Quantum annealing and the Sign Problem

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1. The 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

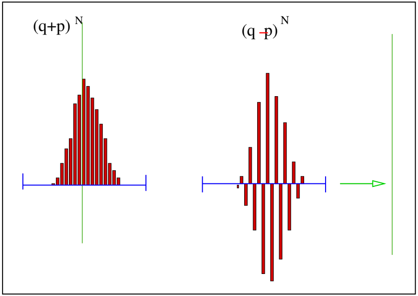
$$\langle O \rangle = \frac{\langle e^{-B}\ O \rangle_{\mathsf{A}}}{\langle e^{-B} \rangle_{\mathsf{A}}}$$

if, e.g. B is exponential in N

An example:

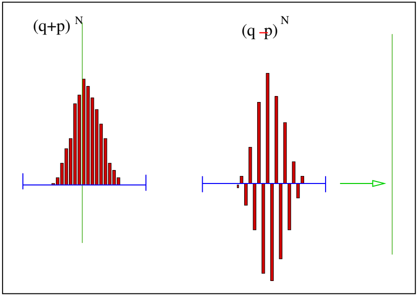
Non-interacting spins in a magnetic field $h_R + i\frac{\pi}{2}$

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



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

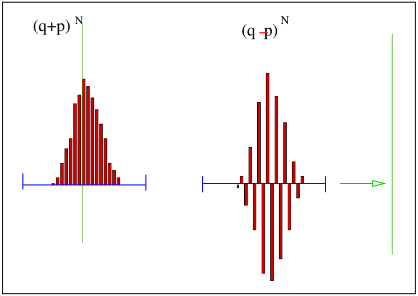
$$(q-p)^N = \sum_r \frac{N!}{r!(N-r)!}\ (-1)^r q^{N-r}p^r$$



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

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

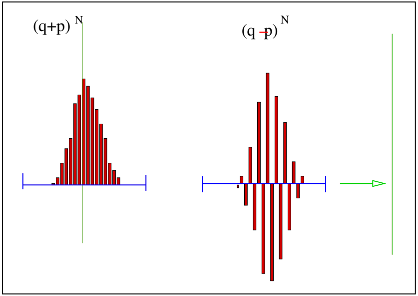
saddle: $\left(\frac{x^*}{1-x^*}\right) = \left(\frac{p}{q}\right) \quad \in \quad [0,1]$



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 $\in$ $[0,1]$

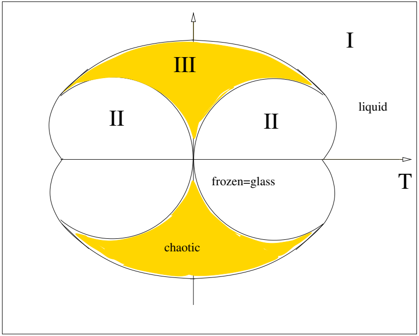


Monte Carlo Sampling of the same problem:

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

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

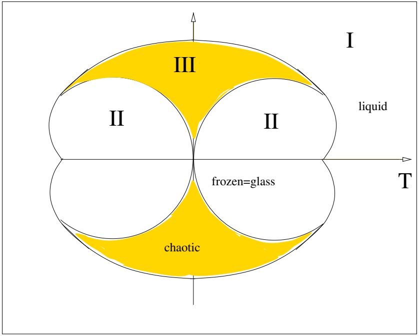
Random Energy Model



Energy levels $E_a = 1, ..., 2^N$ chosen independently from a random Gaussian distribution

and $Z = e^{-\beta E_a}$

Glass models with complex temperature Derrida, Moukarzel, Parga



- **I** Liquid: many states contribute coherently
- **II** Frozen: the lowest states contribute
- **III** Chaotic: many states contribute incoherently. Dense Lee-Yang zeroes.

Simulation time $\frac{\mathcal{T}}{\tau} \sim R \quad \rightarrow \quad R = e^{\gamma N}$ **independent variables**

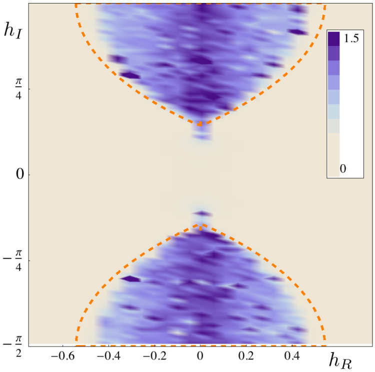
Chosen with distribution $\quad P(s) \sim e^{-W_R}$

Compute the averages: $\langle O \rangle_{estd.} = \frac{\sum_{a=1}^{R} e^{-A(s_a)-iW_I(s_a)} O(s_a)}{\sum_{a'=1}^{R} e^{-A(s_{a'})-iW_I(s_{a'})}}$

A random energy model, generated by partition function

$$\overline{\ln|\mathcal{Z}(j)|} = \sum_{s_1,\ldots,s_R} \Pi_{a=1}^{R} \, P(s_a) \;\; \ln|\mathcal{Z}_j(s_1,...,s_R)| = \overline{\ln|\sum e^{-iW_I(s)}|}$$

There are three phases, dominated by the boundary (II), by the incoherent noise (III) or by the true saddle (I)



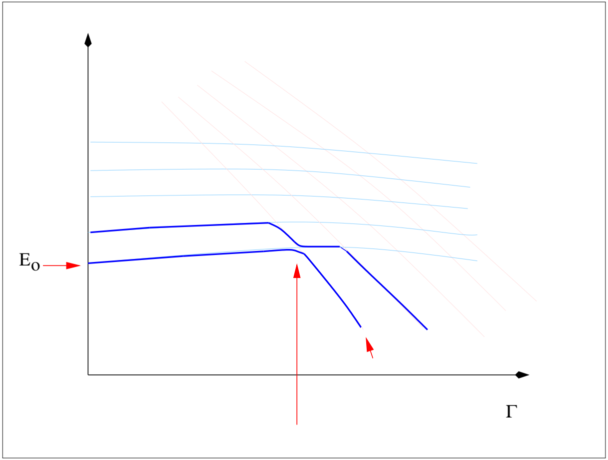
Mean-field ferromagnet in complex magnetic field: **the error.**

The boundary of the phases is: $\frac{Z(\beta,h)}{\sqrt{Z(2\beta_R,2h_R)}} = e^{N\frac{\gamma}{2}} = R^{\frac{1}{2}}$

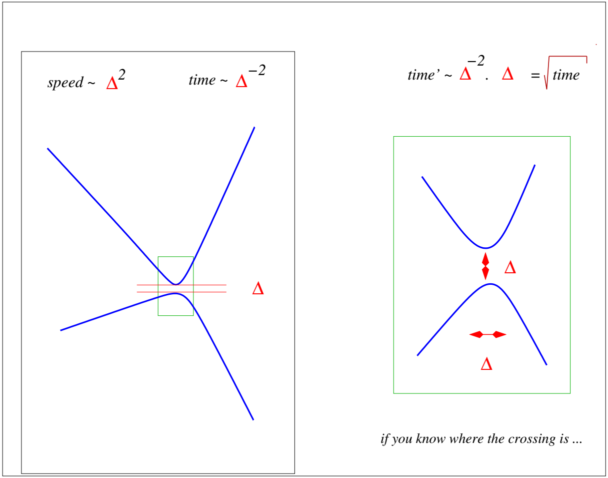
2. Grover-ish advantages

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

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

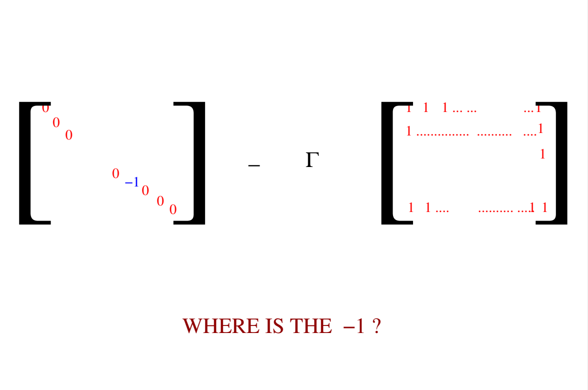


If you know where the crossing takes place, you gain a square root



Grover

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



you may find where the -1 is in $\sqrt{\text{dimension}}$

More generally: quantum amplification Brassard, Hoyer, Mosca, Tapp

For given $|-\rangle$ and output $|\psi\rangle$ you are interested in measuring $|\langle -|\psi\rangle|$

put

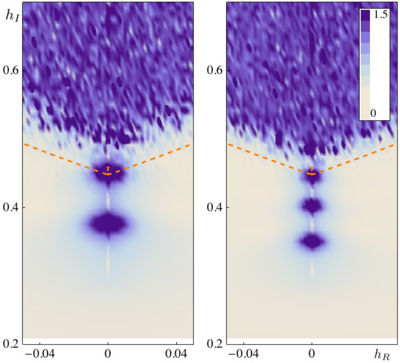
$$\mathcal{H}(\{\sigma\}) = |-\rangle\langle -| + \Gamma\, |\psi\rangle\langle\psi|$$

using the fact that the gap is $|\langle -|\psi\rangle|$, you conclude that you may measure this value in $O(|\langle -|\psi\rangle|)$

i.e. you gained a square-root

The role of the Lee-Yang zeroes

of the original model



is surprisingly not great