A solvable model of quantum random optimization problems

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MIT, November 1, 2010

Based on Phys. Rev. Lett. 105, 167204 (2010)

Outline

Investigation of the performances of quantum adiabatic computations led to two sets of results on the spectrum of quantum constraint satisfaction problems.

Consider a model Hamiltonian acting on N qubits, of the form:

$$H = H_P + \Gamma H_Q = H_P - \Gamma \sum_{i=1}^{N} \sigma_i^x$$

with H_P "problem" Hamiltonian.

1. The existence of a first order transition between a "Quantum Paramagnetic" and a "Classical Paramagnetic"/"Spin Glass" phase at $T = 0$ by varying Γ

- H_p=REM: Goldschmidt 1988; Jörg et al. 2008; Farhi et al. 2010
- H_P=p-spin glass: Nieuwenhuizen and Ritort, 1998; Biroli and Cugliandolo, 2001; Cugliandolo et al. 2001
- H_P=1-in-3-SAT: Young et al. 2009
- H_P=XORSAT: Jörg et al. 2009

2. The existence of level crossings between different ground states (in the spin glass phase), related to "Many Body Localization"

- H_P=WMIS (Weighted Max Independent Set): Amin and Choi, 2009;
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Both phenomena are potentially dangerous for quantum algorithms, since they lead to exponentially small gaps.

Two possible approaches have been used:

- "Worst case": look to particularly dangerous or difficult instances
- "Typical case": choose your favorite ensemble of instances and study properties of typical instances

Here we focus on a typical case study. The advantage is that one can sometimes obtain analytically the typical properties using statistical mechanics.

In natural ensembles of random classical problems H_P (random k-SAT, coloring of random graphs), statistical mechanics investigations showed two distinct phase transitions:

- **SAT-UNSAT phase transition**: typical instances have either an exponential number of solutions (in the SAT phase) or no solutions (in the UNSAT phase)
- **Clustering transition**: the exponentially many solutions are arranged in an exponential number of distinct clusters

Previous studies focused on models that have a unique ground state.
Some studied the first order transition, others the level crossings.

Looking for a unified picture

- Is the first order transition present in typical instances?
- Are level crossings present in typical instances?
- Is it possible to observe the two phenomena in the same model? Are they distinct?
- Do the large degeneracy of solutions and their clustering play a role?

A toy model for random constraint satisfaction problems

- Allows to describe easily the structure of classical problems (k-SAT, COL)... $[H_P]$
- ...and to understand what is the impact of quantum fluctuations! $[H_P + \Gamma H_Q]$

Outline

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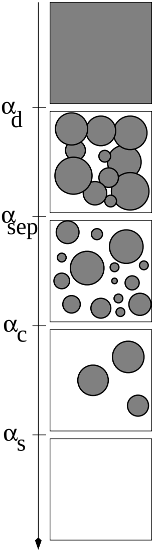
Random Subcubes Model
(Mora and Zdeborová, 2008)

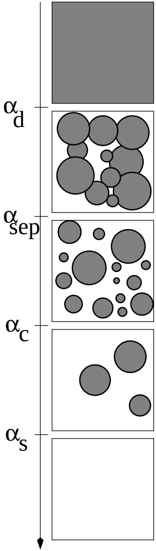


Definition of the Hamiltonian H:

- Hilbert space $\mathcal{H}$ of N qubits, in the basis of σ_i^z: $|\underline{\sigma}\rangle = |\sigma_1 \cdots \sigma_N\rangle$
- Cluster $A = \{|\underline{\sigma}\rangle \,|\, \forall i, \sigma_i \in \pi_i^A\} \subset \mathcal{H}$, π_i^A i.i.d. random
  $\pi_i^A = \{-1\}$ or $\{1\}$ with probability $p/2$ ("frozen")
  $\pi_i^A = \{-1, 1\}$ with probability $1 - p$ ("free")
- $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$, union of $2^{N(1-\alpha)}$ independent clusters
- Assign an energy $Ne(A)$ to each cluster:
  $H_A|\underline{\sigma}\rangle = Ne(A)|\underline{\sigma}\rangle$ if $|\underline{\sigma}\rangle \in A$, $H_A|\underline{\sigma}\rangle = 0$ otherwise
- Assign a penalty NV to configurations that are not in a cluster:
  $H_V|\underline{\sigma}\rangle = NV|\underline{\sigma}\rangle$ if $|\underline{\sigma}\rangle \notin \mathcal{S}$, $H_V|\underline{\sigma}\rangle = 0$ otherwise
- Problem Hamiltonian: $H_P = H_V + \sum_{i=1}^{2^{N(1-\alpha)}} H_{A_i}$
- Total Hamiltonian: $H = H_P - \Gamma \sum_{i=1}^N \sigma_i^x$

Classical model ($\Gamma = 0$). $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{N s_{\rm tot}}$

Topology of the cluster space $\mathcal{S}$



- 2^{Nb} events E_i with $\mathcal{P}(E_i) = 2^{-Na}$
- Union bound: $\mathcal{P}(\cup_i E_i) \leq \sum_i \mathcal{P}(E_i) = 2^{N(b-a)}$
  If $b < a$, the probability of $\cup_i E_i$ is exponentially small
- *If the events are independent*, and $\mathcal{N}$ is the number of true events:
  $\langle \mathcal{N} \rangle = 2^{N(b-a)}$, $\langle \mathcal{N}^2 \rangle = 2^{N(b-a)}(1 - 2^{-Na})$
  Chebyshev's inequality:
  $\mathcal{P}(|\mathcal{N} - \langle \mathcal{N} \rangle| > \epsilon \langle \mathcal{N} \rangle) \leq \frac{\langle \mathcal{N}^2 \rangle}{\langle \mathcal{N} \rangle^2 \epsilon^2} = \frac{1-2^{-Na}}{2^{N(b-a)} \varepsilon^2}$
  If $b > a$, concentration: $\mathcal{N} \sim \langle \mathcal{N} \rangle$, exponentially large

Classical model $(\Gamma = 0)$. $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{N s_{\rm tot}}$
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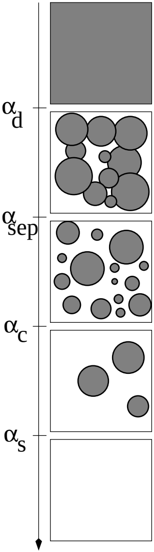

- $\mathcal{P}(|\underline{\sigma}\rangle \in A) = \left(1 - \frac{p}{2}\right)^N$ independently for each A
- $\mathcal{P}(|\underline{\sigma}\rangle \notin \mathcal{S}) = \left[1 - \left(1 - \frac{p}{2}\right)^N\right]^{2^{N(1-\alpha)}} \sim e^{-2^{N[\log_2(2-p)-\alpha]}}$
  $\mathcal{P}(\mathcal{S} \neq \mathcal{H}) = \mathcal{P}(\cup_{\underline{\sigma}}(|\underline{\sigma}\rangle \notin \mathcal{S})) \leq 2^N e^{-2^{N[\log_2(2-p)-\alpha]}}$
- $\mathcal{P}(\mathcal{S} \neq \mathcal{H}) \to 0$ for $\alpha < \log_2(2-p)$
  $\mathcal{P}(|\underline{\sigma}\rangle \notin \mathcal{S}) \to 1$ for $\alpha > \log_2(2-p)$
- $\alpha_d = \log_2(2-p)$
  $\alpha < \alpha_d$ all states are in $\mathcal{S}$: $s_{\rm tot} = 1$
  $\alpha > \alpha_d$ most states are not in $\mathcal{S}$: $s_{\rm tot} < 1$

Classical model ($\Gamma = 0$). $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{N s_{\rm tot}}$

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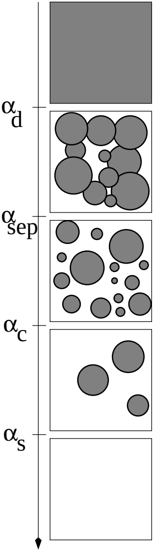

- $\mathcal{P}(A \cap A' \neq \emptyset) = \left(1 - \frac{p^2}{2}\right)^N$
- $\mathcal{P}(\cup_{ij}(A_i \cap A_j \neq \emptyset)) \leq \frac{1}{2} 2^{N(1-\alpha)}(2^{N(1-\alpha)} - 1) \left(1 - \frac{p^2}{2}\right)^N \to 0$
  for $\alpha > \frac{1}{2}(1 + \log_2(2 - p^2))$
- $\alpha_{\rm sep} = \frac{1}{2}(1 + \log_2(2 - p^2))$
  $\alpha > \alpha_{\rm sep}$ all clusters are disjoint

Classical model ($\Gamma = 0$). $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{Ns_{\mathrm{tot}}}$
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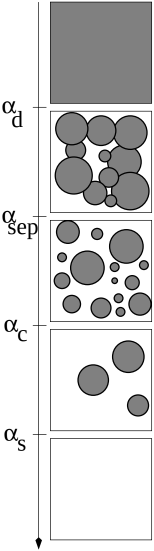
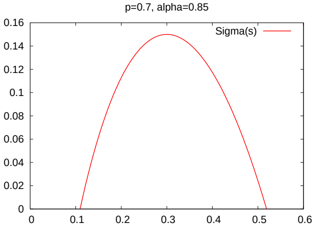


- Entropy of a cluster: $2^{Ns(A)}$, $s(A)$ fraction of free variables.
  $\mathcal{P}(s(A) = s) = \binom{N}{Ns} p^{N(1-s)}(1-p)^{Ns}$ independently for each cluster
- Number of clusters with entropy s:
  $$\mathcal{N}(s) = 2^{N(1-\alpha)}\mathcal{P}(s) = \begin{cases} 2^{N\Sigma(s)} & \Sigma(s) > 0 \\ 0 & \Sigma(s) < 0 \end{cases}$$
  $$\Sigma(s) = 1 - \alpha - s\log_2(s/(1-p)) - (1-s)\log_2((1-s)/p)$$
  $\Sigma(s) > 0$ for $s \in [s_{\min}, s_{\max}]$



Classical model ($\Gamma = 0$). $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{Ns_{\rm tot}}$

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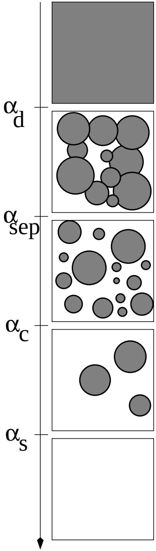

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  $\Sigma(s) > 0$ for $s \in [s_{\rm min}, s_{\rm max}]$

- $2^{Ns_{\rm tot}} = \sum_A 2^{Ns(A)} \sim \int_{s_{\rm min}}^{s_{\rm max}} {\rm d}s\, 2^{N[\Sigma(s)+s]}$
  $s_{\rm tot} = \max_{s\in[s_{\rm min}, s_{\rm max}]}[\Sigma(s) + s]$
- $\alpha_c = p/(2-p) + \log_2(2-p)$
  $\alpha < \alpha_c$: $s^* \in (s_{\rm min}, s_{\rm max})$, $\Sigma(s^*) > 0$ - most states in $\mathcal{S}$ belong to one of the exponentially many clusters of size s^*
  $\alpha > \alpha_c$: $s^* = s_{\rm max}$, $\Sigma(s^*) = 0$ - most states in $\mathcal{S}$ belong to one of the few biggest clusters of size $s_{\rm max}$

Classical model ($\Gamma = 0$). $\mathcal{S} = \cup_{i=1}^{2^{N(1-\alpha)}} A_i$ with $|\mathcal{S}| = 2^{Ns_{\rm tot}}$
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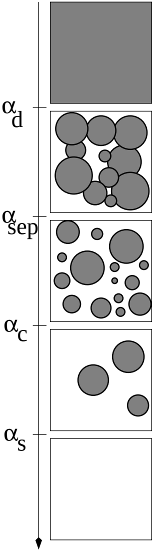
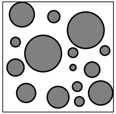


- $\alpha_{\rm d}$ clusterization of the set $\mathcal{S}$
- $\alpha_{\rm sep}$ clusters are well separated
- $\alpha_{\rm c}$ condensation of the set $\mathcal{S}$ in few large clusters
- $\alpha_{\rm s} = 1$ no more clusters

Outline



Quantum model with hard constraints
Simplest case: $V \to \infty$, $\alpha > \alpha_{\text{sep}}$

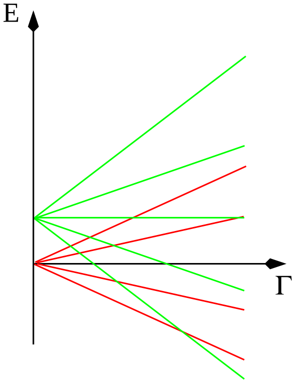
Project out the states outside $\mathcal{S}$
Clusters are disjoint and the quantum term does not connect them

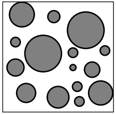
- The quantum Hamiltonian is block diagonal in each cluster
  Diagonal term $Ne(A)$, off-diagonal equal to $Ns(A)$ free spins in transverse field

- Spectrum of a cluster:
$$E(A,k) = Ne(A) + (2k - Ns(A))\Gamma$$
$$k = 0, \cdots, Ns(A)$$

- Ground state of a cluster:
$$e_{GS}(A) = e(A) - s(A)\Gamma$$

- *The energy of a cluster is lowered proportionally to its entropy*



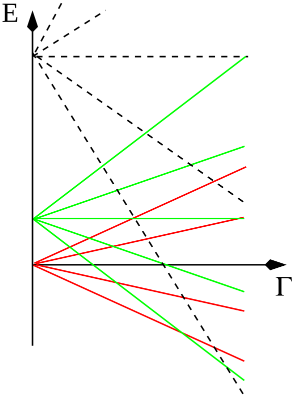


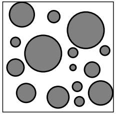
Quantum model with soft constraints
Next-to-simplest case: finite (large) V, $\alpha > \alpha_{\mathrm{sep}}$

At $\Gamma = 0$: $2^{Ns_{\mathrm{tot}}}$ states in $\mathcal{S}$, small energy ($\mathcal{S}$-band)
$2^N - 2^{Ns_{\mathrm{tot}}} \sim 2^N$ not in $\mathcal{S}$, energy NV (V-band)

Perturbation theory for small energy states ($\mathcal{S}$-band)

- Degenerate perturbation theory: start by diagonalizing the perturbation inside each cluster. We already did it in the $V = \infty$ case!
- Clusters are separated, perturbation involves the V-band
- $e_{GS}(A) = e(A) - s(A)\Gamma - \frac{\Gamma^2}{NV}[1 - s(A)] + O\left(\frac{\Gamma^4}{N^2 V^2}\right)$
- Except around crossings $\longrightarrow$ avoided crossings





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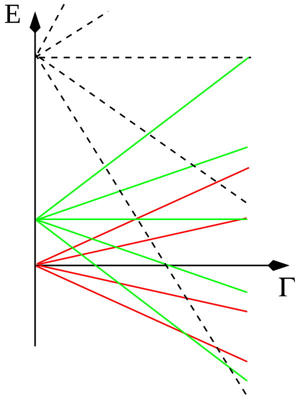
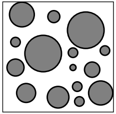
Low-rank perturbation argument for V-band GS

- $$H = \underbrace{NV - \Gamma\sum_i \sigma_i^x}_{H_0} \underbrace{- N\sum_A (V - e(A))|A\rangle\langle A|}_{X}$$
- X is a low rank perturbation: $R = 2^{Ns_{tot}} \ll 2^N$
- $E_n \leq E_n^0 \qquad n = 1, \cdots, R$

  $E_1^0 \leq E_{R+1} \leq E_{R+1}^0$
- In particular: $V - \Gamma \leq e_{GS,V}$





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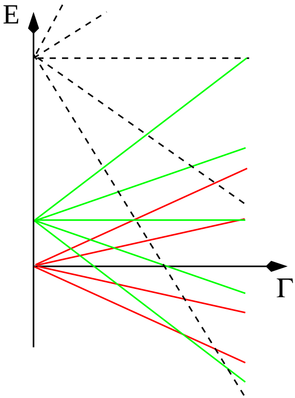
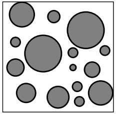
Variational argument for V-band GS

- Consider the state $|QP\rangle = \prod_{i=1}^{N} |\rightarrow\rangle_i$
  $|\rightarrow\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$
- It has scalar product $O(2^{-Ns/2}) \to 0$ with any state in the $\mathcal{S}$-band
- It has energy
  $\langle QP|H|QP\rangle \sim -\Gamma N + NV[1 + O(2^{-Ns_{\mathrm{tot}}})]$
- $e_{GS,V} \leq V - \Gamma$
- Combining with the previous argument:
  $e_{GS,V} = V - \Gamma + O(2^{-\kappa N})$





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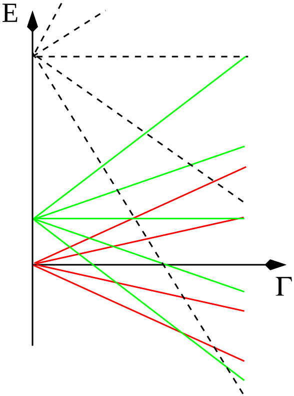
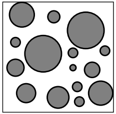
Heuristic argument for V band

- Low rank perturbation X only affects $2^{Ns_{tot}}$ states
- Perturbation "localized" in $|\underline{\sigma}\rangle$ space
- Eigenstates of H_0 are extended
- In the middle of the band there are many states: form localized linear combinations
- Those are mostly affected by X
- All the other states have $O(2^{-\kappa N})$ corrections
- Spectrum of the V-band is that of N free spins in transverse field Γ

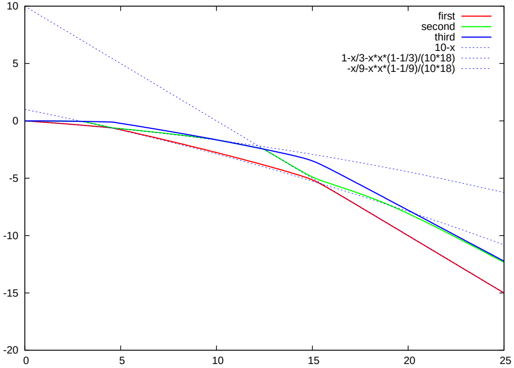


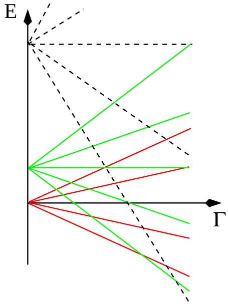


Quantum model with soft constraints
Exact diagonalization of a system of $N = 18$ spins, with $V = 10$

Two clusters ($* = \pm 1$):

$$A1 = (*, *, -1, -1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1) \qquad e(A1) = 0 \qquad s(A1) = 2/18$$
$$A2 = (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, *, *, *, *, *, *) \qquad e(A2) = 1 \qquad s(A2) = 6/18$$





$$e_{GS}(A) = e(A) - s(A)\Gamma - \frac{\Gamma^2}{NV}[1 - s(A)] + O\left(\frac{\Gamma^4}{N^2 V^2}\right)$$

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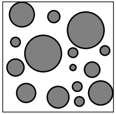
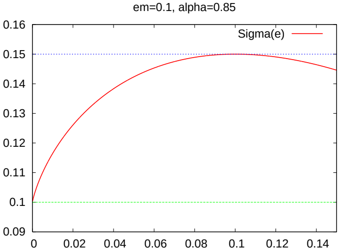


Classical model for $N \to \infty$

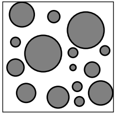
$\alpha > \alpha_{\rm sep}$, fixed V - Distribution of cluster energies

To get an interesting thermodynamic limit we have to assign the distribution of *classical* energy of clusters:

- $\mathcal{N}(e) = 2^{N\Sigma(e)}$
- $\max_e \Sigma(e) = 1 - \alpha$, total number of clusters $2^{N(1-\alpha)}$
- $\Sigma(e = 0) = \frac{2}{3}(1 - \alpha)$, total number of clusters of solutions $2^{N\frac{2}{3}(1-\alpha)}$



$$\Sigma(e) = \frac{1}{3}(1 - \alpha)\left\{2 + e/e_m - (e/e_m)\log(e/e_m)\right\} \text{ for } e \in [0, e_m]$$



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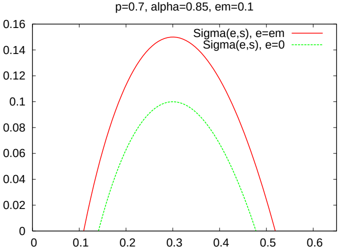
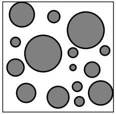
Frozen spins are drawn independently for each cluster:
$\Sigma(e, s) = \Sigma(e) - s \log_2(s/(1 - p)) - (1 - s) \log_2((1 - s)/p)$



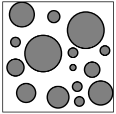
Vanishes for $s = s_{\max}(e)$, increasing function of e: bigger clusters at higher energy



Quantum model for $N \to \infty$

$\alpha > \alpha_{\rm sep}$, fixed V Ground state energy

- $e_{GS}(A) = e(A) - s(A)\Gamma - \frac{\Gamma^2}{NV}[1 - s(A)] + O\left(\frac{\Gamma^4}{N^2V^2}\right)$
- For $N \to \infty$ $e_{GS}(A) = e(A) - \Gamma s(A)$
- $e_{SG}(\Gamma) = \min_A\{e(A) - \Gamma s(A)\} = \min_{e\in[0,e_m]} \min_{s\in[s_{\rm min}(e),s_{\rm max}(e)]}\{e - \Gamma s\}$
- Minimization over s is trivial:
  $e_{SG}(\Gamma) = \min_{e\in[0,e_m]}\{e - \Gamma s_{\rm max}(e)\}$ Solve $\frac{ds_{\rm max}(e)}{de} = \frac{1}{\Gamma}$
- $s_{\rm max}(e)$ is a monotonically increasing function of e, $\frac{ds_{\rm max}(e)}{de} > 0$
- For $\Gamma > \left[\frac{ds_{\rm max}}{de}(e=0)\right]^{-1}$, the minimum is in a different value of e for each Γ
  A continuum of level crossings!



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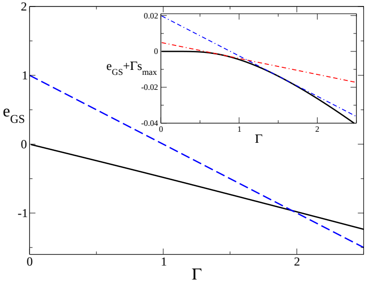
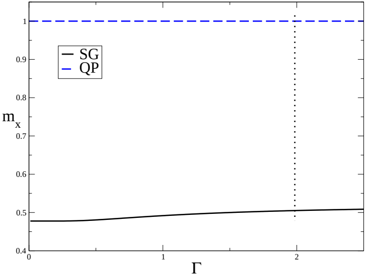
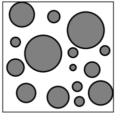




Level crossings in the spin glass phase

- $e_{SG}(\Gamma) = \min_{e\in[0,e_m]}\{e - \Gamma s_{\max}(e)\}$ Solve $\frac{ds_{\max}(e)}{de} = \frac{1}{\Gamma}$
- Inset: $e_{GS} + \Gamma s_{max}(e = 0)$ to highlight the crossings in the *SG* phase
- All thermodynamic functions are analytic in the *SG* phase
- Reminiscent of “chaos” in temperature in classical spin glasses



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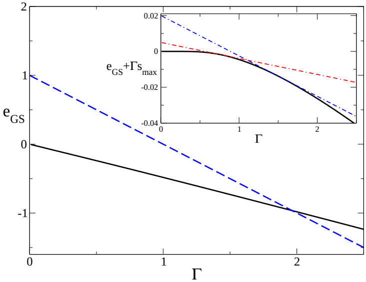
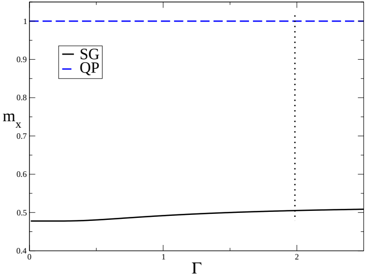
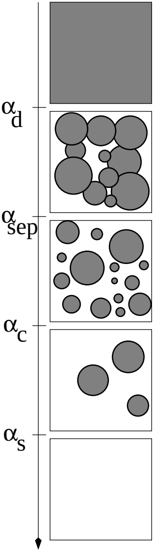




A first order transition between the *SG* (cluster) states and the *QP* state

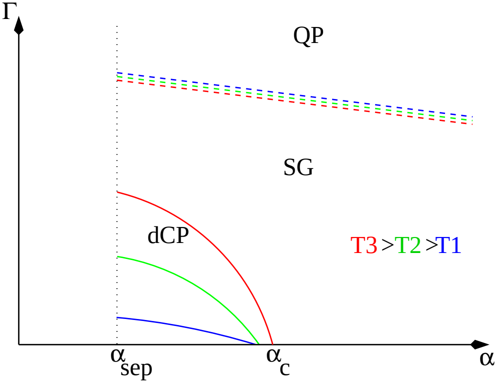
- $e_{QP} = V - \Gamma$
- Transverse magnetization $m_x = s$ classical entropy
  It has a jump at the transition
- Inverse Participation Ratio: $I = \sum_{\underline{\sigma}} |\psi(\underline{\sigma})|^4 = 2^{-Ns}$
  $$\mathcal{I} = -\frac{1}{N} \log_2 I = s = m_x$$

Outline



Finite temperature phase diagram

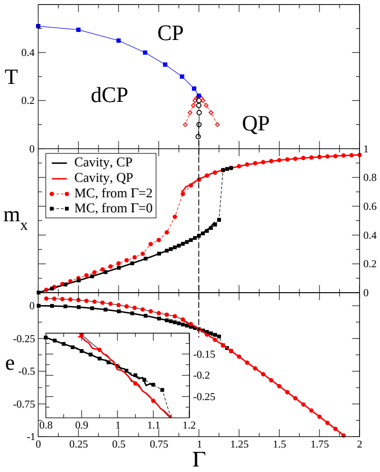
Reentrance of the condensation transition



Remark: similar phenomenon found by Markland et al. (Nature Physics, in press 2010) for quantum hard spheres using a completely different method

Outline

3-XORSAT with $c = 3$



T.Jörg, F.Krzakala, G.Semerjian, FZ, PRL 104, 207206 (2010)

- XORSAT is an easy problem: a solution can be found in polynomial time using Gaussian elimination
- However, it is hard for local search algorithms
- In particular, in the UNSAT phase finding the ground state is hard
- XORSAT on a regular random graph is a "locked" model: solutions are isolated (clusters have no entropy)
- We do not expect level crossings of the type discussed above
- Exact solution in the thermodynamic limit via the cavity method: first order transition
- Comparison with Monte Carlo shows there are no level crossings
- Similar results for 2-in-4-SAT (F.Krzakala, unpublished)

Work in progress:

- Study of a model of lattice glass on the Bethe lattice: the quantum Biroli-Mézard model.
  Here clusters have internal entropy: same phase diagram of the quantum subcubes model.
  (L.Foini, G.Semerjian, FZ, in preparation)
- Preliminary studies of a quantum version of the coloring problem (with G.Semerjian and F.Krzakala)

Outline

A very simple model with a very complex phase diagram

- A spin glass phase, level crossings induced by entropy-energy competition
- A first order transition to a quantum paramagnetic phase
- A re-entrant behavior of the glass transition line

Allow to rationalize previous results

- First order phase transition (signaled by a jump in m_x) is a generic phenomenon: XORSAT, 1-in-3-SAT (Young), coloring, ...
  Is it a many-body localization transition? Jump in $N^{-1}\log_2 I$.
- Two different mechanisms induce level crossings:
  - one based on energetic effects only (Amin-Choi, Altshuler et al., Farhi et al.)
  - the one we identified, based on an energy-entropy competition
  Probably both are at work in typical instances of complicated problems such as k-SAT or coloring.
- In locked problems (XORSAT or 2-in-4-SAT on regular graphs), cluster are points; in this case we don't find evidence for level crossings on typical instances.

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