Ludovic Berthier - Lecture III

i) Algorithm used in glassy field: parallel tempering

Different systems at $\neq T$, exchange configurations at $\neq T$.

$\exists$ quench disorder → • Used in spin glass ⇒ allow to go to low T.
• Bulk glasses → BAD (should be checked). ?

ii) Wang-Landau - Am J Phys '04. Instead of probing Boltzmann $e^{-\beta\epsilon}$, they sample density of state, $g(E)$. No temperature imposed. What does it really do ?

V The Franz-Parisi potential $V(Q)$

~ Landau free energy for glasses as a function of Q (overlap between config.).

Construction:

- Take a ref. eq. $\mathcal{C}_{eq} = \{\vec{r_1}\}$ → quench disorder
- Take a second copy of the same system $\mathcal{C} = \{\vec{r_2}\}$
- Overlap between $\mathcal{C}_{eq}$, $\mathcal{C}$:

$$Q_{12} = \frac{1}{N} \sum_{i,j=1}^{N} \theta\left(a - |\vec{r}_{1,i} - \vec{r}_{2,j}|\right)$$

a coarse grained length $\sim 0.2\,\sigma$

$Q_{12} = 1$ if $1 = 2$

$\simeq 0$ if 1 and 2 are uncorrelated

for uncorrelated $Q_{12} \simeq \frac{4\pi}{3} a^3 \rho \simeq 0.03$ has to be substract.

$V(Q)$ is the average free energy of system 2 having an overlap Q with copy 1 (then average over copy 1).

$$P(Q) \sim \exp\left(-\beta N V(Q)\right)$$

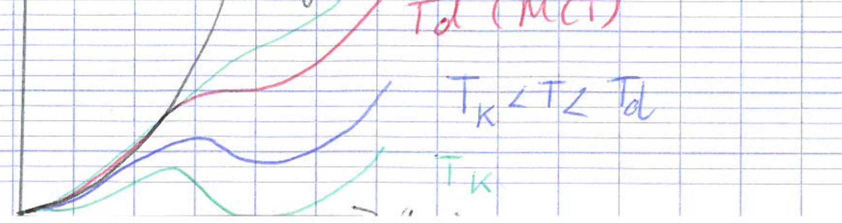
measure fluctuations of the overlap, then log $\times\left(\frac{-1}{\beta N}\right)$ $\rightarrow V(Q)$.

Proba to observe fluctuations in the liquid if $V(Q) \sim 1$ and a few hundred particles $\rightarrow$ very unlikely $\sim 10^{-100}$

$$-\beta N V(Q) = \underbrace{\int d\vec{r}_1^{\,N} \frac{e^{-\beta H(\{\vec{r}_1\})}}{Z_1}}_{\text{disorder average}} \underbrace{\log \int d\vec{r}_2^{\,N} \frac{e^{-\beta H(\{\vec{r}_2\})}}{Z_2} \delta(Q - Q_{12})}_{\text{Free energy at config. 1 fixed}}$$

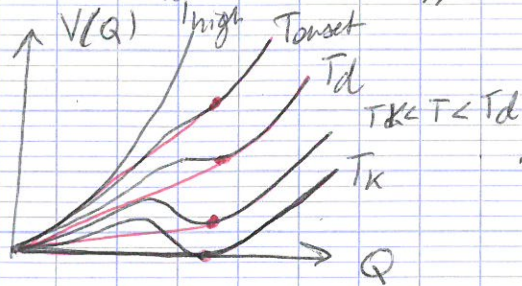
How to access fluctuations that will not happen spontaneously? $\rightarrow$ Have to force them

Mean field behavior:



What about finite dimensions?

↳ Local minimas cannot exist. Appearance of interface:

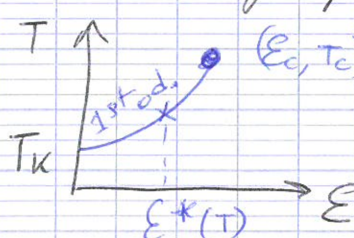


Nothing will happen in $V(Q)$ at T_d.

Consequence of mean field picture

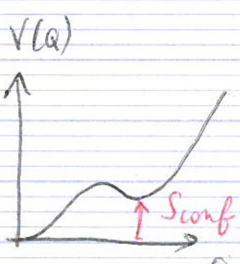
Add a field to Hamiltonian $\Delta H = -\varepsilon Q$ favors large Q. Start to tilt $V(Q)$ with large enough field at $T_d \geq T \geq T_K$.

Will induce a jump in the value of Q increasing ε.



$\varepsilon^*(T)$: energy to pay to create 2 minimas $Q=0$, $Q \neq 0$

$\sim S_{conf}$



Difference of value between low Q and high Q minima $= T S_{config}$ in Biroli's mean field picture.

FP potential: takes care of the mixing entropy.

How to bias the simulation towards unlikely events?

Favor fluctuations with Monte Carlo simulations in a clever way.

Change probability to sample.

Umbrella sampling. bias the equilibrium distribution by a known amount.

→ do biased simu.

→ unbias the system.

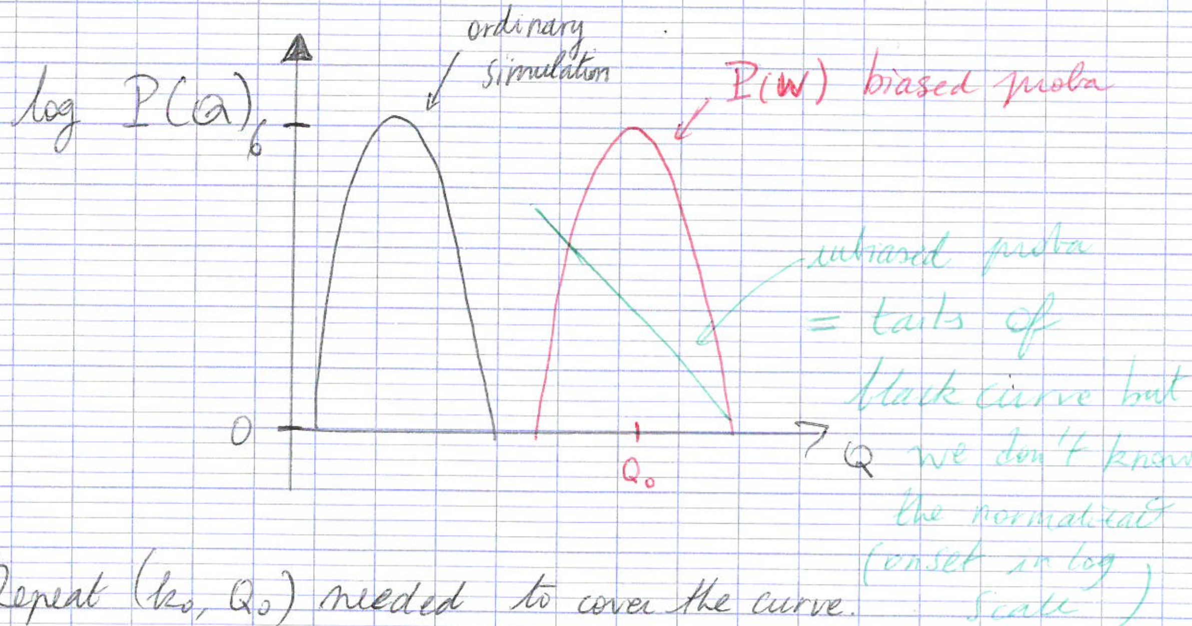
<u>In practice</u>: $\underbrace{H}_{} = \underbrace{\mathcal{H}_0}_{\text{original Ham}} + \underbrace{k_0 \left(Q_{12} - Q_0\right)^2}_{\text{harmonic potential}} = \mathcal{H}_0 + W_0(Q)$

k_0, Q_0: constant and chosen

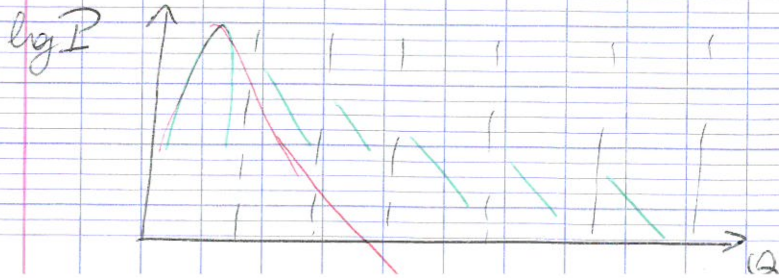
harmonic potential = favors $Q_{12} \sim Q_0$ to minimize the energy.

measure $P(Q_{12} \mid k_0, Q_0 \ldots) = P_W(Q_{12})$ biased fluctuations

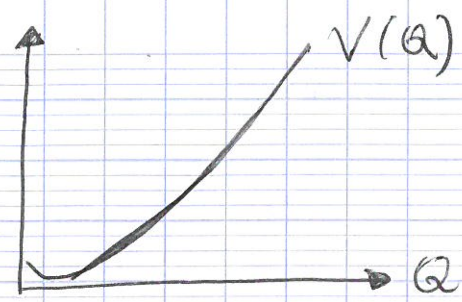
unbiased proba $P(Q_{12}) \propto P_W(Q_{12})\, e^{+\beta k_0 (Q-Q_0)^2}$



Repeat (k_0, Q_0) needed to cover the curve.



$V(Q) \sim -\log P$ gives



How to reconstruct the distribution? (Not by hand)

"Histogram reweighting method"
Reconstruct $\overline{P}$ by indep. n measurements.

$$\overline{P}(Q) = \frac{\sum_{i=1}^{n} P_i / \sigma_i^2}{\sum_{i=1}^{n} 1/\sigma_i^2}$$

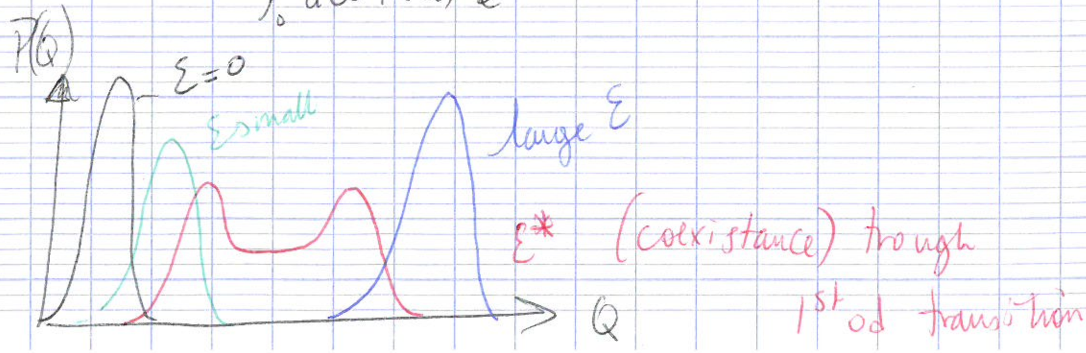
σ_i^2: error in measurm^t
P_i measurement.
form kills large errors.

w_i harmonic.

$$\begin{cases} P(Q) = \dfrac{\sum_{i=1}^{m} P_i(Q)}{\sum_{i=1}^{n} e^{-\beta w_i}/z_i} \\ z_i = \displaystyle\int_0^1 dQ \; \frac{\sum_{j=1}^{m} P_j(Q)}{\sum_j e^{\beta(w_i - w_j)}/z_j} \end{cases}$$

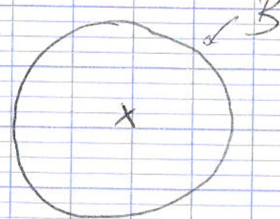
to be solved self-consistently
(guess input and compute next value until convergence)

$$P(Q, \mathcal{E}) = \frac{P(Q)\, e^{-\beta Q \mathcal{E}}}{\int_0^1 dQ\, P(Q)\, e^{-\beta Q \mathcal{E}}}$$



VI Point-to-set correlation length ξ_{PTS}

① Gilles



$\langle O(r)\, f(O\{B\})\rangle$

Static correlation length in dense liquids

② Giulio in the context of RFOT

freeze boundary conditions

$$PTS: \quad \Delta F = \underbrace{-\frac{4\pi R^3}{3} V(Q_{EA})}_{\text{gaining free energy by visiting the cavity}} + \underbrace{4\pi R^2 Y}_{\text{surface tension = energy to pay at the boundary by visiting states}}$$

ξ_{PTS} minimizes ΔF:

$$\xi_{PTS} = \frac{2Y}{V(Q_{EA})} \qquad V(Q_{EA}) \sim S_{conf}$$

Low $S_{conf} \Longleftrightarrow \xi_{PTS}$ diverge.

ξ_{PTS} is the important static length scale. (not about the position of particles but the rarefaction of states).

Idea: • Take $\mathcal{C}_{ref}$ at eq. $= \{\vec{r}_1\}$

• Fix the position of particles outside the cavity of size R.

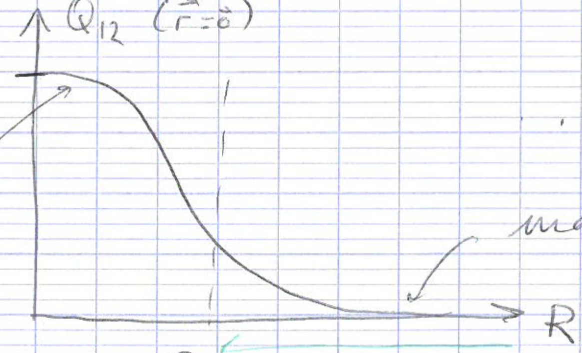
• Thermalize inside the cavity.

+ measure overlap between $\mathcal{C}_{eq}$ and the equilibrated conf inside the cavity $\quad Q_{12}(\vec{r}=0)$ at center of cavity

+ average over $\{\vec{r}_i\}$

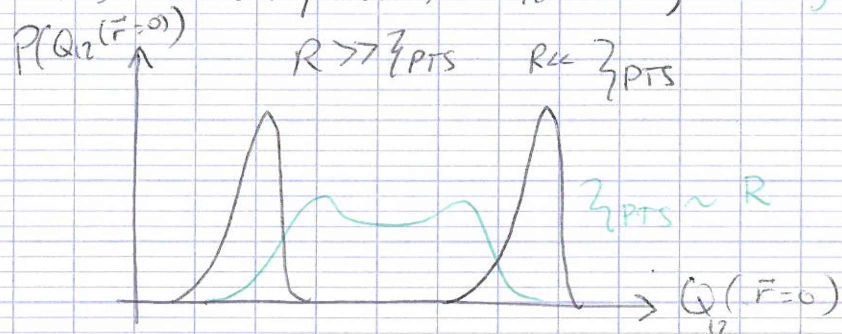
+ repeat for $\neq R_{vas}$ values.

You get 1



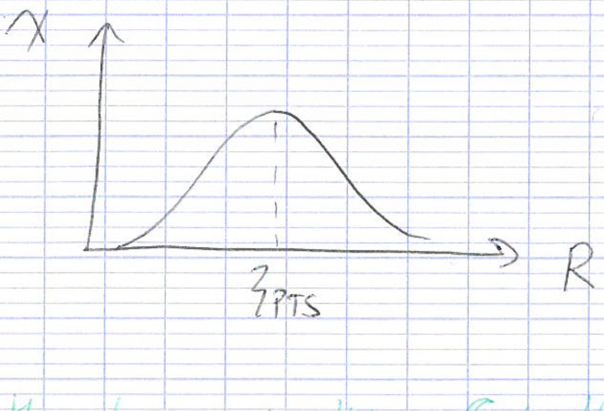
Baby Kauzmann transition
equivalent to lowering T in bulk system.

Could look at proba $P(Q_{12}(\vec{r}=0))$



$$\chi = \langle Q_{12}^2 \rangle - \langle Q_{12} \rangle^2$$

expect a large variance at $R \sim \xi_{PTS}$

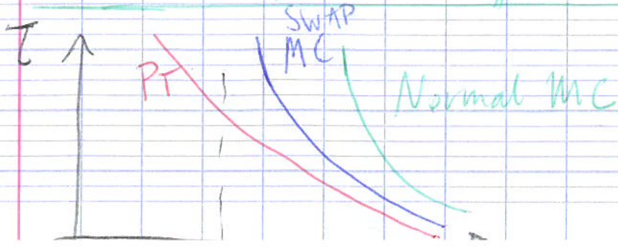


How to sample this efficiently?

We can measure how long it takes to ~~reach~~ reach equilibrium.

PT* = parallel tempering

Sho Yaida



How do we do parallel tempering?

We simulate n copies of the system in parallel.

$(\boxed{\mathcal{C}_1}, \dots, \mathcal{C}_n)$ with same Hamiltonian.

$(\boxed{T_1}, \dots, T_n)$ $\quad T_1 < \dots < T_n$

Original system (Temperature)

$\uparrow$ very large temperature (dynamics very fast)

From time to time, attempt to exchange 2 copies $\mathcal{C}_i, \mathcal{C}_{i+1}$. Accept ~~or~~ reject with detailed balance condition. $\rightarrow$ Reach equilibrium.

Key to thermalize the system in the cavity.

$$\boxed{\xi_{PTS} \simeq \frac{1}{S_{conf}}}$$