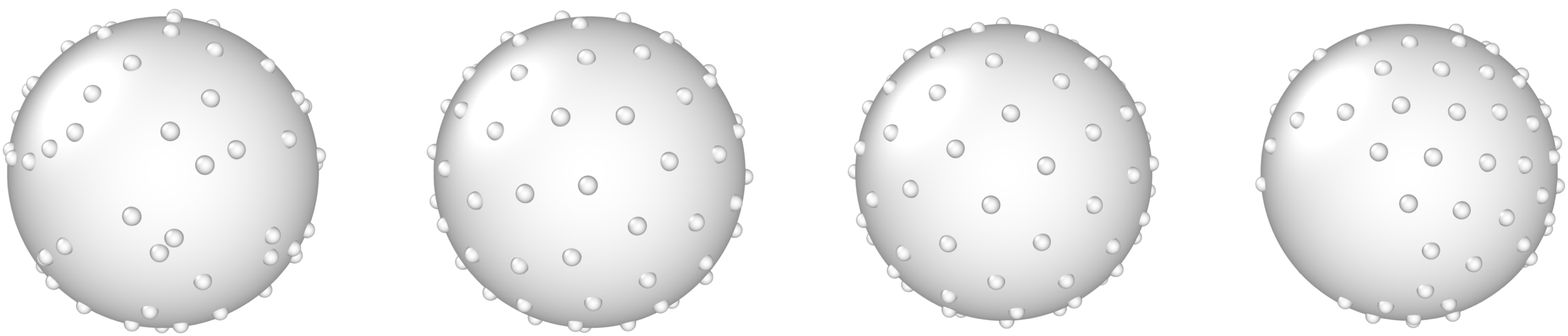
Liquid theory of designs

work with MISAKI OSAWA

SPHERICAL t DESIGNS.

Delsarte, Goethals and Seidel '77

you are asked to place N points on a sphere S^d such that



polynomials of all degrees between 1 and t have the same average

as with the flat measure

$$\frac{1}{N}\sum_{i=1}^{N} r_i^{\alpha_1} r_i^{\alpha_2}\cdots r_i^{\alpha_p} = \int d\mu\, r^{\alpha_1} r^{\alpha_2}\cdots r^{\alpha_p},$$

a const

UNITARY t DESIGNS

Hayden, Leung, Shor, Winter (2004) and many more

$$\int d\mu(U)\, U_{i_1 j_1} \cdots U_{i_t j_t}\, (U^\dagger)_{k_1 l_1} \cdots (U^\dagger)_{k_t l_t} = \int_{\text{Haar}} dU\, U_{i_1 j_1} \cdots U_{i_t j_t}\, (U^\dagger)_{k_1 l_1} \cdots (U^\dagger)_{k_t l_t}$$

$$i_1, \ldots, i_t,\ j_1, \ldots, j_t,\ k_1, \ldots, k_t,\ l_1, \ldots, l_t$$

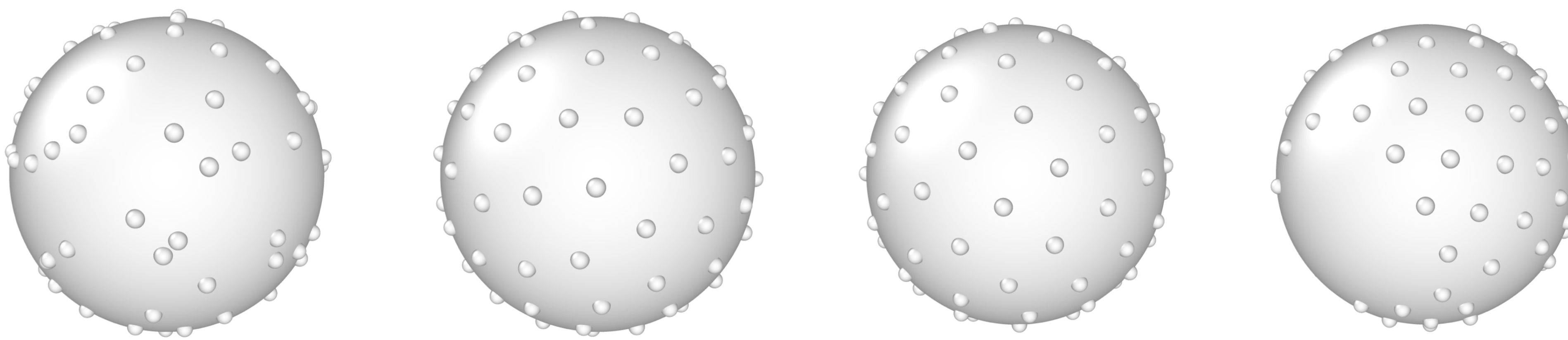
$$\int d\mu(U)\, U^{\otimes t} \otimes (U^\dagger)^{\otimes t} = \int_{\text{Haar}} dU\, U^{\otimes t} \otimes (U^\dagger)^{\otimes t}$$

analog of $\frac{1}{N}\sum_{i=1}^{N} r_i^{\alpha_1} r_i^{\alpha_2} \cdots r_i^{\alpha_p} = \int d\mu\, r^{\alpha_1} r^{\alpha_2} \cdots r^{\alpha_p},$

a const

SPHERICAL t DESIGNS.

S^d



$$\frac{1}{N}\sum_{i=1}^{N} r_i^{\alpha_1} r_i^{\alpha_2} \cdots r_i^{\alpha_p} = \int d\mu\, r^{\alpha_1} r^{\alpha_2} \cdots r^{\alpha_p},$$

a const

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_p} J_{\alpha_1\alpha_2\cdots\alpha_p}\left(\frac{1}{N}\sum_{i=1}^{N} r_i^{\alpha_1} r_i^{\alpha_2}\cdots r_i^{\alpha_p}\right) = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_p} J_{\alpha_1\alpha_2\cdots\alpha_p}\int d\mu\, r^{\alpha_1} r^{\alpha_2}\cdots r^{\alpha_p}.$$

$$h_{\alpha_1\alpha_2\cdots\alpha_p} = \frac{1}{N}\sum_{i=1}^{N} r_i^{\alpha_1} r_i^{\alpha_2}\cdots r_i^{\alpha_p} - \int d\mu\, r^{\alpha_1} r^{\alpha_2}\cdots r^{\alpha_p},$$

a const

a set of equations for r_i (all p<t and all $\alpha_1,\alpha_2,\ldots,\alpha_p$)

this is of the form $\sum$ (equations)^2

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_p} \left(h_{\alpha_1\alpha_2\cdots\alpha_p}\right)^2 = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{r}_i\cdot\mathbf{r}_j)^p - \int d\mu\int d\mu'\,(\mathbf{r}\cdot\mathbf{r}')^p \;\geq\; 0.$$

frame potential   a const

A STAT MECH PROBLEM

$$\sum_{\alpha_1,\alpha_2,\ldots,\alpha_p} \left(h_{\alpha_1\alpha_2\cdots\alpha_p}\right)^2 = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{r}_i\cdot\mathbf{r}_j)^p - \int d\mu \int d\mu' \,(\mathbf{r}\cdot\mathbf{r}')^p \;\geq\; 0.$$

frame potential a const

the solutions form a manifold: a `liquid' or are isolated a `solid'

Of a very particular kind : `constraint satisfaction'

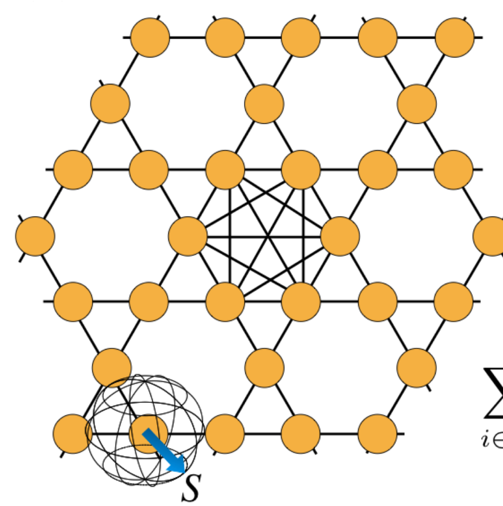
$$\alpha \equiv \frac{\text{number of equations}}{\text{number of unknowns}}$$

this is of the form $\sum$ (equations)^2

a set of equations for r_i (all p<t and all $\alpha_1, \alpha_2, \ldots, \alpha_p$)

equations are polynomial (nonlinear!) :

an intrincate algebraic geometry problem



$$\sum_{i \in \hexagon} \vec{S}_i = 0$$

UNKNOWNS=2d

EQUATIONS

- For $d = 2$ (S^1):

$$D(t,2) = 2t + 1 \;\; so \;\; N_c = 2t$$

- For $d = 3$ (S^2):

$$D(t,3) = (t+1)^2 \qquad - 1$$

- For $d = 4$ (S^3):

$$D(t,4) = \frac{1}{6}(t+1)(t+2)(2t+3) - 1.$$

- For $d = 5$ (S^4):

$$D(t,5) = \frac{1}{24}(t+1)(t+2)(t+3)(t+4) - 1.$$

- For large t,

$$D(t,d) \sim \frac{2}{d!}\, t^{\,d}.$$

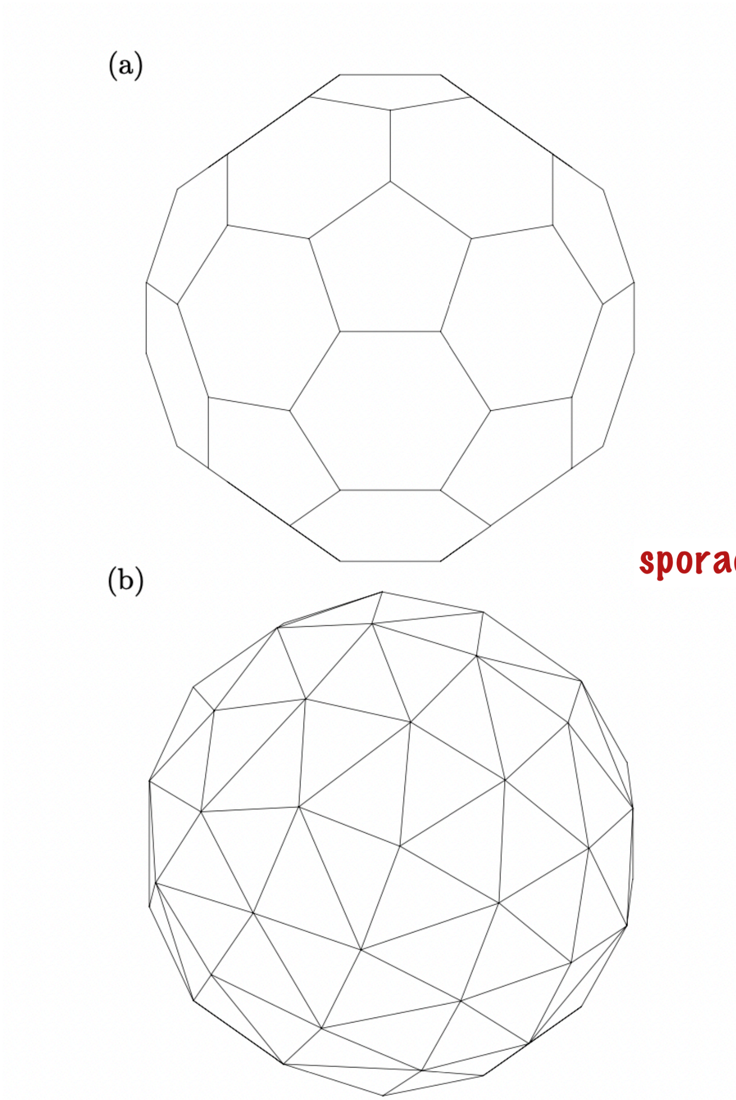
Equating $dN_c \sim \frac{2}{d!}\, t^{\,d}$ one obtains the empirical asymptotic critical N_c for large t.

A rigurous bound with a large constant replacing $\frac{2}{d!}$ was proven by Bondarenko et al

Mathematicians are good at bounds, but also at finding regular, group based, designs. We would call them crystals

and for them it is important to compute things exactly

(Sloane, Bondarenko, Radchenko . Viazovska, ...)



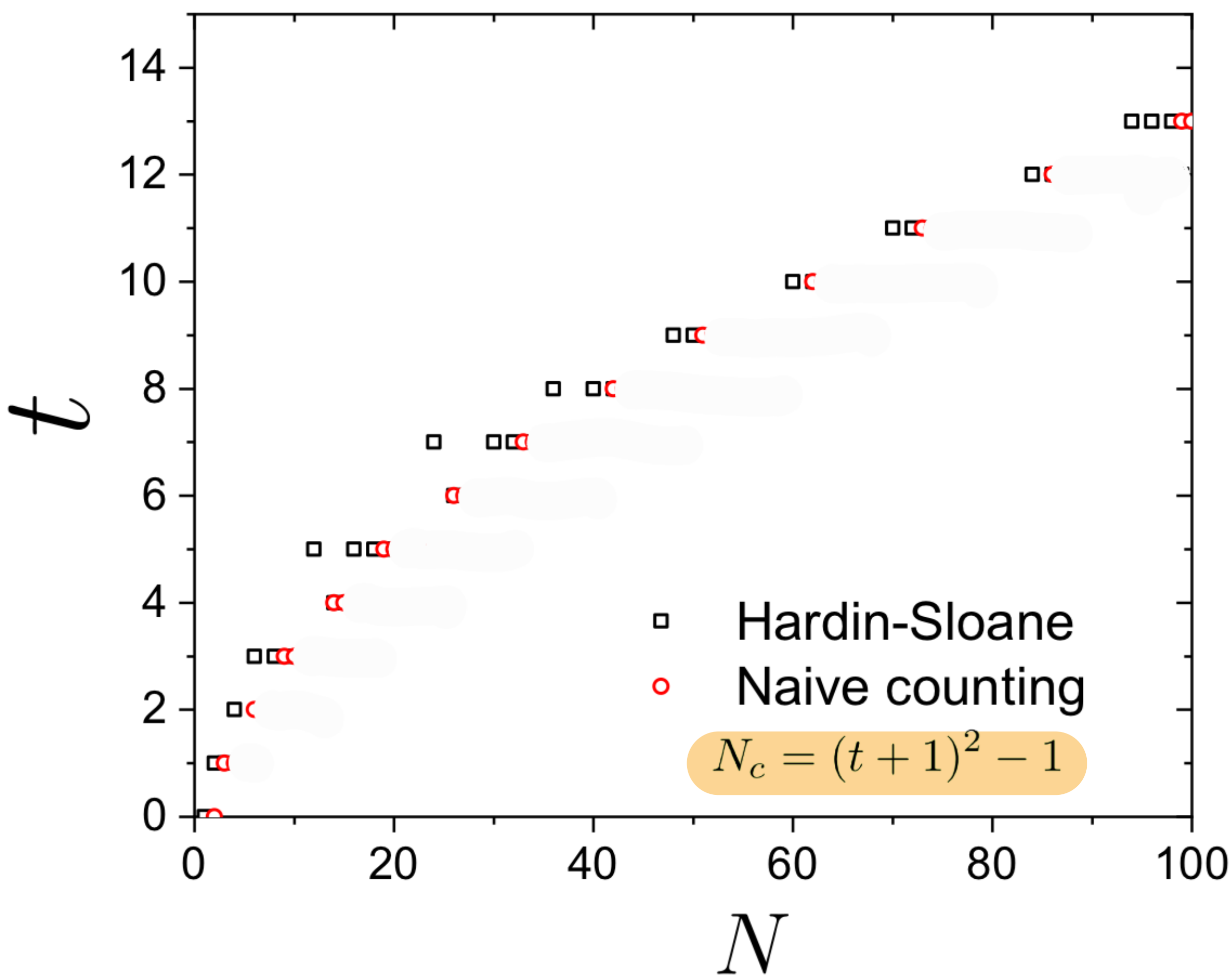
sporadic (vary madly with t) and very hard to find

We concentrate on amorphous (liquid and maybe glass) structures

S^2:

$$\alpha \equiv \frac{\text{number of equations}}{\text{number of unknowns}}$$

$\alpha_c \sim 1$



Naïve ('Maxwell') counting works rather well!

STAT MECH

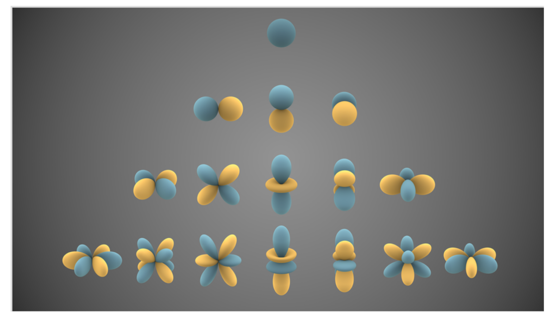
lousy

$$V_t = \sum_{ab} cos^p(\theta) = \sum_{l=1}^{p} a_l P_l(\cos(\theta)) = \sum_{l=1}^{p} \frac{4a_l\pi}{2l+1} \sum_{m=-l}^{l} \langle Y_{lm}\rangle\langle Y_{lm}\rangle$$

imposes

$$\sum_{i=1}^{N} Y_{\ell m}(\Omega_i) = 0$$

for all $\ell = 1, 2, \ldots, t$ and $m = -\ell, -\ell+1, \ldots, \ell$.

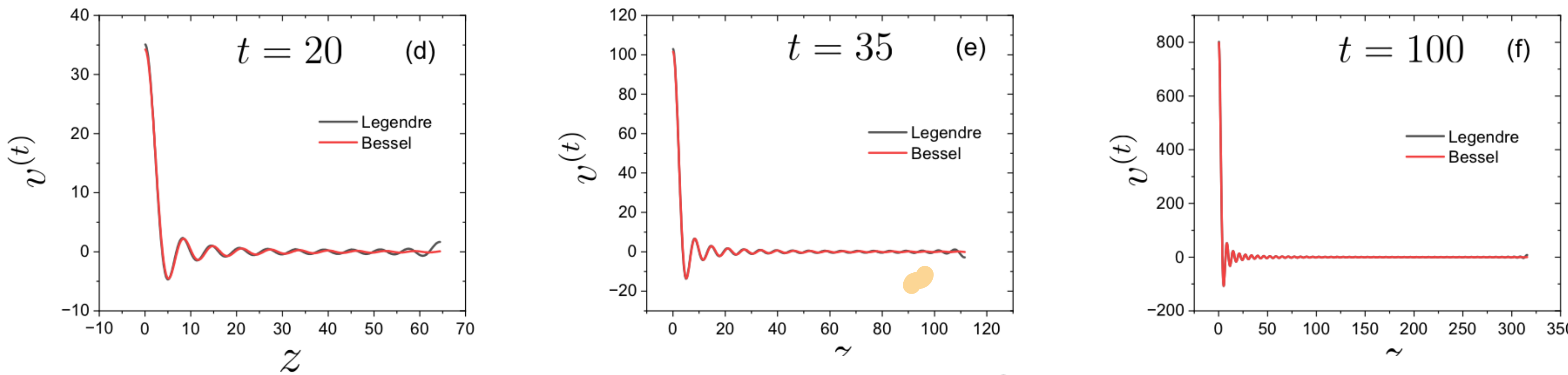


$$\tilde{V} = \sum_{l=1}^{p} \sum_{m=-l}^{l} \left| \sum_{i=1}^{N} Y_{l,m}(\theta_i, \varphi_i) \right|^2 = \frac{+1}{4\pi} \frac{P_{t+1}(\cos\gamma) - P_t(\cos\gamma)}{\cos\gamma - 1}.$$

Christoffel-Darboux summation

Christoffel-Darboux potential

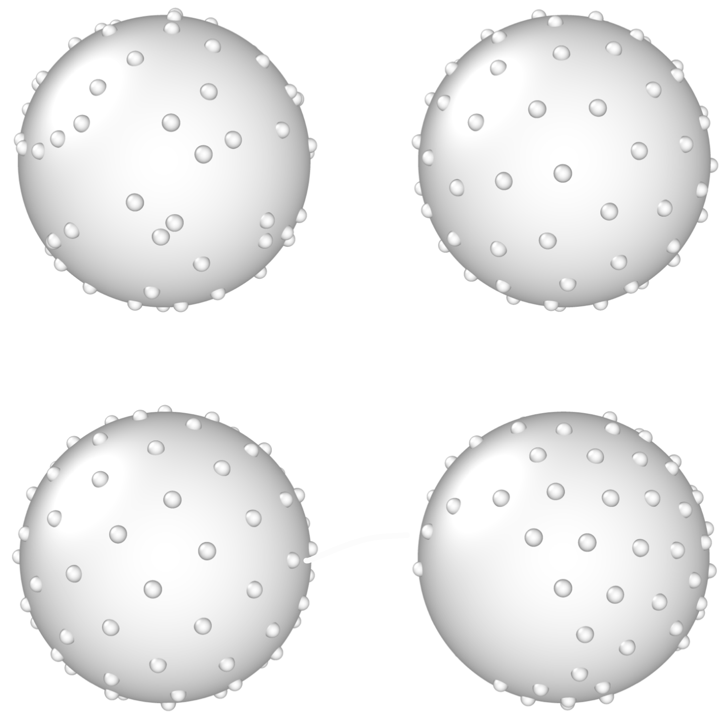
In all these cases before doing anything we need to define a potential that has the same ground states but scales nicely with t,N.



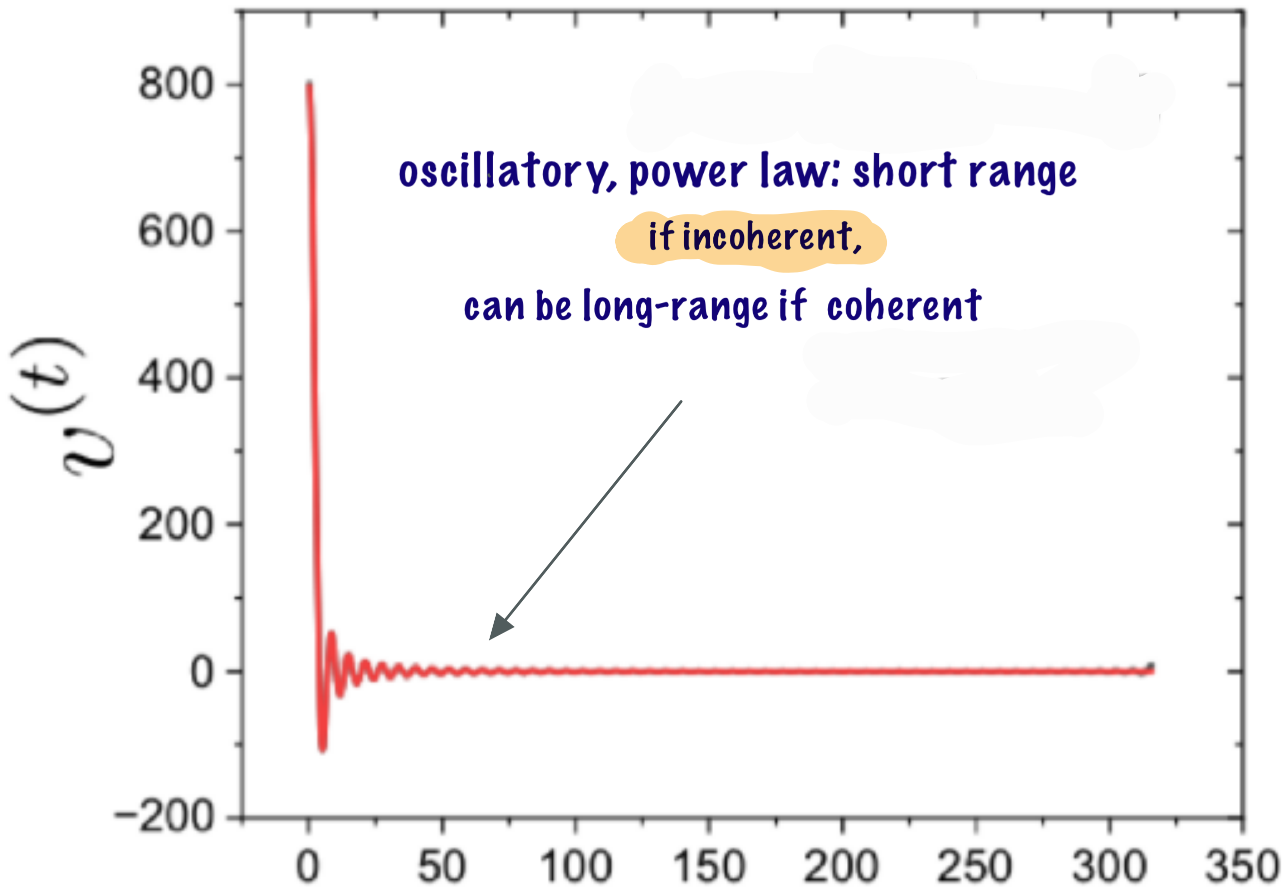
a whole zoo:

crystals
crystal with defects
crystal with particles supperposed

and liquids

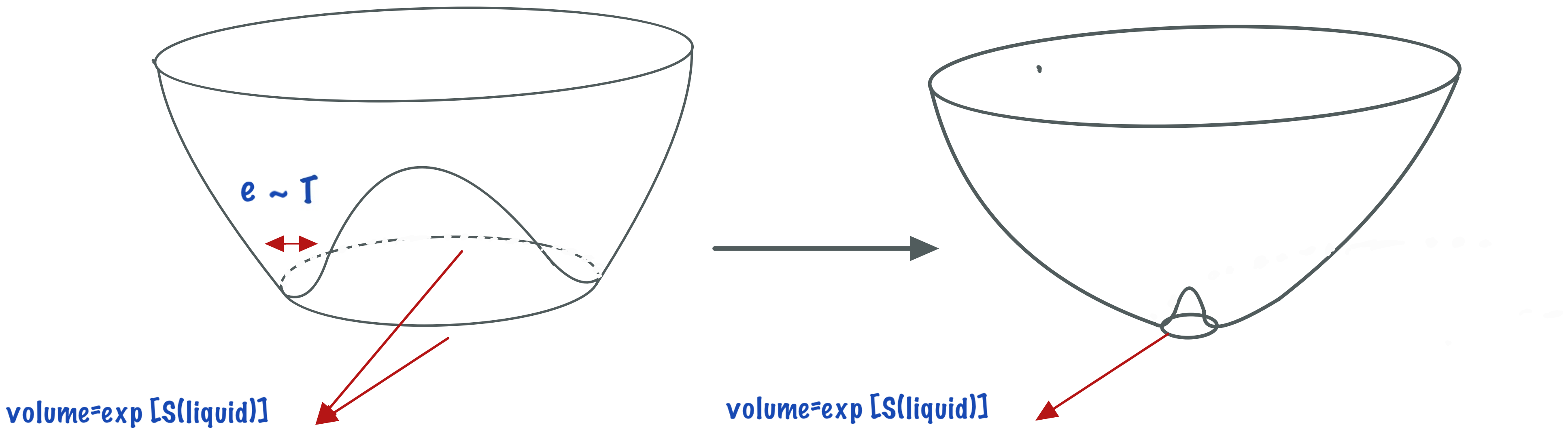


Large t,N liquids

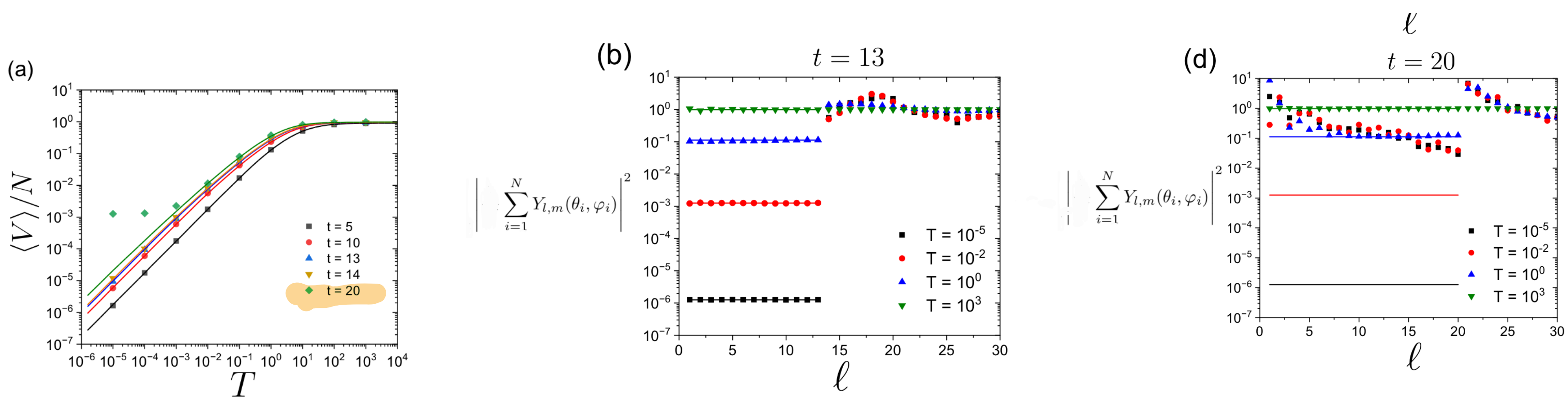


short range interaction liquid

Large t,N liquids



Large t,N liquids



$\alpha \sim 1$

$\alpha > 1$

GENERALIZATION TO S^d IS STRAIGHTFORWARD

$$Y_{\ell\mu}(\hat{\mathbf{r}}) = 0$$

$$\tilde{V}_(\hat{\mathbf{r}}, \hat{\mathbf{r}}') = \sum_{\ell=1}^{t} \sum_{\mu=1}^{d_l} Y_{\ell\mu}(\hat{\mathbf{r}})\, Y^*_{\ell\mu}(\hat{\mathbf{r}}'),$$

d_l is the degeneracy of degree-ℓ hyperspherical harmonics in S^d

The Christoffel–Darboux formula for Gegenbauer polynomials is

$$\tilde{V}_t = = \sum_{\ell=1}^{t} \frac{\ell+\mu}{\mu} \frac{C_\ell^{(\mu)}(x)}{C_\ell^{(\mu)}(1)} = \frac{t+1}{\mu} \frac{C_{t+1}^{(\mu)}(x) C_t^{(\mu)}(1) - C_t^{(\mu)}(x) C_{t+1}^{(\mu)}(1)}{(x-1)\, C_t^{(\mu)}(1)\, C_{t+1}^{(\mu)}(1)}$$

Gegenbauer polynomials reduce to Legendre ones for d=2

LARGE t ASYMPTOTICS

high density fluid

$$\tilde{V}_t^{(d)}(\theta) \sim \text{const} \frac{J_{\frac{d}{2}}(t\theta)}{(t\theta)^{\frac{d}{2}}},$$

range 1/t in distance

Its Fourier transform in $\mathbb{R}^d$ is proportional to the indicator of the unit ball:

$$\widehat{\tilde{V}_t^{(d)}}(k) \propto \mathbf{1}_{\{|k|<1\}}.$$

bear this in mind...

THE FLAT CASE: STEALTHY SYSTEMS

(Torquato, Stillinger...)

$$Y_{\ell\mu}(\hat{\mathbf{r}}) = 0$$

on the sphere

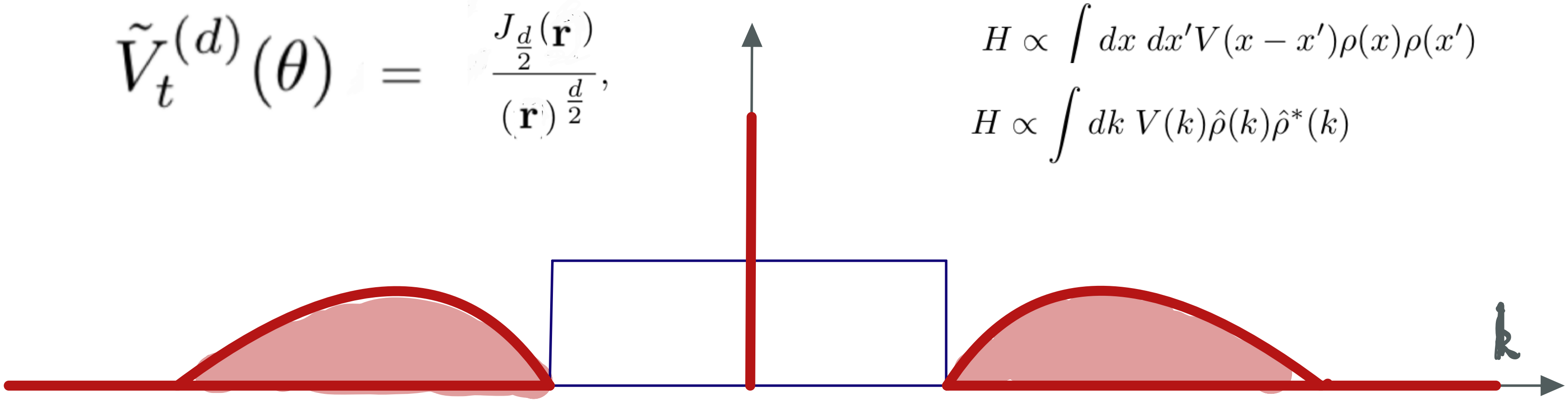
$$\widehat{\tilde{V}_t^{(d)}}(k) \propto \mathbf{1}_{\{|k|<1\}}.$$

in flat space of dimension d (or a torus)

$$\tilde{V}_t^{(d)}(\theta) = \frac{J_{\frac{d}{2}}(\mathbf{r})}{(\mathbf{r})^{\frac{d}{2}}},$$

$$H \propto \int dx\, dx' V(x-x')\rho(x)\rho(x')$$

$$H \propto \int dk\; V(k)\hat{\rho}(k)\hat{\rho}^*(k)$$



a family of ground states!

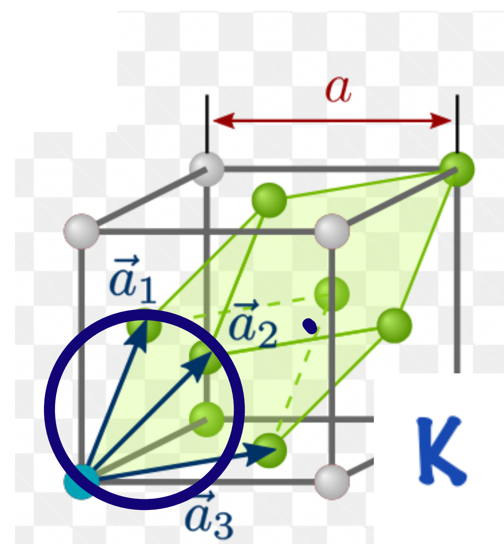
Can we find a $\rho(x)$ as above, that is made of points in real space?

i.e. can we find a set of points on the torus that makes a design?

start with a lattice in x,

Fourier transform of points in a lattice is a lattice in k

make it so the first nonzero |k| is outside the ball



Proof of existence, but not efficient

UNITARY t DESIGNS

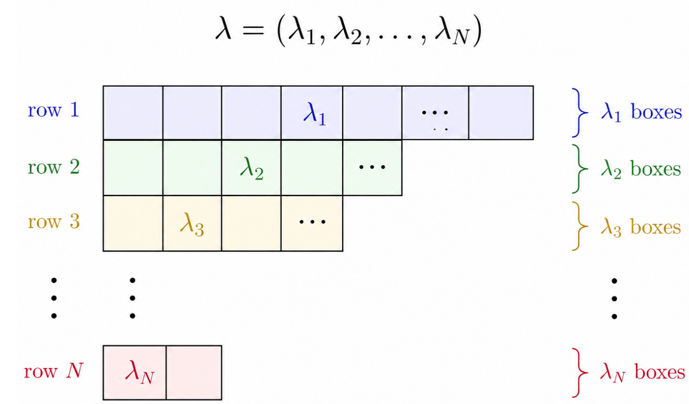
$$V = \sum_{i,j} \left| \mathrm{Tr}(U_i^\dagger U_j) \right|^{2t}$$

frame potential ground state, just as before

Sphere S^d	**Unitary group $U(N)$**
Harmonic functions $Y_{\ell m}(x)$	Matrix elements $D^\lambda_{ab}(U)$ (Peter–Weyl)
Gegenbauer polynomials $C_\ell^{(\alpha)}(\cos\theta)$	Schur polynomials / characters $\chi_\lambda(U)$
Label ℓ	Young tableau λ
Christoffel–Darboux kernel	$\sum_{\lvert\lambda\rvert\le t} d_\lambda\, \chi_\lambda(UV^\dagger)$

analogies

NICE FRAME POTENTIAL FOR UNITARY DESIGNS



lousy

$$V = \sum_{i,j} \left|\mathrm{Tr}(U_i^\dagger U_j)\right|^{2t} = \sum_\lambda m_\lambda \sum_{a,b} \left|\sum_i D^\lambda_{ab}(U_i)\right|^2 = \sum_\lambda m_\lambda \sum_{i,j} \chi_\lambda(U_i^\dagger U_j)$$

$$\tilde{V} = \sum_{i,j} \left|\mathrm{Tr}(U_i^\dagger U_j)\right|^{2t} = \sum_\lambda d_\lambda \sum_{a,b} \left|\sum_i D^\lambda_{ab}(U_i)\right|^2 = \sum_\lambda d_\lambda \sum_{i,j} \chi_\lambda(U_i^\dagger U_j)$$

the analogue of Christoffel-Darboux coefficients

ALL IN ALL:

for large t we get a **LIQUID** phase with a potential =

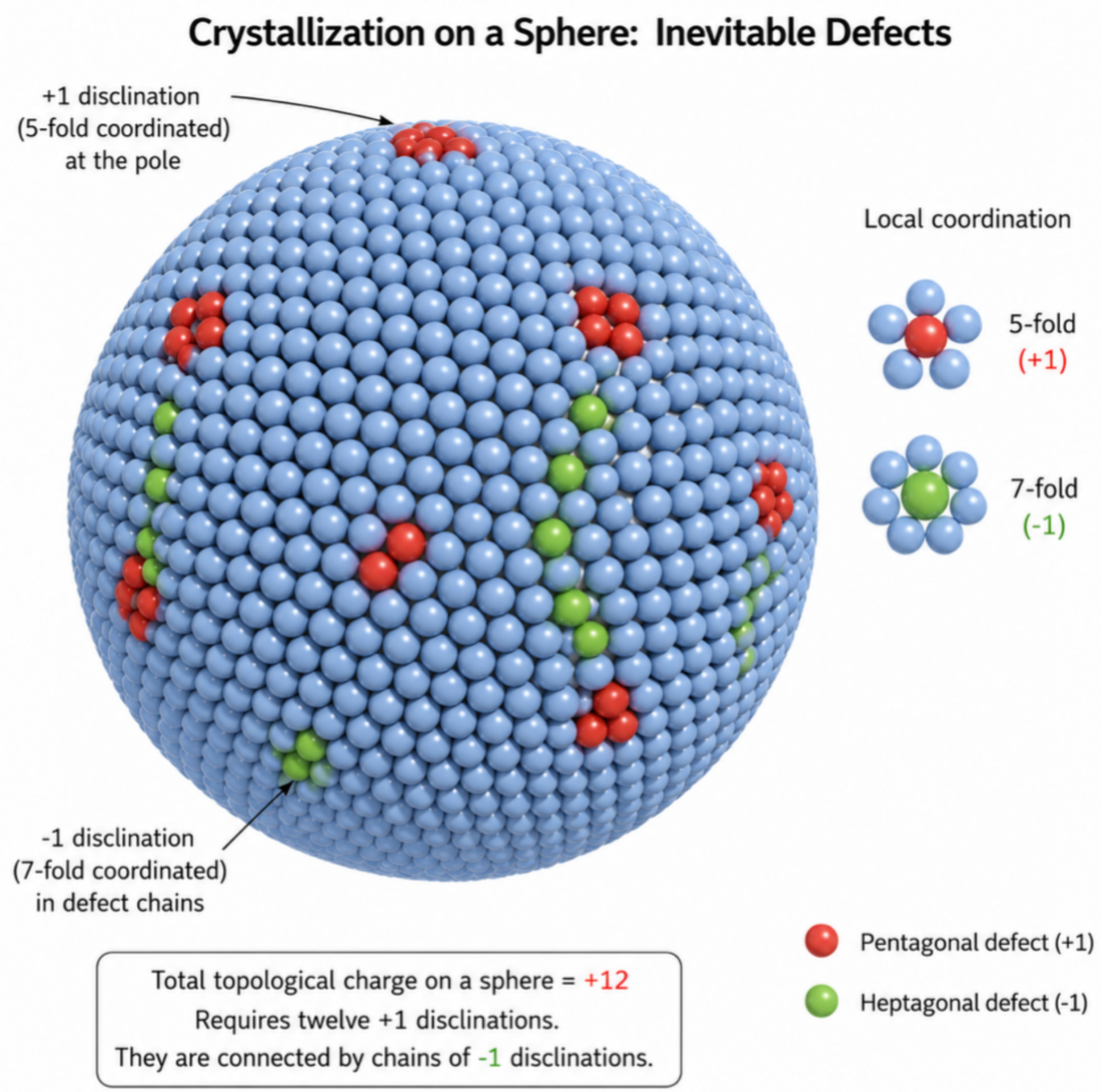
$$\tilde{V}_t^{(d)}(\theta) \sim \text{const} \; \frac{J_{\frac{d}{2}}(t\theta)}{(t\theta)^{\frac{d}{2}}},$$

(asymptotically flat)

range 1/t in distance

where "d" is the dimension of the sphere or the unitary group

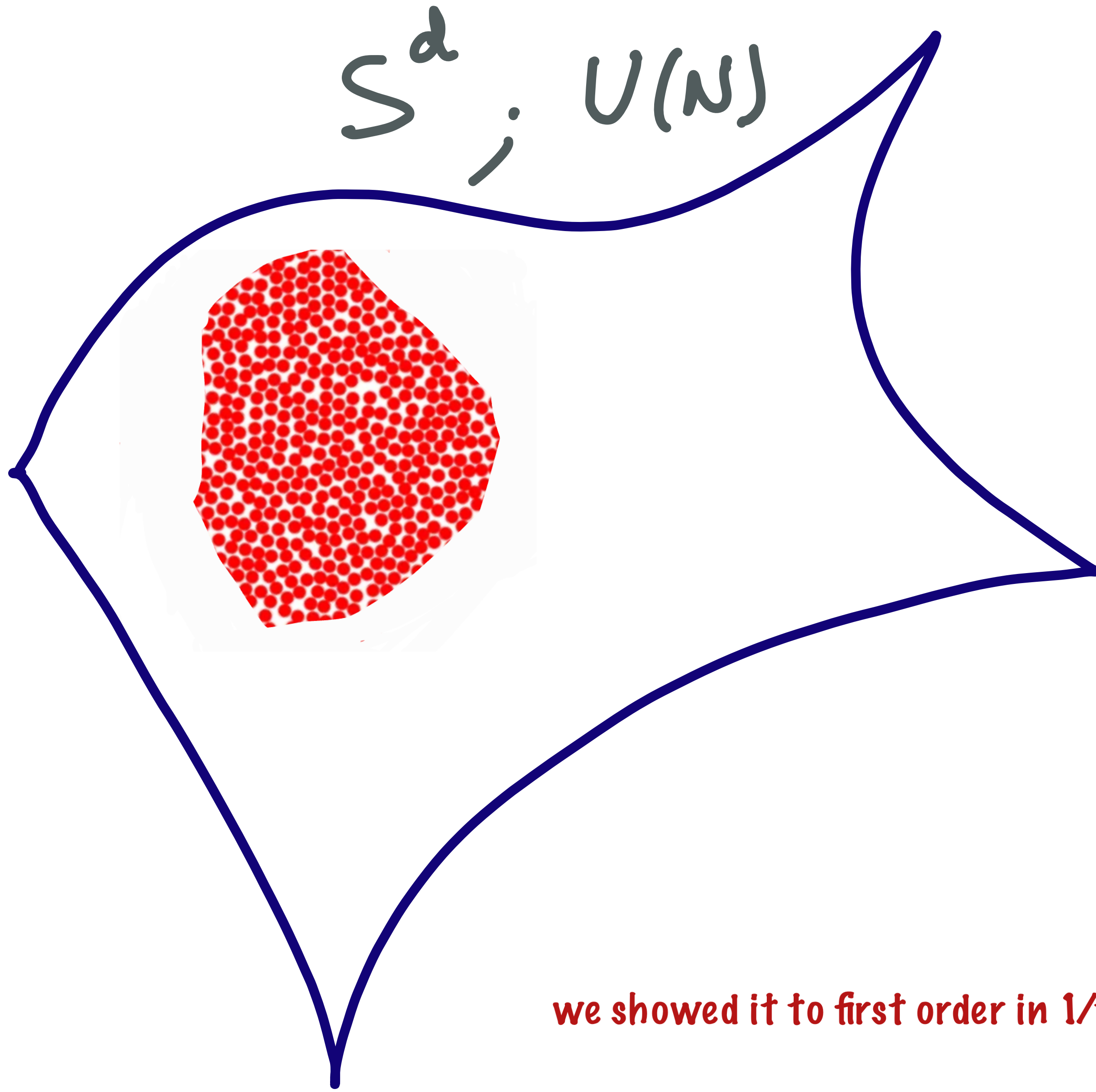
we are `pouring' a liquid into our manifold!



A flat crystal won't work

(but give a good quasi-design)

Conjecture: a liquid can `eat up´ defects, and yield a perfect design in the same range of densitites



we showed it to first order in 1/t

AND:

$$\alpha \equiv \frac{\text{number of equations}}{\text{number of unknowns}}$$

$$\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$$