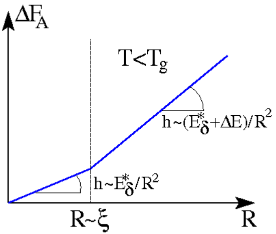
correlation length ξ identified by $\Delta E(R = \xi) \sim S^*(R = \xi)$

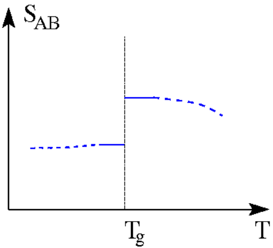
$$\begin{cases} R \ll \xi \\ \Delta F_A \sim E_\delta^*/T + S^* \sim E_\delta^*/T \end{cases} \qquad \begin{cases} R \gg \xi \\ \Delta F_A \sim (E_\delta^* + \Delta E)/T \end{cases}$$

Von Neumann entanglement entropy (III)

$$\begin{cases} R \ll \xi \\ \Delta F_A \sim E_\delta^*/T + S^* \sim E_\delta^*/T \end{cases}$$

$$\begin{cases} R \gg \xi \\ \Delta F_A \sim (E_\delta^* + \Delta E)/T \end{cases}$$





classical argument: requires well-defined metastable states $\rightarrow$ dependent on separation of time scales

quantum entanglement: static + generic

Conclusions

dynamical glass transition $\Leftrightarrow$ *static quantum phase transition*

- massive collapse of eigenstates, divergent local susceptibility
- singularities in the fidelity susceptibility relate directly to the classical heat capacity
- entanglement entropy: static measure to detect glass transitions and growing correlation lengths
- cross-fertilisation between different areas of physics:
  - known glassy systems $\longrightarrow$ new exotic quantum Hamiltonians
  - 'unconventional' quantum systems devoid of local order (e.g., topological order) $\longrightarrow$ insight in glassiness