Quantum annealing and glass problems

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Quantum computers are: a) good for Fourier Transform-based algorithms coherence

b) (obviously) good for avoiding the sign problem

no-coherence ?

c) most probably *bad* for "Golf Course" (=Random Energy=Glassy) systems

Sign Problem

We are asked to compute averages over configurations s

$$\langle O \rangle = \frac{\sum_s e^{-W(s)} O(s)}{\sum_s e^{-W(s)}}$$

and $W = W_R + iW_I$ **is not real.**

- **Quantum mechanics / Field Theory with real time or θ-terms**

- **Hubbard-Stratonovich decoupling** $W = W_o - b \sum C_\alpha^2$

$$Z = \sum_s e^{-W_o(s) - b \sum C_\alpha^2} = \sum_s \int d\lambda \; e^{-W_o(s) + \sqrt{b}\lambda_\alpha C_\alpha - \frac{\lambda_\alpha^2}{2}}$$

The Hubbard-Stratonovich transformation above introduces an imaginary term $W_I = \sqrt{|b|} \sum \lambda_\alpha C_\alpha$ in the repulsive case $b < 0$.

In solid state theory the sign problem is the main obstacle for giving a numerical answer to very urgent questions.

e.g. Hubbard model $H = -t \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$

For definiteness: $W_I = ih_I M(s)$

where $M(s)$ is an integer-valued:

$$Z = \sum_M Z_M \, e^{-ih_I M}$$

$$Z_M = e^{-\beta F(M)} = \sum_s \delta(M(s) - M) \, e^{-W_R}$$

- **Field theory with θ terms. $M =$ a topological number** **'t Hooft, Haldane,...**
- **Fermion systems: $M =$ Fermion world-line crossings** **Muramatsu et al**
- **Hubbard model: $M =$ the number of up Hirsch spins**

  [with a variant of Hubbard-Stratonovich transformation, see: DeForcrand, Batrouni]

Also: If we knew how to deal with the sign problem, we would know how to compute numerically averaged disordered models

using identities of the form

$$\frac{1}{x} = -\lim_{\lambda\to\infty} \frac{1-e^{-\lambda x}}{x} = -\lim_{\lambda\to\infty} \sum_1^\infty (-1)^n \frac{\lambda^n}{n!} x^{n-1}$$

$$\overline{\langle E \rangle} = -\overline{Z^{-1} \frac{\partial Z}{\partial \beta}} = -\lim_{\lambda\to\infty} \frac{\partial}{\partial \beta} \sum_1^\infty \frac{(-1)^n}{n} \frac{\lambda^n}{n!} \overline{Z^n}$$

In practice, what we can do is to compute

$$\langle \mathbf{O} \rangle = \frac{\langle \mathbf{e^{-iW_I}\ O} \rangle_{\mathsf{R}}}{\langle \mathbf{e^{-iW_I}} \rangle_{\mathsf{R}}} \quad ; \quad \text{where} \quad \langle \bullet \rangle_{\mathsf{R}} = \frac{\sum \bullet\ e^{-W_R(s)}}{\sum e^{-W_R(s)}}$$

Note that Monte Carlo is only really good to calculate $\langle O \rangle$ for O non-exponential

and not for

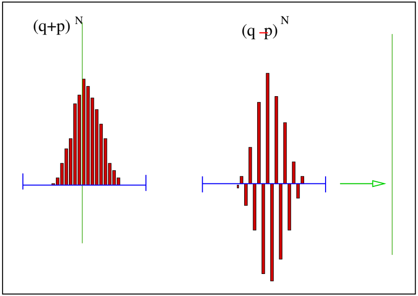
$$\langle O \rangle = \frac{\langle e^{-B}\ O \rangle_{\mathsf{A}}}{\langle e^{-B} \rangle_{\mathsf{A}}}$$

if, e.g. B is exponential in N

An example:

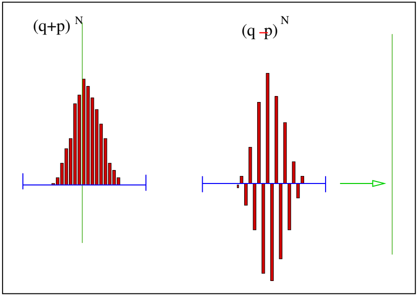
Non-interacting spins in a magnetic field $h_R + i\frac{\pi}{2}$

$$Z = \left(e^{-h-i\frac{\pi}{2}} + e^{h+i\frac{\pi}{2}}\right)^N = e^{-i\frac{N\pi}{2}} \quad \left(e^{-h} - e^{h}\right)^N$$



$$(q+p)^N = \sum_r \frac{N!}{r!(N-r)!} \; q^{N-r} p^r$$

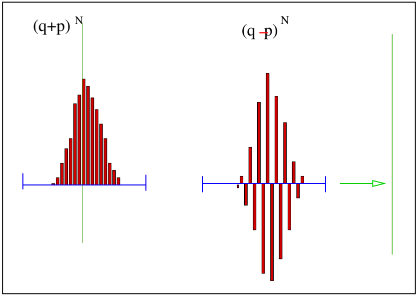
$$(q-p)^N = \sum_r \frac{N!}{r!(N-r)!} \; (-1)^r q^{N-r} p^r$$



put $x = \frac{r}{N}$ and use Stirling:

$$(q+p)^N = \int_0^1 dx \;\; e^{N[-x\ln x-(1-x)\ln(1-x)+(1-x)\ln q+x\ln p]}$$

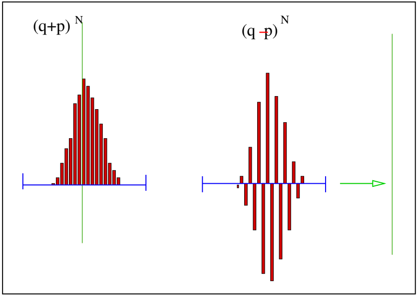
$$\text{saddle: } \left(\frac{x^*}{1-x^*}\right) = \left(\frac{p}{q}\right) \quad \in \quad [0,1]$$



put $x = \frac{r}{N}$ and use Stirling:

$$(q - p)^N = \int_0^1 dx \;\; e^{N[-x \ln x - (1-x)\ln(1-x) + (1-x)\ln q + x \ln p + i\pi x]}$$

saddle: $\left(\frac{x^*}{1-x^*}\right) = -\left(\frac{p}{q}\right)$ not $\in \;\; [0,1]$



Monte Carlo Sampling of the same problem:

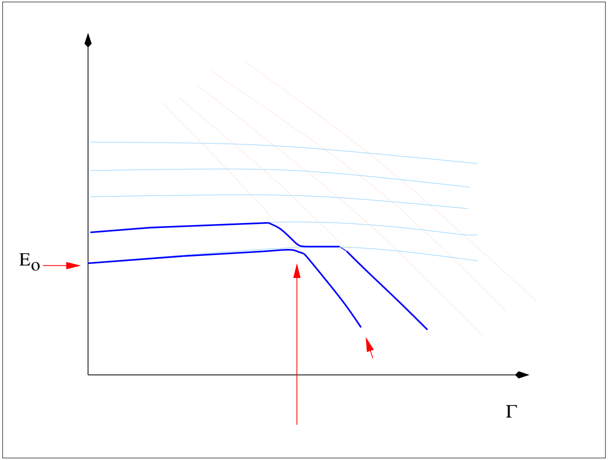
$$(q - p)^N \sim \sum_r \left\{ \frac{N!}{r!(N-r)!} + \sqrt{\frac{N!}{r!(N-r)!}}\eta(r) \right\} \quad (-1)^r q^{N-r} p^r =$$

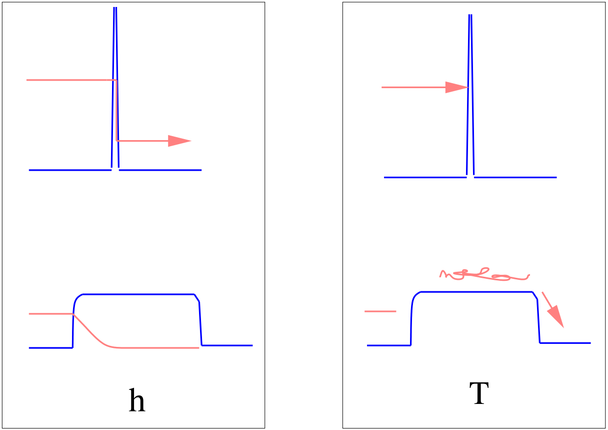
$$(q - p)^N \sim \sum_r \left\{ e^{NS(r)} + e^{N\frac{S(r)}{2}} \eta(r) \right\} \quad (-1)^r q^{N-r} p^r$$ **who wins?**

Quantum Annealing of Hard Problems

$$\mathcal{H}(\{\sigma\}) = E(\{\sigma^z\}) + \Gamma \sum_{i=1}^{N} \sigma_i^x = \mathcal{H}_0 + \Gamma V \qquad (1)$$

Staying in the lowest level without de-railing requires speed Δ^{-2}



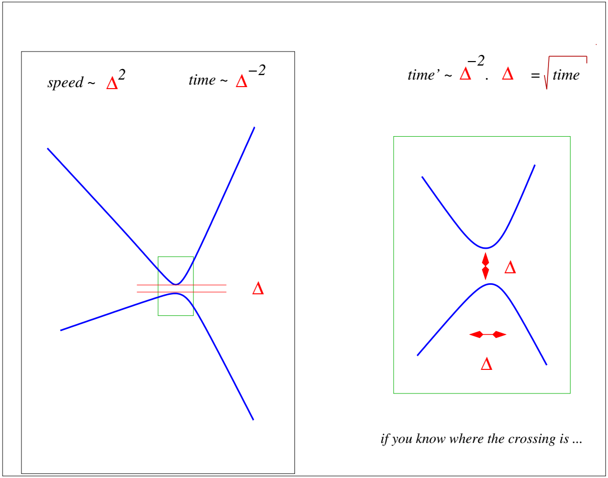


Fat and small versus thin and tall...

The speed is directly given by the minimal gap.

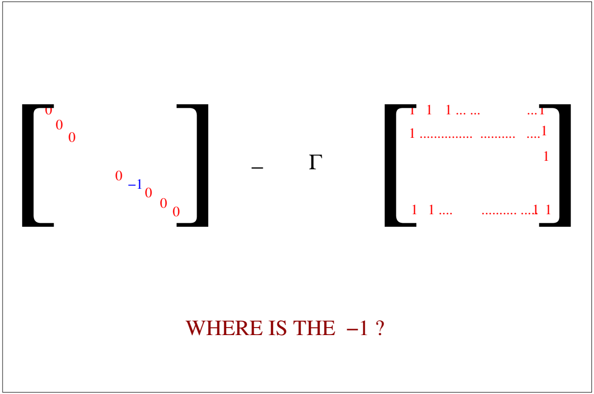
Adiabatic Quantum Computation is Equivalent to Standard Quantum Computation (Aharonov et al)

If you know where the crossing takes place, you gain a square root



Grover

Finding a needle in a haystack, if you know its color...



From N to $\sqrt{N}$, non-trivial yet non miraculous...

The Random Energy Model.

Energies are independent Gaussian random numbers.

An idealization of the $p\ (>2)$-spin model...

$$E(\{\sigma^z\}) = \lim_{p\to\infty} \sum_{i_1,...,i_p} J_{i_1,...,i_p} \sigma^z_{i_1} ... \sigma^z_{i_p}$$

K-SAT...

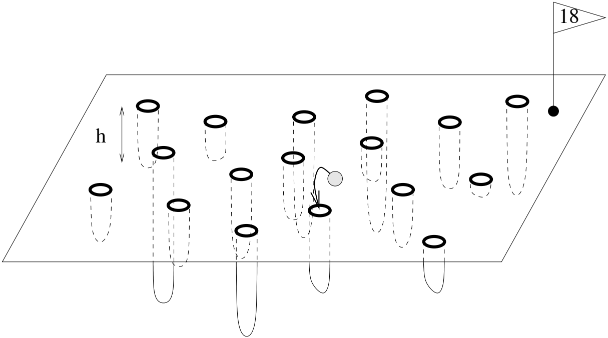
$E(\{\sigma^z\}) = \sum_{clause\ a} C_a$ $\qquad$ $C_a = 0$ iff the clause a is satisfied.

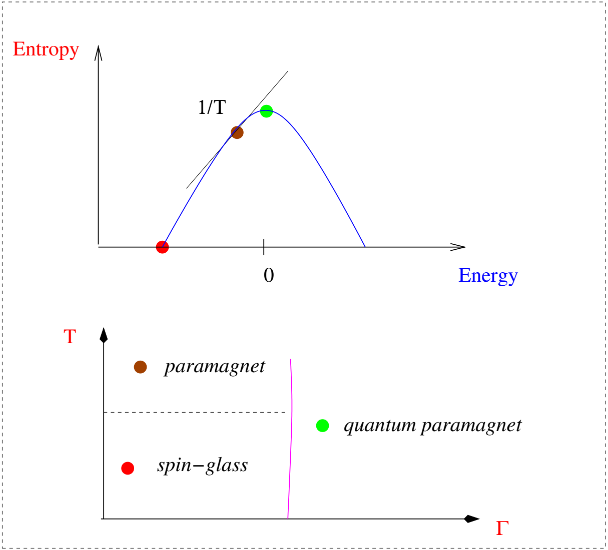
and many other glass models.

The Random Energy Model.

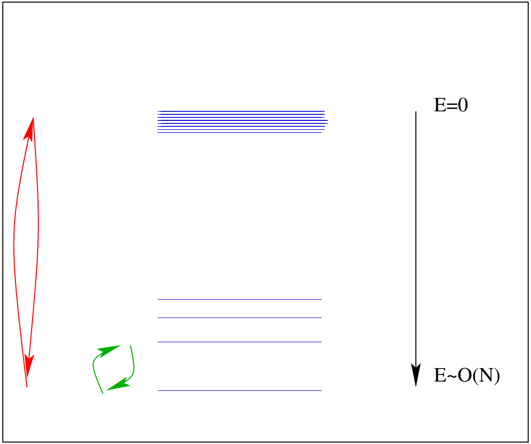
Energies are independent Gaussian random numbers.

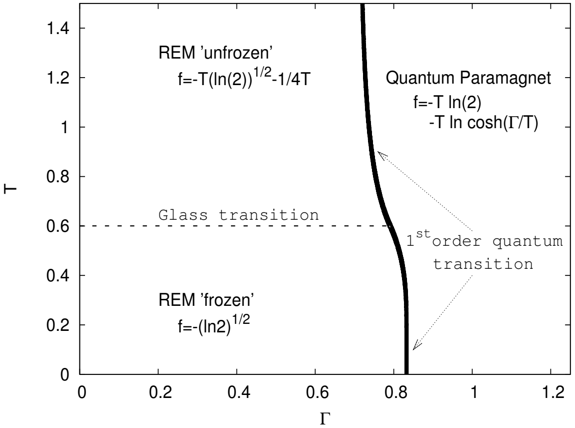
each basin is schematised by a single configuration



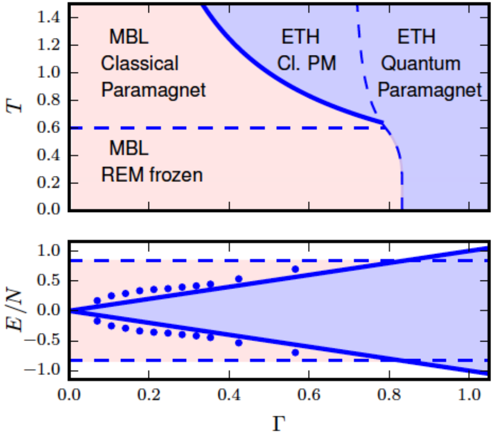

Entropy
1/T
0
Energy
T
paramagnet
quantum paramagnet
spin−glass
Γ

$$E_i(\Gamma) = E_i + \Gamma V_{ii} + \sum_{k \neq i} \frac{\Gamma^2 V_{ik} V_{ki}}{E_i(\Gamma) - E_k} + \ldots = E_i + \frac{N\Gamma^2}{E_i} + O\left(\frac{1}{N}\right)$$




REM 'unfrozen'
f=-T(ln(2))^1/2-1/4T
Quantum Paramagnet
f=-T ln(2)
-T ln cosh(Γ/T)
Glass transition
1st order quantum transition
REM 'frozen'
f=-(ln2)^1/2
T
Γ
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2

Lauman, Pal, Scardicchio

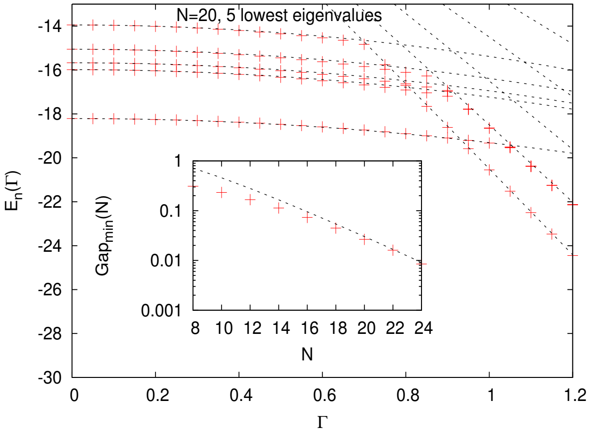


To compute the gap, we just have to diagonalise:

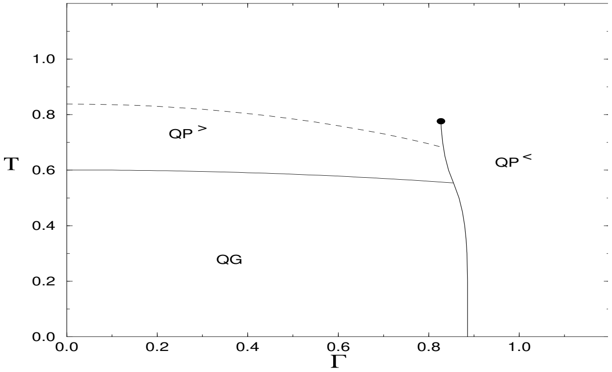
$$\mathcal{H}|\phi\rangle = [\ E_o|SG\rangle\langle SG| - \Gamma N|QP\rangle\langle QP|\ ]|\phi\rangle = \lambda|\phi\rangle$$

The gap is exponentially small

$$\Delta_{\min}(N) = 2|E_o|2^{-N/2}$$


N=20, 5 lowest eigenvalues
$E_n(\Gamma)$
Γ
-14
-16
-18
-20
-22
-24
-26
-28
-30
0
0.2
0.4
0.6
0.8
1
1.2
$Gap_{min}(N)$
N
1
0.1
0.01
0.001
8
10
12
14
16
18
20
22
24

Generic Random First Order random $p > 2$-spin, Potts, etc etc

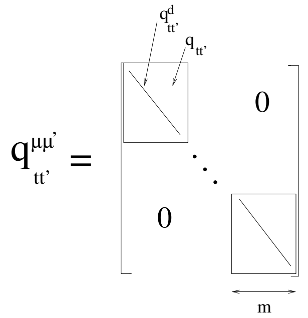


Suzuki-Trotter + Replica Approach

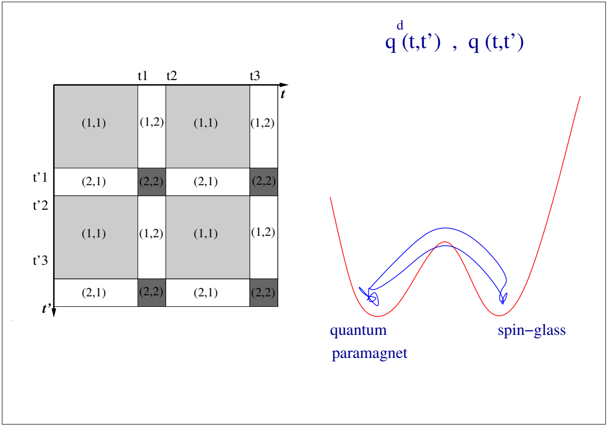
Order parameter: $q^{\mu\nu}(t, t')$

A replicated closed polymer in a random potential!

One-step RSB ansatz



A two-time instanton Approach



In general, the Gap is (minus) the exponential of the free-energy cost of a two-tme wall

It is hence the exponential of a negative extensive quantity

One can easily recover the result of the REM

In conclusion, this class of hard problems remains exponentially hard in Quantum Annealing

Not surprising: you do not thermalize a glass in real life by making it quantum.

Sign problem is more mysterious

it is understandably not hard for a quantum computer, but does not seem to require coherence (?)