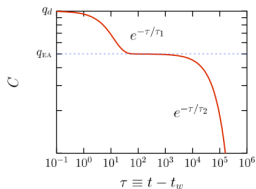


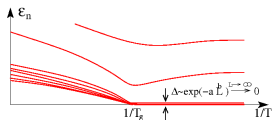
Quantum mechanical view on dynamical glass transitions



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EPSRC
Engineering and Physical Sciences
Research Council

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Outline

- ▶ (very!) brief overview of **classical glassy systems**
- ▶ **quantum mechanical perspective**: why is it interesting?
 - ▶ **classical dynamical transition**
 - ⇒ **static (zero-temperature) quantum transition**
 - ▶ quantum measures that do not require an order parameter:
 - ▶ **fidelity susceptibility** \Leftrightarrow **heat capacity**
 - ▶ **von Neumann entanglement entropy** \Leftrightarrow **detects glass transition and growing correlation length**
- ▶ analogies between **topological spin Hamiltonians** and **kinetically-constrained models**
- ▶ conclusions

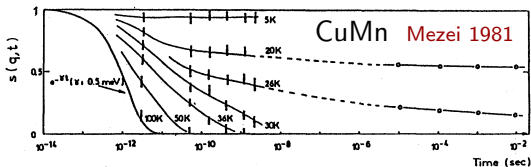
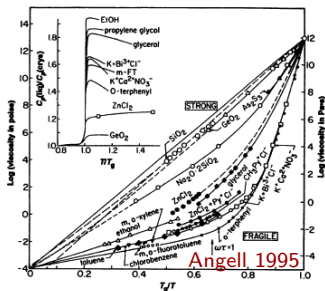
Classical glass transition

experimentally:

$T < T_g \Leftrightarrow$ viscosity
larger than 10^{13} Poise

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

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

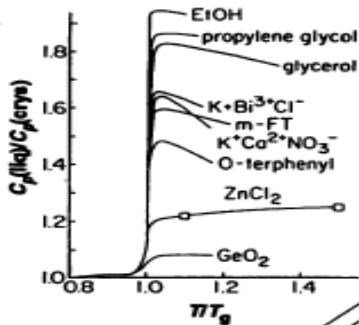


theoretically:

actual singularity
in the time scales
at $T = T_g$

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?



Open issues

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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: $\{C\}$, energy E_C

$$P_C^{(\text{eq})} = \frac{e^{-\beta E_C}}{Z} \quad Z = \sum_C e^{-\beta E_C} \quad \left(\beta = \frac{1}{k_B T} \right)$$

$$\frac{d}{dt} P_C(t) = \sum_{C' \neq C} \left[W_{C,C'} P_{C'}(t) - W_{C',C} P_C(t) \right]$$

$$W_{C,C'} e^{-\beta E_C} = W_{C',C} e^{-\beta E_{C'}}$$

$P^{(\text{eq})}$ is the *null right eigenvector* of W : $\sum_{C'} W_{C,C'} P_{C'}^{(\text{eq})} = 0$
 \rightarrow no decay

QM perspective (I)

- ▶ symmetrise W by similarity transformation

Felderhof 1970

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

- ▶ promote \mathcal{C} to orthonormal basis $|C\rangle$, $\langle C|C'\rangle = \delta_{CC'}$
- ▶ quantum mechanical interpretation $\langle C|\hat{H}|C'\rangle \equiv H_{C,C'}$:

Rokhsar + Kivelson 1998; Henley 2004

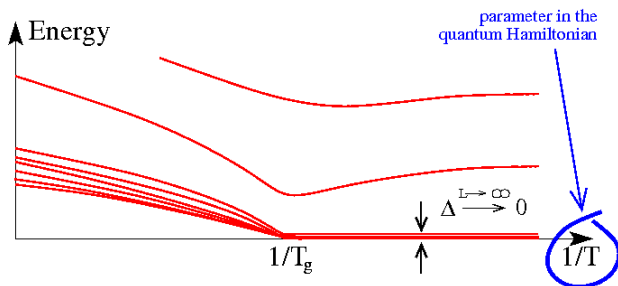
Ardonne *et al.* 2004; Castelnovo *et al.* 2005-2006

$$\hat{H} = \sum_{C \neq C'} w_{CC'} \left[e^{\beta(E_C - E_{C'})/2} |C\rangle \langle C| - |C\rangle \langle C'| \right]$$

$$\hat{H} |\psi_n\rangle = \varepsilon_n |\psi_n\rangle \quad \varepsilon_0 = 0 < \varepsilon_1 \leq \varepsilon_2 \leq \dots$$

$$|\psi_0\rangle = \frac{1}{\sqrt{Z}} \sum_C e^{-\beta E_C/2} |C\rangle \quad Z = \sum_C e^{-\beta E_C}$$

QM perspective (II)



- ▶ *local* energy E_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 ?

▶ details

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

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

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

Henley 2004

At $T = T_g$, $q_{\text{EA}} = \lim_{\tau \rightarrow \infty} C_c(\tau)$ becomes finite

$\Rightarrow \underline{\chi^{\text{loc}}(\omega = 0)}$ diverges

Fidelity susceptibility

quantum measure not based on an order parameter!

$$|\psi_0(\beta)\rangle = \sum_c \frac{e^{-\beta E_c/2}}{\sqrt{Z}} |C\rangle$$

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

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

Castelnuovo, Chamon, Sherrington 2010

local Hamiltonian + closing of a gap \longrightarrow singularity in $\chi_{\mathcal{F}}(\beta)$
specific heat singularity expected at a (local) glass transition!

Fidelity susceptibility

quantum measure not based on an order parameter!

$$|\psi_0(\beta)\rangle = \sum_c \frac{e^{-\beta E_c/2}}{\sqrt{Z}} |C\rangle$$

new tools to study the dynamical transitions of QDTs.

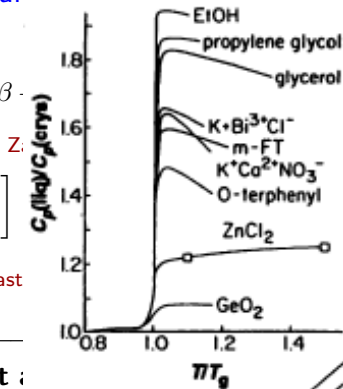
fidelity

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

fidelity susceptibility

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

local Hamiltonian + closing of a gap —
specific heat singularity expected at :

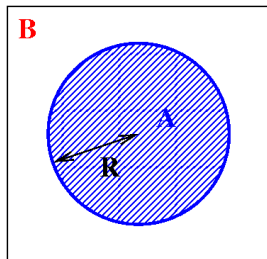


von Neumann entanglement entropy

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

$$\hat{\rho}_A = \text{Tr}_B \hat{\rho}$$

$$\begin{aligned} S_{AB} &= -\text{Tr} \left[\hat{\rho}_A \log \hat{\rho}_A \right] \\ &= \alpha L^{d-1} + \dots \end{aligned}$$



$$\hat{\rho}(\beta) = \frac{1}{Z(\beta)} \sum_{C, C'} e^{-\beta(E_C + E_{C'})/2} |C\rangle\langle C'|$$

$$\begin{aligned} \Rightarrow S_{AB}(T) &= \beta F_A + \beta F_B - \beta F_{A \cup B} + \beta \langle E^{\partial} \rangle_{\text{th}} \\ \beta F_{A, B} &= -\ln Z_D^{A, B} \quad \text{and} \quad \beta F_{A \cup B} = -\ln Z \end{aligned}$$

Fradkin, Moore 2006, Castelnovo, Chamon 2007

von Neumann entanglement entropy

Castelnovo, Chamon, Sherrington 2010

$$S_{AB}(T) = \beta \left[\Delta F_A(T) + \Delta F_B(T) \right] + S_{AB}^F(T)$$

$$\Delta F_A(T) = -\frac{1}{\beta} \ln \left(\frac{Z_A^D}{Z_A^F} \right)$$

$$S_{AB}^F(T) = \ln \left\langle \exp \left[\beta \left(E^\delta - \langle E^\delta \rangle_{\text{th}} \right) \right] \right\rangle_{\text{th}}$$

von Neumann entanglement entropy (I)

consider $S_{AB}^F(T) = \ln \langle \exp [\beta (E^\delta - \langle E^\delta \rangle_{\text{th}})] \rangle_{\text{th}}$

- ▶ cumulant-generating function for the **fluctuations of the boundary energy**
- ▶ e.g., second moment \propto boundary heat capacity
 \Rightarrow **detects thermodynamic singularities**
(like the fidelity susceptibility)

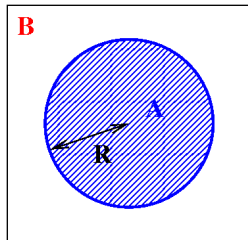
What if there are truly no thermodynamic singularities?

von Neumann entanglement entropy (II)

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

- ▶ 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 energy minima
 - one minimum preferred by the fixed B.C. ($E_\delta \simeq E_\delta^*$)
 - all others **equally disfavoured** ($E_\delta \simeq E_\delta^* + \Delta E$)

Biroli, Bouchaud 2004



$$\begin{aligned}\Delta F_A &\simeq -T \ln \left[\frac{\sum_{i=1}^{\mathcal{N}} e^{-\beta E_i}}{\mathcal{N}} \right] \\ &\simeq -T \ln \left[e^{-\beta E_\delta^*} \frac{(\mathcal{N}-1)e^{-\beta \Delta E} + 1}{\mathcal{N}} \right] \\ &\simeq E_\delta^* - T \ln \left[e^{-\beta \Delta E} + e^{-S^*} \right], \quad S^* \equiv \ln \mathcal{N}\end{aligned}$$

von Neumann entanglement entropy (II)

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

- ▶ above T_g : the system adapts to the fixed B.C. $\rightarrow \Delta F_A \sim E_\delta^*$
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$$\Delta F_A \sim E_\delta^* - T \ln \left(e^{-\Delta E/T} + e^{-S^*} \right)$$

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

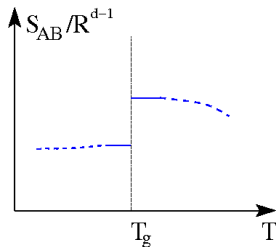
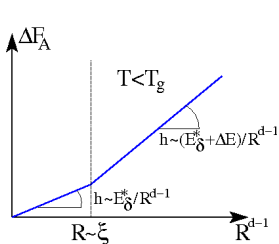
correlation length ξ identified by $\Delta E(R = \xi) \sim S^*(R = \xi)$

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

von Neumann entanglement entropy (II)

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

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



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

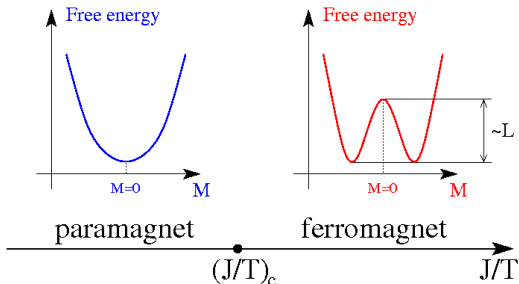
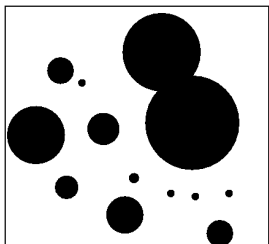
quantum entanglement: static + generic

Castelnovo, Chamon, Sherrington 2010

Example I: the 2D Ising ferromagnet

$$\mathcal{C} \equiv \{\sigma_i = \pm 1\}$$

$$E_C \equiv J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$



under single spin flip dynamics (Glauber)

$$W_{C'C} = \frac{e^{-\beta(E_{C'} - E_C)/2}}{2 \cosh[\beta(E_{C'} - E_C)/2]}$$

energy barriers $\sim L$ from positive to negative magnetisation

Example I: the 2D Ising ferromagnet

$$\hat{H} = \sum_{(c,c')} \frac{1}{2 \cosh[\beta(E_{c'} - E_c)/2]} \left\{ e^{-\beta(E_{c'} - E_c)/2} |c\rangle\langle c| - |c\rangle\langle c'| \right\}$$

single spin flip: $E_{c'} - E_c = 2 \sum_j J_{ij} \sigma_i \sigma_j$

$$\hat{H} = \sum_{i,c} \frac{1}{2 \cosh[\beta \sum_j J_{ij} \sigma_j]} \left\{ e^{-\beta \sum_j J_{ij} \sigma_j \sigma_i} |c\rangle\langle c| - |c\rangle\langle c| \hat{\sigma}_i^x \right\}$$

$$\Rightarrow \hat{H} = \sum_i \frac{1}{2 \cosh[\beta \sum_j J_{ij} \hat{\sigma}_j^z]} \left\{ e^{-\beta \sum_j J_{ij} \hat{\sigma}_j^z \hat{\sigma}_i^z} - \hat{\sigma}_i^x \right\}$$

Castelnovo, Chamon, Pujol, Mudry 2005

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 \rightarrow new exotic quantum Hamiltonians
 - ▶ 'unconventional' quantum systems devoid of local order (e.g., topological order) \rightarrow insight in glassiness

Conclusions

potential **advantages** and open questions

- ▶ can we fully characterise dynamical transitions **using static** (zero-temperature) **techniques**?
- ▶ can we use the **scaling exponents** of the fidelity susceptibility to classify dynamical glass transitions?
- ▶ ability to construct **(off-diagonal) order parameters**, which correspond to ‘dynamical’ quantities in the original classical system

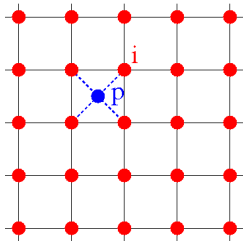
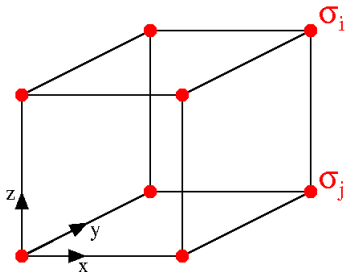
Example II: the gonihedric model

Jonsson, Savvidy 1999-2000, Savvidy 2000

$$E = -J_{xy} \sum_i \sigma_i \sigma_{i+\hat{x}} \sigma_{i+\hat{x}+\hat{y}} \sigma_{i+\hat{y}}$$

$$-J_{yz} \sum_i \sigma_i \sigma_{i+\hat{y}} \sigma_{i+\hat{y}+\hat{z}} \sigma_{i+\hat{z}}$$

$$-J_{zx} \sum_i \sigma_i \sigma_{i+\hat{z}} \sigma_{i+\hat{z}+\hat{x}} \sigma_{i+\hat{x}}$$



$$J_{xy} = J', \quad J_{yz} = J_{zx} = 0:$$

square plaquette kinetically constrained model

$$E = -J' \sum_p \prod_{i \in p} \sigma_i$$

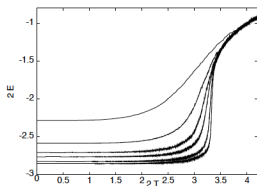
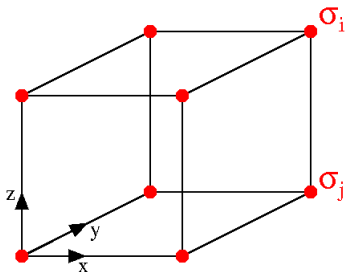
no transition; time scales diverge for $T \rightarrow 0$

Jack *et al.* 2005

Example II: the gonihedric model

Jonsson, Savvidy 1999-2000, Savvidy 2000

$$E = -J_{xy} \sum_i \sigma_i \sigma_{i+\hat{x}} \sigma_{i+\hat{x}+\hat{y}} \sigma_{i+\hat{y}}$$
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$$-J_{zx} \sum_i \sigma_i \sigma_{i+\hat{z}} \sigma_{i+\hat{z}+\hat{x}} \sigma_{i+\hat{x}}$$



$J_{xy} = J_{yz} = J_{zx} = J$: gonihedric model

- ▶ first order phase transition at finite T_c
- ▶ glass transition at $T_g \sim T_c$

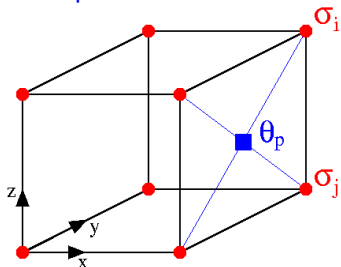
Johnston *et al.* 2007

Example II: the gonihedric model

convenient description using **plaquette dual spins**

$$\theta_p \equiv \prod_{i \in p} \sigma_i$$

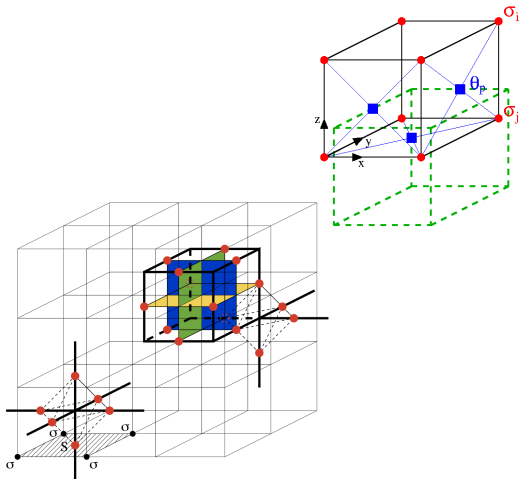
$$E = -J \sum_p \prod_{i \in p} \sigma_i = -J \sum_p \theta_p$$



- ▶ **kinetically constrained model**: trivial thermodynamics, cooperative dynamics
- ▶ not all θ spin configurations are allowed

Example II: the goniohedric model

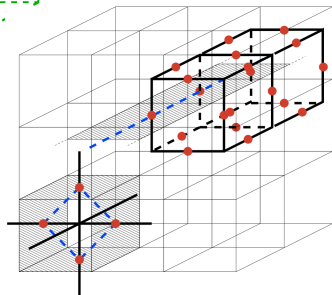
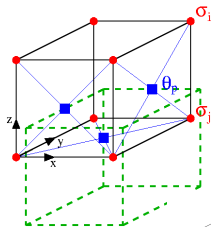
the θ spins live on the bonds of the body-centered dual lattice



$$\sum_{\text{cubes } c} \prod_{p \in c} \theta_p^x$$

Example II: the goniohedric model

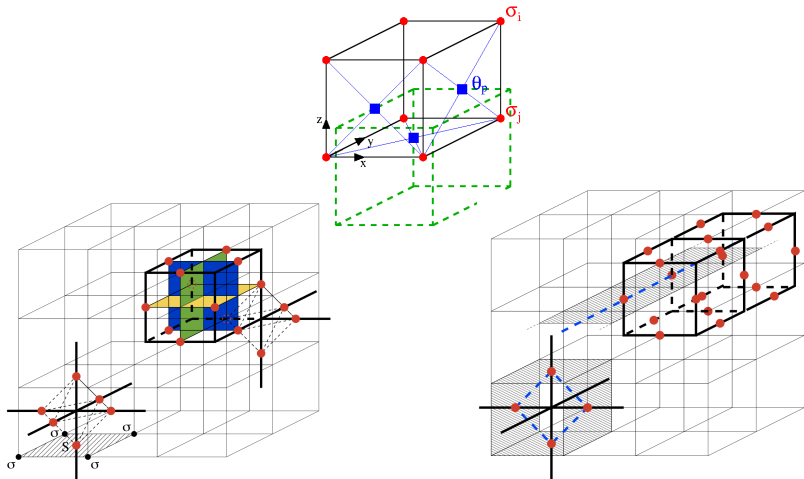
the θ spins live on the bonds of the body-centered dual lattice



$$-\lambda \left[\sum_{\text{stars } s} \prod_{p \in s} \theta_p^z + \sum_{\text{strip } t} \prod_{p \in t} \theta_p^z \right]$$

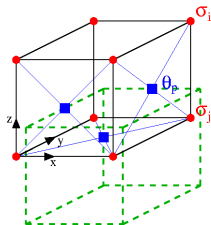
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Example II: the goniohedric model

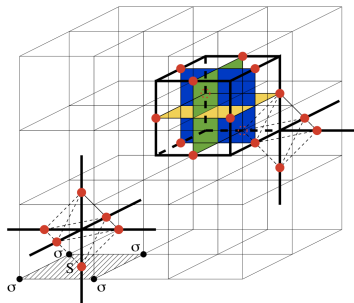
the θ spins live on the bonds of the body-centered dual lattice



$$\hat{H} = \sum_c \frac{1}{2 \cosh(\beta J M_c)} \left\{ \exp(-\beta J M_c) - \prod_{p \in c} \theta_p^x \right\} - \lambda \left[\sum_s \prod_{p \in s} \theta_p^z + \sum_t \prod_{p \in t} \theta_p^z \right]$$

Example II: the goniuhedric model

the high temperature ($\beta \rightarrow 0$) limit gives an odd toric code



$$\hat{H} = - \sum_c \prod_{p \in c} \theta_p^x - \lambda \sum_s \prod_{p \in s} \theta_p^z - \lambda \sum_t \prod_{p \in t} \theta_p^z$$

- ▶ (sub)extensive topological degeneracy
- ▶ the last term selects a unique topological sector

Variational approach to the lowest energy states

$$|\psi_0\rangle = \sum_{\mathcal{C}} \frac{e^{-\beta E_{\mathcal{C}}/2}}{\sqrt{Z}} |\mathcal{C}\rangle = \sum_{\mathcal{C}} \frac{\exp\left\{\frac{\beta}{2} \sum_{ij} J_{ij} \sigma_j^z \sigma_i^z\right\}}{\sqrt{Z}} |\mathcal{C}\rangle$$

variational approach to the collapsing excited states:

- ▶ find $|\psi_1\rangle$ s.t. $\langle\psi_0|\psi_1\rangle = 0$
- ▶ compute $\langle\psi_1|H|\psi_1\rangle$
- ▶ $\Rightarrow \exists$ at least one excited state with energy $\Delta_1 < \langle\psi_1|H|\psi_1\rangle$

for the 2D Ising ferromagnet:

$$|\psi_1\rangle \propto \sum_{\mathcal{C}} \tanh\left[\sum_i \sigma_i^z\right] \exp\left\{\frac{\beta}{2} \sum_{ij} J_{ij} \sigma_j^z \sigma_i^z\right\} |\mathcal{C}\rangle$$

$$\text{and } \Delta_1 < \frac{\sum e^{-|M(\mathcal{C})|} e^{-\beta E_{\mathcal{C}}}}{\sum e^{-\beta E_{\mathcal{C}}}} \sim \exp(-\alpha L) \quad \text{for } T < T_c$$

Other advantages of the quantum language

- ▶ access to “*off-diagonal*” observables in a static formalism (e.g., using a rotated basis: $\langle \psi_0 | \hat{\sigma}_i^x | \psi_0 \rangle, \dots$)
→ new order parameters?
- ▶ different angle to look at conventional techniques for glassy systems: large deviation functions (\Leftrightarrow quantum perturbation theory); four-point dynamical correlation functions; ...
- ▶ intriguing connections between very diverse areas of physics
 - ▶ glassiness ‘=’ massive collapse of states that are statistically ‘similar’
 - ▶ topological order ‘=’ finite collapse of states that are exactly indistinguishable by local operators

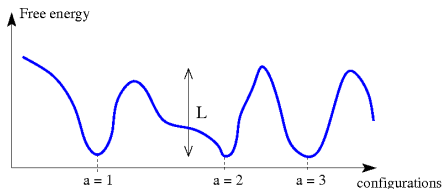
Compare with the Sherrington-Kirkpatrick model

$$E(\{\sigma\}) \equiv - \sum_{ij} J_{ij} \sigma_i \sigma_j \quad \overline{J_{ij}} = 0, \quad \overline{J_{ij}^2} = J^2/N$$

using Parisi's picture at low temperatures:

$$Z = \sum_{a=1}^{\mathcal{N}} Z_a$$

$$\left\{ \begin{array}{l} \tau_{a \rightarrow b} \xrightarrow{L \rightarrow \infty} \infty \\ \mathcal{N} \sim \exp L \end{array} \right.$$



Compare with the Sherrington-Kirkpatrick model

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using Parisi's picture at low temperatures:

$$|\psi_0\rangle = \sum_{a=1}^{\mathcal{N}} \sqrt{\frac{Z_a}{Z}} |\phi_a\rangle \quad |\phi_a\rangle = \frac{1}{\sqrt{Z_a}} \sum_{C \in a} e^{-\beta E_C/2} |C\rangle$$

$$\langle \phi_a | \phi_b \rangle = \delta_{ab}$$

Compare with the Sherrington-Kirkpatrick model

$$E(\{\sigma\}) \equiv - \sum_{ij} J_{ij} \sigma_i \sigma_j \quad \overline{J_{ij}} = 0, \quad \overline{J_{ij}^2} = J^2/N$$

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$$\langle \phi_a | \phi_b \rangle = \delta_{ab}$$

\Rightarrow extensive ($N \sim \exp(L)$) set of collapsing eigenstates
(the known result $q_{\text{EA}}(\mathcal{O}) = \sum_{a=1}^{\mathcal{N}} \sqrt{Z_a/Z} \langle \sigma_i^z \rangle_a^2$ is indeed recovered)

What happens at T_g ? (I)

the **gap closes**: is it a quantum phase transition?

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

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

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

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

What happens at T_g ? (II)

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

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

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

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