From the hopping crystal to the cluster glass

Rogelio Díaz-Méndez, Fabio Mezzacapo, Wolfgang Lechner, Fabio Cinti, Egor Babaev and Guido Pupillo

UNIVERSITÉ DE STRASBOURG

Ordering in 2D

Ordering processes in a system of interacting particles in 2D behave in different ways depending on the uniformity of its constituents: **Monodisperse** ensembles crystallize very well, not only by slow annealing but also after temperature quenches. **Polydisperse** ensembles, instead, are good glass-formers, not only through quenching protocols but also with annealing, so avoiding crystallization.

Cluster-forming ability

Systems of particles interacting via potentials with a negative minimum in the *effective* Fourier transform, develop cluster structures. While these structures are known to form crystals and quasicrystals in 2D, **its dynamics is still unknown**, both in the equilibrium and non-equilibrium regimes.

The model

We consider a system of **monodisperse** particles interacting via a generic ultrasoft repulsive interaction of the form

$$U(r) = U_0\left[1 + (r/r_c)^6\right]^{-1} \quad (1)$$

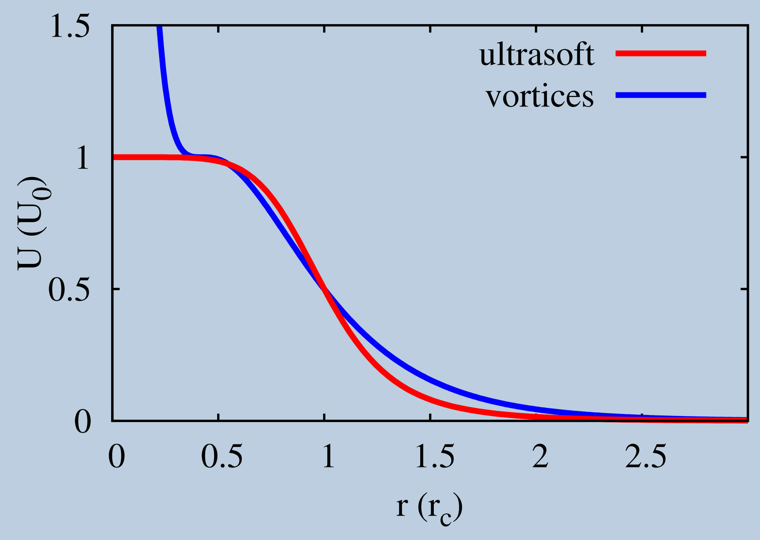

Figure 1: Pair-wise interaction potentials with cluster-forming ability. Red line: generic interaction of Eq. (1). Blue line: specific interaction [Eq. (2)] of relevance to 1.5 superconductors.

We study the physical properties of this ensemble following **annealing** and **temperature quenches**, by means of molecular dynamics simulations with a Langevin thermostat.

Findings

1. The cluster-crystal at equilibrium presents a **two-step relaxation**, similar to that in glass forming liquids. It arises from the hopping of individual particles over the ordered array of clusters. This picture is a classical analog of the quantum supersolid phase. *A solid with diffusion.*

2. The non-equilibrium regime develops a (cluster) **crystal-to-glass transition**. The disordered phase establishes below certain temperature, via a self-generated polydispersity of the clusters, for which particles hopping is arrested. *A glassy phase in a 2D monodisperse isotropic system without quenched disorder.*

3. The phenomenology described here can be addressed in many real experiments, from colloidal suspensions to 1.5-superconductor layers. *It may be also of interest for phase change materials.*

Further readings

[1] R. Díaz-Méndez, F. Mezzacapo, F. Cinti, W. Lechner, and G. Pupillo. *Phys. Rev. E*, 92:052307, 2015.

[2] R. Díaz-Méndez, F. Mezzacapo, W. Lechner, F. Cinti, E. Babaev, and G. Pupillo. *arXiv:1605.00553v1*, 2016.

Equilibrium dynamics: The hopping crystal

We compute the mean square displacement $MSD(t) = \langle \Delta r^2(t) \rangle = \langle \sum_j |\mathbf{r}_j(0) - \mathbf{r}_j(t)|^2/N \rangle$ as well as the self-intermediate scatter function $F_s(k^*, t) = \langle \sum_j e^{ik^*[\mathbf{r}_j(0)-\mathbf{r}_j(t)]}/N \rangle$.

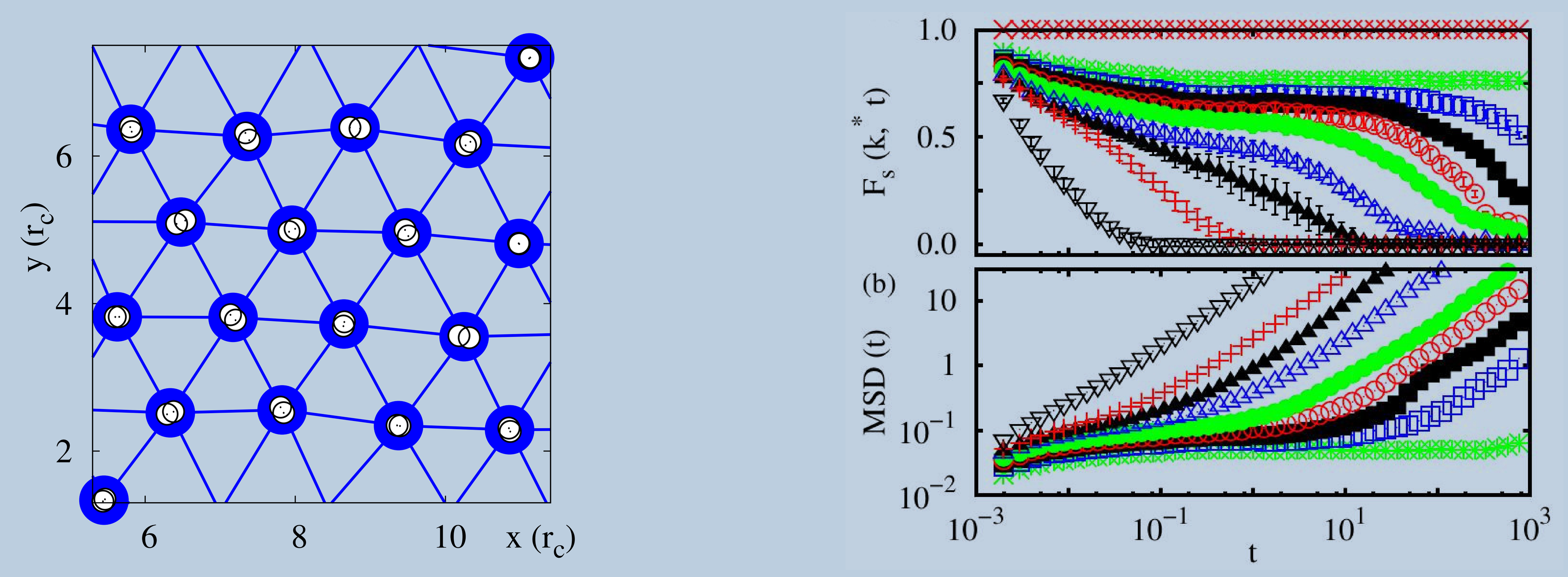

Figure 2: Left: snapshot of the system at equilibrium, signaling the clusters array. Right: F_s and MSD for the equilibrium crystal (left), a two step decorrelation can be observed. Temperature increase from up to down in the upper panel.

Non-equilibrium dynamics: crystal-to-glass transition

The hexatic order is estimated via the bond-order parameter of the clusters, $\Psi_6 = \langle | \sum_j^{N_c} \sum_l^{N_j} e^{i6\theta_{jl}} / (N_c N_j) | \rangle$.

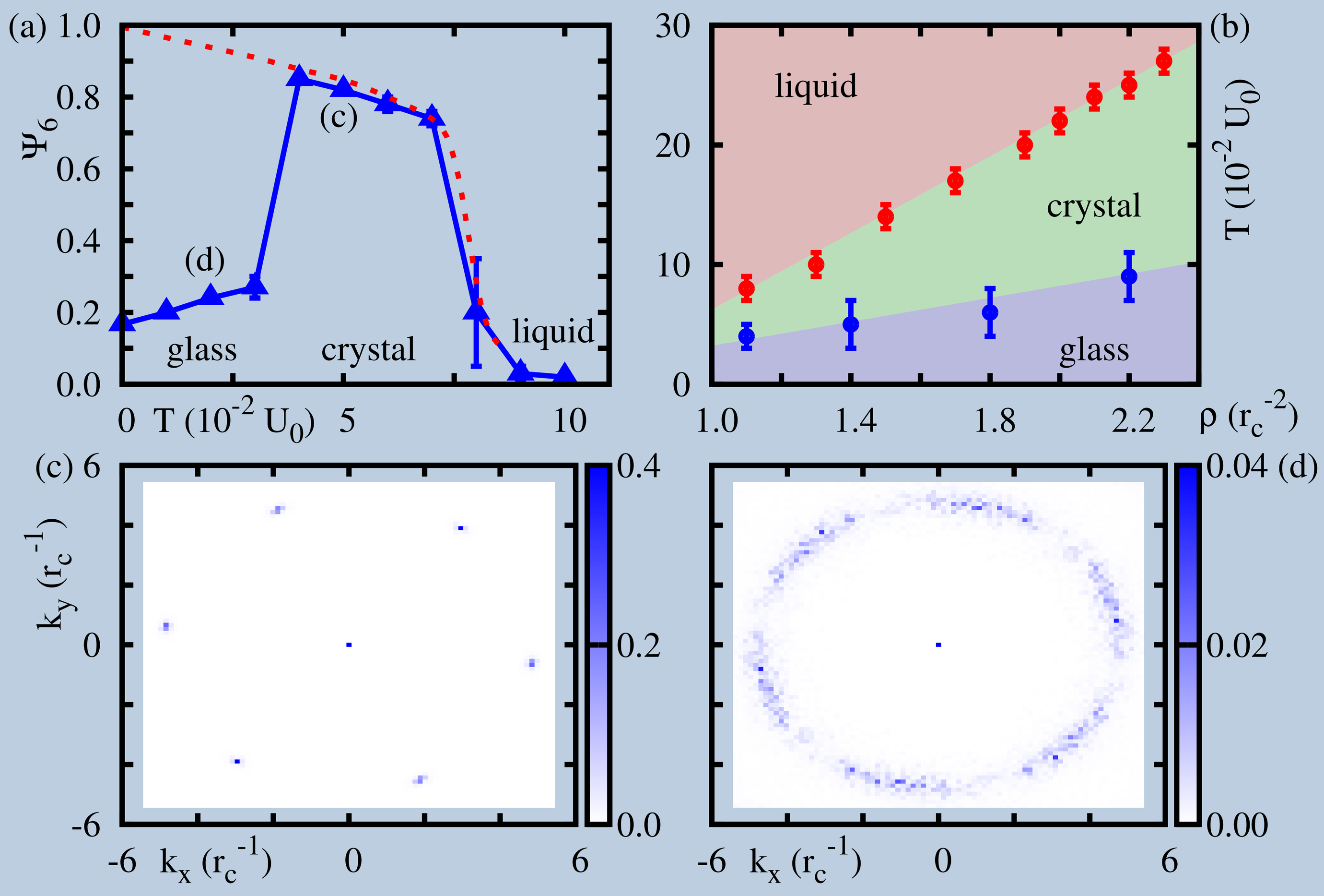

Figure 3: a) Hexatic order versus temperature, after quenches from high temperature (blue line), and by slow cooling (red dashed line). c) and d) are typical structure factors at the temperatures signaled in (a). b) Dynamic phase diagram including the crystal-to-glass transition.

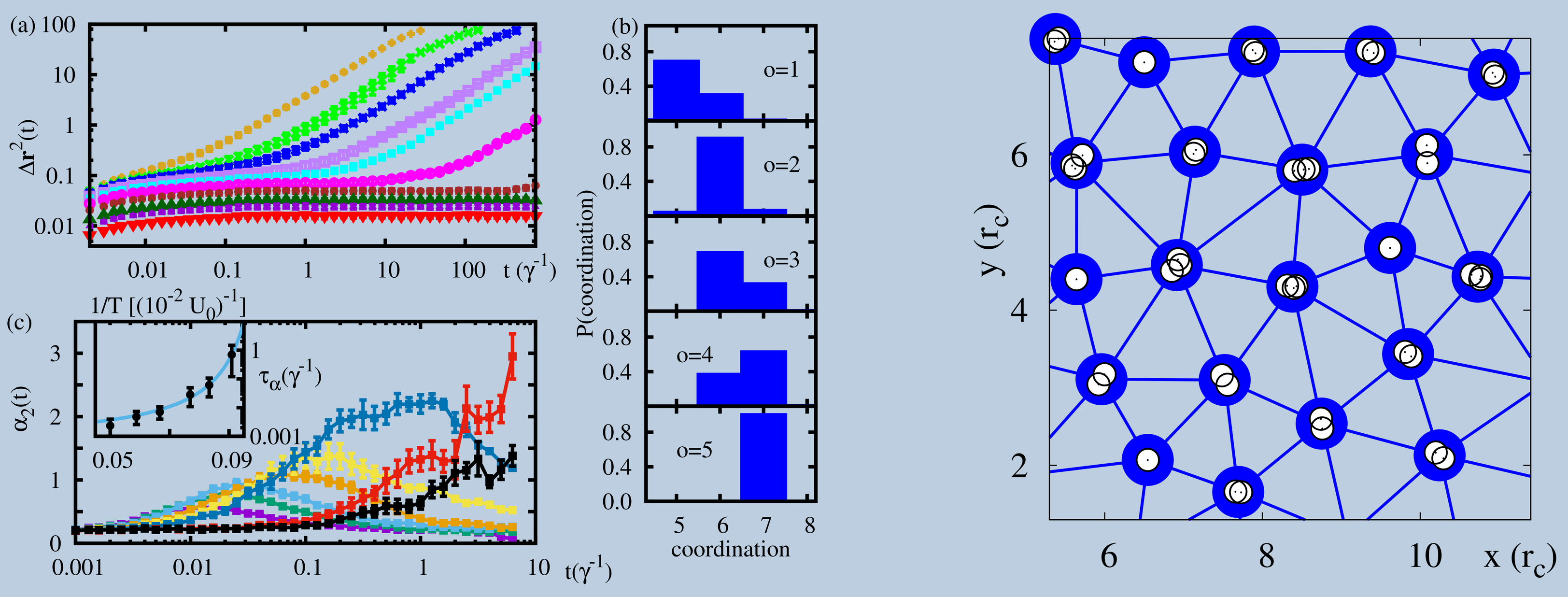

Figure 4: Left: a) MSD, temperature decrease from up to down; c) non-gaussian parameter $\alpha_2 = [\langle \Delta r^4(t) \rangle / 2 \langle \Delta r^2(t) \rangle^2] - 1$, evidence of dynamic heterogeneity; b) distribution of coordination number for clusters with different occupation (number of particles) in the glassy phase. Right: snapshot of the glassy phase.

Application: 1.5-Superconductors

Vortices in layered 1.5-superconductors can interact via an effective potential of the form

$$U(r) = \sum_{i=1,2} C_{B_i}^2 K_0\left(\frac{r}{\lambda_i}\right) - C_i^2 K_0\left(\frac{r}{\xi_i}\right) \quad (2)$$

see the blue line in Fig (1). All above-discussed phenomenology is reproduced by this model of experimental relevance.