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Workshop on Supersolid 2008

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Supersolidity and disorder: quantum dislocations and superglass phase

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Supersolidity and Disorder: quantum dislocations and the superglass phase

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JP Bouchaud and GB: arXiv 0710.3087
GB, C. Chamon, F. Zamponi: arXiv 0807.2458

Outlook

- Recent experimental and numerical results on 'supersolids': basic facts and assumptions.
- A scenario for dislocation induced supersolidity.
- Analysis of the superglass phase (quantum jamming).

Basic Facts & Assumptions

- Starting from Kim & Chan (04) mounting evidence of a phase transition (or cross-over) in He_4: supersolid phase?
- Perfect He_4 crystals are not supersolids: no vacancy-induced supersolidity (Ceperley et al., Boninsegni et al.).
- Very strong annealing effect: the role of disorder is crucial (Rittner & Reppy, Kim & Chan).

Two perspectives on disorder-induced ‘supersolidity’.

- Disorder $\rightarrow$ dislocations in He_4 crystals: dynamics of quantum dislocation, dislocation defects and supersolidity (motivated by PG de Gennes (06)).
- Disorder $\rightarrow$ glass: superglass phase (motivated by Boninsegni et al (06), see also Nussinov et al (06)).

Two perspectives on disorder-induced ‘supersolidity’.

- Disorder $\Rightarrow$ dislocations in He_4 crystals: a scenario for quantum plasticity and dislocation-induced supersolidity (motivated by PG de Gennes (06)).
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A reminder on vacancy induced supersolidity

- Classically, $Z_{1\,vacancy} = Z_{no\,vacancy} e^{-\beta E_v}$
- Quantistically:

$$Z = \frac{1}{N!} \sum_P \int \prod_i \mathrm{d}\vec{z}_i \int_{x_i(0)=z_i}^{x_i(\beta)=z_{P_i}} \mathcal{D}\vec{x}_i(t) \exp S(\{\vec{x}_i(t)\})$$

$$S = \left[- \int_0^\beta \mathrm{d}t \left\{ \sum_i \frac{m}{2\hbar^2} \left(\frac{\partial \vec{x}_i}{\partial t} \right)^2 + \sum_{i<j} V(\vec{x}_i - \vec{x}_j) \right\} \right]$$

Classical path: all particles (and so the vacancy) stay fixed
Quantum paths: the vacancy moves along a closed path (the final configuration is a permutation of the initial one)

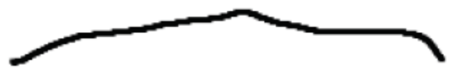
$$Z_{1\,vacancy} = Z_{no\,vacancy} e^{-\beta E_v} \sum_{n=0}^{\infty} w_n$$

w_n is the weight of a vacancy path of length n.

The vacancy creation energy is renormalized

$$e^{-\beta F_v} = e^{-\beta E_v} \sum_{n=0}^{\infty} w_n$$

High T



Low T

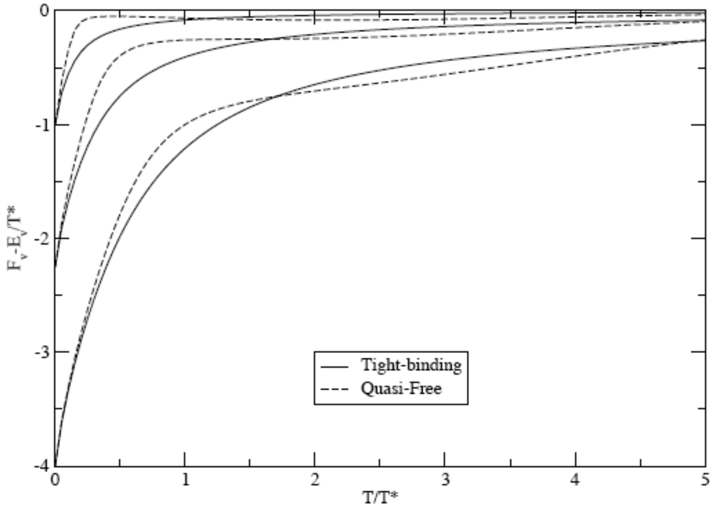
Free energy obtained summing on the number and the positions of the vacancies

$$\mathcal{F} = \mathcal{F}_0 + T\phi_v \left[\ln\left(\frac{\phi_v a^3}{\mathrm{e}} \right) - 1 \right] + \phi_v F_v + O(\phi_v^2)$$

$$F_v|_{T=0} > 0 \to \phi_v \propto e^{-\beta F_v}$$

$$F_v|_{T=0} < 0 \to \phi_v > 0$$

T_v, where F_v=0, is the characteristic tempererature for the evolution of the vacancy density



Recover Andreev Lifschitz model

$$F_v = E_v - 3T \ln \left(\int_0^{2\pi} \frac{d\theta}{2\pi} \exp\left(2\beta K \cos(\theta)\right) \right) \qquad (T^* \equiv \hbar^2/2ma^2)$$

Supersolidity: infinite permutation cycles (Feynman-Ceperley)

Vacancy paths 'concatenate' $a\sqrt{n^*} = a\ \sqrt{3K/T}\Big|_{T=T_c} \sim a\phi_v^{*\,-1/3}$

$$f_s = \frac{T}{T^*}\frac{N\langle \vec{W}^2\rangle}{6a^2} \approx \frac{T}{T^*}\phi_v n^* \approx \frac{3K}{T^*}\phi_v \qquad \vec{W} = N^{-1}\sum_i \int_0^\beta \mathrm{d}t\, \frac{\partial \vec{x}_i}{\partial t}$$

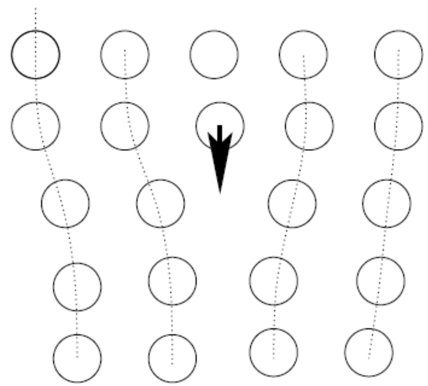
- Numerical simulations have shown that $F_v>0$ so no vacancy induced supersolidity is expected.

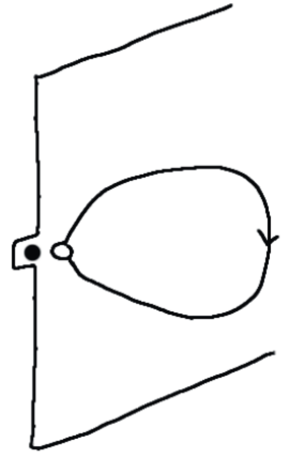
- He_4 crystals contain quenched-in dislocations.

- The dislocation network can become superfluid (Boninsegni et al., Shevchenko) however superfluidity along dislocation cores leads to too small superfluid density compared to experiments (cf Balibar, Caupin).

- Dislocation can be a source of vacancies. Transverse fluctuations of dislocations may be very important.

Dislocation defects are a source of vacancies with smaller E_v





2 important changes repeating the previous analysis:

- Smaller E_v may lead to a negative zero temperature F_v.*
- Vacancies paths start and end on dislocations.

*Classically well known (pipe diffusion); quantistically (Boninsegni et al 07,08)

First temperature regime: $T_c<T<T_v$

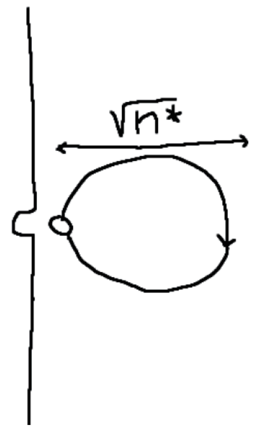
- For $T<T_v$ dislocation defects and vacancies start to ‘proliferate’.
- The defect and vacancy proliferation is limited (no quantum roughening) by the elastic energy cost to create them: elastic repulsion between dislocation defects.
- In this regime the dislocation network resonates (or move) between different distorted configurations.

Dimensional argument to estimate the number of atoms belonging to the resonating dislocation network

$$f \approx F_k \phi_d + \frac{1}{2} G a^3 \phi_d^2 \rightarrow \phi_d \sim 10^{-3}$$

Supersolidity at $T<T_c$

- Vacancies generated along dislocation lines lead to transverse permutation cycles.
- The number of 'superfluid' atoms is enhanced compared to the estimate of Balibar and Caupin because dislocations resonate.
- At a certain temperature, T_c , the permutation cycles from different dislocation may 'concatenate' and lead to supersolidity. What's the value of T_c? Maybe too low?



Consequences & Predictions

- At T_v the elastic properties of the system change (analogy with polymer melts predict a stiffening).
- At T_v change in the specific heat that gets an extra contribution.
- Supersolidity sets in at a smaller temperature T_c.
- T_c, T_v affected substantially by He_3 impurities (how?).
- In He_3 crystals there will be no T_c but there may be a T_v!

Quantitative studies of quantum dislocations (kink-antikink energy, dislocation motion, etc) are crucial!

Two perspectives on disorder-induced 'supersolidity'.

- Disorder $\longrightarrow$ dislocations in He_4 crystals: a scenario for quantum plasticity and dislocation-induced supersolidity (motivated by PG de Gennes (06)).
- Disorder $\longrightarrow$ glass: superglass phase (motivated by Boninsegni et al (06), see also Nussinov et al (06)).

The superglass phase

- Study a model that shows unambiguosly a superglass phase.
- Obtain the basic static and dynamic properties of the superglass phase.
- Strategy: use a mapping between classical Brownian motion and quantum dynamics (Rokshar-Kivelson, Jastrow, etc...).

Classical-Quantum Mapping

$$\gamma_i \frac{d\mathbf{x}_i}{dt} = -\frac{\partial}{\partial \mathbf{x}_i} U_N(\mathbf{x}_1, \ldots, \mathbf{x}_N) + \boldsymbol{\eta}_i(t) \ , \qquad i = 1, ..., N \ ,$$

$$U_N(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{2} \sum_{i \neq j} V_{ij}(\mathbf{x}_i - \mathbf{x}_j) \ , \qquad \langle \eta_i^\alpha(t) \eta_j^\beta(t') \rangle = 2T \, \gamma_i \, \delta_{ij} \, \delta_{\alpha\beta} \, \delta(t - t')$$

- The probability distribution satisfies the Fokker-Planck equation:

$$\partial_t P = -H_{FP} P \qquad H_{FP} = -\sum_i \frac{1}{\gamma_i} \frac{\partial}{\partial \mathbf{x}_i} \left[\nabla_i U_N + T \frac{\partial}{\partial \mathbf{x}_i} \right]$$

- Define the quantum Hamiltonian:

$$H = e^{\frac{1}{2T} U_N} \; H_{FP} \; e^{-\frac{1}{2T} U_N} = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \mathcal{V}_N(\{\mathbf{x}\})$$

$$\mathcal{V}_N(\{\mathbf{x}\}) = -\frac{1}{2} \sum_{j \neq i} \frac{1}{\gamma_i} \nabla^2 V_{ij}(\mathbf{x}_i - \mathbf{x}_j) + \frac{1}{4T} \sum_{i;j(\neq i);j'(\neq i)} \frac{1}{\gamma_i} \nabla V_{ij}(\mathbf{x}_i - \mathbf{x}_j) \cdot \nabla V_{ij'}(\mathbf{x}_i - \mathbf{x}_{j'})$$

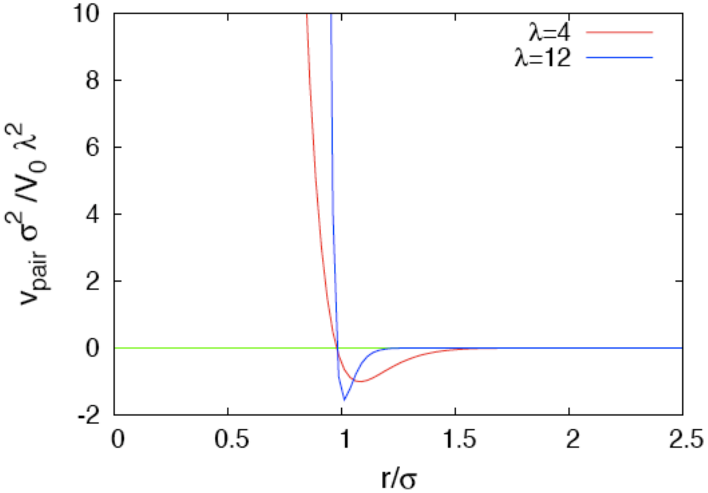
- The ground state wavefunction is $\psi(\{\mathbf{x}\}) = e^{-\frac{U_N}{2T}}$ (quantum averages become classical thermodynamic averages).
- Condensate fraction, correlation functions can be obtained from classical correlation function (a la Jastrow).
- Quantum real time dynamics can be obtained as analytic continuation of the classical Brownian one (Henley).

Our model

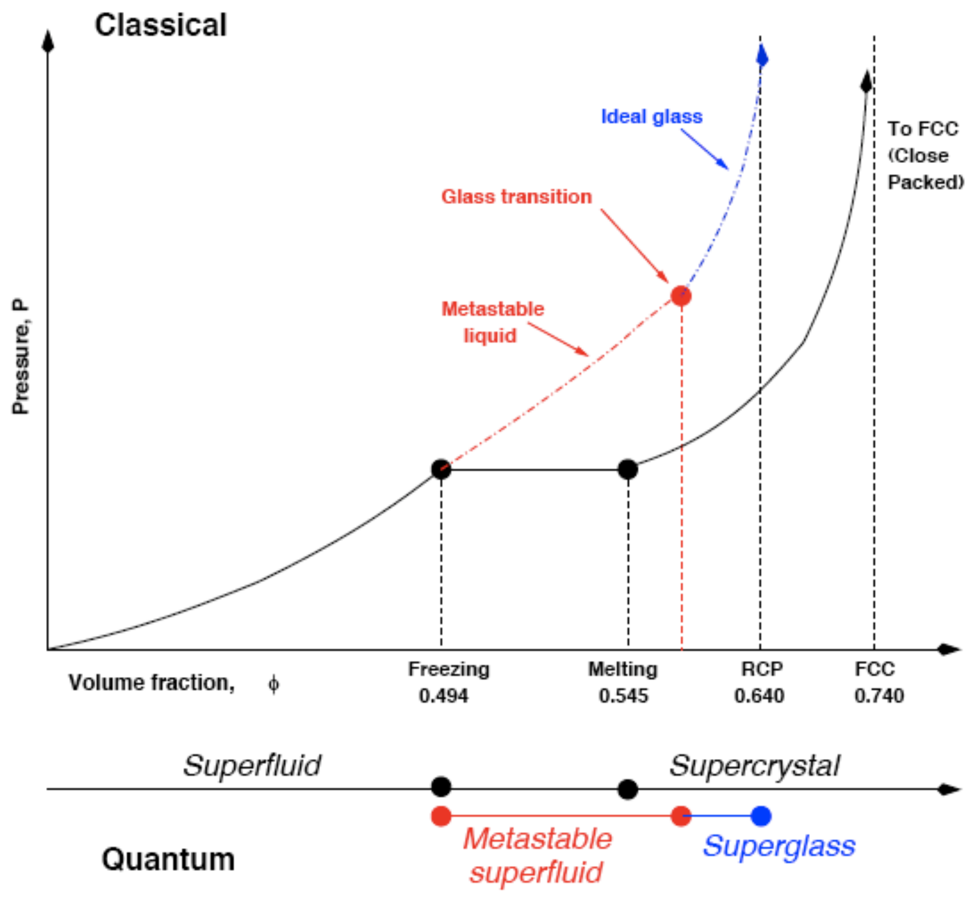
- Quantum counterpart of Brownian hard spheres:

$$V(r) = V_0 \lim_{\lambda\to\infty} \exp(-\lambda[(r/\sigma)^2 - 1])$$

- Quantum 2 and 3 body interaction: hard sphere plus sticky part at contact.



Phase diagram

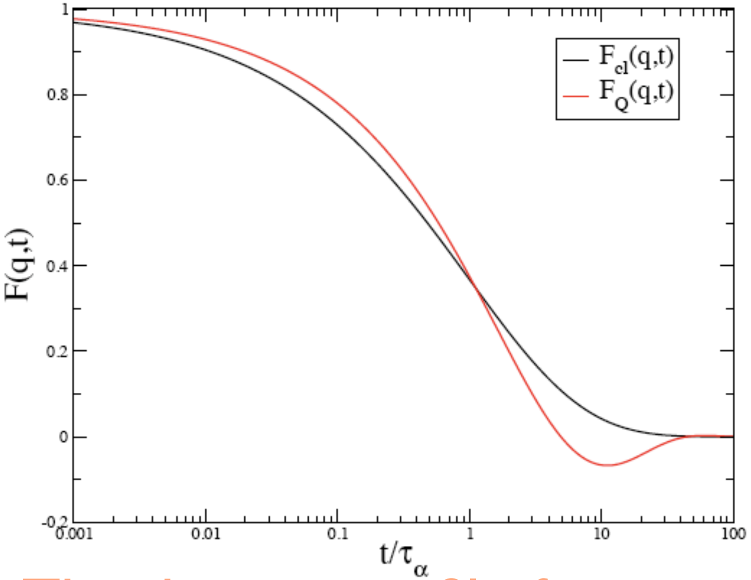


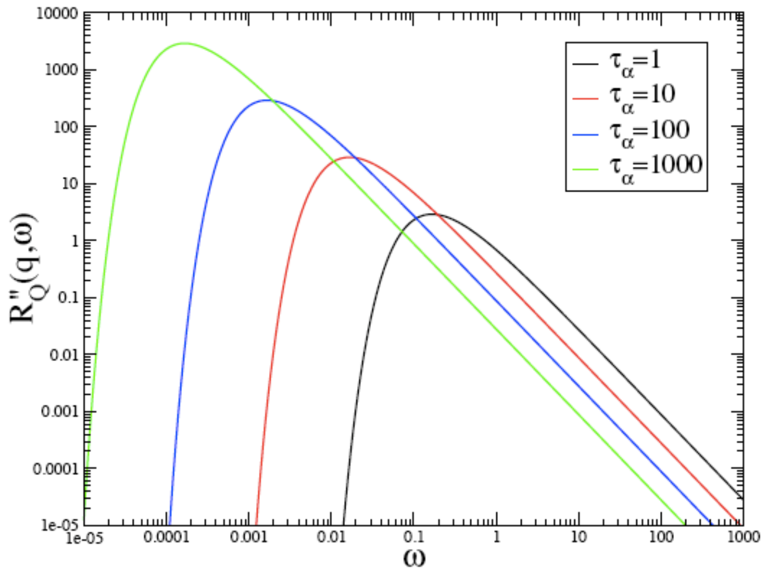
$$\phi = \pi \rho D^3/6$$

Real time dynamics and freezing

Dynamical structure factor and imaginary part of the density response function

$$F(\mathbf{q},t) = \langle \rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)\rangle$$





The density profile freezes gradually into an amorphous profile (and similarly do the condensate fluctuations). The transition superfluid-superglass is first order.

Amorphous condensate profile

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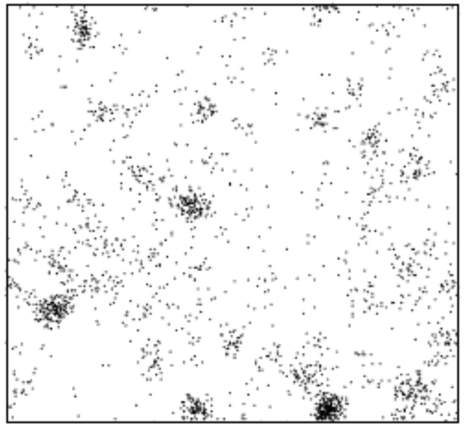
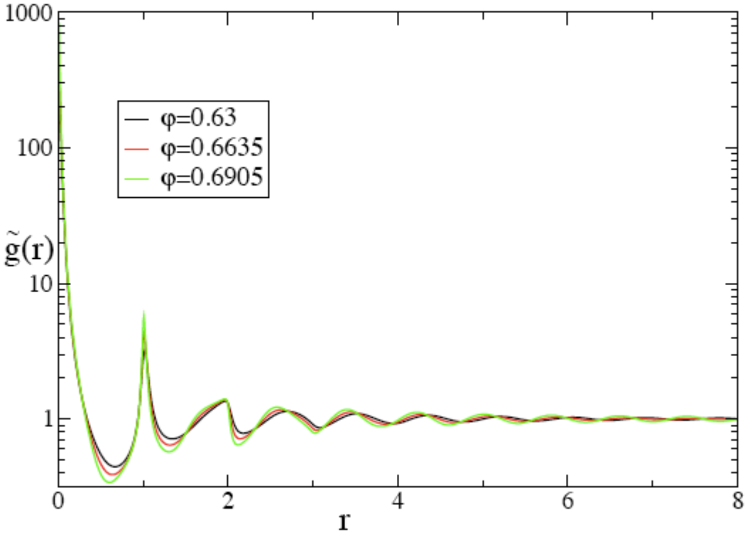
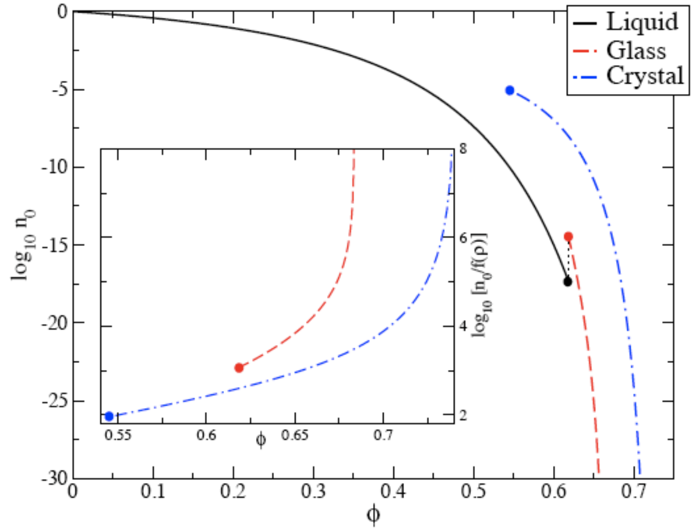
Superglass Phase of ^{4}He

Massimo Boninsegni,[1] Nikolay Prokof'ev,[2,3,4] and Boris Svistunov[2,3]







$$\tilde{g}(\mathbf{r}) = \mathcal{N}\frac{1}{V}\int_V d\mathbf{r}'\,\Psi(\mathbf{r}'+\mathbf{r})\Psi(\mathbf{r}')$$

Conclusion & Perspectives

- Model with unambiguous superglass phase.
- Preliminary analytical computations on He_4 show the existence of metastable superglass phase (cf Boninsegni et al.).
- Properties of the superglass transition at finite temperature?
- Analysis of more realistic superglasses.