Coexistence of Ordinary Elasticity and Superfluidity in a Model of a defect-free Supersolid

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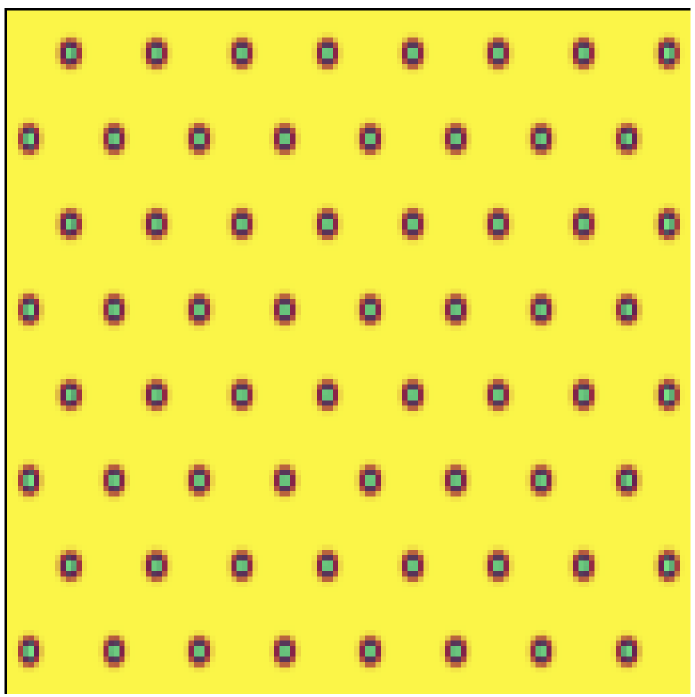

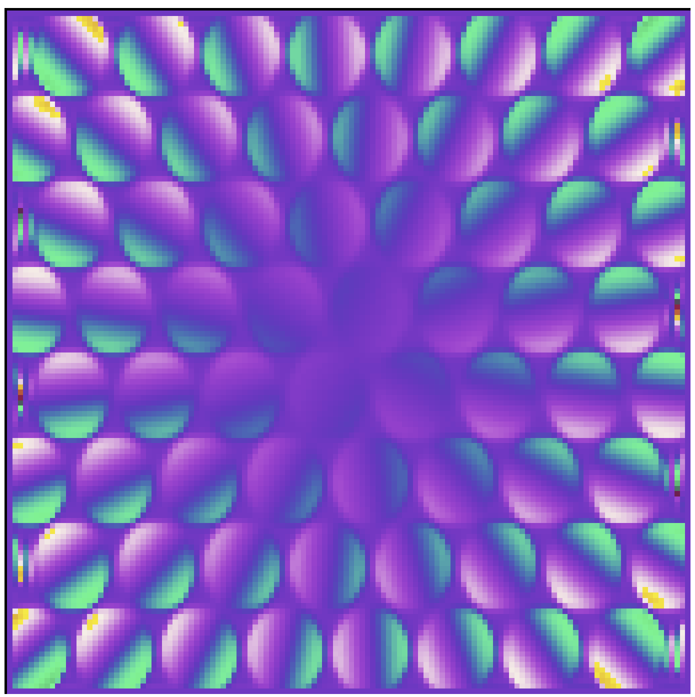

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Outline

- Motivations: Supersolid experiments
- Gross-Pitaevskii model
- Ground state and perturbations
- NCRI and Elasticity
- Perspectives

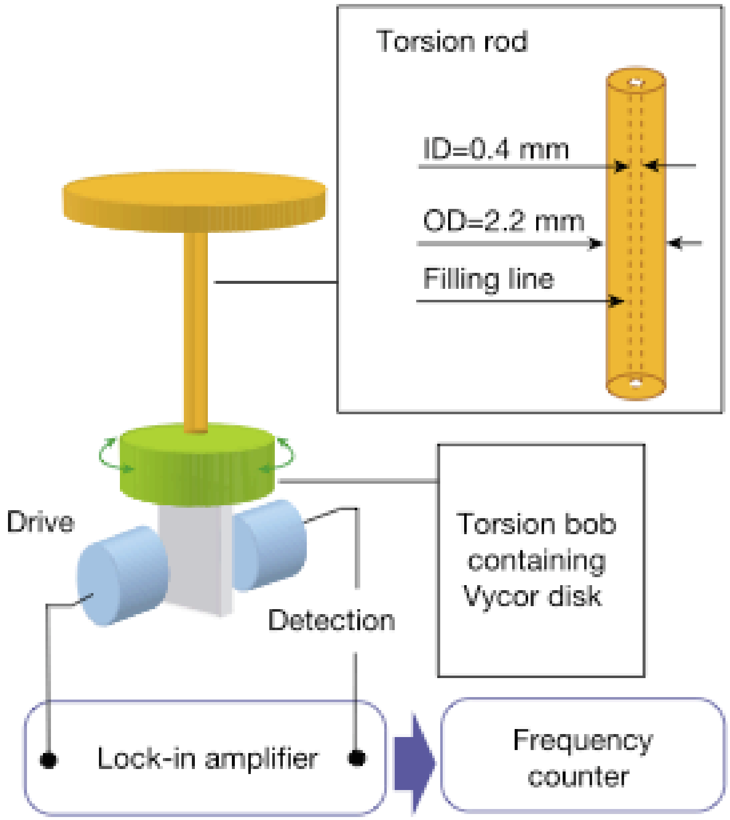


Figure 1 Torsional oscillator used in this experiment. The design of the oscillator follows those used by Reppy and collaborators[18]. The Vycor glass disk has a diameter of 15 mm and a thickness of 4 mm. The cylindrical drive and detection electrodes are aligned off-centre from, and are capacitively coupled to, the central electrode attached to the torsion bob. The signal from the detection electrode (proportional to the amplitude) is sent to the lock-in amplifier through a current preamplifier. The lock-in provides a driving voltage, which controls the amplitude of oscillation, to complete the phase-locked loop and keep the oscillator in resonance. The mechanical Q of the oscillator is 10^6 at low temperature, allowing the determination of the resonant period to a precision of 0.2 ns. The resonant period is 967,640 ns when the Vycor disk is empty, and is 971,900 ns near 0.2 K when pressurized with solid ^{4}He at 62 bar. Measurements were also made with a dummy torsional cell with the Vycor glass disk replaced by a solid brass disk.

E. Kim & M. Chan
Nature 427, 225-227 (2004)

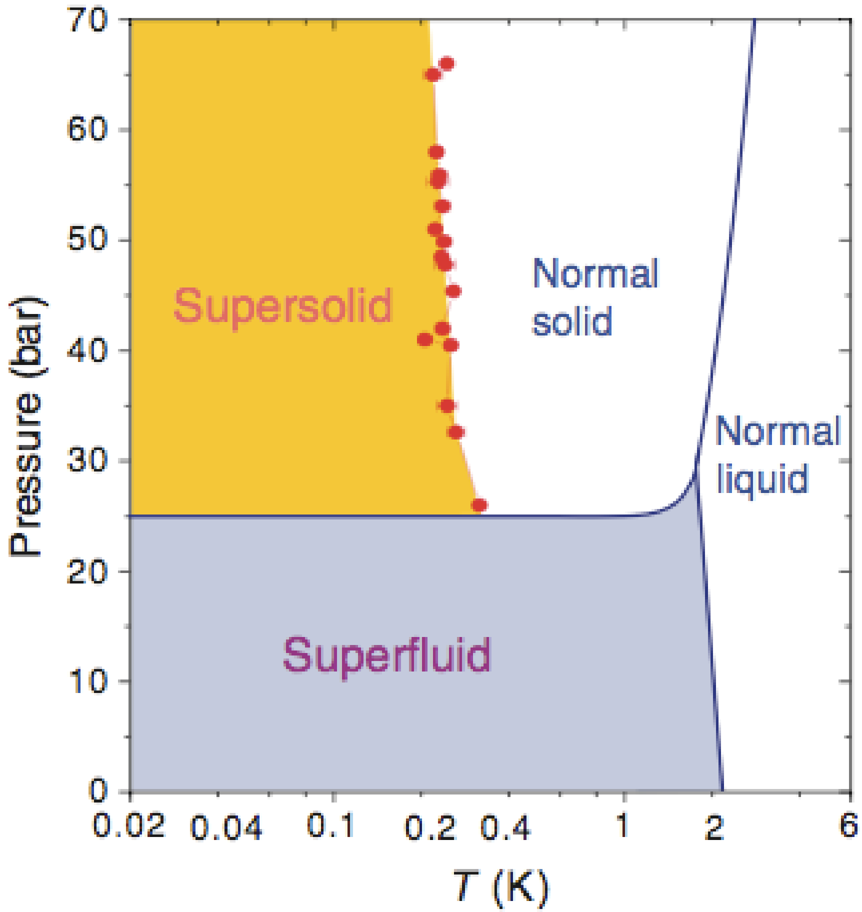
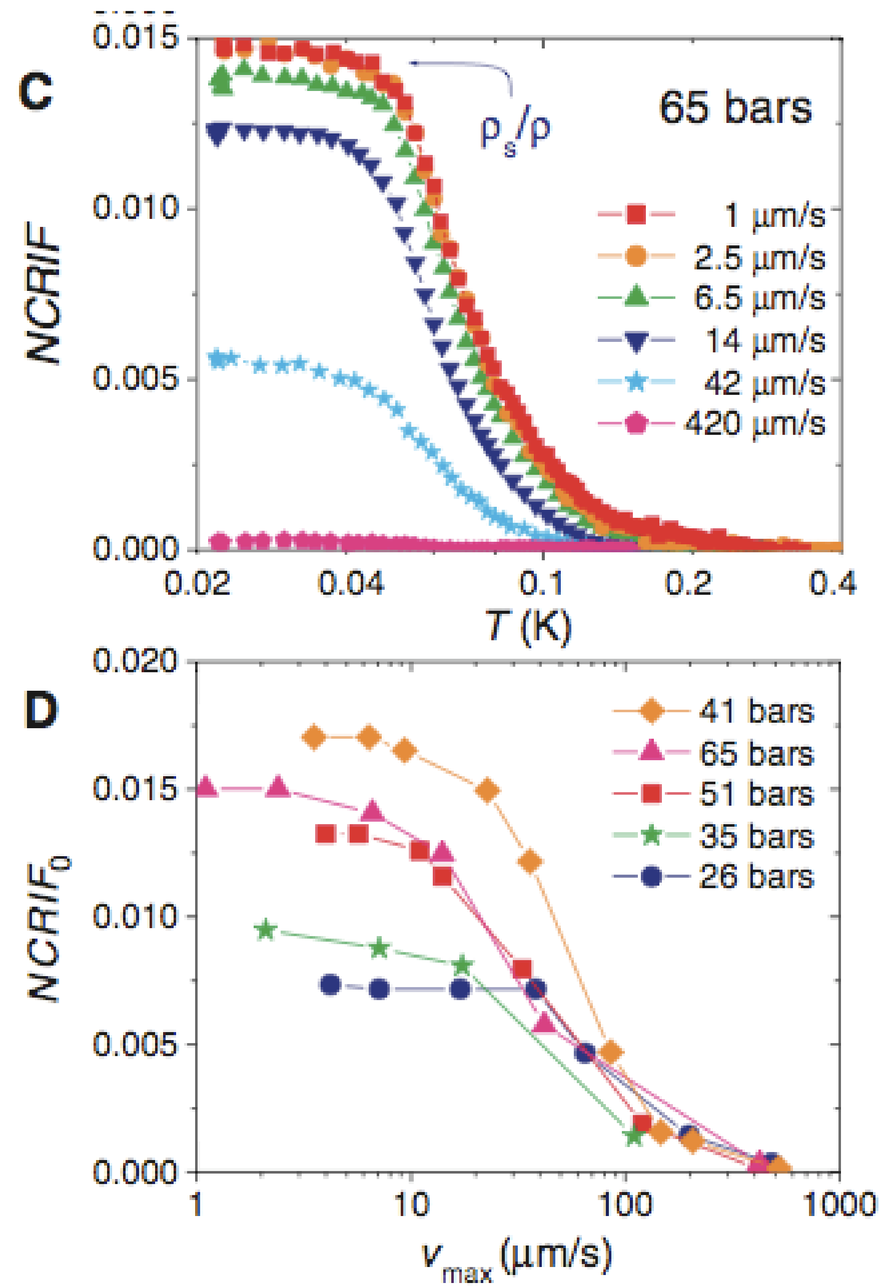


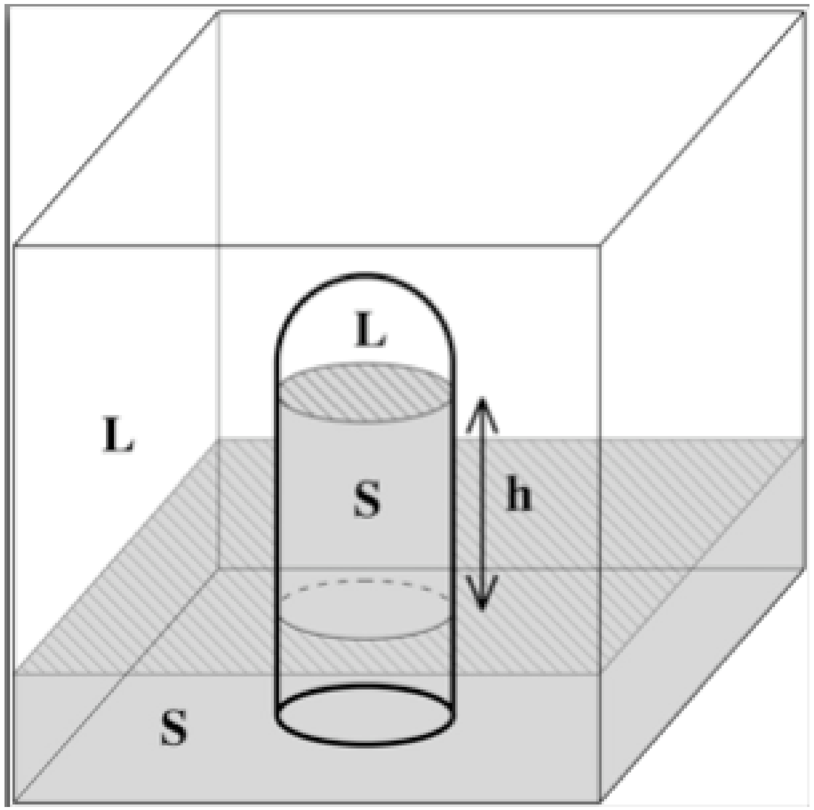
Fig. 4. Phase diagram of liquid and solid helium.

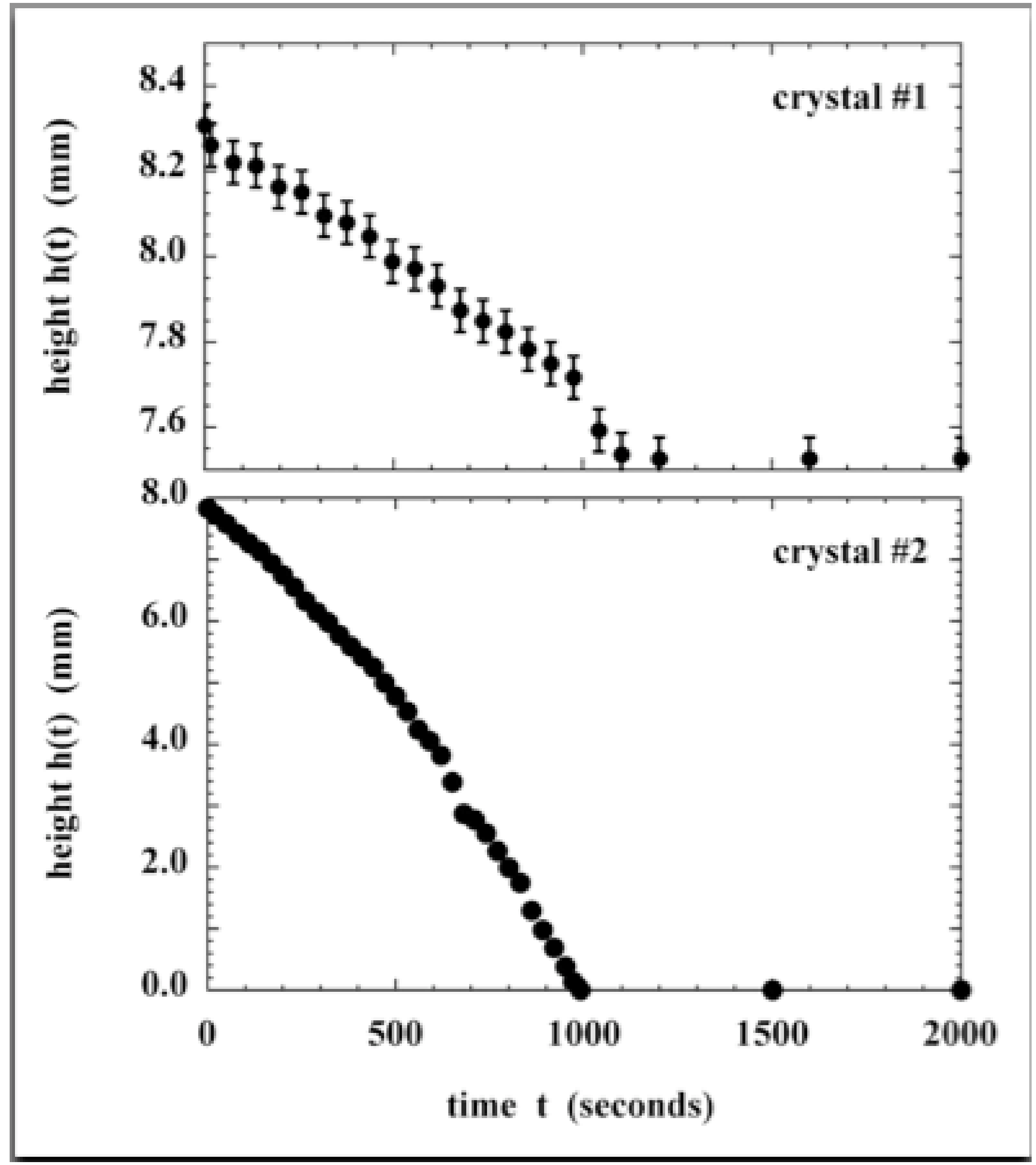


K-C, Science 305, 1941-1944 (2004)

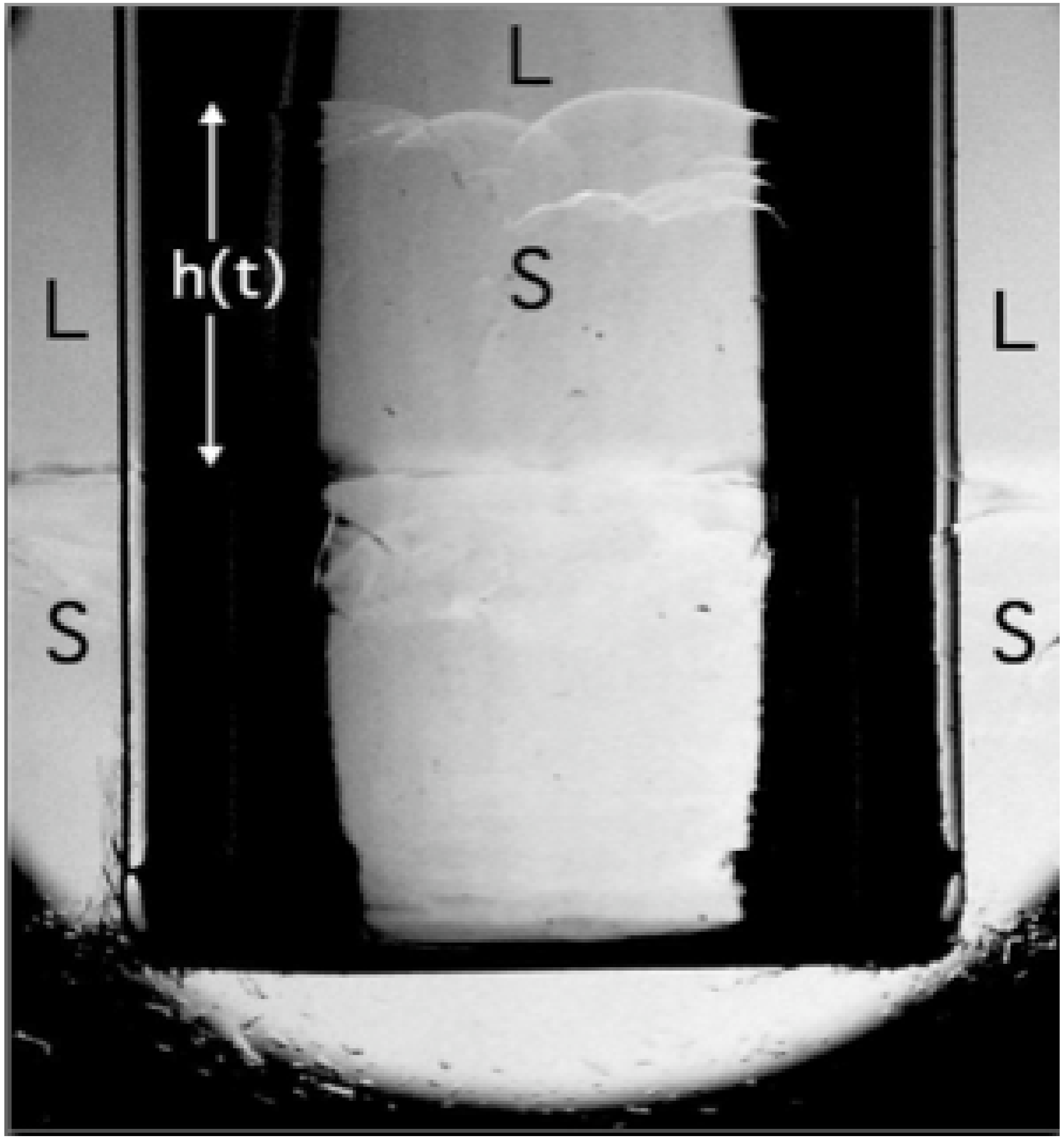
Remarks

- Can we have a Supersolid? (Penrose and Onsager 1956, Andreev and Lifshitz (1969), Chester (1970), Prokof'ev and Svistunov (2005)...)
- What should be a Supersolid? (Leggett (1970)...)
- Role of the disorder (Rittner and Reppy (2006)).





S. Sasaki, R. Ishiguro, F. Caupin, H.J. Maris and S. Balibar, Science 313, 1098-1100 (2006).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- experimental puzzle
- paradox between NCRI and absence of flow out of grain boundaries
- annealing effects and role of the disorder
- Gross-Pitaevskii approach for describing supersolid state

G-P Equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + \psi\int \mathrm{d}\boldsymbol{r}' U(\boldsymbol{r}' - \boldsymbol{r})|\psi(\boldsymbol{r}', t)|^2,$$

- Mean-field approach
- valide in the dilute gas limit
- semi-classical equation: $\Psi = \sqrt{\rho}e^{i\Phi}$
- NLS limit for Dirac potential
- Quantitative agreement with BEC and qualitative description of liquid He4.

- Hamiltonian system (or also Lagrangian structure)
- Conservation of the number of particle

$$\imath \partial_t \psi = \frac{\delta H}{\delta \psi^*}$$

$$H = \frac{1}{2} \int dr \left(|\nabla \psi|^2 + |\psi|^2 \int dy |\psi(r')|^2 U(r - r') \right)$$

$$N = \int dr |\psi|^2$$

- Hydrodynamic form of the equation
- Bernoulli-like equation with quantum pressure

For: $U(r) = g\delta(r)$

$$\frac{\partial \rho}{\partial t} + \frac{\hbar}{m}\nabla \cdot (\rho \nabla \phi) = 0,$$

$$\hbar \frac{\partial \phi}{\partial t} + \frac{\hbar^2}{2m}(\nabla \phi)^2 + g\rho + \frac{\hbar^2}{4m}\left(\frac{(\nabla \rho)^2}{2\rho^2} - \frac{\nabla^2 \rho}{\rho}\right) = 0.$$

- Dispersion law by perturbation around homogenous solution

$$\hbar\omega = \frac{\hbar^2}{m}\sqrt{\frac{k^4}{4} + \frac{m}{\hbar^2}\rho_0 \hat{U}(k) k^2}$$

$$\hbar\omega = \frac{\hbar^2}{m}\sqrt{\frac{k^4}{4} + \frac{m}{\hbar^2}\rho_0 k^2}$$

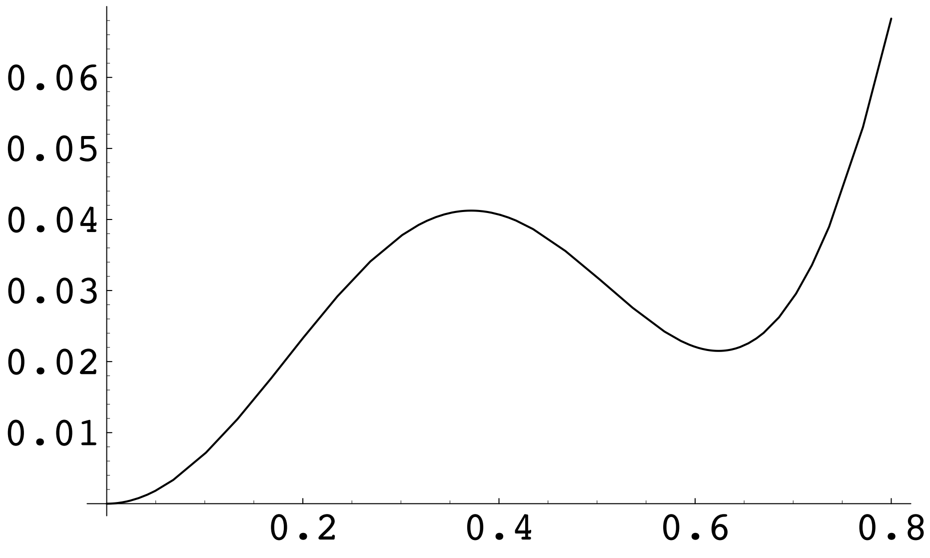
For the Dirac potential

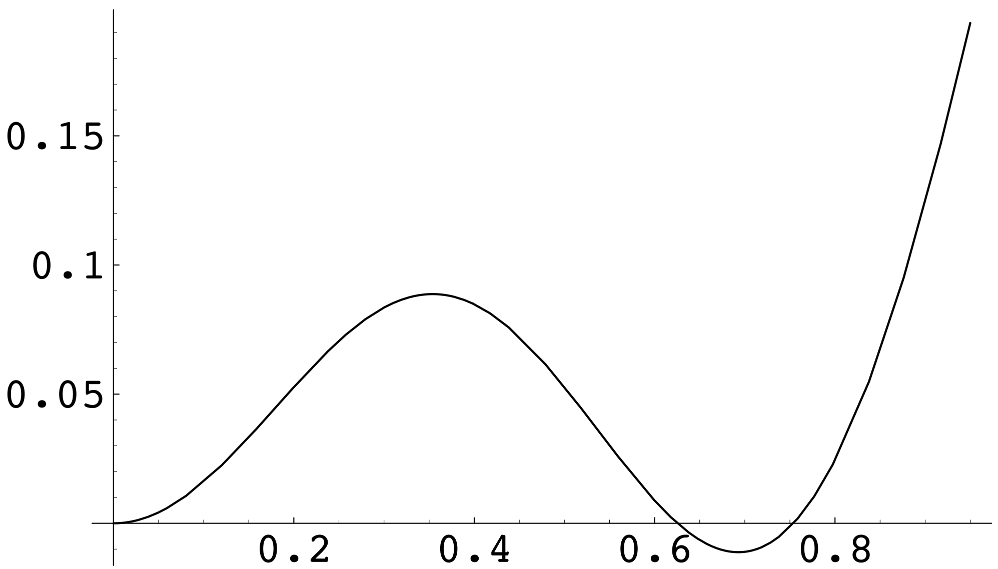
For soft core interaction $U(x) = U_0 \Theta(x-a)$

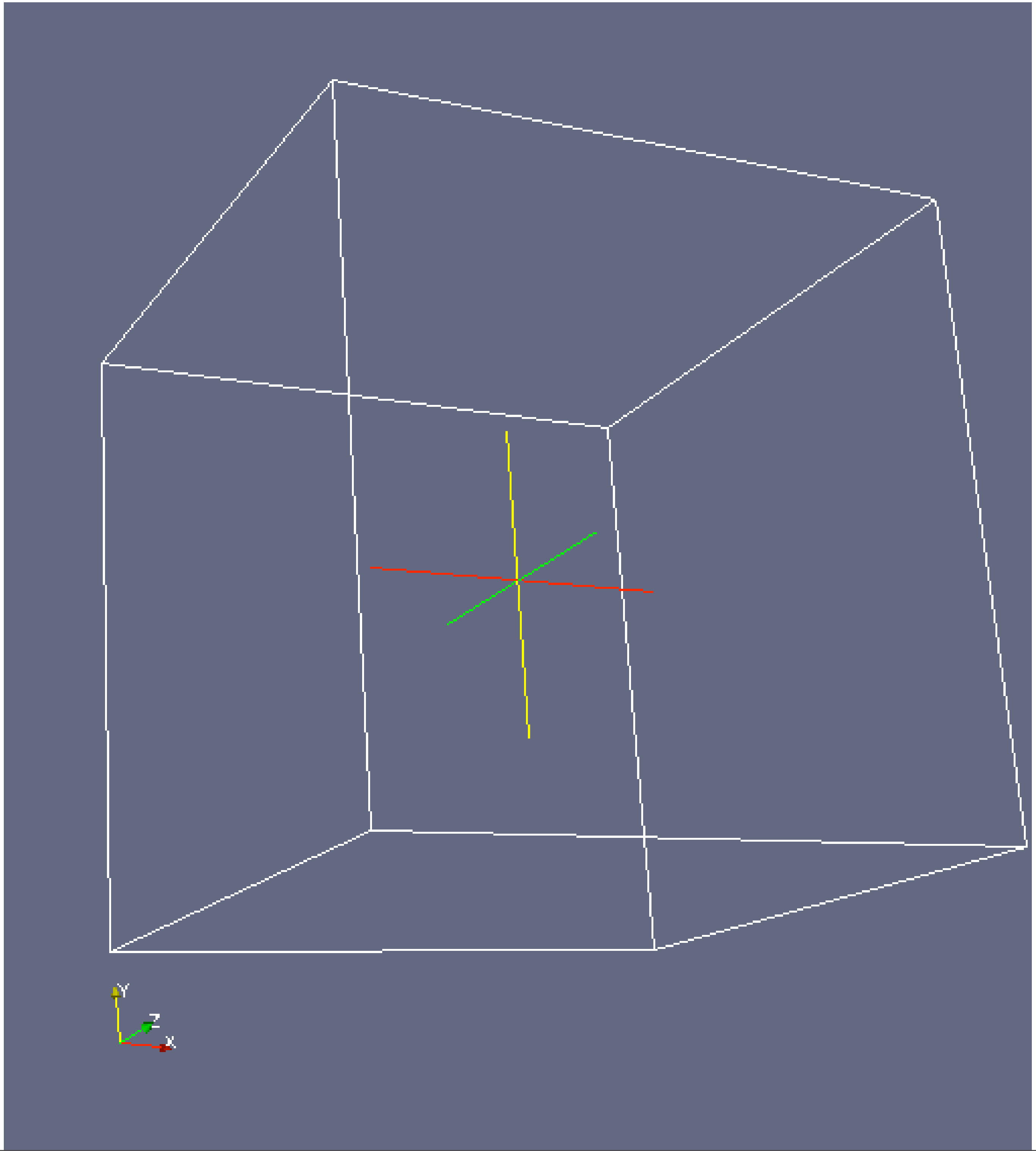
$$\hat{U}(k) = 4\pi a U_0 (sin(k \cdot a)/(k \cdot a) - cos(k \cdot a))/k^2$$ in 3-D

$$\hat{U}(k) = 2\pi a \cdot J1(k \cdot a)/k$$ in 2-D

- roton minimum as precursor of crystallization
- pattern formation



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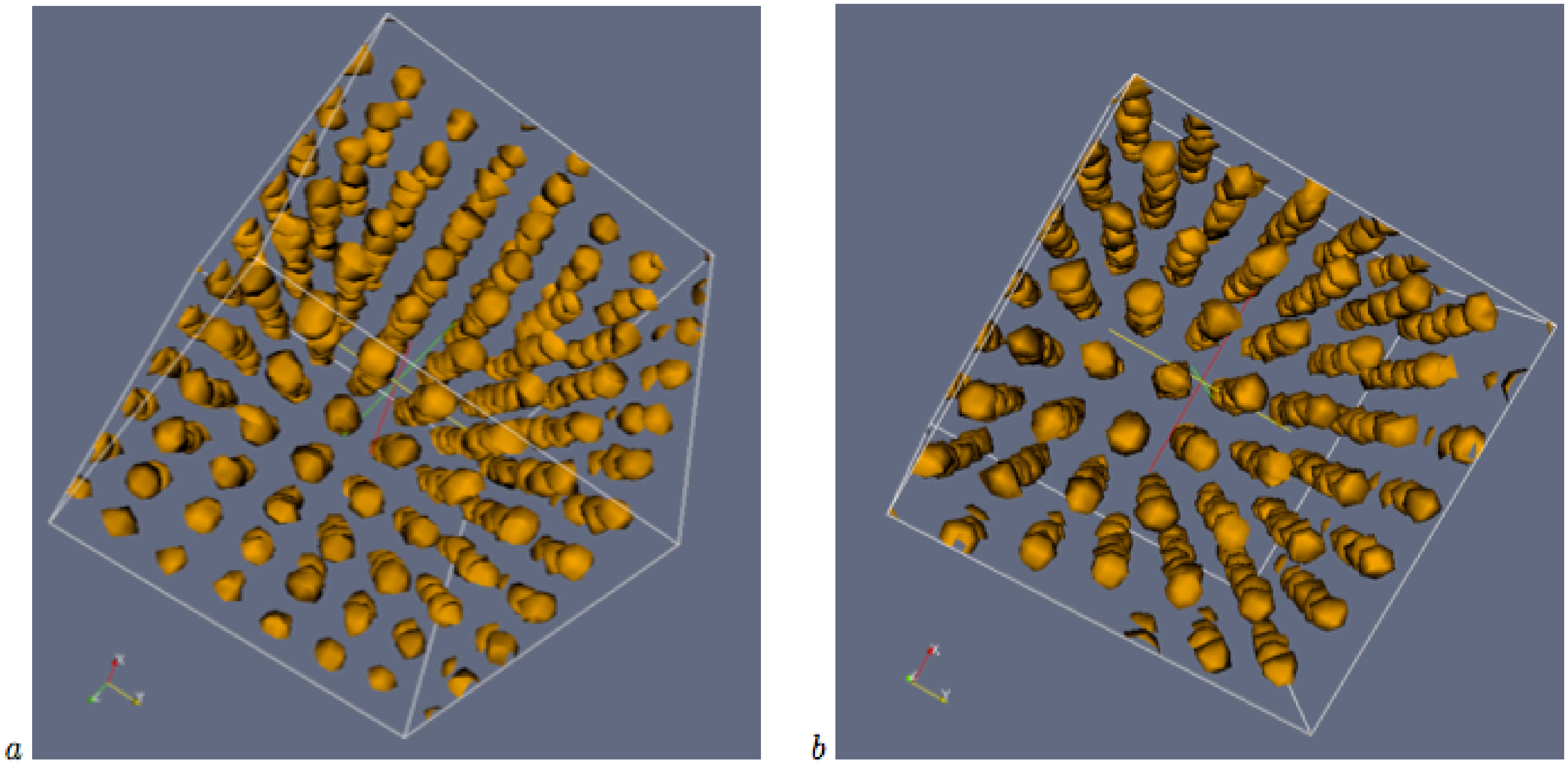
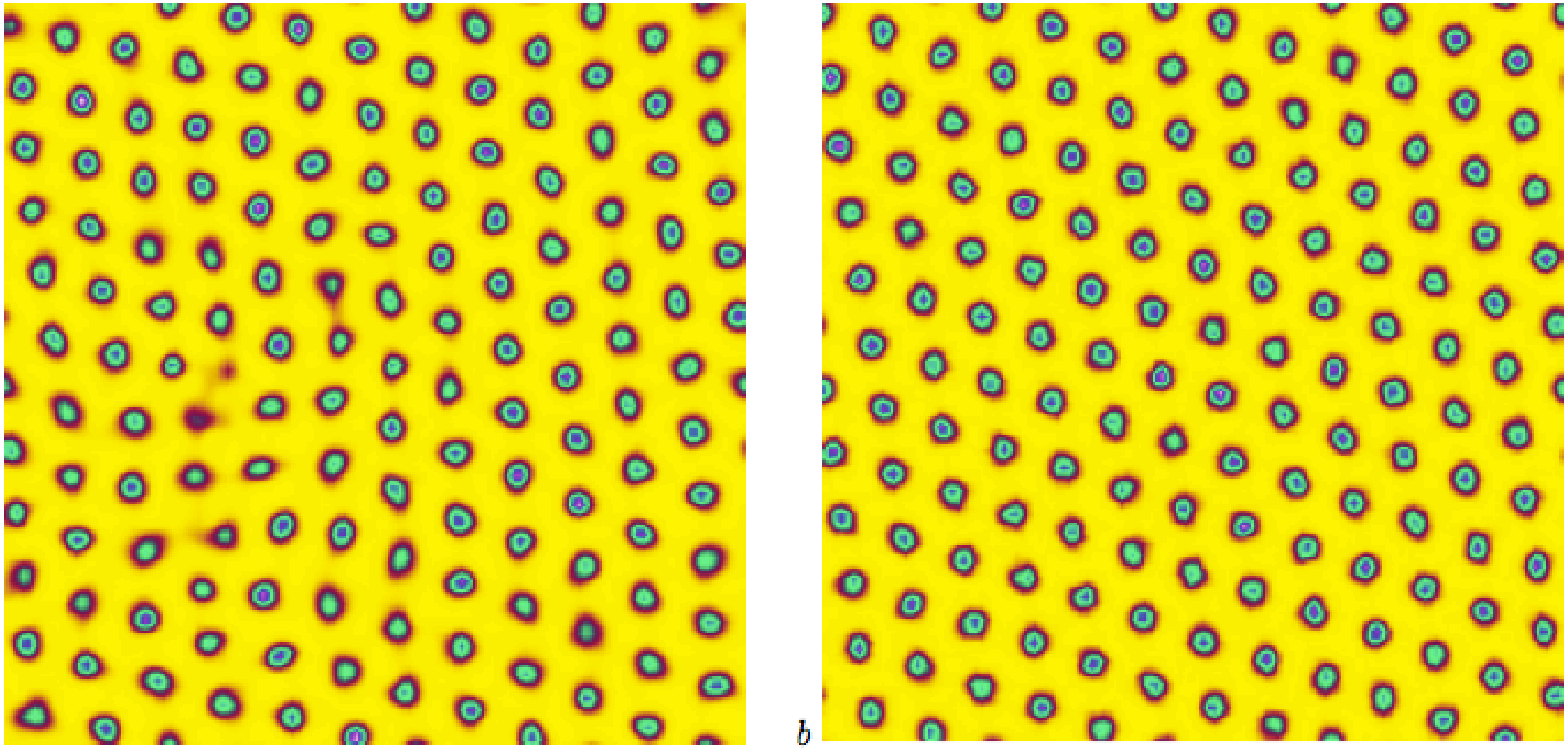


Fig. 2. A three dimensional contour plot of density $|\psi|^2 = 0.3$ of a numerical Simulation of eqn. (1) in a 32^3 box with periodic boundary conditions. As before the scheme conserves the total energy and mass and all conditions are the same as Fig. 1 but $U_0 = 0.02$ and $a = 4$. *a* and *b* are two different view directions.



a b

Fig. 1. We plot the density modulations $|\psi|^2$ (the dark points means a large mass concentration) of a numerical Simulation of eqn. (1) in a 128^2 with periodic boundary conditions. We use a Crank-Nicholson scheme that conserves the total energy and mass. The potential interaction is modeled as a soft core interaction: $U(|\boldsymbol{r}-\boldsymbol{r}'|) = U_0\theta(a-|\boldsymbol{r}-\boldsymbol{r}'|)$, with $\theta(s)$ the Heaviside function. The mesh size is $dx = 1$, the non-local interaction parameters are chosen as $a = 8$ and $U_0 = 0.01$ (physical constants $\hbar$ and m are 1), finally the initial condition is an uniform solution $\psi = 1$ plus small fluctuations. In a) is an early stage of crystallization with the presence of dislocations while in b) is a late stage one gets a free-defect state.

- Regular pattern (hexagons in 2D, hcp in 3D)
- non commensurate crystal (not one atom per peak, similar to Nepomnyashchii)
- Long-wave/slow-time, short-scale/fast scale separation
- Homogenization technique
- Calculation of an Effective Lagrangian for the long/slow perturbations

$$\mathcal{L} = -\int \left[\hbar\rho\frac{\partial\phi}{\partial t} + \frac{\hbar^2}{2m}\left(\rho(\boldsymbol{\nabla}\phi)^2 + \frac{1}{4\rho}(\boldsymbol{\nabla}\rho)^2\right)\right]\mathrm{d}\boldsymbol{r} - \frac{1}{2}\int U(|\boldsymbol{r}-\boldsymbol{r}'|)\rho(\boldsymbol{r})\rho(\boldsymbol{r}')\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'.$$

$$\rho(\boldsymbol{r},t) = \rho_0(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r},t)|n(\boldsymbol{r},t)) + \tilde{\rho}(\boldsymbol{r}-\boldsymbol{u},n,t) + \ldots$$
$$\phi(\boldsymbol{r},t) = \Phi(\boldsymbol{r},t) + \tilde{\phi}(\boldsymbol{r}-\boldsymbol{u},n,t) + \ldots$$

Where n, u and Phi are slow and large scale varying functions while ˜ functions are rapid and short scale (on the order of the peak scale) varying functions.

Effective Lagrangian

$$\mathcal{L}_{eff} = -\hbar n \frac{\partial \Phi}{\partial t} - \frac{\hbar^2}{2m}\left[n\left(\nabla\Phi\right)^2 - \varrho_{ik}(n)\left(\nabla\Phi - \frac{m}{\hbar}\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right)_i\left(\nabla\Phi - \frac{m}{\hbar}\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right)_k\right] + \\ - \mathcal{E}(n) - \frac{1}{2}\lambda_{iklm}\epsilon_{ik}\epsilon_{lm}$$

where

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\hbar}{m}\nabla\Phi\cdot\nabla\boldsymbol{u}.$$

where the new parameters (rho, Epsilon, lambda's) come from explicit calculations based on the ground state solution on a cell unit.

Hamiltonian:

$$\begin{aligned} H &= \Phi_t \frac{\delta\mathcal{L}}{\delta\Phi_t} + \boldsymbol{u}_t\cdot\frac{\delta\mathcal{L}}{\delta\boldsymbol{u}_t} - \mathcal{L}, \\ &= \frac{\hbar^2}{2m}(n - \varrho(n))\left(\nabla\Phi\right)^2 + \frac{m\varrho}{2}\left(\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right)^2 + \mathcal{E}(n) + \frac{1}{2}\lambda_{iklm}\epsilon_{ik}\epsilon_{lm}. \end{aligned}$$

Calculations for ρ_{ij}

- Lagrangian for the fast and short phase:

$$\mathcal{L}_{\tilde{\phi}} = -\frac{\hbar^2}{2m}\int \left(2\rho_0 \boldsymbol{A}\cdot\boldsymbol{\nabla}\tilde{\phi} + \rho_0(\boldsymbol{\nabla}\tilde{\phi})^2\right)\, d\boldsymbol{r}, \qquad \text{where } \boldsymbol{A} = \left(\boldsymbol{\nabla}\Phi - (\boldsymbol{\nabla}\Phi\cdot\boldsymbol{\nabla})\boldsymbol{u} - \tfrac{m}{\hbar}\partial_t \boldsymbol{u}\right)$$

- Euler-Lagrange equation: $\boldsymbol{A}\cdot\boldsymbol{\nabla}\rho_0 + \boldsymbol{\nabla}\cdot\left(\rho_0\boldsymbol{\nabla}\tilde{\phi}\right) = 0.$
- Periodic solution for the phase: $\tilde{\phi} = K_i A_i$ $\qquad \nabla_i\rho_0 + \boldsymbol{\nabla}\cdot(\rho_0\boldsymbol{\nabla}K_i) = 0.$
- So that the effective contribution (slow, large scale):

$$\mathcal{L}_{\tilde{\phi}} = \frac{\hbar^2}{2m}\int \varrho_{ij} A_i A_j \, d\boldsymbol{r} \qquad \rho_{ij} = \frac{1}{V}\int_V \rho_0(r)\nabla K_i\cdot\nabla K_j\, dr$$

- for isotropic ground-state solutions we can assume: $\varrho_{ij} = \varrho(n)\delta_{ij}$

Superfluid dynamics at T=0

$$\hbar \frac{\partial \Phi}{\partial t} + \frac{\hbar^2}{2m}\left[(\nabla \Phi)^2 - \varrho'(n)\left(\nabla \Phi - \frac{m}{\hbar}\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right)^2\right] + \mathcal{E}'(n) + \frac{1}{2}\lambda'_{iklm}\epsilon_{ik}\epsilon_{lm} = 0$$

$$m\frac{\partial}{\partial t}\left[\varrho(n)\left(\frac{\mathrm{D}u_i}{\mathrm{D}t} - \frac{\hbar}{m}\frac{\partial \Phi}{\partial x_i}\right)\right] - \frac{\partial}{\partial x_k}\left(\lambda_{iklm}\epsilon_{lm}\right) + \hbar\frac{\partial}{\partial x_k}\left[\varrho\left(\frac{\mathrm{D}u_i}{\mathrm{D}t} - \frac{\hbar}{m}\frac{\partial \Phi}{\partial x_i}\right)\frac{\partial \Phi}{\partial x_k}\right] = 0$$

$$\frac{\partial n}{\partial t} + \frac{\hbar}{m}\nabla \cdot (n \nabla \Phi) - \frac{\hbar}{m}\frac{\partial}{\partial x_k}\left(\varrho(n)(\delta_{ik} - \partial_k u_i)\left(\partial_i \Phi - \frac{m}{\hbar}\frac{\mathrm{D}u_i}{\mathrm{D}t}\right)\right) = 0$$

General Lagrangian structure besides the particular G-P calculations (Son (2005))

Intimous-Implicit coupling between elasticity and quantum phase

With the B.C.

$$\frac{\hbar}{m}\left(n\partial_k \Phi - \varrho(\delta_{ik} - \partial_k u_i)\left(\partial_i \Phi - \frac{m}{\hbar}\frac{\mathrm{D}u_i}{\mathrm{D}t}\right)\right)\hat{e}_k = nV_k \hat{e}_k.$$

Sound waves

- small perturbations around u=0, zero phase gradient and constant peak density n.
- decoupling between shear waves and phase-compressive waves
- phase mode disappears at the transition supersolid-solid (when rhon-->n)

$$\frac{\partial^2 \Phi}{\partial t^2} = \frac{\mathcal{E}''(n)}{m}\left(\varrho(n)\nabla^2\Phi + (n-\varrho(n))\frac{\partial \boldsymbol{\nabla}\cdot\boldsymbol{u}}{\partial t}\right)$$

$$K\nabla^2(\boldsymbol{\nabla}\cdot\boldsymbol{u}) = (n-\varrho(n))\left(\frac{\partial^2(\boldsymbol{\nabla}\cdot\boldsymbol{u})}{\partial t^2} - \frac{\hbar}{m}\frac{\partial\nabla^2\Phi}{\partial t}\right)$$

$$\left(v^2 - \frac{K+4\mu/3}{m(n-\varrho)}\right)\left(v^2 - \frac{\mathcal{E}''(n)}{m}\varrho\right) = v^2\left((n-\varrho)\frac{\mathcal{E}''(n)}{mn}\right)$$

NCRI

- rotation of a container at constant angular velocity

$$\nabla^2 \Phi = 0 \quad \text{in} \quad \Omega \quad \text{with} \quad \boldsymbol{\nabla}\Phi \cdot \hat{e} = (m/\hbar)(\boldsymbol{\omega} \times \boldsymbol{r}) \cdot \hat{e} \quad \text{on} \quad \partial\Omega.$$

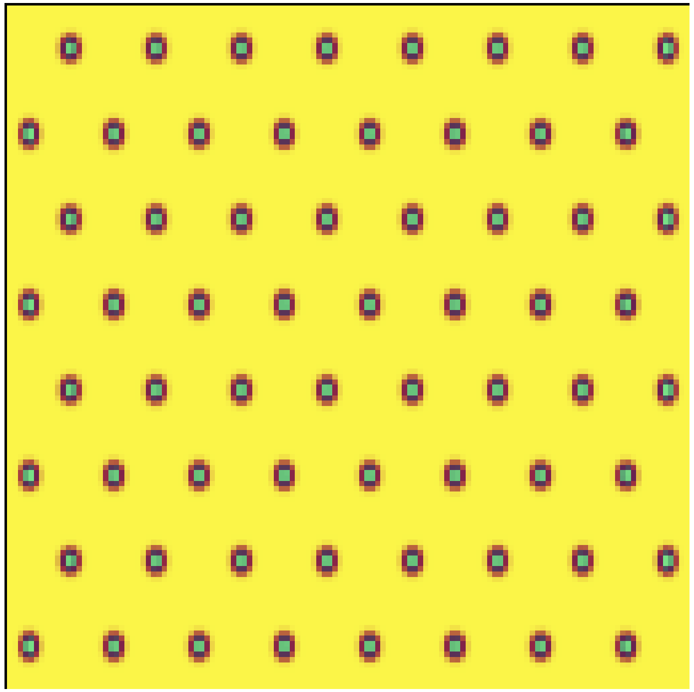
- Moment of Inertia defined from the Energy: $E = \frac{1}{2} I_{ss} \omega^2$

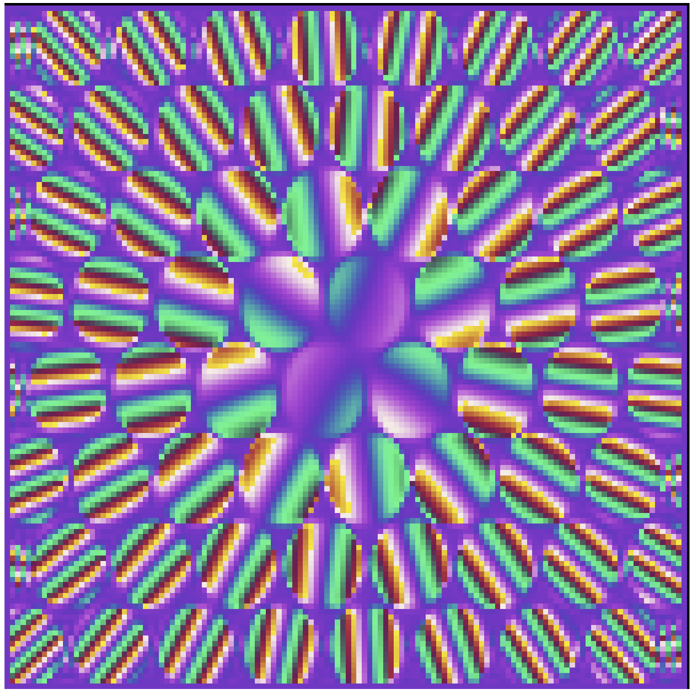
$$I_{ss} = m(n - \varrho(n))\mathcal{I}_{pf} + m\varrho(n)\mathcal{I}_{rb}$$

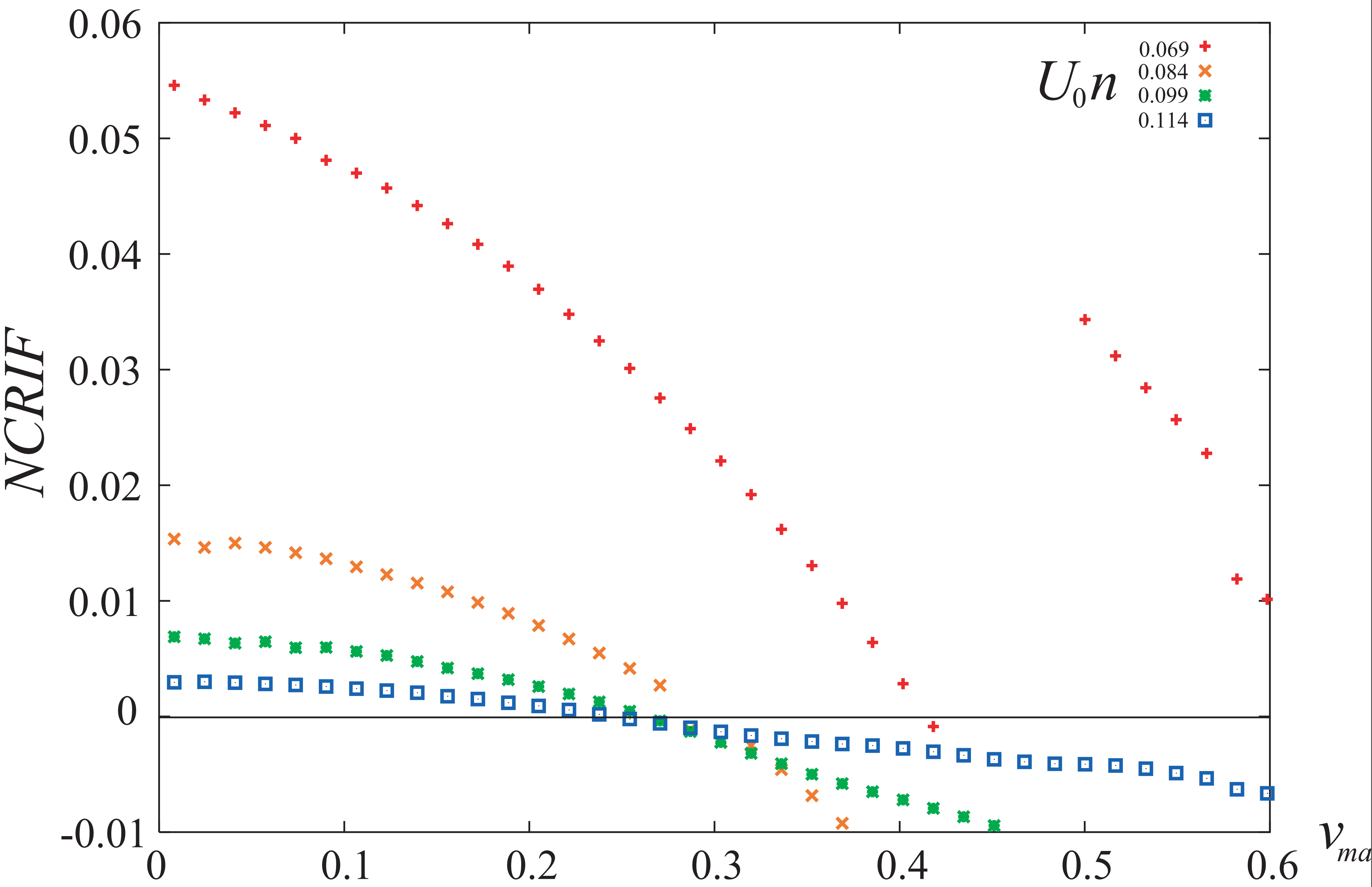
- Relative change of moment of inertia as Supersolid phase appears:

$$(I_{ss} - I_{rb})/I_{rb} = -(1 - \varrho(n)/n)(1 - \mathcal{I}_{pf}/\mathcal{I}_{rb})$$

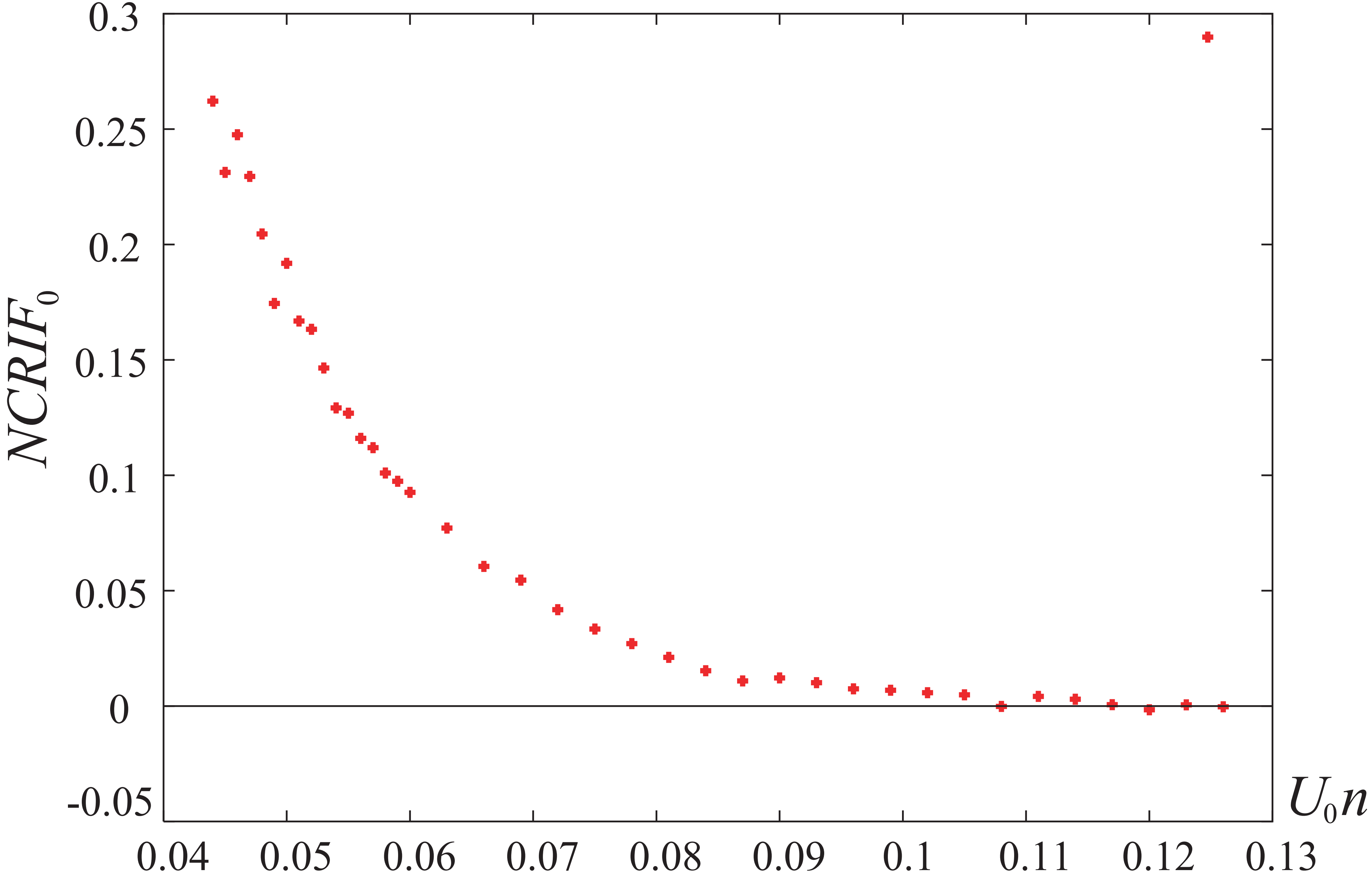
Numerical simulation of G-P at 2D





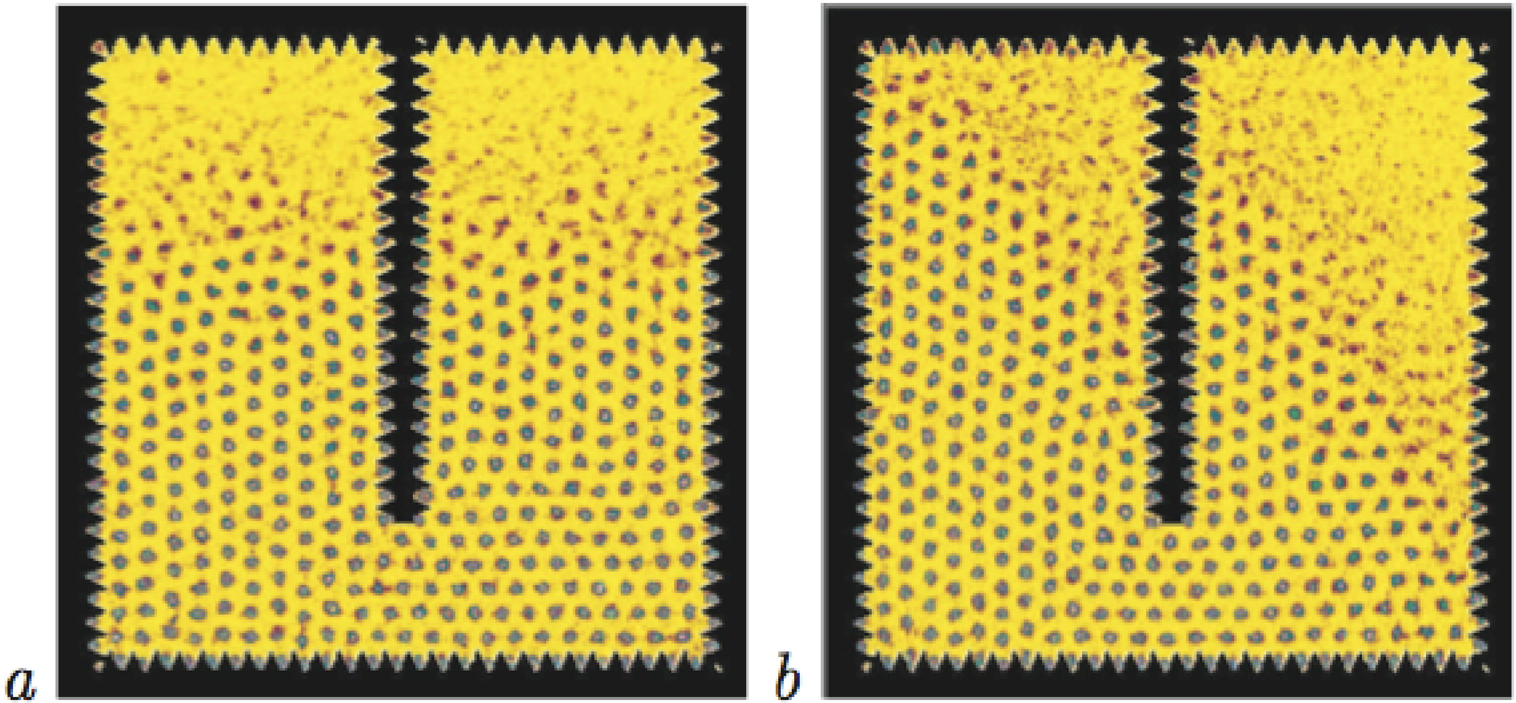


0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
NCRIF
0
0.1
0.2
0.3
0.4
0.5
0.6
v_{ma}
$U_0 n$
0.069
0.084
0.099
0.114



NCRIF0
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
U0n
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13

No mass flow under pressure gradients



Conclusions-Perspectives

- Model of Supersolid with a complex coupling between elasticity and phase
- shows the apparent paradoxal effects of NCRI and absence of mass flow under stress
- 3D simulations
- Role of the disorder
- Annular geometry (1D calculations)