The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization
IAEA

2162-26

Advanced Workshop on Anderson Localization, Nonlinearity and Turbulence: a Cross-Fertilization

23 August - 3 September, 2010

Chaos in space? The case of glasses. (Chaos / Glasses)

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chaos / glasses

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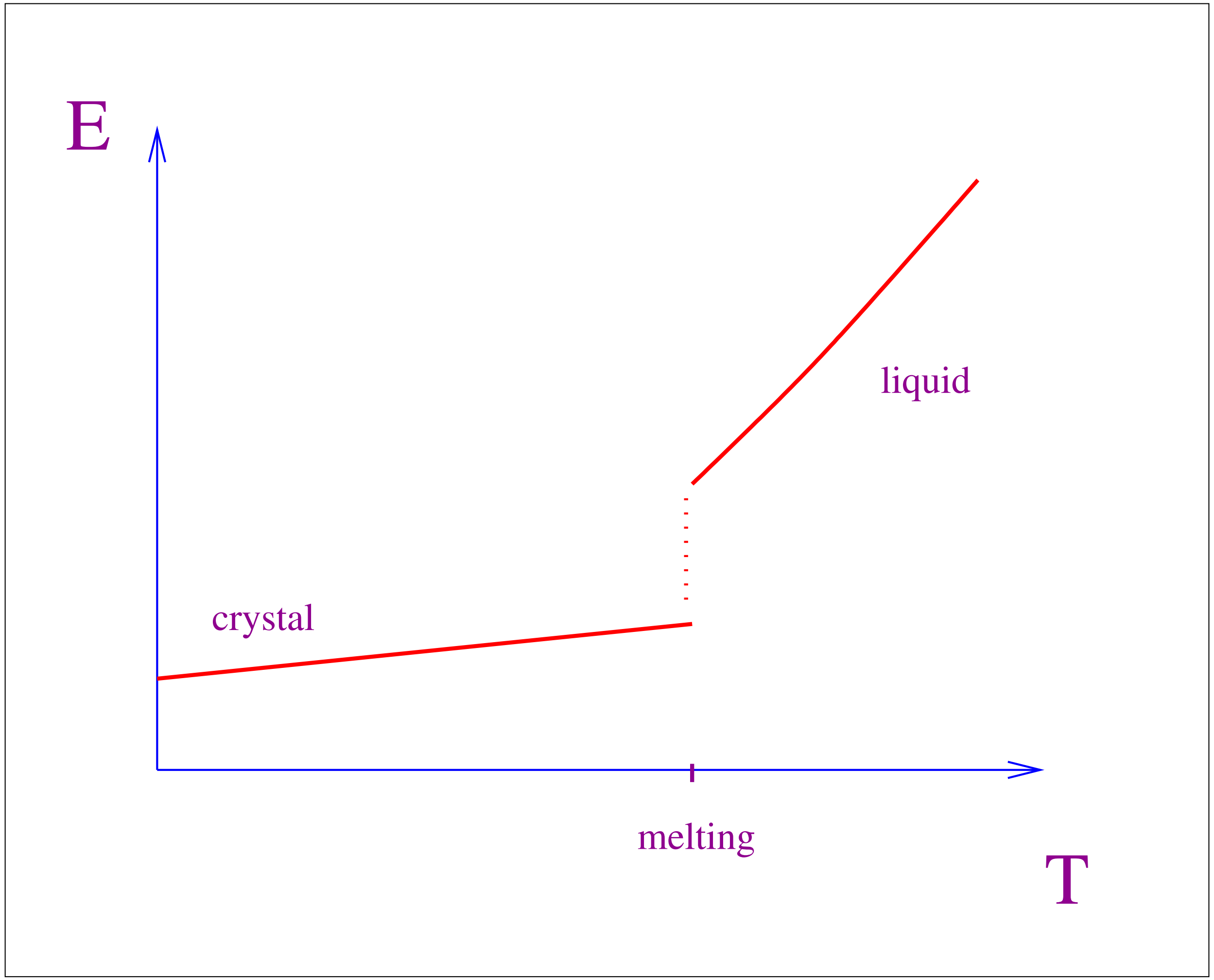
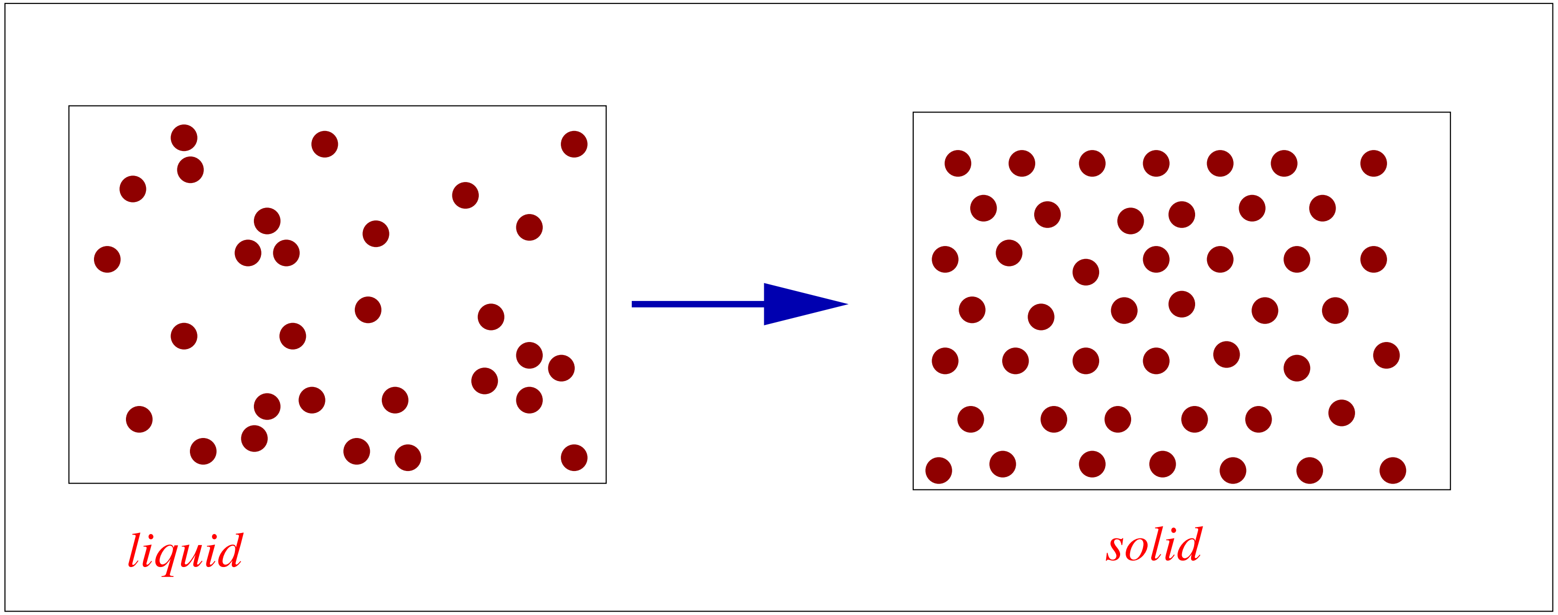
trieste

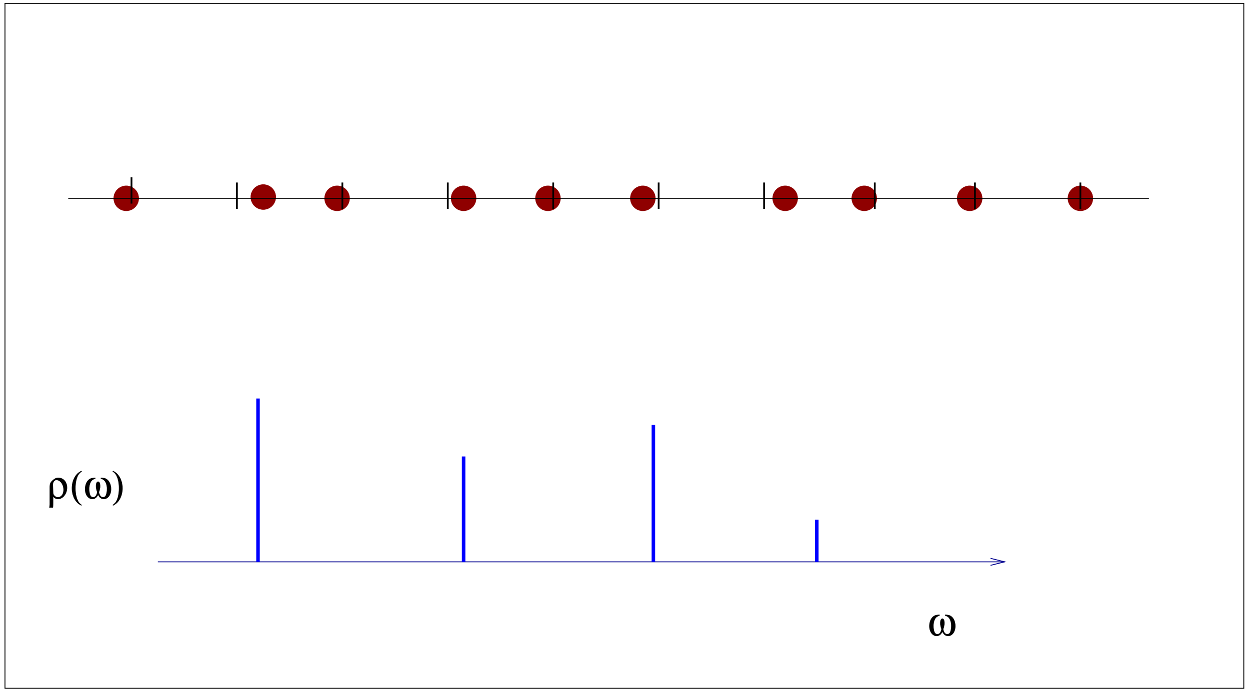


E versus T – or V versus $1/P$.

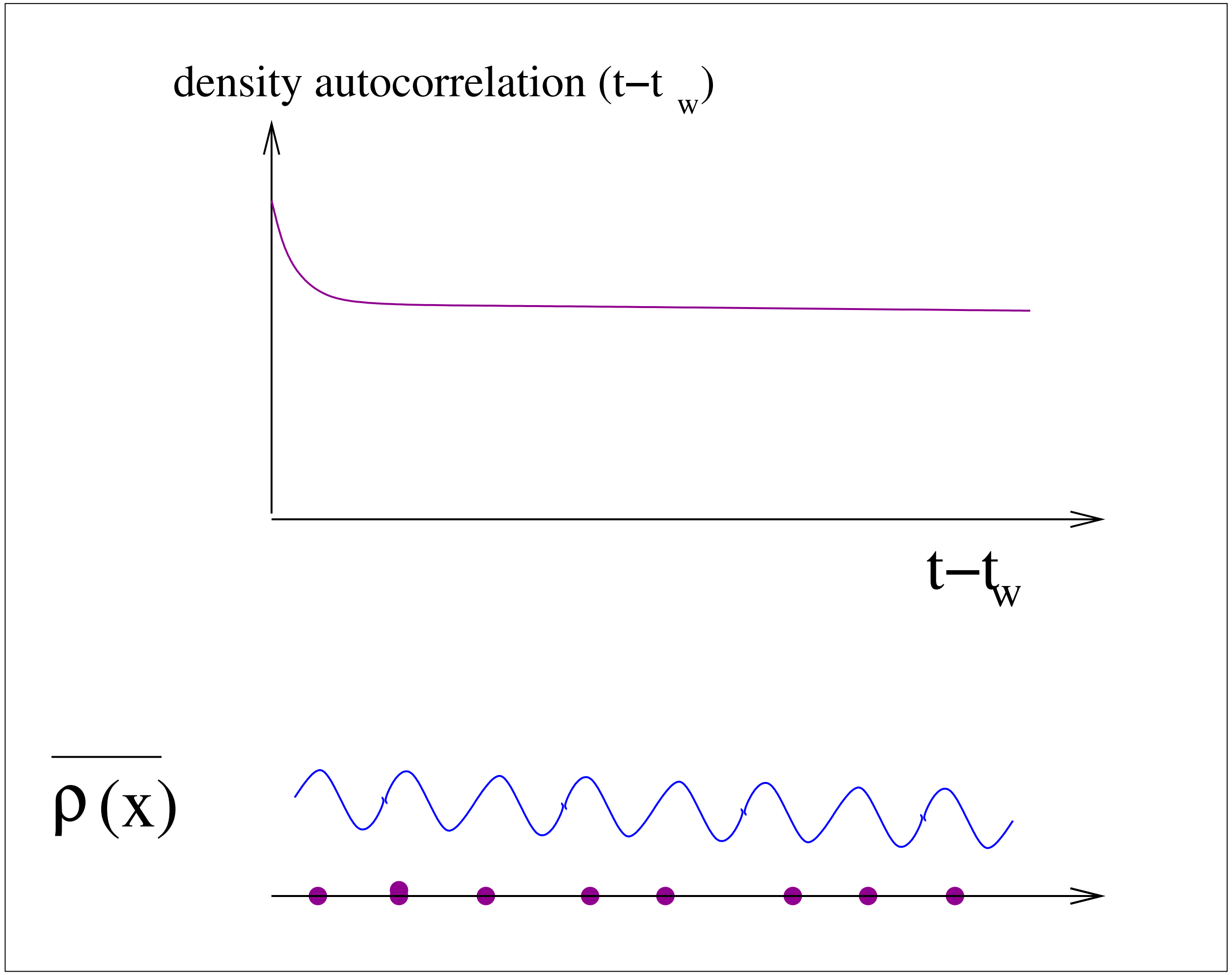
Solidification: a magic trick of crystallisation



Bragg peaks

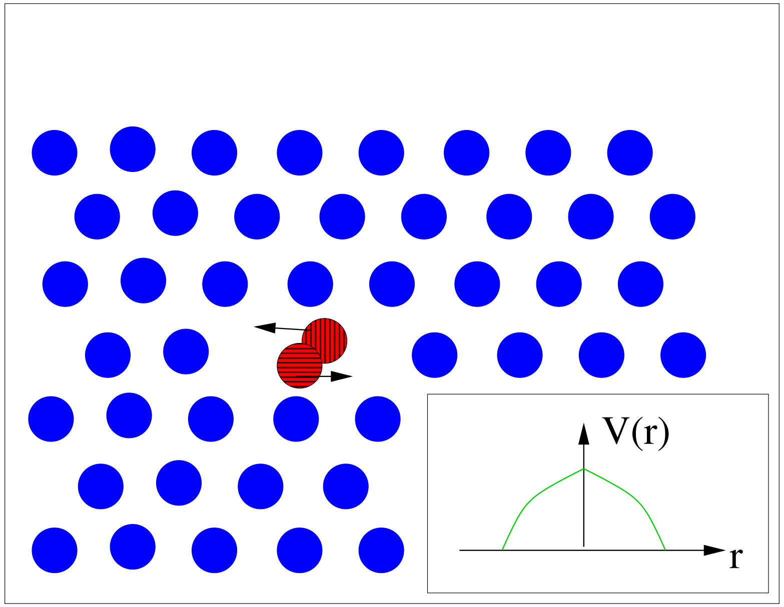


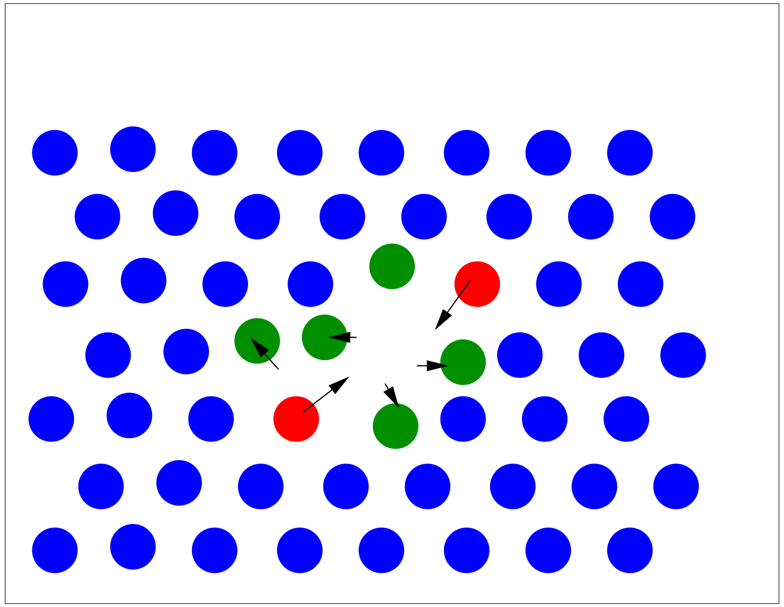
$$\bar{\rho}(x) = \tau^{-1} \int_0^{\tau} dt \; \rho(x,t) \; = \frac{1}{N\tau} \int_0^{\tau} dt \; \Sigma_a \; \delta[x_a(t) - x]$$



$$C(t,t_w) = V^{-1} \int dx \; [\rho(x,t)\rho(x,t_w) - \rho_o^2]$$

Soft (and even hard) particles may rearrange

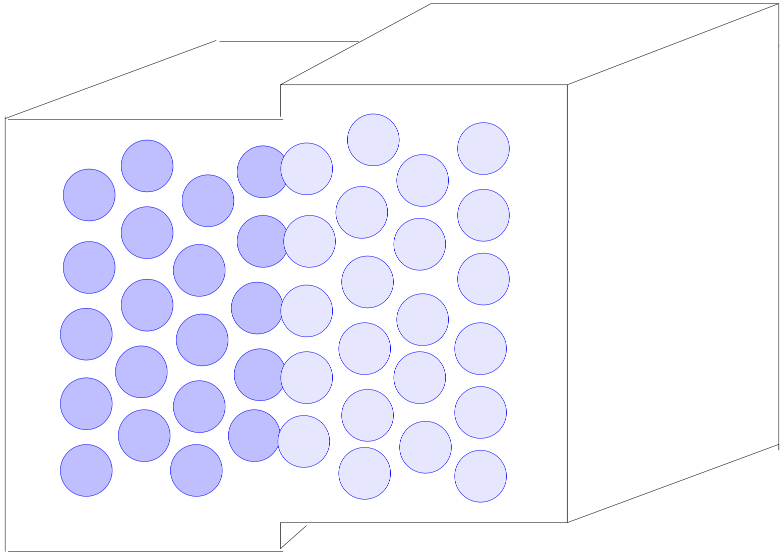


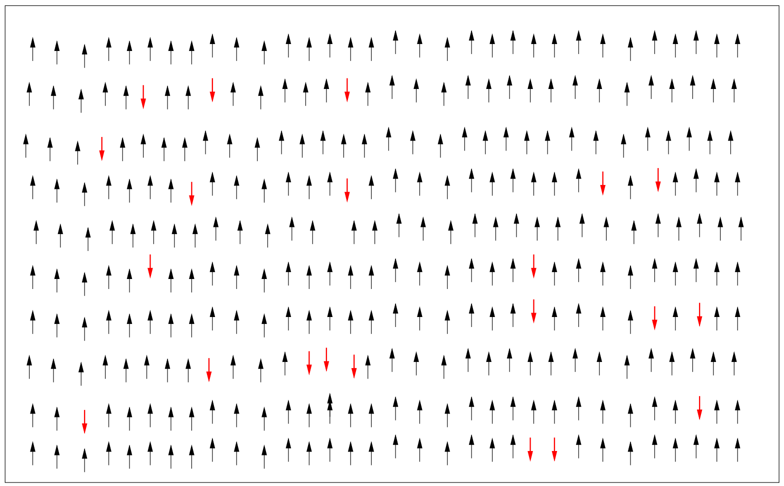


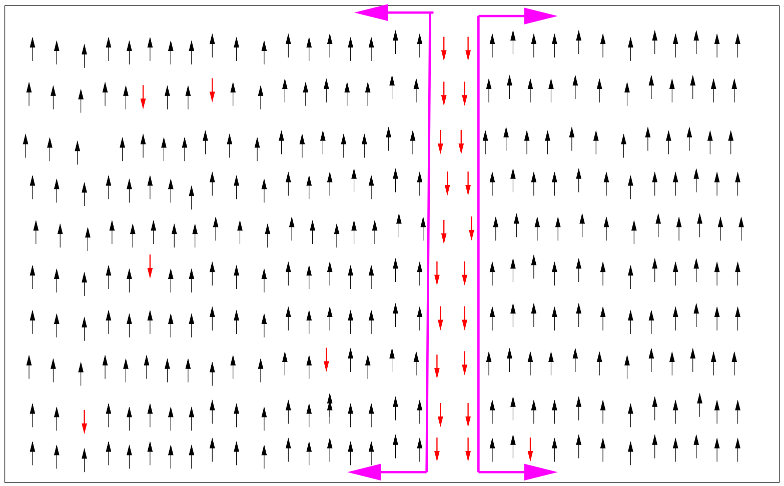
It is a conspiracy of soft constituents that makes a solid

How to make a hard building with soft bricks

energetic

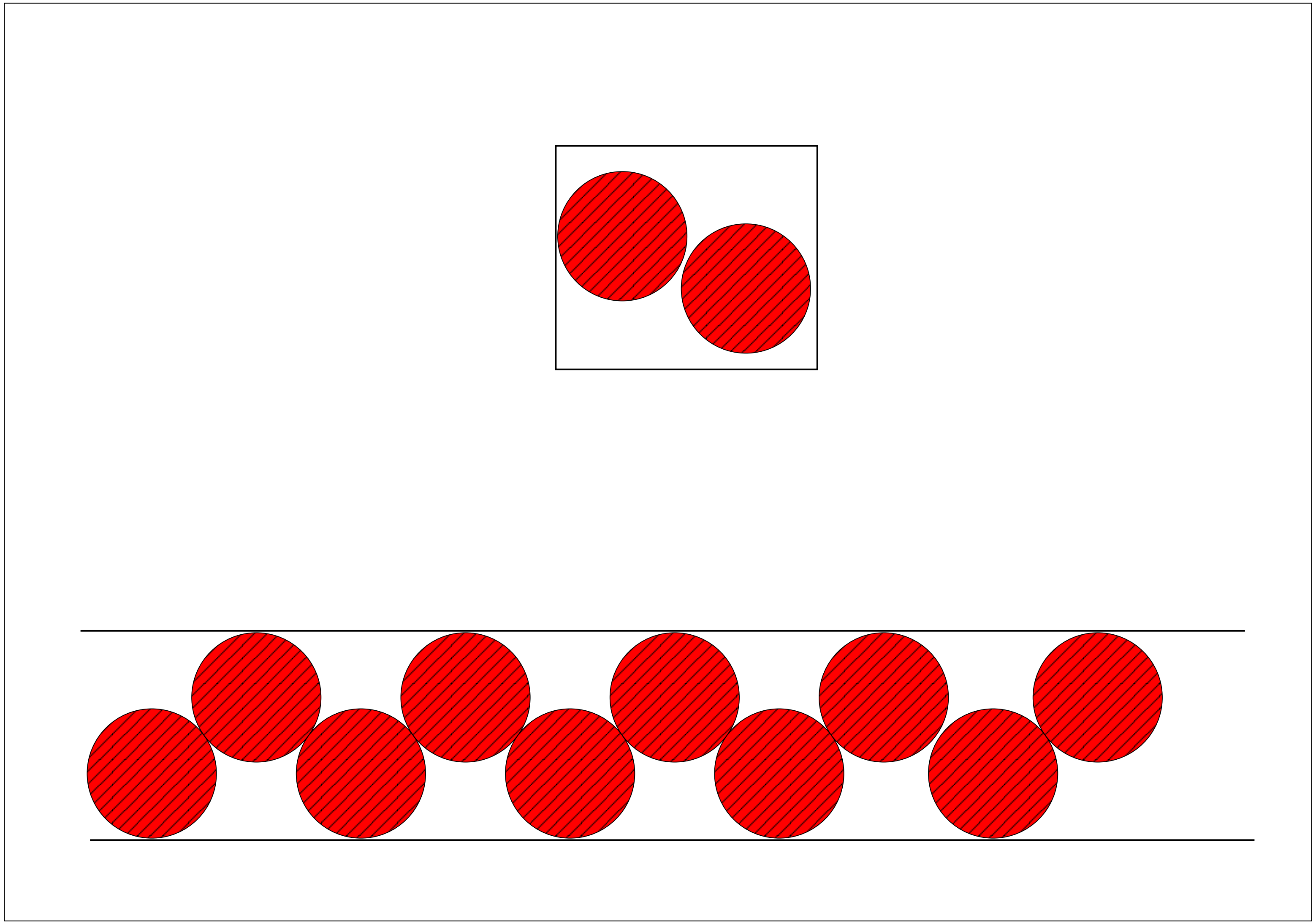




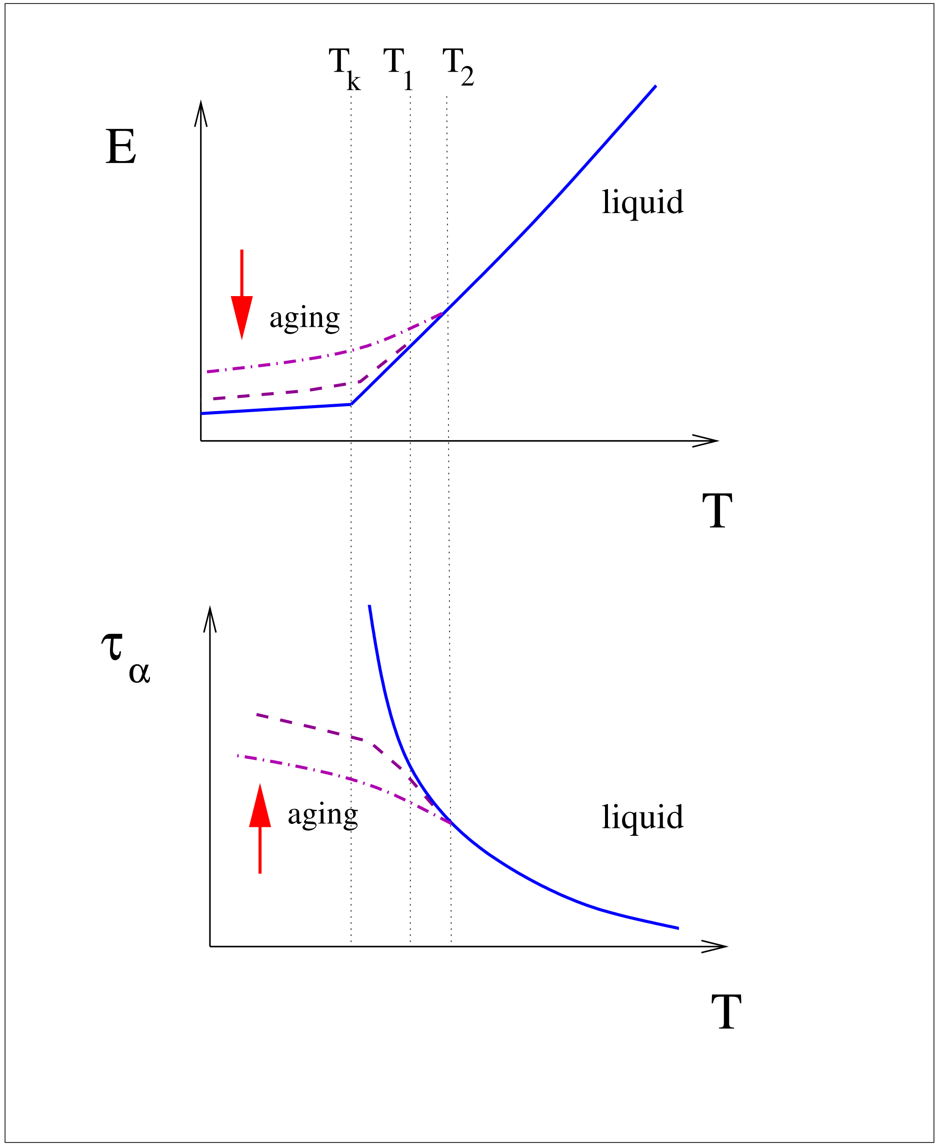


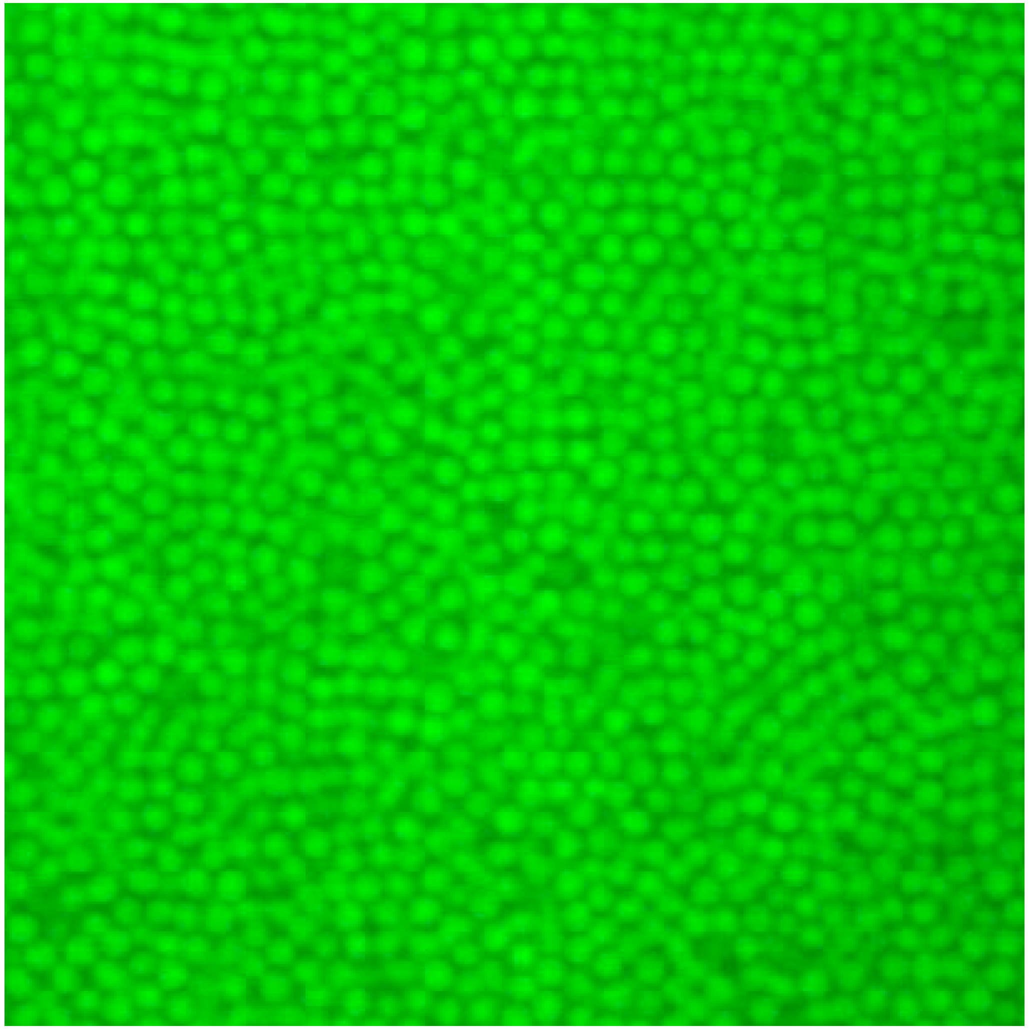
entropic

Jammed non-thermodynamc solidity

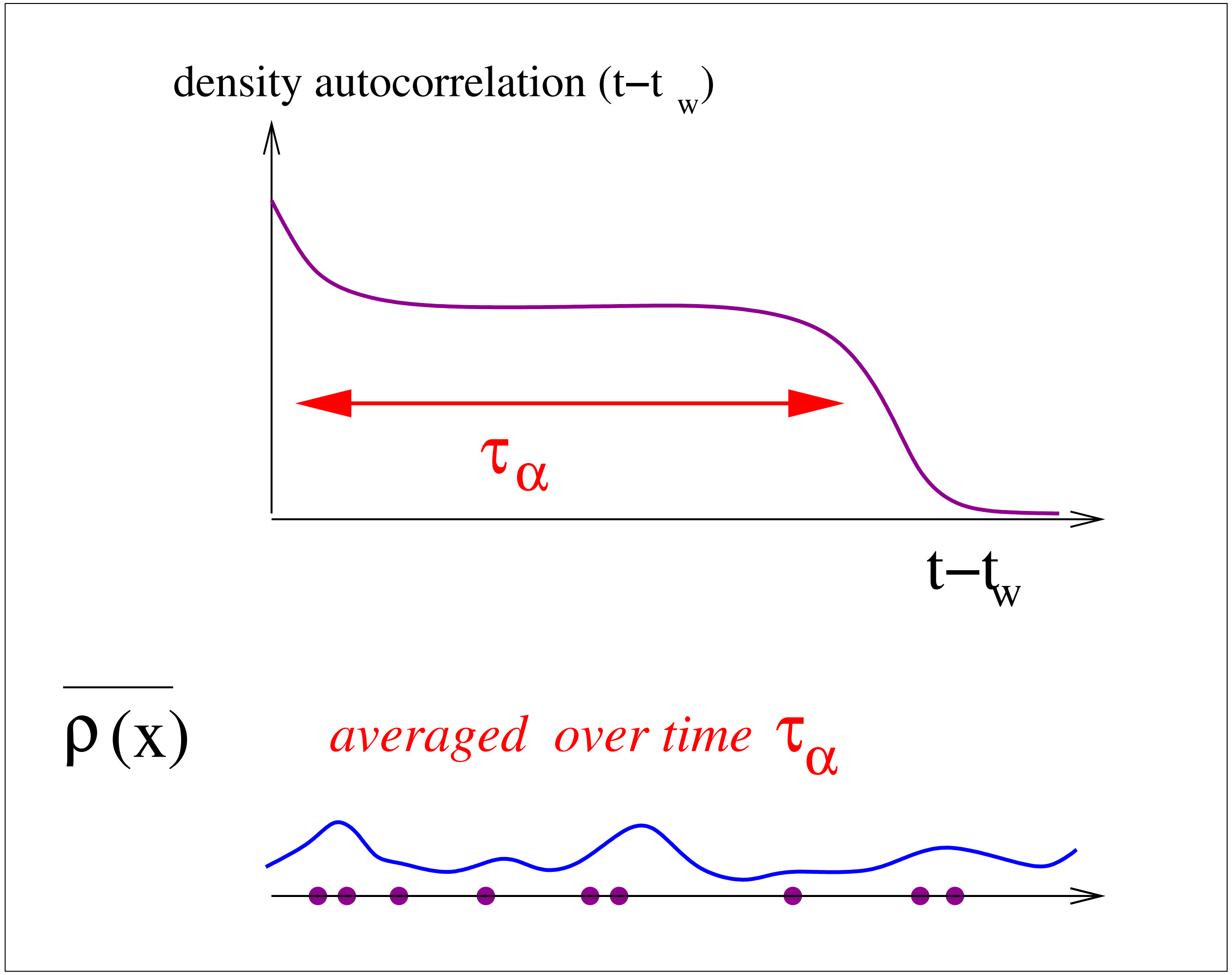


Glassy solid: a trick without a magician?

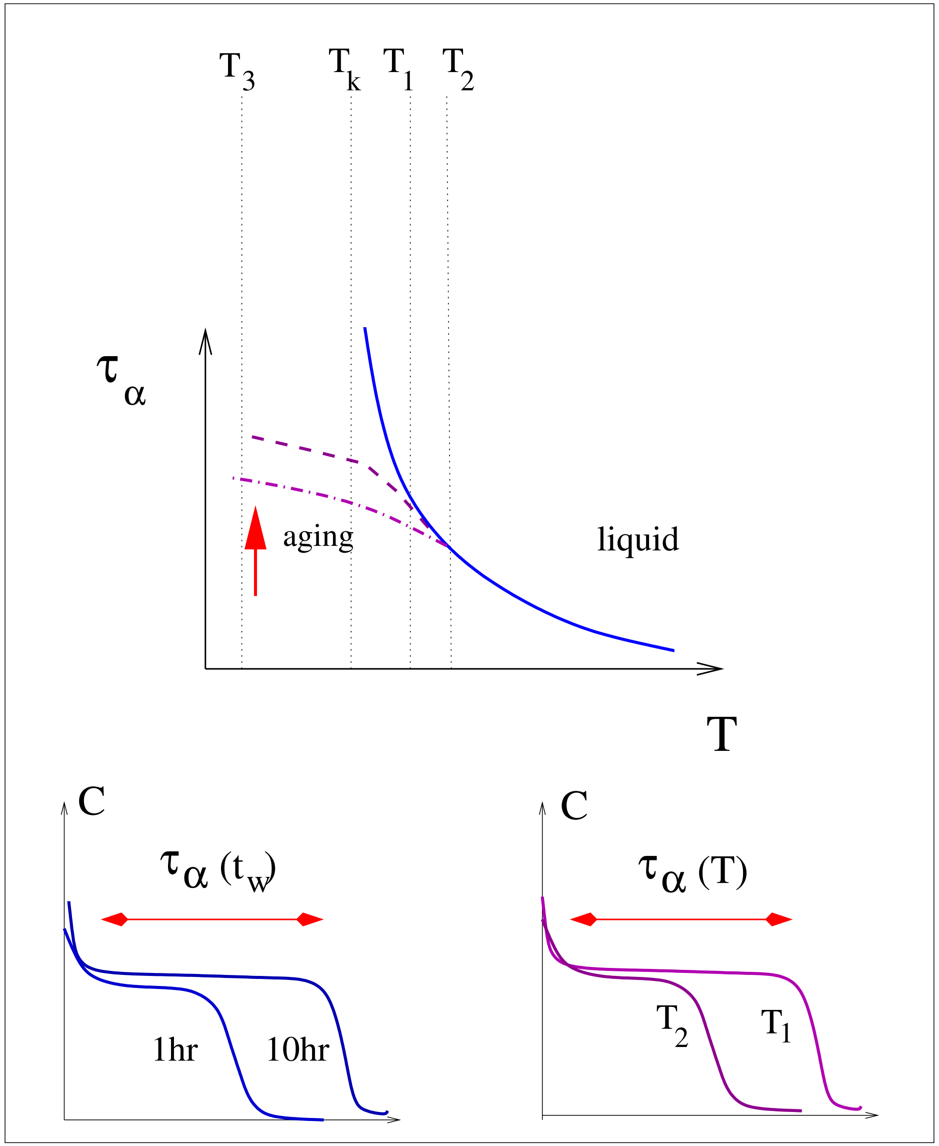


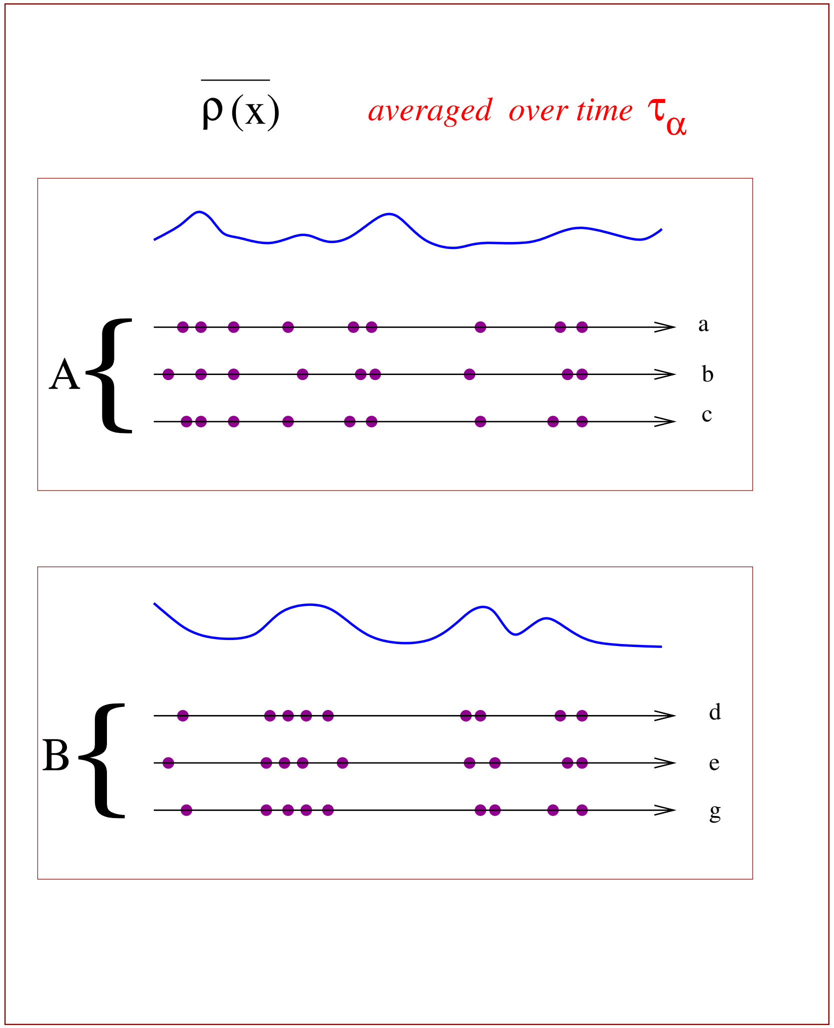


(less and less) transient density profiles

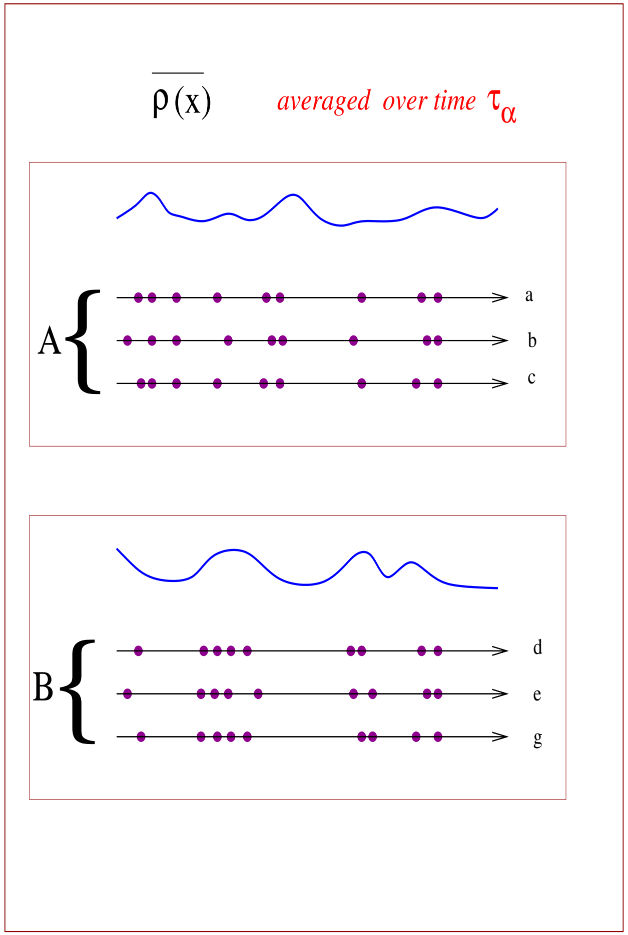


The α scale, in and out of equilibrium

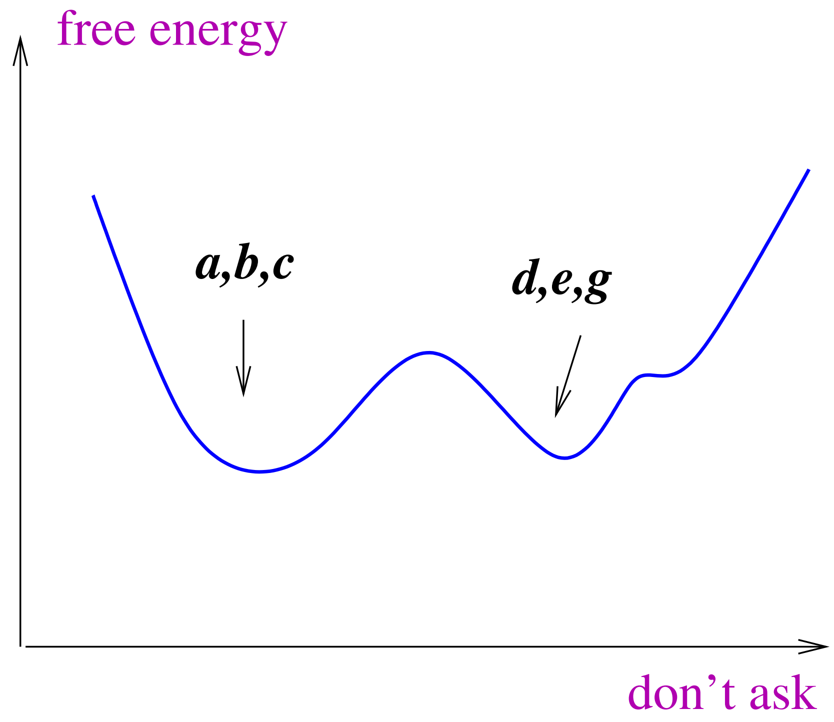




If $\tau_\alpha = \infty$ we have true states


$\overline{\rho}(x)$
averaged over time τ_α
A
a
b
c
B
d
e
g

landscape


free energy
a,b,c
d,e,g
don't ask

Density functional theory $\leftrightarrow$ Random First Order

a mean-field free energy

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\ \rho[\ln\rho(\mathbf{x}) - 1] - \frac{1}{2}\int d^3\mathbf{x}\ d^3\mathbf{x}'\ [\rho(\mathbf{x}) - \rho_o] C(\mathbf{x} - \mathbf{x}') [\rho(\mathbf{x}') - \rho_o]$$

has many local minima, solutions of

$$\frac{\delta F[\rho(\mathbf{x})]}{\delta \mathbf{x}} = \ln\rho(\mathbf{x}) - 1 - \int d^d\mathbf{x}'\ C(\mathbf{x} - \mathbf{x}', \rho_o)[\rho(\mathbf{x}') - \rho_o] = 0$$

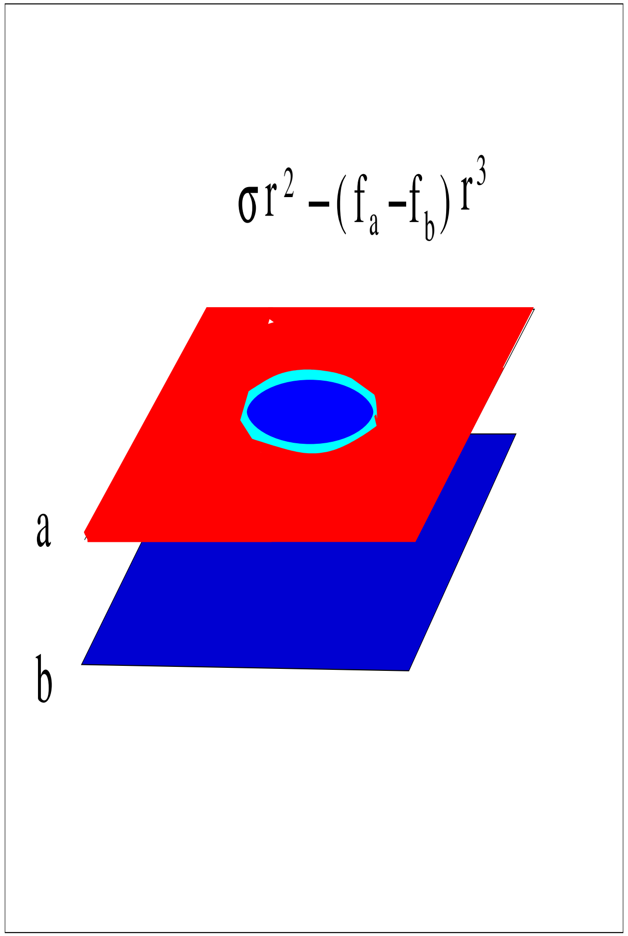
liquid – crystal + many amorphous

Two nucleation arguments show that it is impossible to have

- **stable states with free energy density higher than equilibrium**

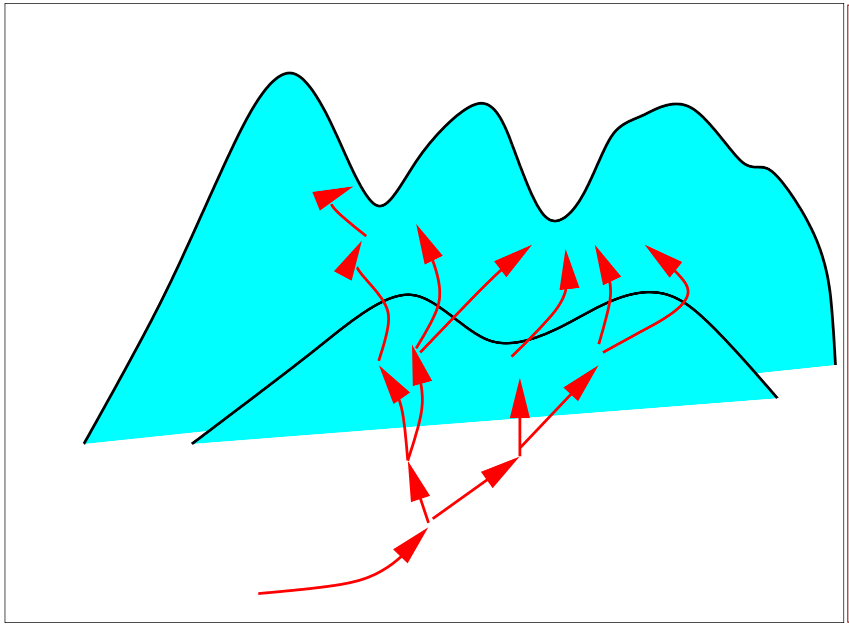
or

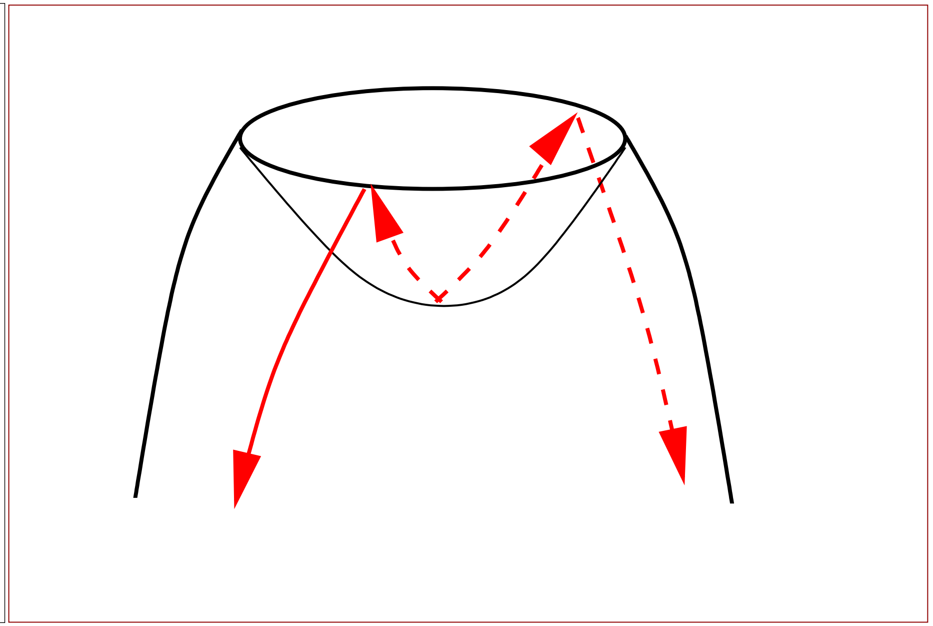
- **exponential in number**



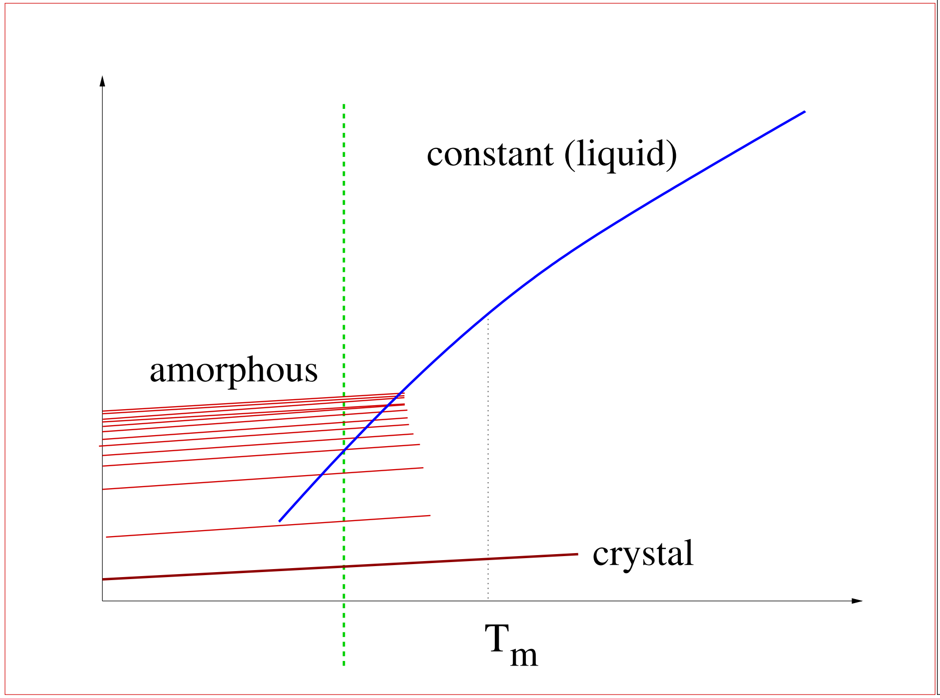
$$r^* = \frac{(2)\sigma}{3(f_a - f_b)} \quad \rightarrow \quad f(r^*) \propto \frac{\sigma^3}{(f_a - f_b)^2}$$

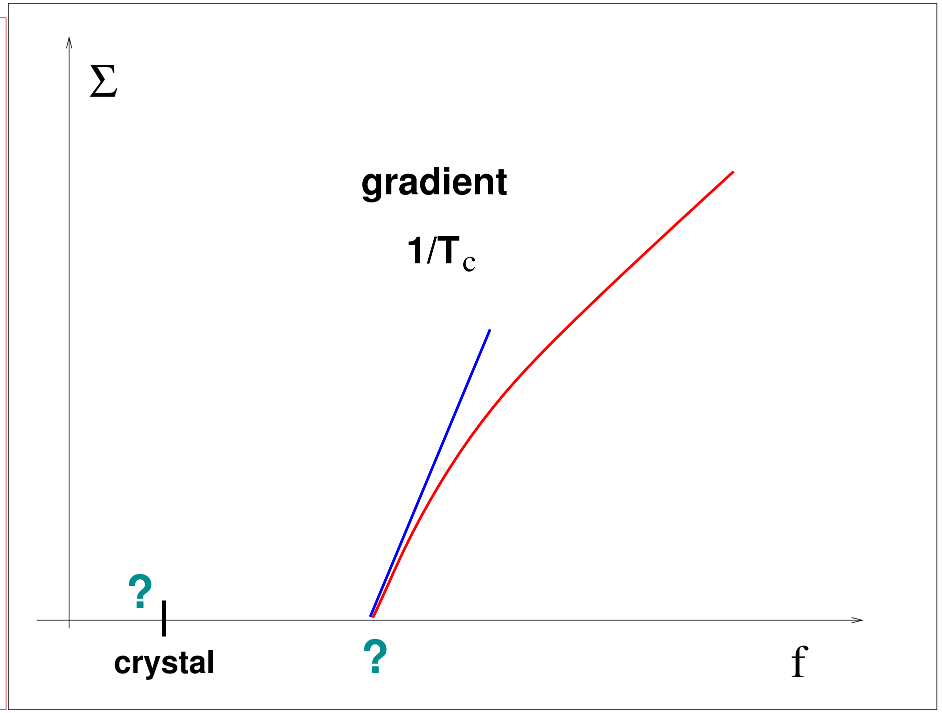
Entropic pressure: multiplication of possibilities helps climb high mountains





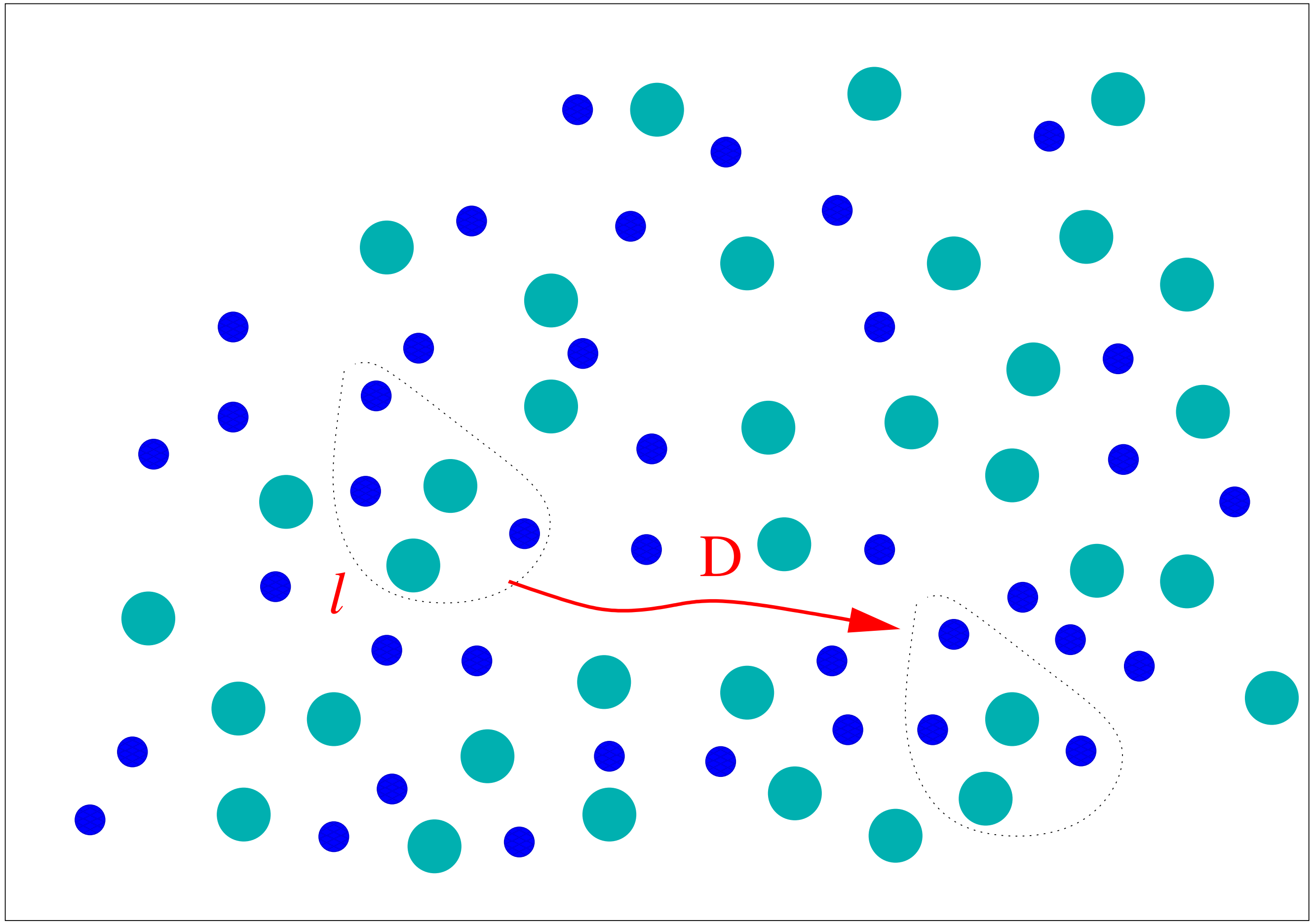
$$V_{eff} = V(r) - T(d-1)\ln r$$





$$\mathbf{Z} = \mathbf{\Sigma_{solutions}} \quad \mathbf{e}^{\mathbf{V}[\mathbf{\Sigma(f)}-\beta\mathbf{f}]}$$

$$\frac{\mathbf{d\Sigma}}{\mathbf{df}} = \frac{\mathbf{1}}{\mathbf{T}}$$



Complexity measurable from pattern repetition in $\rho(x)$

$$D \sim e^{\ell^d/\Sigma}$$

$\Sigma = 0$ **implies patterns of all sizes repeat *often*** (more later)

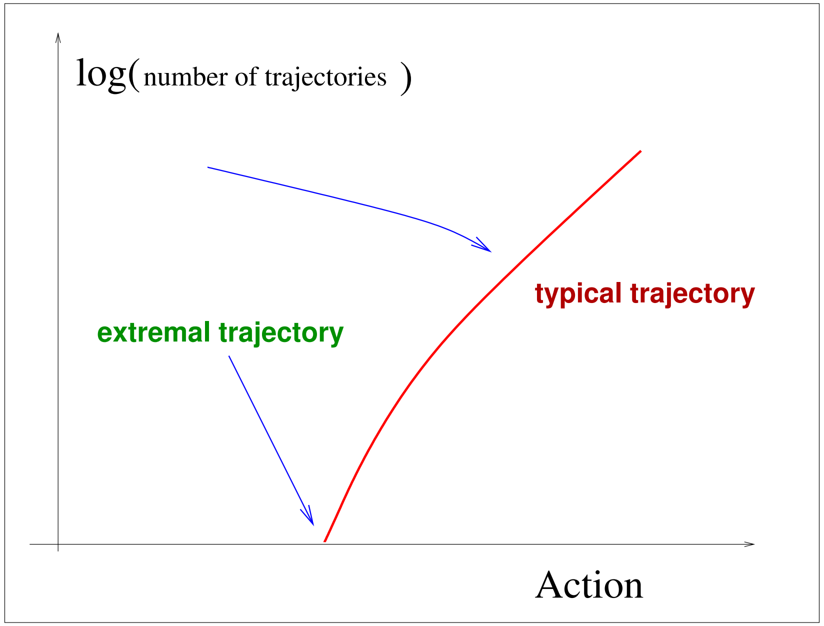
Analogy with dynamic systems Ruelle + Aubry-Mather theory

space	$\longrightarrow$	time
$-\int d^d\mathbf{x}'\ C(\mathbf{x}-\mathbf{x}',\rho_o)[\rho(\mathbf{x}')-\rho_o] + \ln\rho(\mathbf{x}) = 1$	$\longrightarrow$	$\ddot{x}_i = f_i$

$\rho(x) = \rho_o$ liquid	$\longrightarrow$	fixed point
crystal	$\longrightarrow$	periodic solution
amorphous	$\longrightarrow$	chaotic solution

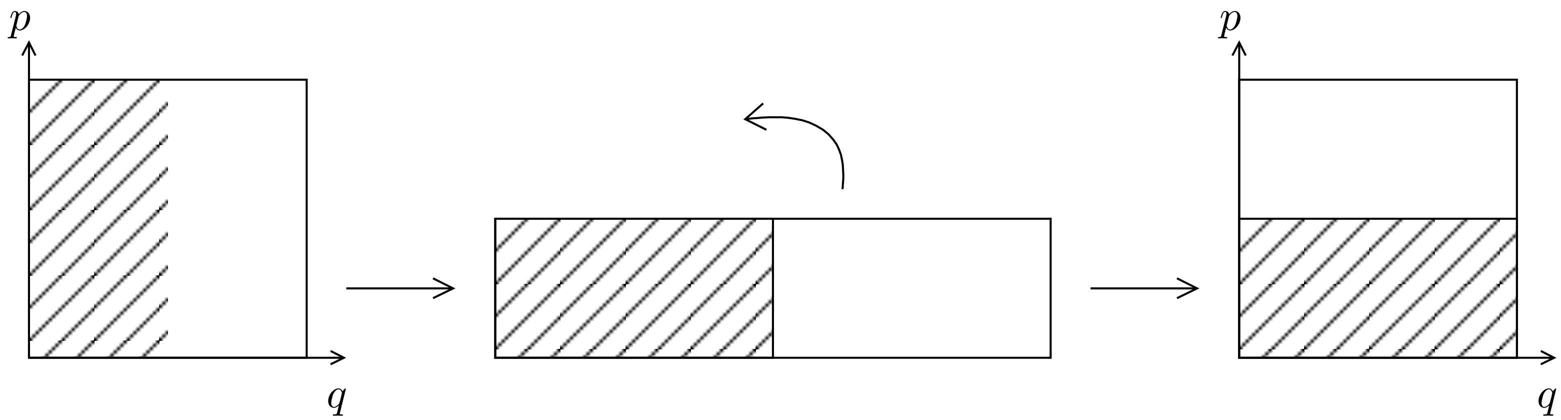
Are glasses then chaotic solutions in space?

yes and no!



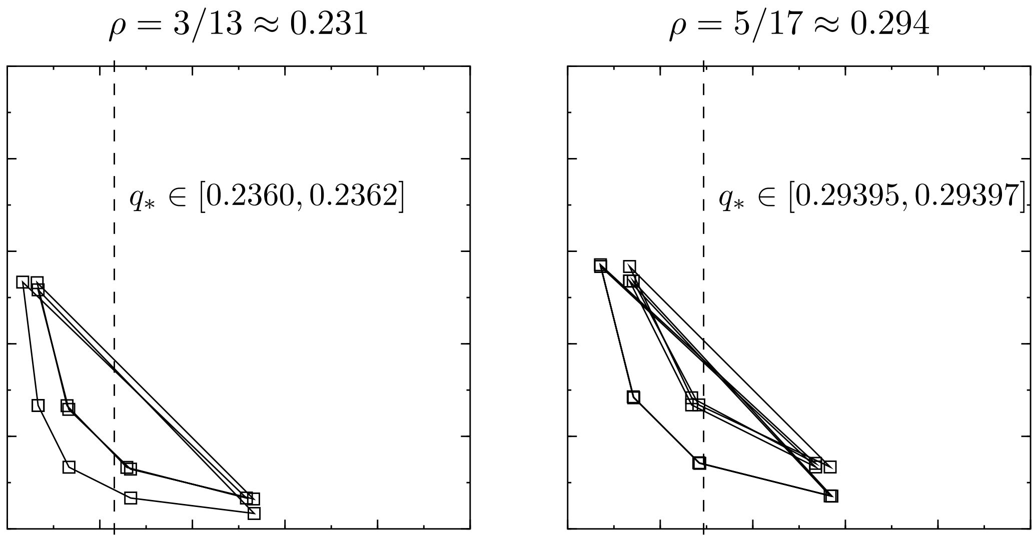
Because we are looking for solutions that are global minima of the free energy, the analogue is to look for trajectories that have globally minimal action $S = \int dt\ L(q, \dot{q})$, or are extrema of some functional $\mathcal{A} = \int dt\ A(q, \dot{q})$

The baker's map



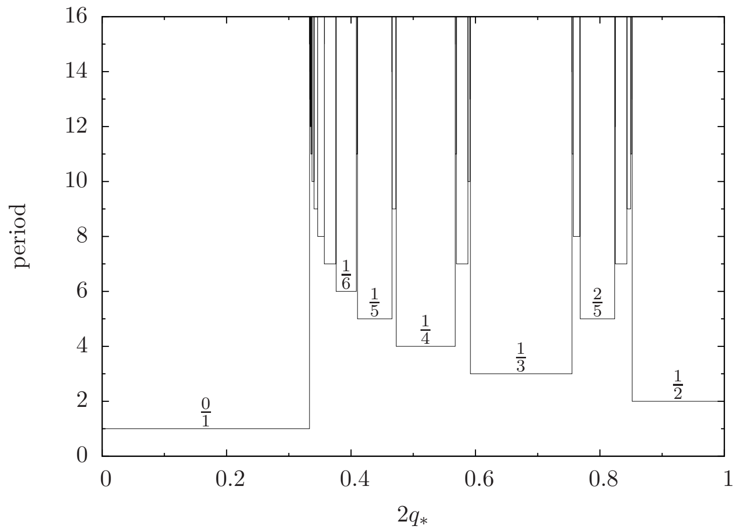
... is as chaotic as you can be.

And yet, orbits minimising a 'free energy' function, e.g. $\mathcal{A} \equiv \int dt\ (q(t) - q_*)^2$



are periodic or quasiperiodic

Hunt and Ott — Khan-Dang Nguyen Thu Lam, JK , D Levine



Period versus q^*

Density functional theory reduced to the essential

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\; \rho[\ln \rho(\mathbf{x}) - 1] - \frac{1}{2}\int d^3\mathbf{x}\, d^3\mathbf{x}'\; [\rho(\mathbf{x}) - \rho_o] C(\mathbf{x} - \mathbf{x}') [\rho(\mathbf{x}') - \rho_o]$$

$$\downarrow$$

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\, V(\rho) - \frac{1}{2}\int d^3\mathbf{x}\;\; \rho(\mathbf{x})(a_o + a_1\nabla^2 + a_2\nabla^4 + \ldots)\rho(\mathbf{x})$$

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\, V(\rho) - \frac{1}{2}\int d^3\mathbf{x}\;\; (a_o\rho^2 - a_1(\nabla\rho)^2 + a_2(\nabla^2\rho)^2 + \ldots)$$

What are then the stationary solutions of

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\, V(\rho) - \frac{1}{2}\int d^3\mathbf{x}\ \ (a_o\rho^2 - a_1(\nabla\rho)^2 + a_2(\nabla^2\rho)^2)$$

and , in particular, its ground state?

One dimension

$$F[\rho(\mathbf{t})] = \int dt\; V(\rho) - \frac{1}{2}\int dt\;\; (a_o\rho^2 - a_1(\dot{\rho})^2 + a_2(\ddot{\rho})^2)$$

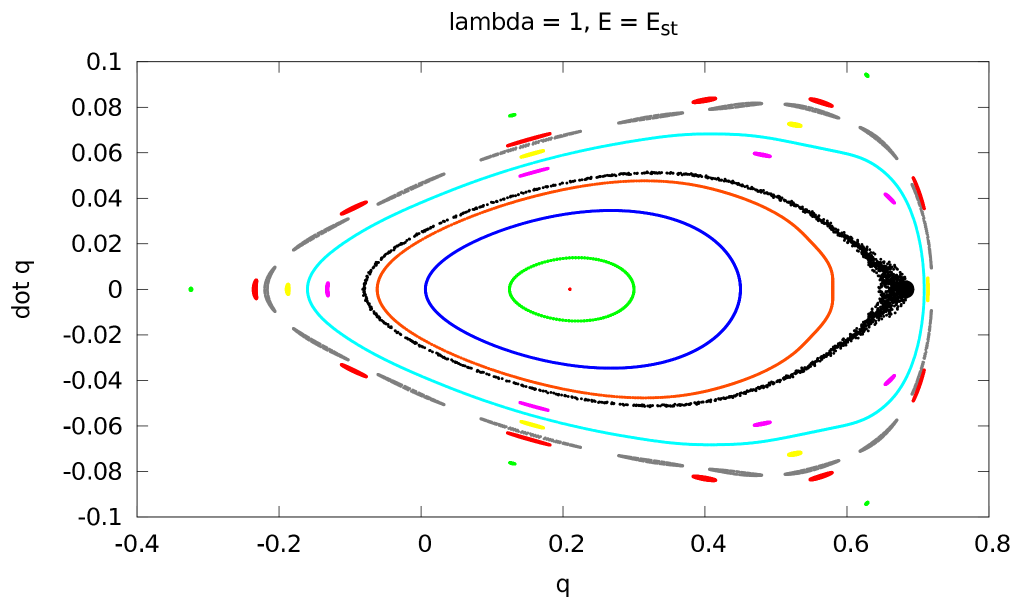
ad nauseam Legendre transform $(\rho, \hat{\rho})$ and $(w, \hat{w})$

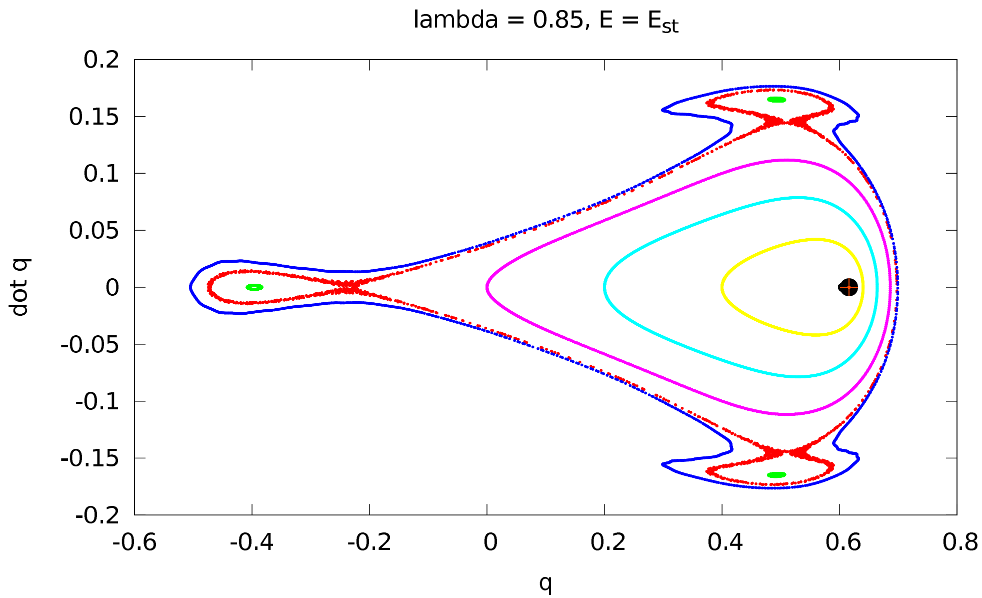
$$\mathcal{H} = V(\rho) + \tfrac{1}{2}a_o\rho^2 - \tfrac{1}{2}a_1 w^2 + w\hat{\rho} - \tfrac{1}{2}\hat{w}^2$$

a non-linear, unbounded, Hamiltonian with more than one degree of freedom

Chaos allows to have amorphous solutions

Unboundedness allows to have isolated periodic solutions


lambda = 1, E = E_st
dot q
q
0.1
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.4
-0.2
0
0.2
0.4
0.6
0.8


lambda = 0.85, E = E_st
dot q
q
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8

Density functional theory in higher dimension:

Chaos with several variables *and* **three dimensional time...**

The ideal glass state might well be periodic or quasiperiodic

...what matters is whether it is *isolated* or not.

glasses $\leftrightarrow$ spatio-temporal chaotic scattering