IHP lectures

0 Intro

* Cavity method : a method to solve stat mech models on random graphs (improved Bethe approximation)

Why ?

Mot. 1 Standard mean field : fully connected graph. (e.g. Curie-Weiss, Fisher-Fisher for Bose-Hubbard)

$$H = -\sum_{ij} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i$$

Corresponds to $d \to \infty$

But : no localization !

Random graph : leading order in a $\frac{1}{d}$ expansion (refined mean field)

THERE CAN BE LOCALIZATION : Abou-Chacra, Thouless, Anderson → Biroli

Mot. 2 Better quantitative accuracy on finite d

Mot. 3 Random graph problems are natural benchmarks for optimization algorithms. → For quantum annealing

Mot. 4 (related to 3) Entropy-driven glass transitions (e.g. in hard spheres) cannot be described by fully connected models

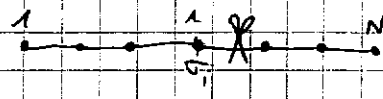
IHP Lectures

0. Intro
1. The classical cavity method & relation with large d
2. The quantum cavity method. (QQC / PIQC)
3. & some selected results

1 THE CLASSICAL CAVITY METHOD

1a- Start with 1d transfer matrix

$$H = -\sum_{i=1}^{N-1} J_i \sigma_i \sigma_{i+1} - \sum_{i=1}^{N} h_i \sigma_i$$



$$Z^i_{1\to i+1}(\sigma_i) = \sum_{\sigma_1 \dots \sigma_{i-1}} e^{+\beta \sum_{k=1}^{i-1} J_k \sigma_k \sigma_{k+1} + \beta \sum_{k=1}^{i} h_k \sigma_k}$$

Partition function when we cut the link $i \to i+1$ with fixed σ_i

$$= \sum_{\sigma_{i-1}} e^{\beta \sigma_i h_i + \beta J_{i-1} \sigma_{i-1} \sigma_i} \sum_{\sigma_1 \dots \sigma_{i-2}} e^{\beta \sum_{k=1}^{i-2} J_k \sigma_k \sigma_{k+1} + \beta \sum_{k=1}^{i-1} h_k \sigma_k}$$

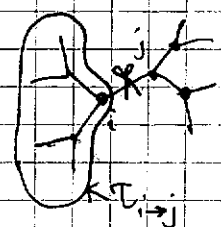
$$= e^{\beta \sigma_i h_i} \sum_{\sigma_{i-1}} e^{\beta J_{i-1} \sigma_{i-1} \sigma_i} Z_{i-1 \to i}(\sigma_{i-1})$$

Recurrence relation - [transfer matrix]

$$\vec{Z}_{1 \to i+1} = \hat{T}_i \vec{Z}_{1 \to i}$$

N matrix multiplications instead of a sum over 2^N $\{\sigma_i\}$

1b- Similarly on a tree graph.



$$H = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - \sum_{i=1}^{N} h_i \sigma_i$$

$\tau_{i\to j}$ subtree rooted at i in absence of $\langle ij \rangle$

$$Z_{1_i \to j}(\sigma_i) = \sum_{\{\sigma_k\}, k \in \{\tau_{i\to j}\} \setminus i\}} e^{-\beta H(\tau_{i\to j})}$$

Recursion:

$$Z_{1 i \to j}(\sigma_i) = e^{\beta h_i \sigma_i} \prod_{k \in \partial i \setminus j} \sum_{\sigma_k} Z_{k \to i}(\sigma_k) e^{\beta J_{ik} \sigma_i \sigma_k}$$

Note: 1 equation for each $Z_{i\to j}$

operations = # of directed links of the tree.

Computation of the free energy

Introduce "cavity messages"

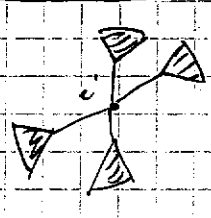
$$\eta_{i\to j}(\sigma_i) = \frac{z_{i\to j}(\sigma_i)}{\sum_{\sigma_i} z_{i\to j}(\sigma_i)} \longrightarrow \left\{ \text{marginal probability of } \sigma_i \text{ on } \tau_{i\to j} \right\}$$

$$\begin{cases} \eta_{i\to j}(\sigma_i) = \dfrac{e^{\beta h_i \sigma_i}}{z_{i\to j}} \prod_{k\in\partial i\setminus j} \sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \\ z_{i\to j} = \sum_{\sigma_i} e^{\beta h_i \sigma_i} \prod_{k\in\partial i\setminus j} \sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \end{cases}$$

recursion for η

also called "Belief Prop." BP equations

Introduce true marginals:



$$\begin{cases} z_i(\sigma_i) = e^{\beta h_i \sigma_i} \prod_{k\in\partial i} \sum_{\sigma_k} z_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \\ \eta_i(\sigma_i) = \dfrac{z_i(\sigma_i)}{\sum_{\sigma_i} z_i(\sigma_i)} = \dfrac{e^{\beta h_i\sigma_i}}{z_i} \prod_{k\in\partial i} \sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \\ z_i = \sum_{\sigma_i} e^{\beta h_i\sigma_i} \prod_{k\in\partial i} \sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \end{cases}$$

Introduce:

$$z_{ij} = \sum_{\sigma_i\sigma_j} \eta_{i\to j}(\sigma_i)\,\eta_{j\to i}(\sigma_j)\, e^{\beta J_{ij}\sigma_i\sigma_j} = \frac{z_j}{z_{j\to i}} = \frac{z_i}{z_{i\to j}}$$

obtained by using the recursion for $\eta_{i\to j}$ or $\eta_{j\to i}$

Choose any site i

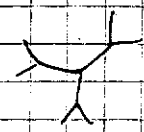
$$z_i = \sum_{\sigma_i} z_i(\sigma_i) = z_i \prod_{j\in\partial i} \left(\frac{z_{j\to i}}{z_{j\to i}} \prod_{k\in\partial j\setminus i} z_{k\to j} \cdots \right) = z_i \cdot \prod_{\substack{\text{directed links} \\ k\to j \\ \text{towards } i}} z_{k\to j} = z_i \prod_{\substack{\text{links} \\ \langle jk\rangle}} \frac{z_k}{z_{jk}}$$

$$= \frac{\prod_i z_i}{\prod_{\langle ij\rangle} z_{ij}} \longrightarrow \boxed{F = -T\log Z = -T\sum_i \log z_i + T\sum_{\langle ij\rangle} \log z_{ij}}$$

So we know how to solve models on trees. Now what?

1c. From trees to random graphs

Problem 1 On a Cayley tree a finite fraction of sites is on the boundary.



$$N = 1 + c + c(c-1) + c(c-1)^2 + \cdots c(c-1)^\ell$$

$$N_b = c(c-1)^\ell$$

$$\frac{N_b}{N} = \frac{1}{1 + \frac{1}{c-1} + \frac{1}{(c-1)^2} + \cdots} = \frac{1}{\sum_{\ell=0}^{\infty} \left(\frac{1}{c-1}\right)^\ell}$$

$$= \frac{1}{\frac{1}{1 - \frac{1}{c-1}}} = 1 - \frac{1}{c-1} > 0 \quad \text{(except if } c=2\text{)}$$

(1a) Boundary conditions are crucial

(1b) Free energy is dominated by the boundary

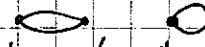
Problem 2 On a Cayley tree there is no frustration!

Partition function can be computed using $O(\#\text{directed links})$ operations

(sometimes) We want difficult problems where finding the GS takes $O(e^N)$ operations.

Random graphs: Can be easily generated.

Regular. 1 2 3 ···· $N-2$ $N-1$ N → Random permutation

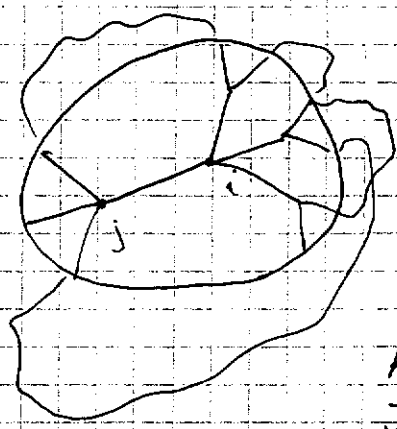
Check if  if YES reject and restart.

Erdős-Rényi: Put each link at random with prob. $p = c/N-1$

Locally tree-like: Pick a node. # of neighbors at distance ℓ: $w_\ell \sim (c-1)^\ell$

If i is a neighbor of itself: $w_\ell \sim N \rightarrow \ell \sim \frac{\log N}{\log(c-1)}$

1d Recursions on a random graph



Cut $\langle ij \rangle$.

$$\eta_{i\to j}(\sigma_i) = \frac{e^{\beta h_i \sigma_i}}{z_{i\to j}} \sum_{\{\sigma_k\}_{k\in\partial i\setminus j}} e^{\beta \sum_k J_{ik}\sigma_i\sigma_k} \eta_{(\partial i)\to i}(\{\sigma_k\})$$

The recursion is not closed.

Approximated closure: (factorization)

$$\eta_{(\partial i\setminus j)\to i}(\{\sigma_k\}) \approx \prod_{k\in\partial i\setminus j} \eta_{k\to i}(\sigma_k)$$

The cavity method consists in using the Bethe equations on random graphs, under the assumption of factorization.

Justification: ⊛ loops are long ($\log N$)

⊛ if the system is in a pure state ⇒ correlations decay with the distance ⇒ factorization is OK.

NOTE: We can try to use the cavity equation even when the approximation is not justified a priori ⇒ Belief Propagation algorithm in computer science

1e Summary RANDOM GRAPHS HAVE MANY NICE PROPERTIES

- Easy to construct numerically, easy to simulate by Monte Carlo because of finite connectivity (easier than fully connected models)
- "Translationally invariant" (better than Cayley tree: "a tree with no boundary")
- For $N\to\infty$ mean field solution via Bethe equations is correct if there is one single pure state
- Loops are there ⇒ frustration ⇒ one can construct models where finding the ground state is $\exp(N)$ (unlike on Cayley trees)

1f. **Ising ferromagnet**

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

$$\eta_{i\to j}(\sigma_i) = \frac{1}{Z_{i\to j}} \prod_{k \in \partial i \setminus j} \sum_{\sigma_k} e^{\beta J \sigma_i \sigma_k} \eta_{k\to i}(\sigma_k)$$

For $N \to \infty$ all sites are equivalent:

$$\eta_c(\sigma_i) = \frac{1}{Z_c} \left(\sum_{\sigma'} e^{\beta J \sigma' \sigma} \eta_c(\sigma') \right)^{c-1}$$

$$\eta_c(\sigma) = \frac{1 + m_c \sigma}{2} \Rightarrow m_c = \tanh\left[(c-1) \operatorname{atanh}\left(m_c \tanh(\beta J) \right) \right]$$

$$\Downarrow$$

$$m_c \approx (c-1)\, m_c \tanh(\beta J)$$

$$\Downarrow$$

$$1 = (c-1) \tanh(\beta_c J) \Leftarrow T_c = \frac{J}{\operatorname{atanh}\left(\frac{1}{c-1}\right)}$$

Choose $J = 1/c$ and $c = 2d$ to approximate a d-dimensional lattice:

$$T_c(d) = \frac{1}{2d \operatorname{atanh}\left(\frac{1}{2d-1}\right)}$$

d	$T_c^{(CM)}$	$T_c^{(exact)}$
2	0.721	0.567
3	0.822	0.752
4	0.869	0.835
5	0.896	0.878
6	0.914	0.902
7	0.926	0.919

COMPARE WITH USUAL MF THEORY:

$$m = \tanh(2\beta J m) \Rightarrow \boxed{T_c = 1}$$

1g. **Correlations**

Cavity method.

$$\langle \sigma_0 \sigma_d \rangle = \sum_{\sigma_0 \sigma_d} \sigma_0 \sigma_d \psi(\sigma_0) e^{\beta J \sigma_0 \sigma_1} \psi(\sigma_1) e^{\beta J \sigma_1 \sigma_2} \psi(\sigma_2) \cdots \psi(\sigma_{d-1}) e^{\beta J \sigma_{d-1} \sigma_d}$$

Simplest way

$$\frac{\partial \langle \sigma_0 \rangle}{\partial h_{d,m}} = \beta \langle \sigma_0 \sigma_{d,m} \rangle - \beta \langle \sigma_0 \rangle \langle \sigma_{d,m} \rangle = \beta \langle \sigma_0 \sigma_{d,m} \rangle_c$$

$$\beta \langle \sigma_0 \sigma_{d,m} \rangle_c = \frac{\partial \langle \sigma_0 \rangle}{\partial h_{d,m}} = \frac{\partial m_0}{\partial m_1} \cdot \frac{\partial m_1}{\partial m_2} \frac{\partial m_2}{\partial m_3} \cdots \frac{\partial m_{d-1}}{\partial m_d} \cdot \frac{\partial m_d}{\partial h_{d,m}}$$

$$m_0 = \tanh\left[\sum_k a\tanh\left(m_k \tanh \beta J \right) \right]$$

$$\left. \frac{\partial m_0}{\partial m_1} \right|_{m=0} = \left[1 + \tanh^2(\cdots) \right] \tanh(\beta J) = \tanh(\beta J)$$

$$\eta_d(\sigma_d) = \frac{1 + m_d \sigma}{2} = \frac{e^{\beta h_d \sigma_d}}{z} \sum_{\sigma} \left(\sum_{\sigma'} \eta(\sigma') e^{\beta J \sigma \sigma'} \right)^{c-1}$$

$$\frac{\left[2 \cosh(\beta J) \right]^{c-1}}{z} \left(1 + \beta h_d \sigma_d \right)$$

$$m_d \approx \beta h_d$$

$$\frac{\partial m_d}{\partial h_d} = \beta \longrightarrow \boxed{\langle \sigma_0 \sigma_d \rangle_c = \left[\tanh(\beta J) \right]^d}$$

NOTE: $\langle \sigma_0 \sigma_d \rangle \sim e^{-m/\xi}$ $\quad \xi = -\frac{1}{\log[\tanh(\beta J)]}$ Always finite.

However:

$$\chi = \frac{dm}{dh} = \beta \sum_{m,d=0}^{\infty} \langle \sigma_0 \sigma_{d,m} \rangle \mathcal{N}_{d,m} \qquad \text{At } \beta_c \quad \boxed{\tanh(\beta J) = \frac{1}{c-1}}$$

$$\chi \sim \sum_{m,d=0}^{\infty} \left(\frac{1}{c-1} \right)^{d,m} (c-1)^{d,m} \longrightarrow \infty$$

Correlation function in Mean field (MF++)

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \sum_i h_i \sigma_i \longrightarrow H_i = -J \sigma_i \sum_{k \in \partial i} m_k - h_i \sigma_i$$

MF equation: $m_i = \tanh\left[\beta\left(J \sum_{k \in \partial i} m_k + h_i\right)\right]$

$$\sim \beta J \sum_{k \in \partial i} m_k + \beta h_i$$

$$\sum_k \left(\delta_{ik} - \beta J A_{ik}\right) m_k = \beta h_i$$

$$\begin{cases} m(q) = \sum_k e^{Ikq} m_k & q = \frac{2\pi}{L}(n_x, n_y, \dots) \quad q \in (-\pi, \pi) \quad n_\alpha \in \left(-\frac{L}{2}, \frac{L}{2}\right) \\ m_k = \frac{1}{L^d} \sum_q e^{-Ikq} m_q \end{cases}$$

$$\frac{1}{L^d} \sum_q m_q \left(e^{-Iiq} - \beta J e^{-Iiq} \sum_\alpha 2\cos q_\alpha\right) = \frac{1}{L^d} \sum_q e^{-Iiq} \beta h_q$$

$$m_q = \beta h_q \cdot \frac{1}{1 - \beta J \sum_\alpha 2\cos q_\alpha} \longrightarrow m_k = \frac{1}{L^d} \sum_q e^{-Ikq} \frac{\beta h_q}{1 - \beta J \sum_\alpha 2\cos q_\alpha}$$

$$= \frac{\beta}{L^d} \sum_q e^{-Ikq} \frac{\sum_i e^{Iiq} h_i}{1 - \beta J \sum_\alpha 2\cos q_\alpha}$$

$$\beta \langle \sigma_i \sigma_k \rangle_c = \frac{dm_k}{dh_i} = \frac{\beta}{L^d} \sum_q e^{I(i-k)q} \frac{1}{1 - \beta J \sum_\alpha 2\cos q_\alpha} \longrightarrow \frac{\beta}{(2\pi)^d} \int dq \frac{e^{I(i-k)q}}{1 - \beta J \sum_\alpha 2\cos q_\alpha}$$

$$\longrightarrow \langle \sigma_0 \sigma_n \rangle_c = \frac{1}{(2\pi)^d} \int dq \frac{e^{I(n)q_x}}{1 - \beta J \sum_\alpha 2\cos q_\alpha} = \frac{1}{(2\pi)^d} \int dq\, e^{I(n)q_x} \int_0^\infty d\lambda\, e^{-\lambda\left(1 - 2\beta J \sum_\alpha \cos q_\alpha\right)}$$

$$= \int_0^\infty d\lambda\, e^{-\lambda} \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} dq\, e^{Inq + 2\beta J \lambda \cos q}\right)^{d-1} = \int_0^\infty d\lambda\, e^{-\lambda} \left[I_0(2\beta J\lambda)\right]^{d-1} \times \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} dq\, e^{2\beta J \lambda \cos q}\right)$$

$$I_n(2\beta J\lambda)$$

Remember $J = \frac{1}{2d} \longrightarrow T_c = 1$

Comparison of correlations

Bethe lattice

$$C(n) = \left[\tanh\left(\frac{\beta}{2d}\right)\right]^n$$

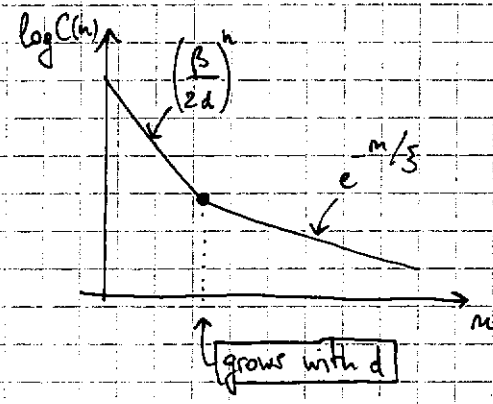
Mean field

$$C(n) = \int_0^\infty d\lambda\, e^{-\lambda} I_0\left(\frac{\beta\lambda}{d}\right)^{d-1} I_n\left(\frac{\beta\lambda}{d}\right)$$

$$\begin{cases} n,\ \beta<1 \text{ fixed} \\ d\to\infty \end{cases} \qquad C(n) \approx \left(\frac{\beta}{2d}\right)^n$$

$$\begin{cases} d,\ \beta<1 \text{ fixed} \\ n\to\infty \end{cases} \qquad C(n) \approx e^{-n/\xi}$$

$$\xi = \frac{\beta/2d}{(1-\beta)^{1/2}}$$



Lecture 2

Summary

1. Statistical models on random graphs
   - ⊛ Mean field models (MF)
   - ⊛ Easy to construct
     Easy to simulate numerically
   - ⊛ "Translationally invariant"
   - ⊛ Loops are there → there can be frustration
     (exp N to find the ground state)
     Good MF models for glasses
   - ⊛ In quantum models there can be localization.

2. (RS) Cavity method: use equation for trees on random graphs under the assumption that
   a) loops are long ($\log N$)
   b) correlations decay fast enough

$$\begin{cases} \eta_{i\to j}(\sigma_i) = \dfrac{1}{z_{i\to j}} e^{\beta h_i \sigma_i} \prod_{k\in\partial i\setminus j} \left(\sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \right) \\ \qquad\qquad = F_{i\to j}\left[\{\eta_{k\to i}\} \right] \\ z_i = \sum_{\sigma_i} e^{\beta h_i \sigma_i} \prod_{k\in\partial i} \left(\sum_{\sigma_k} \eta_{k\to i}(\sigma_k)\, e^{\beta J_{ik}\sigma_i\sigma_k} \right) \\ Z_{ij} = \sum_{\sigma_i,\sigma_j} \eta_{i\to j}(\sigma_i)\, \eta_{j\to i}(\sigma_j)\, e^{\beta J_{ij}\sigma_i\sigma_j} \\ F = -T \sum_{i=1}^{N} \log z_i + T \sum_{\langle ij\rangle} \log Z_{ij} \end{cases}$$

↑ On a given graph it allows to compute the partition function in $\mathrm{poly}(N)$ operations

- exact on trees
- approximate on a given RG

3. $N \to \infty$ on an ensemble of random graphs

3a. Ordered models: $\eta_{i\to j} \longrightarrow \eta_c$ for all i,j

- Mean-field-like self-consistent equation for η_c
- Ferromagnetic transition
- Correlations give the correct result when $d \to \infty$

3b. Disordered models: $H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i$

$P(J)$, $P(h)$, $P(g)$ distribution of the disorder

$\Downarrow$ induces a

$P[\eta]$ distribution of $\eta_{i\to j}$ over the disorder for a given link (but it must be the same for all links)

Self consistency equation:

$$\begin{cases} \eta \overset{d}{=} F[\eta_1 \cdots \eta_{c-1}] \\ P[\eta] = \int dP[\eta_1]\cdots dP[\eta_{c-1}]\ \delta\left(\eta - F[\eta_1 \cdots \eta_{c-1}]\right) \end{cases} \quad \{J, h, c-1\}$$

3c. 1RSB

Assume that there are many pure states.

Each pure state is a solution of BP

$$\eta^{(\alpha)}_{i\to j} = F_{i\to j}\left[\eta^{(\alpha)}_{k\to i}\right] \qquad f^{(\alpha)} = \frac{1}{N} F[\eta^{(\alpha)}]$$

Count all the solution:

$$\mathcal{Z} = \int D\eta\ e^{-\beta F^{(\alpha)}} \cdot \delta\left[\eta^{(\alpha)}_{i\to j} - F[\eta^{(\alpha)}_{\cdot\to i}]\right]$$

"Messages on messages"

Many quantum cavity works.

Motivations: 1) Localization (Many-Body)
2) Quantum glasses
3) Quantum algorithms

equations. In Sec. 6.2 and 6.3 we shall present explicit results on two models of random constraint satisfaction problems obtained in this way.

It is however important to mention the limitations of the method. As already explained at the beginning of this section, it can only handle quantum systems that do not suffer from the sign problem, and it is a finite temperature method; the ground state properties are necessarily obtained by an extrapolation to zero temperature. Moreover the numerical resolution of the quantum cavity equations is a numerically costly task. The generic quantum 1RSB case involves indeed a representation by $\mathcal{N}_{\rm ext} \times \mathcal{N}_{\rm int} \times \mathcal{N}_{\rm traj}$ imaginary time trajectories[3] (recall the discussion of Sec. 5.1.5 in the classical case and the additional population level due to the quantum nature of the model explained in Eq. (94)). Fortunately for factorized models (with regular degrees) this is reduced with $\mathcal{N}_{\rm ext} = 1$, see the end of Sec. 5.1.5. In any case the memory available on present days computers limit the numbers $\mathcal{N}_{\rm int}$ and $\mathcal{N}_{\rm traj}$ to relatively small values (examples will be given on concrete cases in Sec. 6.2 and 6.3). This induces both systematic deviations of the empirical mean from the exact value and noise in its estimation; extrapolations to $\mathcal{N}_{\rm int}, \mathcal{N}_{\rm traj} \to \infty$ via finite size analysis can however be performed to reduce these effects. A specific difficulty comes from the weighted representations of probability distributions used in Eq. (94) for instance; one must take care by resampling methods of the tendency that these weights have to flow towards very inhomogeneous repartitions, which leads to situation where the number of effective representants of the distribution becomes much smaller than $\mathcal{N}_{\rm traj}$ [234].

In the following sections we shall describe alternative approaches to quantum models on sparse random graphs that, even if approximate, allow to bypass some of these limitations.

5.3. Operator quantum cavity methods

In this section we shall describe alternative formulations of the quantum cavity method that do not make use of the path integral formulation but work directly with quantum operators [242, 221, 222, 223, 224, 225, 243, 226]. These approaches have been sometimes called "quantum belief propagation" but we will refer to them here as Operator Quantum Cavity (OQC) methods. They all share common features and ideas whose connections are still only partially understood. They represent approximated methods, and their level of accuracy is not completely controlled yet. However, compared to path integral methods they have the important advantage that the $T = 0$ limit can be taken explicitly. Moreover, the cavity messages are represented as finite matrices, therefore there are no sampling errors, unlike in the PIQC where the messages are represented through finite samples of probability distributions over an infinite-dimensional space.

[3] An alternative approach, that will not be further discussed here, consists in a systematic perturbative expansion in the transverse field Γ; any finite order of the expansion can be expressed in terms of the classical cavity computation, thus strongly reducing the numerical cost with respect to the fully quantum approach. This however does not give access to non-perturbative effects like phase transitions

For the sake of simplicity, we will present these methods in the simpler case of an Hamiltonian that is the sum of two-body interactions:

$$\widehat{H} = \sum_{\langle i,j \rangle} \widehat{H}_{i,j} \,. \tag{107}$$

The sum over $\langle i,j \rangle$ runs on the links of a regular lattice of degree c. We will mainly focus on the case $c = 2$ of a one dimensional chain, and $c = 3$ with the underlying lattice being a 3-regular random graph. Moreover we will consider the case of an Ising model in a transverse field for which $\widehat{H}_{i,j} = -J_{ij}\widehat{\sigma}_i^z\widehat{\sigma}_j^z - (\Gamma_i\widehat{\sigma}_i^x + \Gamma_j\widehat{\sigma}_j^x)/c$. The generalization to more complex Hamiltonians is straightforward.

5.3.1. Operator cavity messages

We start our presentation by following the derivation of [223] and considering for simplicity a finite one-dimensional chain with open boundaries. The quantum partition function is

$$Z = \mathrm{Tr}\, e^{-\beta\widehat{H}} = \mathrm{Tr}\left(e^{-\beta\widehat{H}_{1,2}} \odot e^{-\beta\widehat{H}_{2,3}} \odot \cdots \odot e^{-\beta\widehat{H}_{N-1,N}}\right) , \tag{108}$$

where $e^A \odot e^B = e^{A+B}$. As in the classical case, we can define an operatorial message that acts on the Hilbert space of spin i only:

$$\eta_{i\to i+1} = \frac{1}{z_{i\to i+1}} \mathrm{Tr}_{1,\cdots,i-1}\, e^{-\beta\sum_{k=1}^{i-1}\widehat{H}_{k,k+1}} , \tag{109}$$

where the normalization is determined by $\mathrm{Tr}_i\, \eta_{i\to i+1} = 1$.

We can derive an approximate recurrence equation for these messages by following the same steps as in the classical case:

$$\begin{aligned}
\eta_{i\to i+1} &\propto \mathrm{Tr}_{1,\cdots,i-1}\left(e^{-\beta\sum_{k=1}^{i-2}\widehat{H}_{k,k+1}} \odot e^{-\beta\widehat{H}_{i-1,i}}\right) \\
&= \mathrm{Tr}_{i-1}\left\{\mathrm{Tr}_{1,\cdots,i-2}\left[e^{-\beta\sum_{k=1}^{i-2}\widehat{H}_{k,k+1}} \odot e^{-\beta\widehat{H}_{i-1,i}}\right]\right\} \\
&\sim \mathrm{Tr}_{i-1}\left\{\left[\mathrm{Tr}_{1,\cdots,i-2} e^{-\beta\sum_{k=1}^{i-2}\widehat{H}_{k,k+1}}\right] \odot e^{-\beta\widehat{H}_{i-1,i}}\right\} \\
&\propto \mathrm{Tr}_{i-1}\left(\eta_{i-1\to i} \odot e^{-\beta\widehat{H}_{i-1,i}}\right) ,
\end{aligned} \tag{110}$$

and the proportionality constant is determined by normalization as in the classical case. The crucial point is that, unlike in the classical case, here we made an approximation when we changed the position of the square brackets moving from the second to the third line of the above equation.

Indeed, consider a system made of three parts a, b, c and operators $\widehat{H}_{a,b}$, $\widehat{H}_{b,c}$, acting only on $a \otimes b$ and $b \otimes c$ respectively. Due to quantum entanglement

$$\mathrm{Tr}_a\left[e^{-\beta\widehat{H}_{a,b}} \odot e^{-\beta\widehat{H}_{b,c}}\right] \neq \left[\mathrm{Tr}_a e^{-\beta\widehat{H}_{a,b}}\right] \odot e^{-\beta\widehat{H}_{b,c}} . \tag{111}$$

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However, the above equation is an equality if the "conditional mutual information" $I(a:c|b) = S(a,c) + S(b,c) - S(b) - S(a,b,c)$ vanishes (here S is the von Neumann entropy), indicating that all correlations between a and c are mediated through b (as in the classical case). It has been argued that this condition holds when the region b is sufficiently "thick" [223]. The problem is that in Eq. (110) the region b coincides with a single spin, $b = \{i-1\}$.

This observation motivates the introduction of new messages, that are operators on the space of spins $\{i-\ell+1, \cdots, i\}$. Repeating the above derivations:

$$\begin{aligned} \eta^{(\ell)}_{i\to i+1} &= \frac{1}{z_{i\to i+1}} \mathrm{Tr}_{1,\cdots,i-\ell} e^{-\beta \sum_{k=1}^{i-1} \widehat{H}_{k,k+1}} \\ &\propto \mathrm{Tr}_{i-\ell} \left\{ \mathrm{Tr}_{1,\cdots,i-\ell-1} \left[e^{-\beta \sum_{k=1}^{i-2} \widehat{H}_{k,k+1}} \odot e^{-\beta \widehat{H}_{i-1,i}} \right] \right\} \\ &\sim \mathrm{Tr}_{i-\ell} \left\{ \left[\mathrm{Tr}_{1,\cdots,i-\ell-1} e^{-\beta \sum_{k=1}^{i-2} \widehat{H}_{k,k+1}} \right] \odot e^{-\beta \widehat{H}_{i-1,i}} \right\} \\ &\propto \mathrm{Tr}_{i-\ell} \left(\eta^{(\ell)}_{i-1\to i} \odot e^{-\beta \widehat{H}_{i-1,i}} \right) \end{aligned} \tag{112}$$

The crucial difference is that now the region $b = \{i-\ell, \ldots, i-1\}$ has thickness ℓ and one can hope that the error is much smaller. An argument in favor of this has been discussed in [223]. The drawback is of course that now the messages are operators acting on ℓ spins, and therefore they have to be represented by matrices of size 2^ℓ.

The generalization of this procedure to a tree is straightforward. Let us call $\mathcal{T}_{i\to j}$ the partial tree rooted at i obtained by cutting the link $\langle i,j\rangle$, and $d(i,j)$ the distance on the tree between i and j. The message from i to j is defined as

$$\eta^{(\ell)}_{i\to j} = \frac{1}{z_{i\to j}} \mathrm{Tr}_{\{k\in\mathcal{T}_{i\to j}, d(i,k)\geq \ell\}} e^{-\beta \sum_{\langle k,l\rangle \in \mathcal{T}_{i\to j}} \widehat{H}_{k,l}} , \tag{113}$$

and we get as in the classical case:

$$\eta^{(\ell)}_{i\to j} \propto \mathrm{Tr}_{\{k\in\mathcal{T}_{i\to j}, d(i,k)=\ell\}} \left\{ \bigodot_{k\in\partial i\setminus j} \left(\eta^{(\ell)}_{k\to i} \odot e^{-\beta \widehat{H}_{k,i}} \right) \right\} . \tag{114}$$

Here, the messages are operators acting on $1+(c-1)+(c-1)^2+\cdots+(c-1)^{\ell-1}$ spins, so they must be represented by matrices whose size $2^{\sum_{k=0}^{\ell-1}(c-1)^k}$ grows much faster than in the one dimensional case.

With similar reasonings one can obtain the approximate expression for the free energy, which is exactly the same as in the classical case (here specialized to a system with two-body interactions only), with sums replaced by traces and the normal product replaced by the $\odot$ product:

$$\begin{aligned} -\beta F &= \sum_i \log z_i - \sum_{\langle i,j\rangle} \log z_{ij} , \\ z_i &= \mathrm{Tr}_{i, \cup_{j\in\partial i}\{k\in\mathcal{T}_{j\to i}, d(j,k)<\ell\}} \left[\bigodot_{j\in\partial i} \left(\eta^{(\ell)}_{j\to i} \odot e^{-\beta \widehat{H}_{j,i}} \right) \right] , \\ z_{ij} &= \mathrm{Tr}_{\{k\in\mathcal{T}_{i\to j}, d(i,k)<\ell\}\cup\{k\in\mathcal{T}_{j\to i}, d(j,k)<\ell\}} \left(\eta^{(\ell)}_{i\to j} \odot \eta^{(\ell)}_{j\to i} \odot e^{-\beta \widehat{H}_{i,j}} \right) . \end{aligned} \tag{115}$$

5.3.2. Explicit equations for single-spin messages

Let us now consider more explicitly the above OQC formulation on a tree with $\ell = 1$. In this case the messages are operators on a single spin, i.e. 2×2 Hermitian matrices normalized to have trace 1. We can parametrize them by two local fields:

$$\eta_{i\to j} = \frac{1}{z_{i\to j}} e^{\beta(b_{i\to j}\widehat{\sigma}^x_i + h_{i\to j}\widehat{\sigma}^z_i)} , \tag{116}$$

omitting a term proportional to $\widehat{\sigma}^y_i$ that vanishes by symmetry. Equivalently we can describe the message $\eta_{i\to j}$ in terms of the magnetizations

$$\begin{aligned} m^x_{i\to j} &= \mathrm{Tr}_i(\widehat{\sigma}^x_i \eta_{i\to j}) = \frac{b_{i\to j}}{\sqrt{h^2_{i\to j} + b^2_{i\to j}}} \tanh\left[\beta\sqrt{h^2_{i\to j} + b^2_{i\to j}}\right] \\ m^z_{i\to j} &= \mathrm{Tr}_i(\widehat{\sigma}^z_i \eta_{i\to j}) = \frac{h_{i\to j}}{\sqrt{h^2_{i\to j} + b^2_{i\to j}}} \tanh\left[\beta\sqrt{h^2_{i\to j} + b^2_{i\to j}}\right] \end{aligned} \tag{117}$$

Plugging this in Eq. (114) with $\ell = 1$ we obtain

$$e^{\beta(b_{i\to j}\widehat{\sigma}^x_i + h_{i\to j}\widehat{\sigma}^z_i)} \propto \mathrm{Tr}_{k\in\partial i\setminus j} e^{\beta \sum_{k\in\partial i\setminus j}[b_{k\to i}\widehat{\sigma}^x_k + h_{k\to i}\widehat{\sigma}^z_k - \widehat{H}_{k,i}]} \tag{118}$$

which can be recast in the following form:

$$m^x_{i\to j} = \frac{\mathrm{Tr}_{i,k\in\partial i\setminus j}(\widehat{\sigma}^x_i e^{-\beta \widehat{H}_{\mathrm{eff}}})}{\mathrm{Tr}_{i,k\in\partial i\setminus j}(e^{-\beta \widehat{H}_{\mathrm{eff}}})} , \tag{119}$$

and similarly for $m^z_{i\to j}$, where

$$\begin{aligned} \widehat{H}_{\mathrm{eff}} &= \sum_{k\in\partial i\setminus j} \widehat{H}_{k,i} - b_{k\to i}\widehat{\sigma}^x_k - h_{k\to i}\widehat{\sigma}^z_k \\ &= -\sum_{k\in\partial i\setminus j} \left[J_{ik}\widehat{\sigma}^z_i\widehat{\sigma}^z_k + (\Gamma_i\widehat{\sigma}^x_i + \Gamma_k\widehat{\sigma}^x_k)/c + b_{k\to i}\widehat{\sigma}^x_k + h_{k\to i}\widehat{\sigma}^z_k \right] \end{aligned} \tag{120}$$

is an effective Hamiltonian acting on spin i and its neighbors (except j). Iteration of these equations then requires at each step the diagonalization of a Hamiltonian acting on c spins. Note that taking the $T = 0$ limit is straightforward and simplifies the computation, because in this case we only need to find the ground state of $\widehat{H}_{\mathrm{eff}}$.

One can actually take a different approach and substitute Eq. (116) in the free energy Eq. (115), obtaining then a function of the set of all fields $b_{i\to j}$ and $h_{i\to j}$. One can then derive equations for these fields by imposing stationarity of the free energy with respect to variations of any field, as in the classical case. However, because the OQC is only approximate, the stationarity equations *do not coincide* with the equations obtained from cavity iteration, Eqs. (117), (119), (120). It can be shown on specific examples (e.g. the ferromagnetic case $J_{ij} = J$ and $\Gamma_i = \Gamma$) that imposing stationarity of the free energy is slightly more accurate than the iteration scheme.

Let us also mention a further approximation that has been proposed in [225, 243, 226], which amounts to replace the operators $\widehat{\sigma}_k^x, \widehat{\sigma}_k^z$ in Eq. (120) by their averages $m_{k\to i}^x, m_{k\to i}^z$ in Eq. (117). One thus obtains the following equations:

$$b_{i\to j} = \frac{c-1}{c}\Gamma_i \ ,$$

$$h_{i\to j} = \sum_{k\in\partial i\setminus j} J_{ki} m_{k\to i}^z = \sum_{k\in\partial i\setminus j} \frac{J_{ki} h_{k\to i}}{\sqrt{h_{k\to i}^2 + b_{k\to i}^2}} \tanh\left[\beta\sqrt{h_{k\to i}^2 + b_{k\to i}^2}\right] \ .$$

These are closed and relatively simple equations for the fields $h_{i\to j}$ and have been exploited in [225, 243] to obtain detailed information on a disordered system that would have been extremely hard to obtain from the numerical solution of the OQC or PIQC equations. Additionally, it is clear from these equations that one can take the $\beta \to \infty$ limit without problems just by dropping the hyperbolic tangent term. A drawback of this approach is that these equations are approximate, even in the classical case $\Gamma_i = 0$. It has been argued in [225, 243] that they become exact for $c \to \infty$, see [226] for a detailed discussion. However, this is only true for weakly frustrated models: in situations where frustration is strong enough that messages can lead to contradictions (e.g. in XORSAT at zero temperature) this approximation is not reliable.

5.3.3. Relation with the PIQC

The OQC has been introduced in [225, 243], independently from [223], to study the metal-insulator transition in disordered superconductor and later used in [226] to discuss the properties of disordered ferromagnets. The derivation of [225, 243, 226] starts from the PIQC formulation and makes a simple ansatz on the functional form of the distribution of imaginary time trajectories. In turn, this can be reinterpreted as an ansatz over the Hamiltonian governing a reduced part of the system, consisting of neighboring spins, and gives back the OQC.

The PIQC leads to the following equation (which is the specialization of the treatment of Sec. 5.2 to Ising spins, see also [220]):

$$\eta_{i\to j}(\sigma_i) = \frac{\Gamma_i^{|\sigma_i|}}{z_{i\to j}} \prod_{k\in\partial i\setminus j} \int D\sigma_k \, \eta_{k\to i}(\sigma_k) e^{J_{ik}\int_0^\beta \sigma_i(t)\sigma_k(t)\mathrm{d}t} \ , \qquad (121)$$

where $|\sigma_i|$ is the number of spin flips in the imaginary time trajectory σ_i. In order to simplify the solution of these self-consistent equations, in [225, 243, 226] it was suggested to consider the following ansatz:

$$\eta_{i\to j}(\sigma_i) \propto (b_{i\to j})^{|\sigma_i|} e^{\int_0^\beta h_{i\to j}\sigma_i(t)\mathrm{d}t} \ . \qquad (122)$$

Once inserted in the right hand side of Eq. (121) this ansatz doesn't give back in the left hand side a message of the same form. However one can take its "projection" over the distributions of trajectories described by (122), by fixing

the new fields $h_{i\to j}$ and $b_{i\to j}$ in such a way that the expectation values of $\widehat{\sigma}_i^x$ and $\widehat{\sigma}_i^z$ on the two sides of Eq. (121) are the same. Not surprisingly, it is easy to show that this procedure gives back[4] the same equations as the OQC for $\ell = 1$, Eqs. (117), (119), (120). It was shown in [226] that this approximation gives quite good results when compared with the exact PIQC solution, and the quality of the approximation increases with increasing connectivity c.

For $\ell > 1$, the connection between OQC and PIQC is less obvious. We will not discuss it in detail, but roughly speaking the idea is the following. The Markovian ansatz in Eq. (122) neglects all imaginary time correlations in the path integral description of spin i. Therefore, a more refined ansatz would include, for instance, a Gaussian term $\int_0^\beta \mathrm{d}t\mathrm{d}t' G_{i\to j}(t-t')\sigma_i(t)\sigma_i(t')$ in the exponent [219]. In presence of such a term, the PIQC equations cannot be cast in an operator formulation using only local operators. The reason is that these imaginary time correlations are obtained by tracing out the neighboring spins. In the PIQC representation, this could be represented by consider a Markovian ansatz acting not only on i but also on a neighboring shell of size ℓ, and then integrating out the neighbors to obtain an imaginary time correlated message on spin i. In the OQC language, this should correspond indeed to an operator message acting on spin i and a set of neighbors. We conclude that messages with $\ell > 1$ in the OQC should roughly correspond to adding some imaginary time correlations in the PIQC. This is very reminiscent of what is done in dynamical mean field theory where imaginary time correlations are often represented by an Hamiltonian thermal bath of phonons [244].

5.3.4. Discussion

OQC [242, 221, 222, 223, 224, 225, 243, 226] (or Quantum Belief Propagation) is a very promising approach to the solution of spin glass models on locally tree-like graphs. First of all, this method is not affected by the "sign problem" and therefore can be applied to Hamiltonians that do not admit a path integral representation with positive weights (e.g. the QSAT problem [54]). Another important advantage is that for a given ℓ the cavity messages are finite matrices that can be parametrized by a finite set of real numbers. The accuracy of this representation is only limited by machine precision, unlike in the case of PIQC where sampling introduces systematic numerical errors and noise. For a given ℓ, the limit $T = 0$ can be taken easily by replacing everywhere the traces at finite temperature by a ground state average.

Its main drawback is that it is an approximate method: its accuracy is expected to increase with the size of the block ℓ. If one requires a given accuracy, then the block size must be increased when decreasing T and $\ell \to \infty$ for $T \to 0$ [223] (however, there is some hope to combine OQC with local renormalization

[4] Actually, there is a slight difference due to the fact that in the OQC formulation above we chose to symmetrize the local Hamiltonian $\widehat{H}_{i,j}$. The PIQC leads naturally to a non-symmetric formulation where $\widehat{H}_{i,j} = -J_{i,j}\widehat{\sigma}_i^x\widehat{\sigma}_j^x - \Gamma_j\widehat{\sigma}_j^x/(c-1)$. This difference should not be crucial, especially for large c where approximation (122) is better justified.

SUMMARY OF OQC

1. Any possible Hamiltonian
2. Finite matrices messages are a finite numb. of reals
3. Approximate
4. Quality increases with ℓ (but 2^ℓ)
5. Can be used directly at $T=0$

LECTURE 3

Fermions, PIQC

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \sum_i \mu_i n_i$$

$$Z_i = \int d\bar{a}_i \, da_i \; e^{-\int_0^\beta d\tau \left[\sum_i \bar{a}_i (\partial_\tau - \mu_i) a_i - t \sum_{\langle ij \rangle} (\bar{a}_i a_{i+1} + \bar{a}_{i+1} a_i) \right]}$$

Cavity equations

$$m_{i \to j}(\bar{a}_i, a_i) = \frac{e^{-\int_0^\beta d\tau \, \bar{a}_i (\partial_\tau - \mu_i) a_i}}{Z_{i \to j}} \prod_{k \in \partial i \setminus j} \left[\int d\bar{a}_k \, da_k \, m_{k \to i}(\bar{a}_k, a_k) \times e^{t \int_0^\beta d\tau (\bar{a}_k a_i + \bar{a}_i a_k)} \right]$$

Gaussian

$$m_{i \to j}(\bar{a}_i, a_i) \propto e^{-\int_0^\beta d\tau \, d\tau' \, \bar{a}_i(\tau) \, G^{-1}_{i \to j}(\tau - \tau') \, a_i(\tau')}$$

$$\int d\bar{a}_k \, da_k \; e^{-\int_0^\beta d\tau \, d\tau' \, \bar{a}_k(\tau) \, G^{-1}_{k \to i}(\tau - \tau') \, a_k(\tau') + t \int_0^\beta d\tau (\bar{a}_k a_i + \bar{a}_i a_k)}$$

$$\propto e^{t^2 \int_0^\beta d\tau \, d\tau' \, \bar{a}_i(\tau) \, G_{k \to i}(\tau - \tau') \, a_i(\tau)}$$

$$\rightarrow \quad G^{-1}_{i \to j}(\tau - \tau') = (\partial_\tau - \mu_i) \, \delta(\tau - \tau') - t^2 \sum_{k \in \partial i \setminus j} G_{k \to i}(\tau - \tau')$$

$$\boxed{\frac{1}{G_{i \to j}(i\omega_n)} = i\omega_n - \mu_i - t^2 \sum_{k \in \partial i \setminus j} G_{k \to i}(i\omega_n)}$$

$$\Downarrow$$

$$P\left[G^{(0)}_{i \to j}(i\omega_n) \right] = \int dP[G_1] \cdots dP[G_{c-1}] \cdot \delta\left(t \, G_0 = \frac{1}{i\omega_n - \mu_0 - t^2 \sum_{\ell=1}^{c-1} G_\ell} \right)$$

Abou-Chakra
Anderson
Thouless 1973

Bosons

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + U \sum_i n_i(n_i - 1)$$

$$\psi = (\bar{a}, a)$$

$$\eta_c(\psi) = \frac{1}{Z_c} w(\psi)\, e^{(c-1)\Gamma[J\psi]}$$

$$\Gamma[\phi] = \log\left[\int D\psi\ \eta_c(\psi)\, e^{\int_0^\beta d\tau (\psi^\dagger \phi)}\right] \rightarrow$$ Generating functional of connected correlations of ψ on $\eta_c(\psi)$

$$\begin{cases} \Gamma[\phi] = \int_0^\beta d\tau\ \phi_c^\dagger(\tau) \cdot \phi(\tau) + \int_0^\beta d\tau\, d\tau'\ \phi^\dagger(\tau)\ \hat{G}_c(\tau - \tau')\ \phi(\tau) + \cdots \\ \quad \begin{cases} \phi_c^\dagger(\tau) = \langle \psi^\dagger(\tau) \rangle_{\eta_c} \\ \hat{G}_c(\tau) = \langle \psi(\tau)\psi^\dagger(\tau') \rangle_{\eta_c} - \langle \psi(\tau) \rangle_{\eta_c} \langle \psi^\dagger(\tau') \rangle_{\eta_c} \end{cases} \end{cases}$$

$$\rightarrow \eta_c(\psi) = \frac{1}{Z_c} w(\psi)\, e^{(c-1)\left[J \int d\tau\ \phi_c^\dagger \cdot \phi + J^2 \int d\tau d\tau'\ \phi^\dagger \cdot \hat{G}_c \phi + \cdots\right]}$$

$\Downarrow$

Compute self-consistently ϕ_c and $\hat{G}_c$ $\Rightarrow$ DMFT equations

→ Semerjian Tarzia Zamponi
PRB 80, 014524 (2009)

→ Anders, Gull, Pollet, Troyer, Werner
New J. Phys. 13, 075013 (2011)
[arXiv 1103.0017]

For spins, Laumann-Scardicchio-Sondhi PRB 78, 134424 (2008)
[First paper on quantum cavity method]
for disordered systems

a supplementary "discrete imaginary time" coordinate (which becomes a continuous parameter in the $N_s \to \infty$ limit). The important point is that the spatial structure of the graph of interactions is preserved in this construction, at the price of the introduction of imaginary time-dependent classical degrees of freedom. In particular, if the interactions of the quantum model are defined on a tree-like graph, the cavity method still applies to this extended classical model. This line of thought was first followed for quantum spin models in [32] (see also [33]) for a finite number N_s of Suzuki-Trotter slices, the continuous imaginary time limit was then taken in [34]. In this paper we shall extend this method to deal with lattice bosons models.

In this case the decomposition of the identity operator in the Suzuki-Trotter can be expressed using either coherent states or occupation numbers. The latter has the advantage of being discrete, and we shall use it in the rest of the paper. For the sake of clarity and in order to make contact with the recently proposed B-DMFT [23, 24] we discuss first the application of the cavity method within the coherent states representation in the rest of this subsection. Inserting such a decomposition of the identity for each of the N sites at each of the N_s Suzuki-Trotter slices leads, in the continuous time limit $N_s \to \infty$, to the coherent state path integral expression of the partition function of the Bose-Hubbard model [35]:

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + U \sum_i n_i(n_i - 1)$$

$$Z = \int \prod_{i=1}^{N} D\boldsymbol{a}_i D\bar{\boldsymbol{a}}_i \, e^{-S} , \tag{19}$$

$$S = \int_0^\beta \mathrm{d}\tau \left[\sum_{i=1}^{N} \left(\bar{a}_i(\tau)(\partial_\tau - \mu) a_i(\tau) + \frac{U}{2} (\bar{a}_i(\tau) a_i(\tau))^2 \right) - J \sum_{\langle i,j \rangle} (\bar{a}_i(\tau) a_j(\tau) + \bar{a}_j(\tau) a_i(\tau)) \right] . \tag{20}$$

Here and in the following we use bold symbols to denote imaginary-time dependent quantities. $a_i(\tau)$ and $\bar{a}_i(\tau)$ are two (formally conjugate) complex numbers indexing the coherent state at site i and imaginary time τ, with $D\boldsymbol{a}_i D\bar{\boldsymbol{a}}_i$ the path-integral measure of this site. Following the same steps as in the study of the Ising model, the cavity method for a Bethe lattice of connectivity c leads to the following self-consistency equation:

$$\eta_{\mathrm{cav}}(\boldsymbol{a}, \bar{\boldsymbol{a}}) = \frac{1}{z_{\mathrm{cav}}} w(\boldsymbol{a}, \bar{\boldsymbol{a}}) \int \prod_{i=1}^{c-1} D\boldsymbol{a}_i D\bar{\boldsymbol{a}}_i \, \eta_{\mathrm{cav}}(\boldsymbol{a}_i, \bar{\boldsymbol{a}}_i) \, \exp \left\{ J \int_0^\beta \mathrm{d}\tau \left[\bar{a}(\tau) \sum_{i=1}^{c-1} a_i(\tau) + a(\tau) \sum_{i=1}^{c-1} \bar{a}_i(\tau) \right] \right\} , \tag{21}$$

with the on-site weight of the path $(\boldsymbol{a}, \bar{\boldsymbol{a}})$ given by

$$w(\boldsymbol{a}, \bar{\boldsymbol{a}}) = \exp \left[- \int_0^\beta \mathrm{d}\tau \left(\bar{a}(\tau)(\partial_\tau - \mu) a(\tau) + \frac{U}{2} (\bar{a}(\tau) a(\tau))^2 \right) \right] . \tag{22}$$

This self-consistent equation on η_{cav} is formally similar to the corresponding Eq. (14) of the Ising model. It is however much more complicated: the Ising degree of freedom σ could only take two distinct values, whereas $(\boldsymbol{a}, \bar{\boldsymbol{a}})$ belongs to a space of functions of the imaginary time τ. Therefore $\eta_{\mathrm{cav}}(\boldsymbol{a}, \bar{\boldsymbol{a}})$ is a functional measure whose representation is much more difficult; a complete parametrization requires the knowledge of all n, m-points correlations $\langle a(t_1) \cdots a(t_n) a^\dagger(s_1) \cdots a^\dagger(s_m) \rangle$. On the other hand, this is one of the most interesting features of the quantum cavity method: on-site quantum fluctuations are fully kept into account, without any truncation of higher order correlations.

Unfortunately, an exact solution of (21) can be easily obtained only in the case of free bosons ($U = 0$). η_{cav} acquires in this case a Gaussian form, with averages and two-point functions which can be computed exactly and reproduce the results obtained by direct diagonalization of the adjacency matrix of the Bethe lattice [43].

C. Large connectivity limit and the connection with B-DMFT

In the interacting case ($U > 0$) a solution of (21) can be looked for in the limit of large connectivity, and this is precisely the road followed by the B-DMFT studies [23, 24]. For completeness we shall explain in this subsection how to recover the B-DMFT formalism from Eq. (21), before turning in the next section to the occupation number basis which will allow to solve the model for any connectivity.

To state the large c expansion let us rewrite (21) in a more convenient way, using the lighter Nambu notation $\Psi^\dagger(\tau) = (\bar{a}(\tau), a(\tau))$, and consequently $\boldsymbol{\Psi}^\dagger = (\bar{\boldsymbol{a}}, \boldsymbol{a})$. Then we can rewrite (21) as

$$\eta_{\mathrm{cav}}(\boldsymbol{\Psi}) = \frac{1}{z_{\mathrm{cav}}} w(\boldsymbol{\Psi}) \, e^{(c-1)\Gamma(J\boldsymbol{\Psi})} , \qquad \Gamma(\boldsymbol{\Phi}) = \log \left\{ \int D\boldsymbol{\Psi} \, \eta_{\mathrm{cav}}(\boldsymbol{\Psi}) \exp \left[\int_0^\beta \mathrm{d}\tau \, \Psi^\dagger(\tau) \Phi(\tau) \right] \right\} . \tag{23}$$

$\Gamma(\mathbf{\Phi})$ is the generating functional of the connected correlation functions of a and $\bar{a}$. It can be expanded as

$$\Gamma(\mathbf{\Phi}) = \int_0^\beta \mathrm{d}\tau \, \langle \Psi^\dagger \rangle \, \Phi(\tau) + \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \, \Phi^\dagger(\tau) \widehat{G}_c(\tau - \tau') \Phi(\tau') + O(\Phi^3) \, , \tag{24}$$

where the averages $\langle \cdot \rangle$ are with respect to η_{cav}, we have used the cyclic invariance in imaginary time, and $\widehat{G}_c(\tau - \tau') = \langle \Psi(\tau) \Psi^\dagger(\tau') \rangle - \langle \Psi \rangle \langle \Psi^\dagger \rangle$ is the connected part of the two point correlator of $\mathbf{\Psi}$.

In the large connectivity limit, the superfluid-insulator transition happens for a critical value of $J = \mathcal{J}/c$, with a finite $\mathcal{J}$. This can be argued by looking at Eq. (9), where it is clear that the dependence on hopping and connectivity is only through $\mathcal{J} = Jc$, which is the real control parameter. For large c and $J = \mathcal{J}/c$, the cumulant expansion of $(c-1)\Gamma(\mathcal{J}\mathbf{\Psi}/c)$ thus becomes a systematic expansion in powers of $1/c$. By keeping only a finite number of terms in the cumulant expansion, we obtain an expression of $\eta_{\mathrm{cav}}(\mathbf{\Psi})$ that *is not* Gaussian (because of the U term in $w(\mathbf{\Psi})$); still, we can obtain closed equations for the cumulants by computing them self-consistently as averages over the non-Gaussian η_{cav}.

The leading order in c gives, assuming without loss of generality that the average value of the order parameter is real, $\langle \Psi^\dagger \rangle = (\psi, \psi)$,

$$\eta_{\mathrm{cav}}(\mathbf{\Psi}) = \frac{1}{z_{\mathrm{cav}}} w(\mathbf{\Psi}) \, e^{\int_0^\beta \mathrm{d}\tau \, \mathcal{J} \langle \Psi^\dagger \rangle \Psi(\tau)} \quad \Rightarrow \quad \psi = \frac{1}{z_{\mathrm{cav}}} \int D\boldsymbol{a} D\bar{\boldsymbol{a}} \, a(0) \, e^{-\int_0^\beta \mathrm{d}\tau \left(\bar{a}(\tau)(\partial_\tau - \mu) a(\tau) + \frac{U}{2}(\bar{a}(\tau) a(\tau))^2 - \mathcal{J}\psi(a(\tau) + \bar{a}(\tau)) \right)} \, . \tag{25}$$

This last equation can be rewritten in the operator representation, which gives back the equation for ψ corresponding to the minimization of the variational free-energy (9), up to a multiplicative constant in the definition of ψ. Note that a generalization of the discussion above and of Eq. (25) to the disordered case leads to the stochastic mean field theory devised in [44].

We will now show that the next-to-leading order in the cumulant expansion of (24) gives the B-DMFT equations recently derived in [23, 24]. Note that the truncation at this two-point level was also used in the context of spin models in [32]. Plugging the expansion (24) in (23), we obtain to order $1/c$:

$$\begin{aligned}
&\eta_{\mathrm{cav}}(\mathbf{\Psi}) = \frac{1}{z_{\mathrm{cav}}} \exp\left[- S_{\mathrm{loc}} \right] , \\
&S_{\mathrm{loc}} = \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \, \Psi^\dagger(\tau) \widehat{\mathcal{G}}^{-1}(\tau - \tau') \Psi(\tau') + \int_0^\beta \mathrm{d}\tau \left[\frac{U}{8} (\Psi^\dagger(\tau)\Psi(\tau))^2 - \mathcal{J} \frac{c-1}{c} \langle \Psi^\dagger \rangle \Psi(\tau) \right] , \\
&\widehat{\mathcal{G}}^{-1}(\tau - \tau') = \frac{1}{2} \begin{pmatrix} \partial_\tau - \mu & 0 \\ 0 & -\partial_\tau - \mu \end{pmatrix} \delta(\tau - \tau') - \frac{\mathcal{J}^2}{c} \widehat{G}_c(\tau - \tau') \, .
\end{aligned} \tag{26}$$

Then, $\langle \Psi^\dagger \rangle$ and $\widehat{G}_c(\tau - \tau') = \langle \Psi(\tau) \Psi^\dagger(\tau') \rangle - \langle \Psi \rangle \langle \Psi^\dagger \rangle$ have to be computed self-consistently as averages with the local action S_{loc}. This set of equations correspond exactly to the B-DMFT of [23, 24] for the special case of a Bethe lattice.

Away from these two limits ($U = 0$ and $c \to \infty$) it seems difficult to obtain a solution of the cavity equation (21) as written in the coherent state basis. As a consequence we shall turn in the following to the representation number basis to apply the Suzuki-Trotter formula and thus obtain a more tractable equation for all values of U and c.

IV. THE QUANTUM CAVITY METHOD IN THE OCCUPATION NUMBER BASIS

A. The equations and the procedure for their numerical resolution

The insertion of a decomposition of the identity expressed in the occupation number basis in the Suzuki-Trotter formula (18) leads to an expression of the partition function of the Bose-Hubbard model as a sum over occupation number trajectories in imaginary time, $\{n_i(\tau)\}$. These trajectories are defined on an imaginary time interval of length β, with the periodicity condition $n_i(0) = n_i(\beta)$. The weight (action) of these trajectories has two origins: the local part of the Hamiltonian (1) yields a contribution of the form $\exp[-\int \mathrm{d}\tau \, V(n_i(\tau))]$ for each of the sites, where $V(n) = Un(n-1)/2 - \mu n$ is the local energy term in the Hamiltonian. In addition the hopping term of the Hamiltonian imposes constraints between the occupation number trajectories: each time $n_i(\tau)$ is raised (resp. decreased) by 1, the occupation number $n_j(\tau)$ of one of the neighbors $j \in \partial i$ must decrease (resp. increase) of 1, meaning one particle has jumped from j to i (resp. from i to j). Moreover each hopping event multiplies the weight of the trajectory $\{n_i(\tau)\}$ by J and by a coefficient depending on the instantaneous occupation numbers of the sites involved in the

Exact PIQC (Rosso, Krzakala, Semerjian, Zamponi PRB 2008)

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x$$

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \mathrm{Tr}\left[e^{\beta J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + \beta \Gamma \sum_i \hat{\sigma}_i^x}\right]$$

using
$$e^{\beta(X_1+X_2)} = \sum_{p=0}^{\infty} \int_0^{\beta} dt_1 \int_{t_1}^{\beta} dt_2 \cdots \int_{t_{p-1}}^{\beta} dt_p \; e^{t_1 \hat{X}_1} \hat{X}_2 \, e^{(t_2-t_1)\hat{X}_1} \hat{X}_2 \cdots \hat{X}_2 e^{(\beta-t_p)\hat{X}_1}$$

$$Z = \sum_{p=0}^{\infty} \int_0^{\beta} dt_1 \cdots dt_p \;\mathrm{Tr}\left[e^{J t_1 \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z} \left(\Gamma \sum_i \hat{\sigma}_i^x\right) \cdots \left(\Gamma \sum_i \hat{\sigma}_i^x\right) e^{J(\beta - t_p)\sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z}\right]$$
$t_1 \le t_2 \cdots \le t_p$

$$= \sum_{p=0}^{\infty} \Gamma^p \int_0^{\beta} dt_1 \cdots dt_p \sum_{\underline{\sigma}_1 \cdots \underline{\sigma}_p} e^{J t_1 \sum_{\langle ij \rangle} \sigma_{i,1} \sigma_{j,1}} \langle \underline{\sigma}_1 | \sum_i \hat{\sigma}_i^x | \underline{\sigma}_2 \rangle \cdots \langle \underline{\sigma}_p | \sum_i \hat{\sigma}_i^x | \underline{\sigma}_1 \rangle \cdot e^{J(\beta - t_p)\sum_{\langle ij \rangle} \hat{\sigma}_{i,1}^z \hat{\sigma}_{j,1}^z}$$
$t_1 < \cdots < t_p$

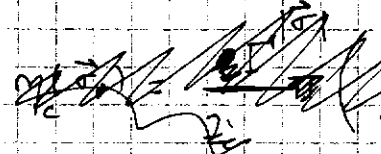
$$= \int D\underline{\sigma}(t) \cdot \Gamma^{(\#\text{jumps})} \, e^{J \int_0^{\beta} dt \sum_{\langle ij \rangle} \sigma_i(t) \sigma_j(t)}$$

Path integrals for spins

Then
$$Z = \int \left(\prod_i D\sigma_i(t)\right) \prod_{i=1}^{N} v(\sigma_i) \prod_{\langle ij \rangle} e^{J \int_0^{\beta} dt \, \sigma_i(t) \sigma_j(t)}$$

$$= \int \left(\prod_i D\sigma_i(t)\right) \prod_{i=1}^{N} e^{|\vec{\sigma}_i| \log \Gamma} \prod_{\langle ij \rangle}^{N} e^{J \vec{\sigma}_i \cdot \vec{\sigma}_j}$$

Cauty equations.



$$\mathcal{M}_c(\vec{\sigma}) = \frac{1}{Z_c} \cdot \Gamma^{|\vec{\sigma}|} \cdot \prod_{i=1}^{c-1} \int D\vec{\sigma}_i \, \mathcal{M}_c(\vec{\sigma}_i) \, e^{J \int_0^\beta \sigma(t) \cdot \sigma_i(t) \, dt}$$

$$= \frac{1}{Z_c} \int D\vec{\sigma}_1 \, \mathcal{M}_c(\vec{\sigma}_1) \cdots D\vec{\sigma}_{c-1} \, \mathcal{M}_{c-1}(\vec{\sigma}_{c-1}) \cdot \Gamma^{|\vec{\sigma}|} \, e^{J \int_0^\beta \sigma(t) \cdot \sum_{i=1}^{c-1} \sigma_i(t) \, dt}$$

$$= \int D\vec{\sigma}_1 \, \mathcal{M}_c(\vec{\sigma}_1) \cdots D\vec{\sigma}_{c-1} \, \mathcal{M}_{c-1}(\vec{\sigma}_{c-1}) \, \frac{Z_c(\vec{h})}{Z_c} \cdot \frac{\Gamma^{|\vec{\sigma}|} \, e^{J \int_0^\beta \sigma(t) \cdot h(t) \, dt}}{Z(\vec{h})}$$

$$\begin{cases} Z(\vec{h}) = \int D\vec{\sigma}(t) \, \Gamma^{|\vec{\sigma}|} \, e^{J \int_0^\beta \sigma(t) \cdot h(t) dt} \\ \vec{h}(t) = \sum_i \vec{\sigma}_i(t) \end{cases}$$

$$\mathcal{M}_c(\vec{\sigma}) = \int D\mathcal{M}(\vec{\sigma}_1) \cdots D\mathcal{M}(\vec{\sigma}_{c-1}) \cdot \frac{Z(\vec{h})}{Z_c} \cdot p(\vec{\sigma} \mid \vec{h})$$

↑ This is a weight associated to the new $\mathcal{M}$

Procedure:

- Encode $\mathcal{M}_c(\vec{\sigma}) = \sum_{\alpha=1}^{w} w_\alpha \, \delta(\vec{\sigma} - \vec{\sigma}^\alpha)$

Repeat w times:

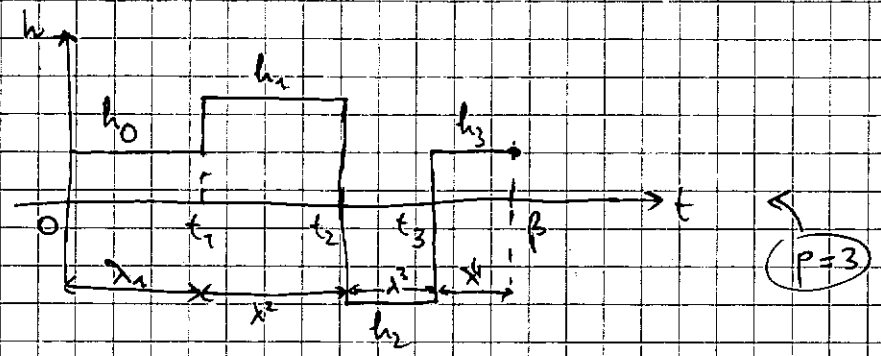
- Pick $c-1$ trajectories with weights w_α
- $\vec{h} = \sum_{i=1}^{c-1} \vec{\sigma}_i(t)$
- Generate $\vec{\sigma}$ from $p(\vec{\sigma} \mid \vec{h})$
- weight $w \propto Z(\vec{h})$

- Normalize the weights

How to compute $Z(\vec{h})$

$$Z(\vec{h}) = \int D\vec{\sigma}(t)\ \pi^{|\vec{\sigma}|-1}\ e^{J\int_0^\beta \sigma(t)\,h(t)\,dt}$$

← This is the path integral of one single spin in a time-dependent external field



$$Z(\vec{h}) = \mathrm{Tr}\left[\prod_{i=0}^{p} e^{\lambda_i\left(h_i\hat{\sigma}^z + \Gamma\hat{\sigma}^x\right)}\right]$$

Can be computed by "diagonalizing" $p+1$ 2×2 matrices

How to extract a trajectory from $p(\vec{\sigma}|\vec{h})$

Call $$W(\sigma_i \to \sigma_{i+1};\ \lambda_i, h_i) = \langle \sigma_i | e^{\lambda_i\left(h_i\hat{\sigma}^z + \Gamma\hat{\sigma}^x_i\right)} | \sigma_{i+1}\rangle$$

$$= \begin{cases} \cosh\left(\lambda_i\sqrt{\Gamma^2+h_i^2}\right) + \sigma\dfrac{h_i}{\sqrt{h_i^2+\Gamma^2}}\sinh\left(\lambda_i\sqrt{\Gamma^2+h_i^2}\right) & \sigma=\sigma' \\ \dfrac{\Gamma}{\sqrt{h_i^2+\Gamma^2}}\sinh\left(\lambda_i\sqrt{\Gamma^2+h_i^2}\right) & \sigma\neq\sigma' \end{cases}$$

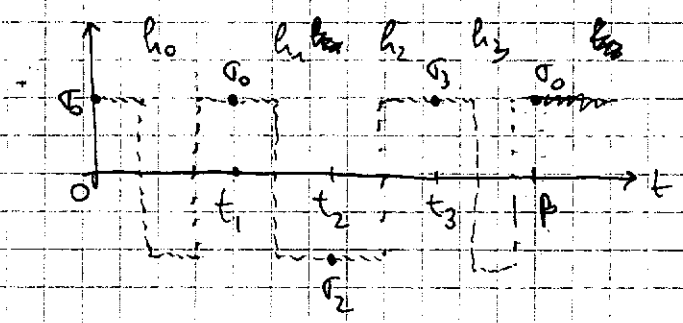
$$Z(\vec{h}) = \sum_{\sigma_0\ldots\sigma_p} W(\sigma_0\to\sigma_1, \lambda_0, h_0)\, W(\sigma_1\to\sigma_2, \lambda_1, h_1)\cdots W(\sigma_p\to\sigma_0, \lambda_p, h_p)$$

Therefore:

$$p(\sigma_0\ldots\sigma_p) = \frac{W(\sigma_0\to\sigma_1, \lambda_0, h_0)\cdots W(\sigma_p\to\sigma_0, \lambda_p, h_p)}{Z(\vec{h})}$$

A 1d Ising chain of length p → generate $\{\sigma_0\ldots\sigma_p\}$ by transfer matrix

Generate a trajectory that goes through $\sigma_0 \dots \sigma_p$



Amounts to generate a trajectory with fixed boundaries in a constant field.

$$p(\sigma(t)) = \frac{1}{W(\sigma \to \sigma', \lambda, h)} \Gamma^{|\vec{\sigma}|} \cdot e^{\int_0^\lambda dt\, \sigma(t) \cdot h} \, dt_1 \dots dt_{|\vec{\sigma}|}$$

Identities:

$$\begin{cases} W(\sigma \to \sigma, \lambda, h) = e^{\sigma h \lambda} + \Gamma \int_0^\lambda du\, e^{\sigma h u}\, W(\sigma \to \sigma, h, \lambda - u) \\ W(\sigma \to -\sigma, \lambda, h) = \Gamma \int_0^\lambda du\, e^{\sigma h u}\, W(-\sigma \to -\sigma, h, \lambda - u) \end{cases}$$

~~or since~~

Algorithm:

If $\sigma = \sigma'$:

- with prob. $e^{\sigma h \lambda} / W(\sigma \to \sigma, \lambda, h)$ set $\sigma(t) = \sigma$ and exit
- otherwise - draw u with

$$p(u) = \frac{\Gamma\, e^{\sigma h u}\, W(\sigma \to \sigma, h, \lambda - u)}{W(\sigma \to \sigma, \lambda, h) - e^{\sigma h \lambda}}$$

- set $\sigma(t) = \sigma$ up to u
- generate a traj $-\sigma \to \sigma$ on $\lambda - u$

If $\sigma = -\sigma'$

- Draw u and set $\sigma(t) = \sigma$ up to u
- generate with $-\sigma \to -\sigma$ up on $\lambda - u$

PIQC

Advantages:

- exact, no approximation
- Computational time is Ok for a given accuracy (but grows with N, with local Hilbert space with c)

Problems:

- only H with no "sign problems"
- only $T>0$ (extrapolation to $T \to 0$ usually possible)
- affected by sampling noise and finite size effects

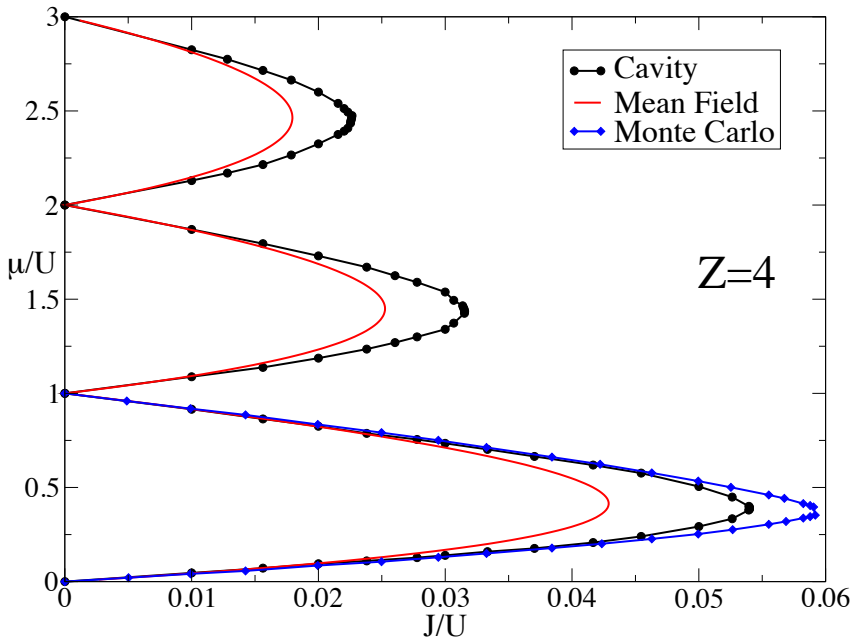
For the moment this is the only method that has been used for problems with frustration.

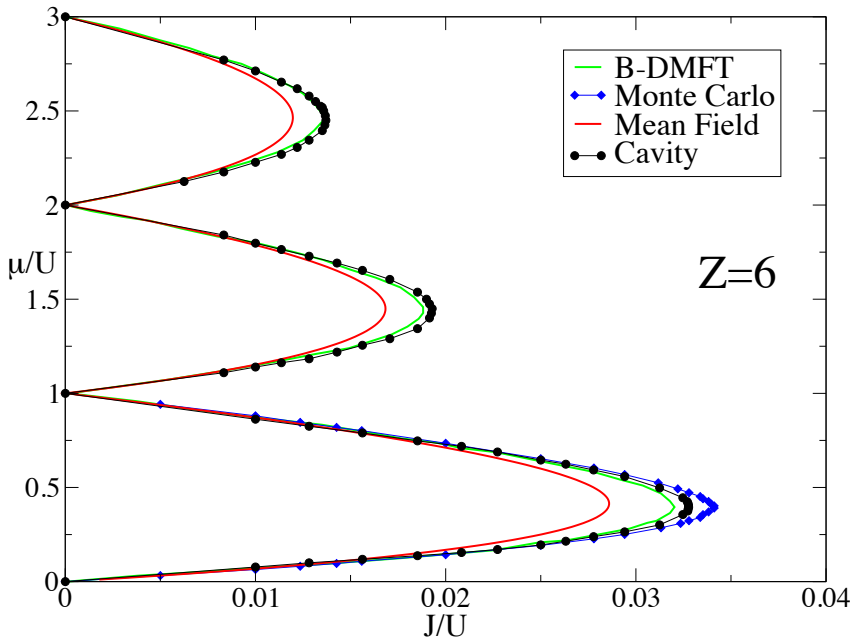
(note that QMC is in trouble when there is frustration)

Study of the Mott transition in the Bose-Hubbard model on RRG

G. Semerjian, M. Tarzia, FZ, PRB 80, 014524 (2009)

$$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2}\sum_i n_i(n_i-1) - \sum_i \mu n_i$$





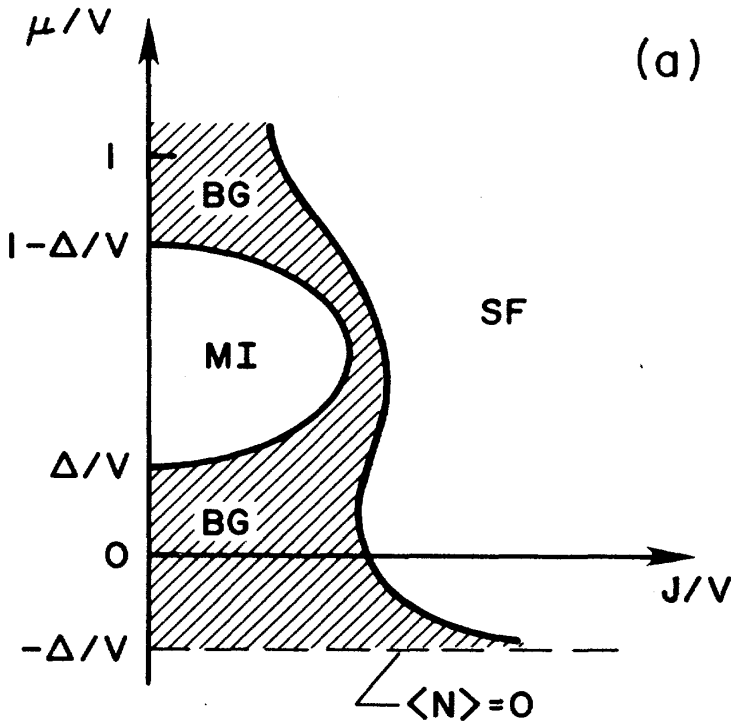
We can compute many observables:

- Local density $\langle n_i \rangle$ and condensate wavefunction $\langle a_i \rangle$
- Local green function $\left\langle a_i^\dagger(\tau) a_i(0) \right\rangle$ and correlation $\langle n_i(\tau) n_i(0) \rangle$
- Spatial correlations $\left\langle a_i^\dagger a_j \right\rangle$

Disordered Bose-Hubbard model: the Bose glass

$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i (\mu + \varepsilon_i) n_i$

$\varepsilon_i \in [-\Delta, \Delta]$ *quenched external disorder*



- Mott insulator: one particle/site
  Strong localization $\Rightarrow$ no BEC, $\rho_c = 0$
  Zero compressibility
- Bose glass: additional defects
  Anderson localization, $\rho_c = 0$
  Finite compressibility

Fisher, Weichman, Grinstein, Fisher, PRB 40, 546 (1989)

No frustration, no RSB

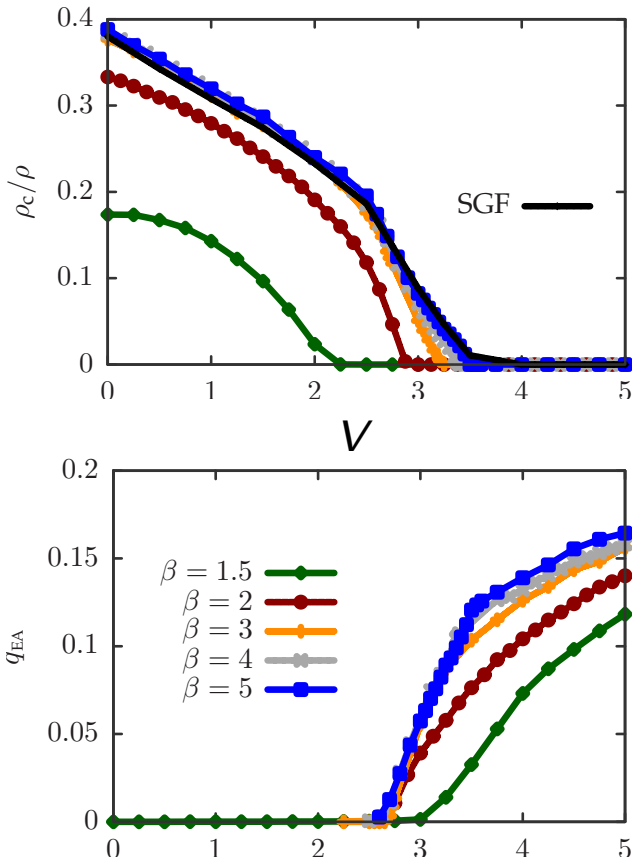
On RRG: Ioffe and Mézard, PRL 105, 037001 (2010) using OQC
Hard with PIQC: very low temperatures, very rare events

A lattice model for the superglass: extended Hubbard model with $U = \infty$ on a RRG

$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V \sum_{\langle i,j \rangle} n_i n_j - \sum_i \mu n_i$

G. Carleo, M. Tarzia, FZ, PRL 103, 215302 (2009)

Half-filling, $J = 1$, several temperatures



Condensate fraction:

$\rho_c = \lim_{|i-j| \to \infty} \langle a_i^+ a_j \rangle = |\langle a \rangle|^2$

Edwards-Anderson order parameter:

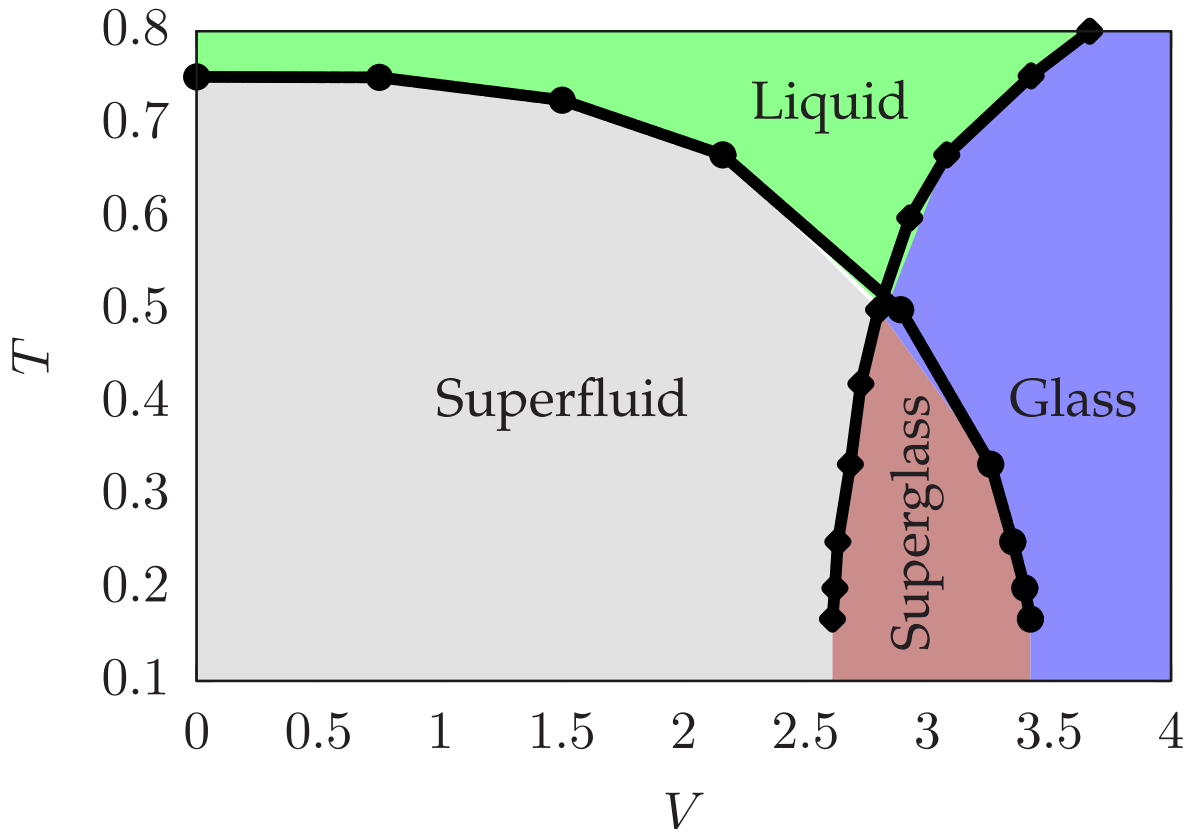
$q_{EA} = \frac{1}{L} \sum_i \langle (\delta n_i)^2 \rangle \qquad \delta n_i = n_i - \langle n_i \rangle$

A lattice model for the superglass: extended Hubbard model with $U = \infty$ on a RRG

$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V \sum_{\langle i,j \rangle} n_i n_j - \sum_i \mu n_i$

G. Carleo, M. Tarzia, FZ, PRL 103, 215302 (2009)

Half-filling, $J = 1$



Same phase diagram for a 3D disordered model:

Tam, Geraedts, Inglis, Gingras, Melko, PRL 104, 215301 (2010)

Quantum Biroli-Mézard model: a lattice glass model

$$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_i n_i q_i \theta(q_i) - \sum_i \mu n_i \qquad q_i = \sum_{j\in\partial i} n_j - \ell$$

Foini, Semerjian, FZ, PRB 83, 094513 (2011)

Classical model ($J = 0$): glass transition similarly to Hard Spheres:

- Random First Order Transition: discontinuous q_{EA}, 2nd order phase transition
- Glassy phase both on 3D cubic and Bethe lattices (quantitatively similar)
- Self-generated disorder and RSB
- Very slow dynamics (divergence stronger than power-law)
- Believed (by some) to be in the same universality class of particle systems (e.g. Lennard-Jones, Hard Spheres): *RFOT theory of the glass transition*

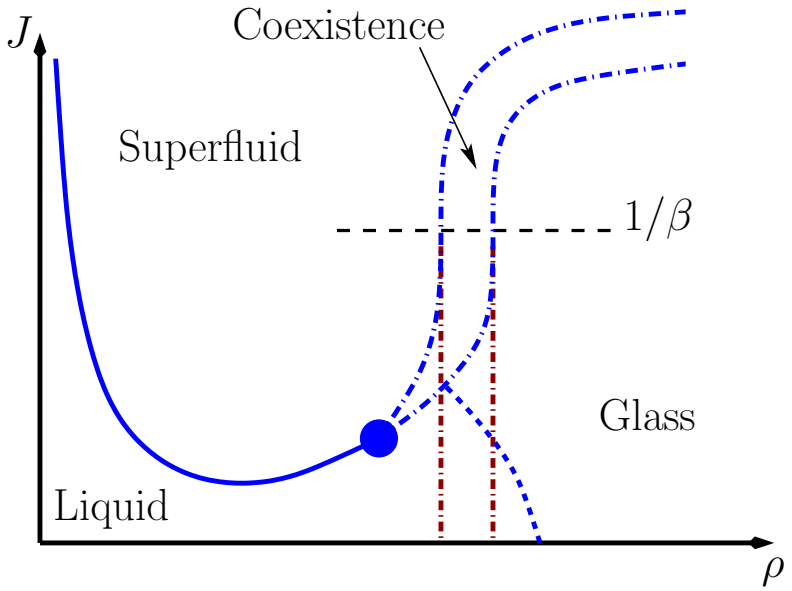
Quantum Biroli-Mézard model: a lattice glass model

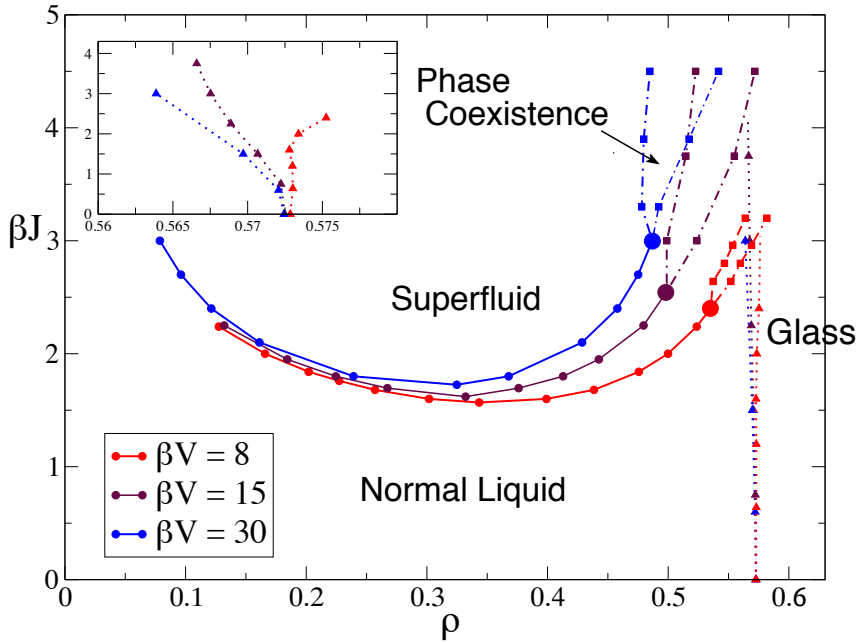
$$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_i n_i q_i \theta(q_i) - \sum_i \mu n_i \qquad q_i = \sum_{j\in\partial i} n_j - \ell$$

Foini, Semerjian, FZ, PRB 83, 094513 (2011)

Quantum model ($J > 0$): a model for quantum Hard Spheres

- A re-entrant glass transition line
- At large J, a first order quantum glass-superfluid transition
- A coexistence region between superfluid and glass





Quantum 3-XORSAT model: a difficult optimization problem

$H = H_P + \Gamma H_Q = \sum_{\langle ijk \rangle} (1 - J_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z) - \Gamma \sum_{i=1}^N \sigma_i^x$

Jörg, Krzakala, Semerjian, FZ, PRL 104, 207206 (2010)

Farhi et al. (including FZ), in preparation

Classical model ($\Gamma = 0$):

- A system of linear equations on Boolean variables
- Random First Order Transition: discontinuous q_{EA}, 2nd order phase transition
- Very hard to find the ground state using any local algorithm (but easy to find with Gaussian elimination): very natural benchmark for classical algorithms

Quantum 3-XORSAT model: a difficult optimization problem

$H = H_P + \Gamma H_Q = \sum_{\langle ijk \rangle} (1 - J_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z) - \Gamma \sum_{i=1}^N \sigma_i^x$

Jörg, Krzakala, Semerjian, FZ, PRL 104, 207206 (2010)

Farhi et al. (including FZ), in preparation

Quantum model:

- A first order glass-paramagnet transition (with histeresis)
- Gap is exponentially small at the transition
- Quantum adiabatic algorithms take an exponential time