SPHERES

① Spheres as constraint satisfaction problem.

ⓐ **Perceptron:** GENERAL FORMULATION

$$\begin{cases} \vec{X} = \{x_1 \cdots x_N\} \qquad \sum_{i=1}^{N} x_i^2 = N \\ h_\mu(\vec{X}) = \vec{\xi}_\mu \cdot \vec{X} - \sigma \geq 0 \end{cases} \qquad \xi_i^\mu \sim \mathcal{N}(0, 1/N)$$

$$\mu = 1 \dots M$$

$$Z = \int \mathcal{D}\vec{X} \prod_{\mu=1}^{M} e^{-\beta v(h_\mu(\vec{X}))}$$

Thermodynamic limit

$N, M \to \infty$

$\alpha = \frac{M}{N}$

Control parameters $\{\alpha, \sigma\}$

Spheres:

$$\vec{X} = \{\vec{x}_1 \dots \vec{x}_N\} \qquad \vec{x}_i \in V \subset \mathbb{R}^d \quad \left[\text{or } \vec{x}_i \in \mathbb{R}^{d+1}, |\vec{x}_i|^2 = R^2\right]$$

$\mu = \langle ij \rangle = 1 \dots \frac{N(N-1)}{2}$

$$h_\mu(\vec{X}) = |\vec{x}_i - \vec{x}_j| - \sigma \geq 0$$

$$Z = \int \mathcal{D}\vec{X} \prod_{\langle ij \rangle} e^{-\beta v(|\vec{x}_i - \vec{x}_j| - \sigma)}$$

Thermodynamic limit

$N, V \to \infty$ or $N, R \to \infty$

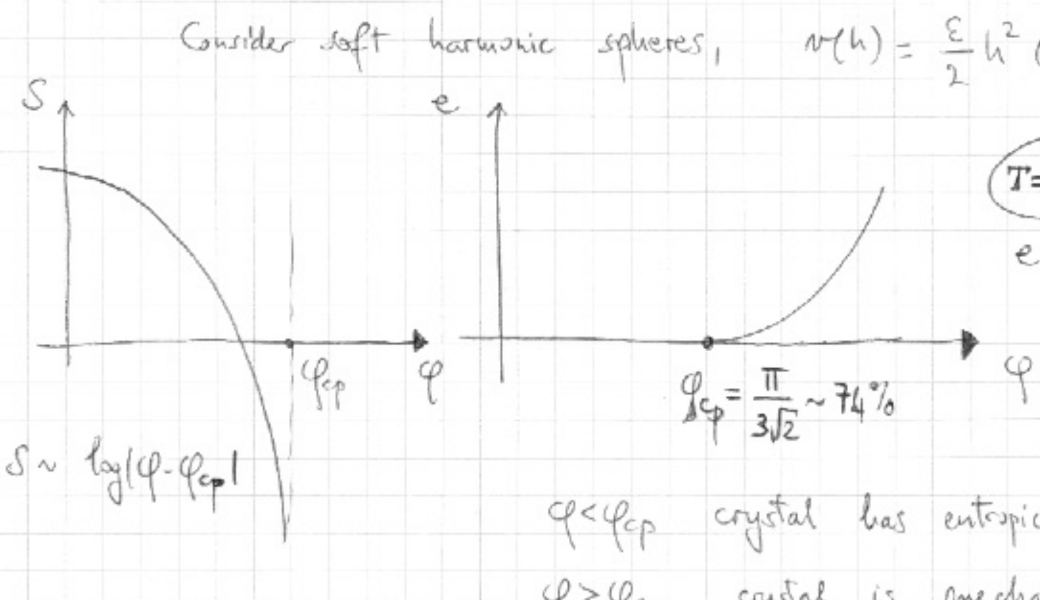
$$\varphi = \frac{N}{V} v_d(\sigma/2) \qquad \text{or} \qquad \varphi = \frac{N\, v_d(\sigma/2)}{\Omega_d(R)}$$

One control parameter φ.

ⓑ DIFFERENCES. Spheres: $\begin{cases} \text{no quenched disorder} \\ \text{crystal state} \end{cases}$

Example: $d = 2, 3$ $(4, 5 \dots ?)$ the sat/unsat transition is the densest packing $\to$ crystal

Consider soft harmonic spheres, $v(h) = \frac{\varepsilon}{2} h^2 \theta(-h)$



$T = 0$

$e \sim (\varphi - \varphi_{cp})^2$

$\varphi < \varphi_{cp}$ crystal has entropic rigidity: $p \propto T$, $\mu \propto T$

$\varphi > \varphi_{cp}$ crystal is mechanically rigid.

$\boxed{\text{Solution 1}}$ Reintroduce disorder: $h_\mu(\vec{x}) = |\vec{x}_i - \vec{x}_j + \vec{A}_{ij}| - \sigma$ $\quad \vec{A}_{ij}$ random vector

$\left\{ \begin{array}{l} \text{Kraichnan 1962 (liquid)} \\ \text{Mari - Krzakala - Kurchan 2008} \\ \text{Mari - Kurchan 2010} \end{array} \right.$ (glass - jamming)

$\boxed{\text{Solution 2}}$ Get rid of the crystal as usual (polydispersity) $h_\mu = |\vec{x}_i - \vec{x}_j| - \sigma_{ij}$

$\boxed{\text{Solution 3}}$ Increase dimension: above $d = 4$ no crystallization is observed

($\rightarrow$ Henry Cohn, very hard to find crystals in large d)

In both cases, there is a bunch of crystalline solutions, but impossible to find $\Rightarrow$ restrict the study to amorphous ones

Ⓒ What about replicas? Why replicas if there is no quenched disorder?

Solution: Franz-Parisi potential.

Reference equilibrium configuration $\vec{R}$
Coupled equilibrium configuration $\vec{X}$

$$f_g(\varphi, T \mid \varphi_g, T_g; Q) = -\frac{T}{N} \int d\vec{R} \, \frac{e^{-\beta_g H(\vec{R})}}{Z_1} \log \int d\vec{X} \, e^{-\beta H(\vec{X})} \, \delta\left(Q - Q(\vec{X}, \vec{R})\right)$$

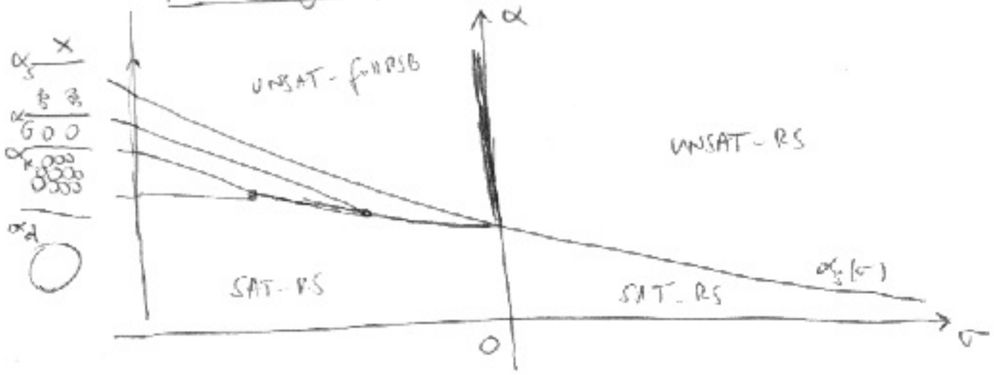
Note: φ, φ_g are controlled by σ, σ_g

Alternative solution: the Monasson method (Monasson, PRL 1995)

We are going to discuss the problem in $d \to \infty$ using the Franz-Parisi potential as our main tool.

$\rightarrow$ does not need any quenched disorder

Summary of ~~lect~~ lecture 2



Perceptron

$\exists \vec{X} \in \mathbb{R}^N$, $\vec{X}\cdot\vec{X} = N$, s.t. $h_\mu(\vec{X}) = \vec{X}\cdot\vec{\xi}_\mu - \sigma \geq 0$

$\mu = 1 \dots M$

$N, M \to \infty$ $\quad \alpha = N/M$

Spheres

$X = \{\vec{x}_1 \dots \vec{x}_N\}$ $\begin{cases} \vec{x}_i \in V \subset \mathbb{R}^d \\ \vec{x}_i \in S_d(R) \subset \mathbb{R}^{d+1} \end{cases}$

Thermodynamic limit $\begin{cases} N, V \to \infty \\ \varphi = \frac{N}{V} V_d(\sigma/2) \end{cases}$

satisfy $h_\mu(\vec{X}) = |\vec{x}_i - \vec{x}_j| - \sigma \geq 0$

$\mu = \langle ij \rangle = 1 \dots \frac{N(N-1)}{2}$

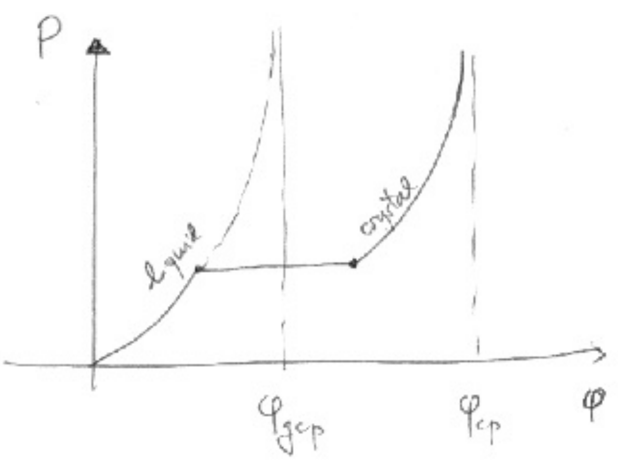
Hamiltonian.
$H = \sum_{ij} v(|\vec{x}_i - \vec{x}_j| - \sigma)$

~~Problems~~. Differences: crystal, no disorder $\Rightarrow$ close packing is ordered, hyperstatic

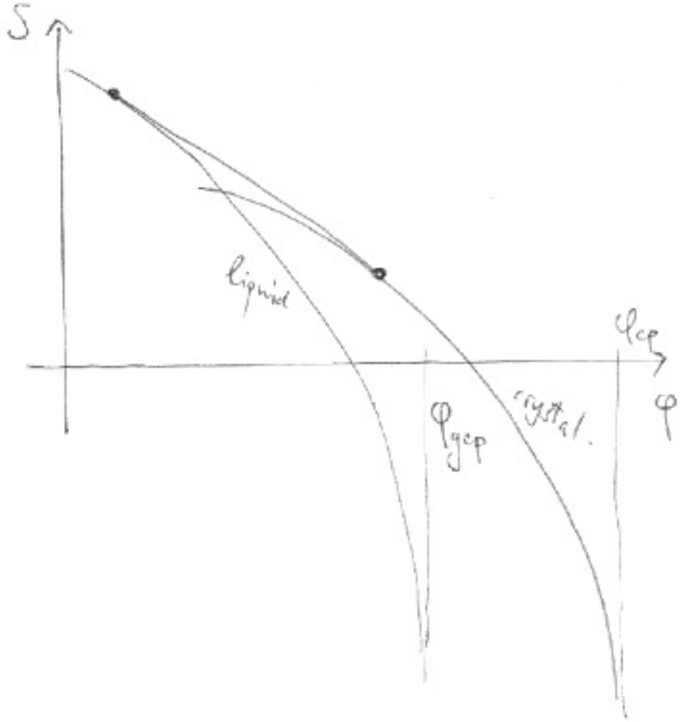
Focus on amorphous states: ① $h_\mu(x) = |x_i - x_j + A_{ij}| - \sigma$

② $h_\mu(x) = |x_i - x_j| - \sigma_{ij}$

③ look at $d \gg 4$ monodisperse



⇑
sat-unsat
transition
when crystal
is not allowed



(2) Spheres in infinite dimension. (book, can be sent privately)

[a physicist perspective]

(a) Liquid [Frisch, Rivier, Klein, Wyler '80s]

[Frisch-Percus PRE '99]

Virial expansion.

$$-\beta F[\rho(x)] = \int dx\, \rho(x)\left[1-\log\rho(x)\right] + \bullet\!-\!\bullet + \triangle + \square + \dots + \boxtimes$$

$f(x) = e^{-\beta v(x)} - 1$, $\rho(x)$

Specialize to $\rho(x) = \rho$ [eliminate crystal]

Define $\bar\varphi = 2^d\varphi$ and specialize to hard spheres $\Rightarrow$ SAT phase.

(*) The series converges for $\bar\varphi_{conv} \geq \dfrac{(W(e/2)-1)^2}{W(e/2)} = 0.144\dots$

$$\left(W(x)\, e^{W(x)} = x \right) \qquad \begin{bmatrix}\text{Lebowitz} \\ \text{Penrose '64}\end{bmatrix}$$

[Remember Minkowski bound $2^d\varphi = \bar\varphi \geq 1$
and best upper bound $\bar\varphi \leq 2^{(1-0.5990\dots)d} = 2^{0.401\dots d}$]

(*) Ring diagrams dominate at each order

$$-\beta f(\rho) = -\beta f^{id}(\rho) + \bullet\!-\!\bullet + \triangle + \square + \pentagon + \dots$$

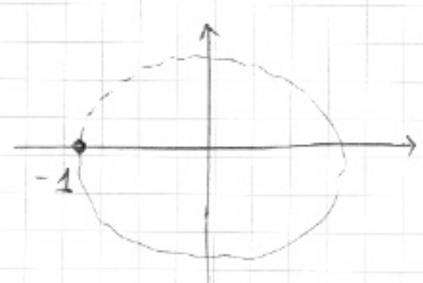
$\Rightarrow$ exact resummation, closed expression for $f(\rho)$

Three important result:

- Strongly suggests that $\bar\varphi_{conv} = 1$

  i.e. the liquid realizes at least the Minkowski bound.

- The pole that makes the series divergent is at $\bar\varphi < 0$

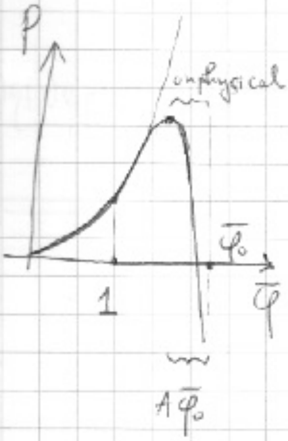


like $\log(1+x)$

(*) The first singularity at $\bar\varphi>0$ is at

$$\bar\varphi_0 = \left(\frac{e}{2}\right)^{\frac{d}{2}} = e^{d\,\frac{1-\log 2}{2}} = 2^{d\,\frac{1}{2}\left[\log_2(e)-1\right]} = 2^{d\,\frac{1}{2}\left[\frac{1}{\ln 2}-1\right]}$$

$$= 2^{0.22135\, d}$$



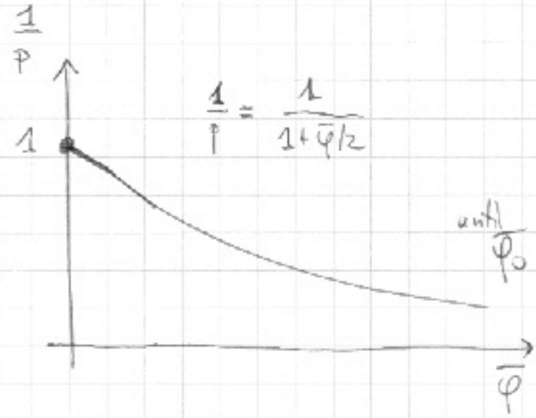
Some kind of liquid spinodal. (remember KL $\bar\varphi < 2^{0.401 d}$)

Aha! The liquid might exist up to $\bar\varphi_0$ and beat exponentially the Minkowski bound.
(Somehow this is Sal Torquato's perspective)

Conclusion. For any $\bar\varphi < \bar\varphi_0$, one can discard all virial diagrams except the first one

$$-\beta F[\rho(x)] = \int dx\, \rho(x)\left[1-\log\rho(x)\right] + \frac{1}{2}\int dx\,dy\, \rho(x)\rho(y)\, f(x,y)$$

$$\Rightarrow \quad p(\rho) = 1 + \frac{\bar\varphi}{2}$$



Liquid dynamics:

Exactly solvable [Stamel.]

MCT like, transition at $\bar\varphi = 4.8\, d$

Change scale: $\bar\varphi = d\hat\varphi \qquad p = 1 + \frac{\bar\varphi}{2} \sim d\,\hat\varphi/2 \qquad \frac{p}{d} \approx \frac{\hat\varphi}{2}$

Note:

$$p = \frac{\beta P}{\rho} = \bar\varphi\,\frac{\partial \beta f}{\partial\bar\varphi} = 1 + \frac{\bar\varphi}{2} - \frac{d}{2\bar\varphi}\,\frac{V_d^2}{(2\pi)^d}\int_0^\infty dq\, q^{d-1}\, L_3\left[\bar\varphi\, J_d(q)\right]$$

$$+ \frac{d}{2\bar\varphi}\,\frac{V_d^2}{(2\pi)^d}\int_0^\infty dq\, q^{d-1}\,\frac{\left[\bar\varphi\, J_d(q)\right]^3}{1+\bar\varphi\, J_d(q)}$$

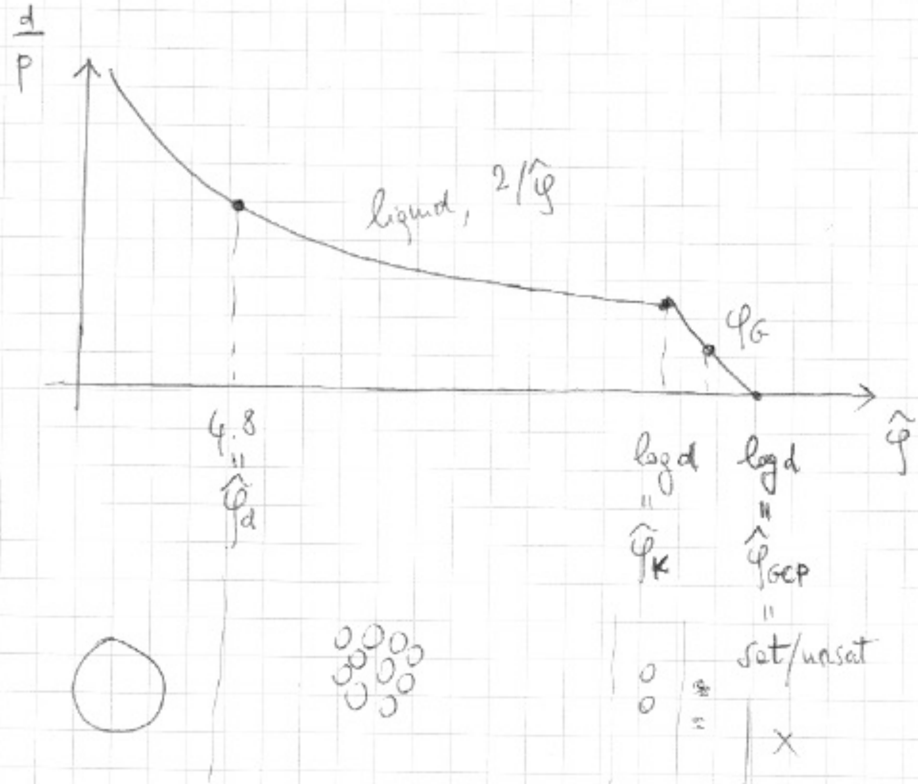
2(b) Franz-Parisi potential, results for the transition densities

Replicas
$$F[\rho(\underline{x})] = \int d\underline{x}\, \rho(\underline{x})\left[1-\log \rho(\underline{x})\right] + \int d\underline{x}\, d\underline{y}\, \rho(\underline{x})\rho(\underline{y}) f(\underline{x},\underline{y})$$

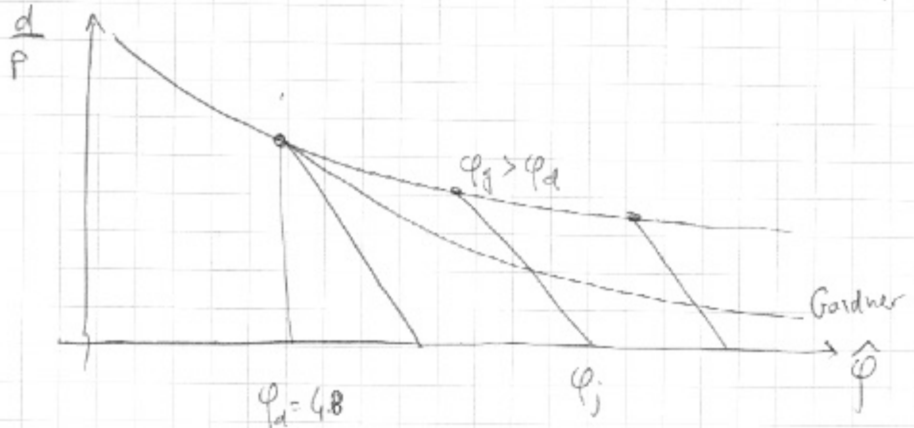
Rotational + translational invariance

+ $\lim_{d\to\infty}$ (central limit theorem)

$\Rightarrow$ exact expression of the Franz-Parisi potential.



(c) Out of equilibrium: following state in density / temperature with the Franz-Parisi potential



Landscape picture

J-line

All packings are in the fullRSB phase

~~(2) Criticality of jamming~~

- Very slow compression: $\varphi \sim \frac{d \log d}{2^d}$
  beats best lower bound (but not exponentially)
- Slow compression (but poly(N)): $\varphi \sim 7.2^d / 2^d$
  also beats some lower bounds
- Very fast compression: $\varphi \sim d/2^d$ unknown prefactor
- Sampling of all solutions stops at $\varphi_d \simeq 4.8\, d/2^d$

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(3) Criticality of jamming only found at fullRSB level
~ not true at any KRSB ~

(*) The jammed states are isostatic ~~(only true at~~

(*) $P(h) \sim 2\,\delta(h) + h^{-\gamma}$

(*) $P(f) \sim f^{\theta}$

(*) Away from jamming, $\Delta \sim p^{-\kappa}$

three critical exponents, two scaling relations $\Rightarrow$ one independent exponent

Wyart PRL 2012

Conclusion:

- mention MF theory in 3d [Mézard - Parisi]
- post doc openings
- thanks to { Leo Dakota & co-organizers
  lecturers
  you!