Bose-Einstein condensation in Quantum Glasses

Francesco Zamponi

CNRS and LPT, Ecole Normale Supérieure, Paris, France

Giulio Biroli, FZ, JLTP 168, 101 (2012)
Giulio Biroli, Bryan Clark, Laura Foini, FZ, PRB 83, 094530 (2011)
Laura Foini, Guilhem Semerjian, FZ, PRB 83, 094513 (2011)
Giuseppe Carleo, Marco Tarzia, FZ, PRL 103, 215302 (2009)
Giulio Biroli, Claudio Chamon, FZ, PRB 78, 224306 (2008)

INLN, June 19, 2015

Outline

Outline

The liquid-glass transition

Macroscopically well-known for thousands of years. . .

Dynamical arrest of a liquid into an amorphous solid state
No change in structure, $g(r)$ unchanged
Driven by thermal fluctuations: entropic effects, entropic rigidity

The liquid-glass transition

Macroscopically well-known for thousands of years...

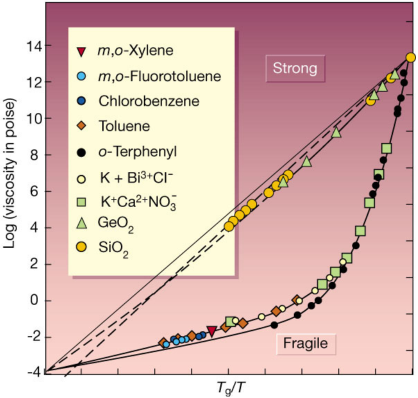
...yet constructing a first-principle theory is a very difficult problem!

- No natural small parameter to construct a perturbative expansion
  Low density virial expansion: fails, too dense
  Harmonic expansion: fails, reference positions are not known
- Several processes simultaneously at work: crystal nucleation, ergodicity breaking, activated barrier crossing, dynamic facilitation
- Laboratory glasses are very far from criticality (if any)
  Theory must take into account strong pre-critical corrections

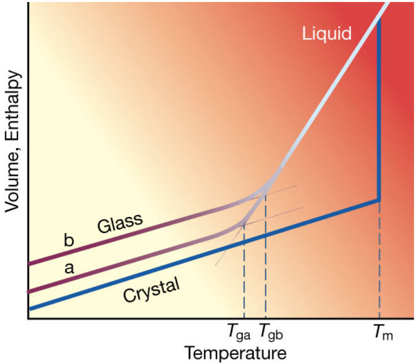
[Berthier, Biroli, RMP 83, 587 (2011)]

The liquid-glass transition

Classical particle system (e.g. Lennard-Jones like potential)

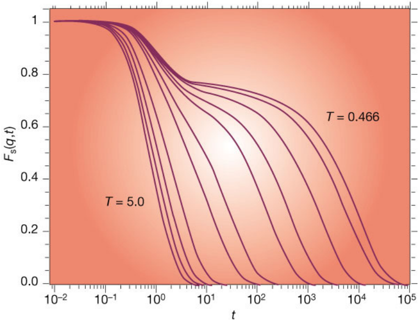


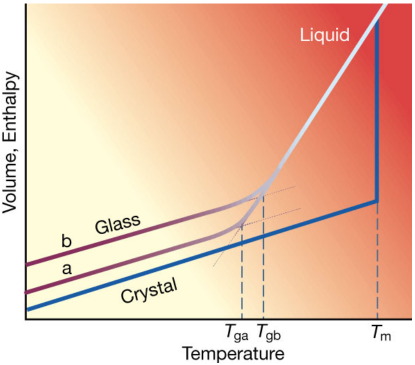
Huge increase of the viscosity in a small range of temperature



Second order phase transition: jump in compressibility

The liquid-glass transition





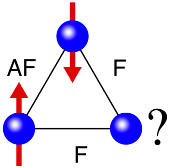
Two steps relaxation:

- Vibrational motion around an amorphous structure
- Structural relaxation: transition between distinct amorphous structures
- Frozen structural relaxation: glass

The number of amorphous structures is exponentially large in system size: $\mathcal{N} \sim e^{NS_{\rm conf}}$

What is a glass?

- A disordered solid
- Many constraints that cannot be easily satisfied simultaneously: e.g. spin glasses



- Many degenerate ground states not related by a simple symmetry
- At low T, the system is confined to a small region around a ground state: glass
- At moderate T, it jumps between distinct ground states: slow dynamics, supercooled liquid

Spin glasses, atomic glasses, colloidal glasses, granular media, random constraint satisfaction problems (SAT, graph coloring...), sphere packings, electron glasses...

Outline

What is a quantum glass?

- A disordered *quantum* solid (like e.g. quantum effects are important in solid Helium 4)
- Many degenerate ground states not related by a simple symmetry
- Simplest recipe: take a classical glassy system and add quantum fluctuations

Why?

- Almost all atomic glasses show anomalies in thermodynamic and transport properties in the low-temperature quantum regime where $\Lambda = \rho^{1/3}\sqrt{2\pi h^2/(mk_B T)} \sim 1$. Phenomenological models based on tunnelling two-level systems. A more microscopic theory?
- Can quantum fluctuations help to find ground states of highly frustrated systems? Quantum annealing versus thermal annealing. Application to quantum computers.
- Within the debate on supersolidity in Helium 4 a *superglass* phase was proposed. A new phase of matter displaying at the same time glassiness (slow dynamics) and superfluidity (zero viscosity). Can it really exist? **Focus of the rest of this talk**

Note: computer simulation of classical glasses are extremely hard. For quantum glasses it is even worse: QMC is slow and we do not have access to real-time dynamics. Strong need for analytical results.

What is a quantum glass?

- A disordered *quantum* solid (like e.g. quantum effects are important in solid Helium 4)
- Many degenerate ground states not related by a simple symmetry
- Simplest recipe: take a classical glassy system and add quantum fluctuations

Why?

- Almost all atomic glasses show anomalies in thermodynamic and transport properties in the low-temperature quantum regime where $\Lambda = \rho^{1/3}\sqrt{2\pi h^2/(mk_B T)} \sim 1$. Phenomenological models based on tunnelling two-level systems. A more microscopic theory?
- Can quantum fluctuations help to find ground states of highly frustrated systems? Quantum annealing versus thermal annealing. Application to quantum computers.
- Within the debate on supersolidity in Helium 4 a *superglass* phase was proposed. A new phase of matter displaying at the same time glassiness (slow dynamics) and superfluidity (zero viscosity). Can it really exist? **Focus of the rest of this talk**

Note: computer simulation of classical glasses are extremely hard. For quantum glasses it is even worse: QMC is slow and we do not have access to real-time dynamics. Strong need for analytical results.

What is a quantum glass?

- A disordered *quantum* solid (like e.g. quantum effects are important in solid Helium 4)
- Many degenerate ground states not related by a simple symmetry
- Simplest recipe: take a classical glassy system and add quantum fluctuations

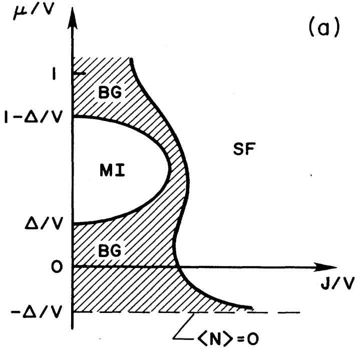
Why?

- Almost all atomic glasses show anomalies in thermodynamic and transport properties in the low-temperature quantum regime where $\Lambda = \rho^{1/3}\sqrt{2\pi h^2/(mk_B T)} \sim 1$. Phenomenological models based on tunnelling two-level systems. A more microscopic theory?
- Can quantum fluctuations help to find ground states of highly frustrated systems? Quantum annealing versus thermal annealing. Application to quantum computers.
- Within the debate on supersolidity in Helium 4 a *superglass* phase was proposed. A new phase of matter displaying at the same time glassiness (slow dynamics) and superfluidity (zero viscosity). Can it really exist? **Focus of the rest of this talk**

Note: computer simulation of classical glasses are extremely hard. For quantum glasses it is even worse: QMC is slow and we do not have access to real-time dynamics. Strong need for analytical results.

The Bose glass is not a quantum glass

$$H = -J\sum_{<i,j>}(a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2}\sum_i n_i(n_i-1) - \sum_i(\mu+\varepsilon_i)n_i \qquad \varepsilon_i \in [-\Delta,\Delta]$$



- Mott insulator: one particle/site, strong localization
  Zero compressibility
- Bose glass: additional defects
  Anderson localization of quasi-particles
  Finite compressibility

No frustration: unique ground state, easy to find
QMC easy to equilibrate
At finite T, a disordered insulator
Dynamics might be slow but not really glassy

Many-body localization versus quantum glassiness

Typical MBL system: a Heisenberg 1d chain $H = \sum_i h_i S_i^z + \sum_i J S_i \cdot S_{i+1}$

- No frustration at all: unique ground state
- MBL is supposed to happen even at $T = \infty$: glassiness only at low temperature
- Transport of energy completely suppressed in MBL, while glasses transport energy
- Both MBL and glassiness lead to slow dynamics and lack of equilibration

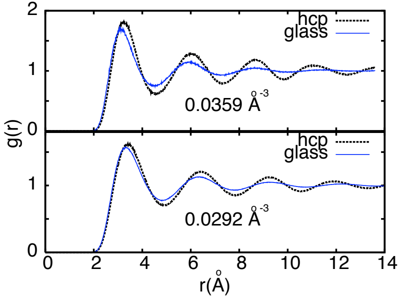
MBL is due to the localization of many-body wavefunctions in Fock space

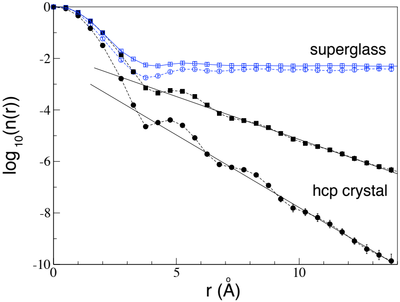
Glassiness corresponds to *clustering* of extended many-body eigenstates: each cluster corresponds to a distinct glass

Outline

Helium 4: Monte Carlo results - I

Quantum Monte Carlo simulation of He^4 at densities where the ground state is a crystal
Quench from the liquid phase down in the solid phase at $T \sim 0.2K$.





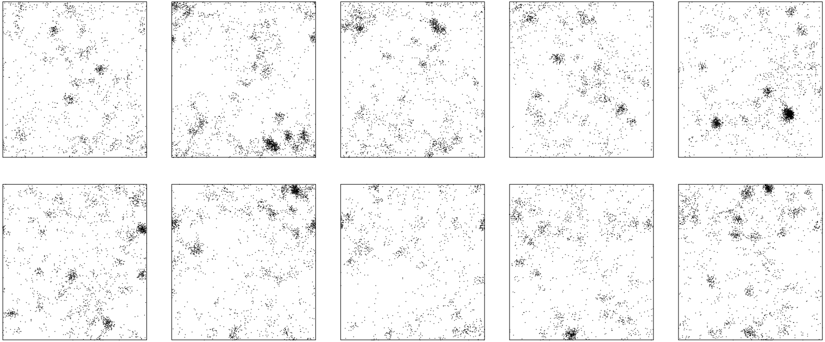
Density-density correlations similar to the liquid (large Lindemann ratio)

ODLRO observed in the one-particle density matrix → BEC, superfluidity
At $\rho = 0.0292 A^{-3}$, $n_0 = 0.5\%$ and $\rho_s/\rho = 0.6$

[Boninsegni, Prokof'ev, Svistunov, PRL 96, 105301 (2006)]

Helium 4: Monte Carlo results - I

Amorphous condensate wavefunction: $n(r-r') \sim n_0 \phi(r)\phi(r')$



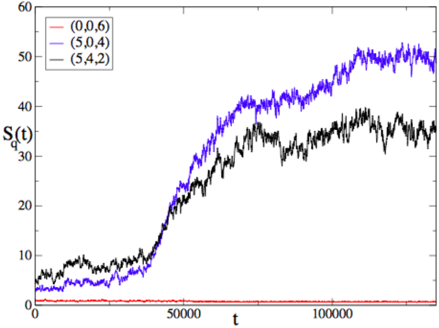
Plot of $\phi(x,y,z)$ on slices at fixed z

Many open problems:

- Is this a long-lived metastable phase?
- What is the nature of the transition?
- Is it accompanied by slow dynamics in the liquid phase?
- Where does superfluidity come from?

Helium 4: Monte Carlo results - II

Quantum Monte Carlo simulation of He^4 at densities where the ground state is a crystal
Quench from the liquid phase down in the solid phase at $T \sim 0.2K$.



After a very short transient, the structure factor starts to grow large Bragg peaks, indicating crystallization

The claimed superfluid fraction of 0.6 is incompatible with a bound due to Legget that gives $\rho_s/\rho \lesssim 0.28$

Conclusion: strong tendency to crystallization, no stable glass phase in pure He^4.

[Biroli, Clark, Foini, FZ, PRB 83, 094530 (2011)]

PIMD simulation of a binary mixture designed to avoid crystallization. Stable glass phase.
Glassiness is promoted by quantum fluctuations. Exchange neglected.
Conclusions: simulations are too heavy to compute the phase diagram.

[Markland et al., Nature Physics 7, 134 (2011)]

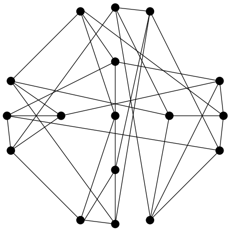
Outline

A lattice model

Extended Hubbard model on a regular random graph at half-filling and $U = \infty$:

$$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V \sum_{\langle i,j \rangle} n_i n_j - \sum_i \mu n_i$$

We study the model on a regular random graph of L sites and connectivity $z = 3$:



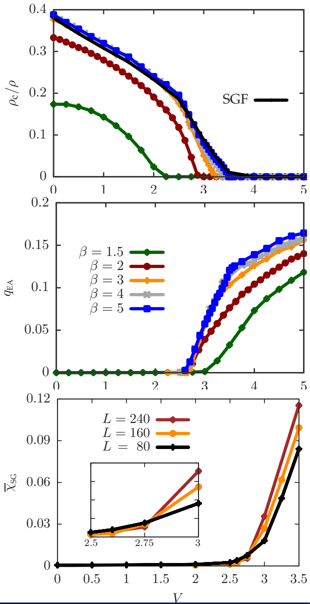
- No disorder in the interactions
- Frustration: loops of even and odd size
- Large loops, locally tree-like graph
- Solution for $L \to \infty$ possible via the cavity method (an extension of DMFT for disordered systems)
- Classical model ($J = 0$): spin glass transition (like Sherrington-Kirkpatrick model)
- Glass phase is thermodynamically stable
- Many degenerate glassy states, slow dynamics

Methods:

- Quantum cavity method: solution for $L \to \infty$
- Stochastic Green Function Monte Carlo: limited to $L < 240$ by ergodicity problems
- Variational calculation (for illustration) + Green Function Monte Carlo

[G. Carleo, M. Tarzia, FZ, PRL 103, 215302 (2009)]

A lattice model - results at half-filling and $J = 1$



Condensate fraction:

$$\rho_c = \lim_{|i-j|\to\infty} \left\langle a_i^+ a_j \right\rangle = |\langle a\rangle|^2$$

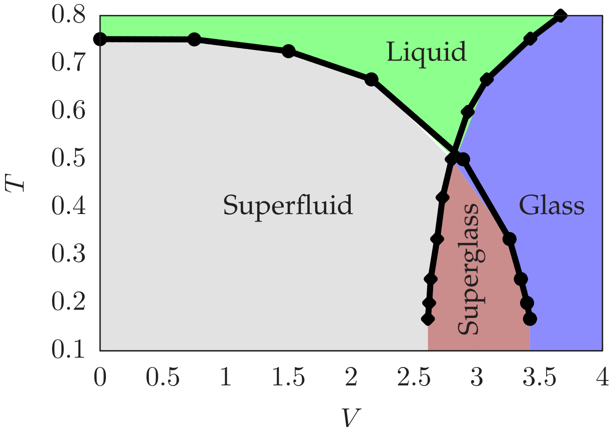
Edwards-Anderson order parameter:

$$q_{EA} = \frac{1}{L}\sum_i \left\langle (\delta n_i)^2 \right\rangle \qquad \delta n_i = n_i - \langle n_i \rangle$$

Spin-Glass susceptibility:

$$\chi_{SG} = \frac{1}{L}\int_0^\beta d\tau \sum_{i,j} \left\langle \delta n_i(\tau)\delta n_j(0) \right\rangle^2$$

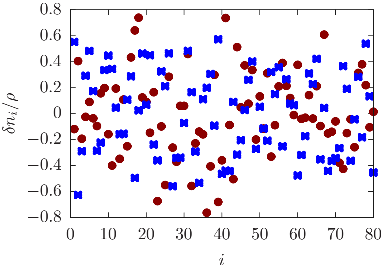
A lattice model - phase diagram at half-filling and $J = 1$



A lattice model - variational argument

Many spin glass states:

- Each spin glass state breaks translation invariance
- Simplest variational wavefunction: $\langle \underline{n} | \Psi \rangle = \exp(\sum_i \alpha_i n_i)$
- A different set of parameters for each spin glass state
- Optimization of the parameters α_i depends on the initial condition



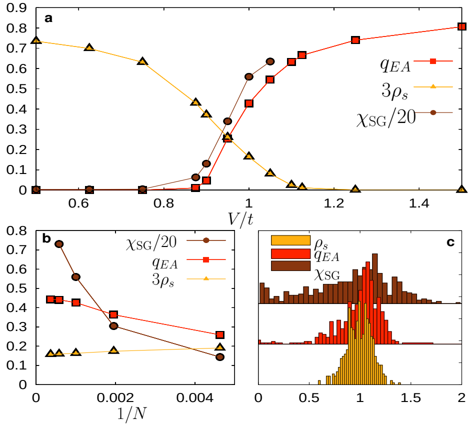
Stability of the glass state:

- Green Function Monte Carlo: $|\Psi(\tau)\rangle = e^{-\tau H} |\Psi\rangle$
- The time τ needed to escape from the initial state $|\Psi\rangle$ increases with system size

A lattice model - 3D version

$$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \sum_{\langle i,j \rangle} V_{ij} (n_i - 1/2)(n_j - 1/2)$$

QMC for the 3D cubic lattice with couplings $V_{ij} = \pm V$:



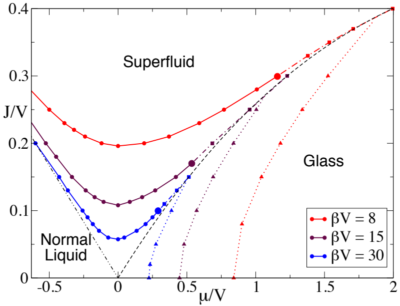
- Same phase diagram
- But frustration is induced by quenched disorder

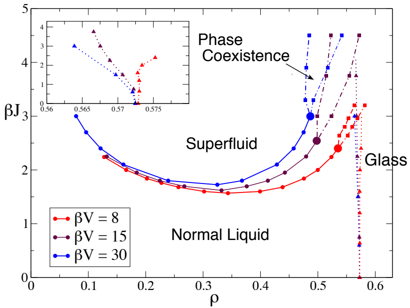
[Tam, Geraedts, Inglis, Gingras, Melko, PRL 104, 215301 (2010)]

Another lattice model

Quantum Biroli-Mézard model:
$H = -J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_i n_i q_i \theta(q_i) - \sum_i \mu n_i \qquad q_i = \sum_{j\in\partial i} n_j - \ell$

We study the model on a regular random graph for $L = \infty$, $z = 3$ and $\ell = 1$.





First order transition, with phase coexistence, between glass and superfluid: no superglass
Re-entrant glass transition line: confirms the results of Markland et al.

[L. Foini, G. Semerjian, FZ, PRB 83, 094513 (2011)]

Outline

Discussion

- Within the debate on supersolidity in Helium 4 a *superglass* phase was proposed. A new phase of matter displaying at the same time glassiness (slow dynamics) and superfluidity (zero viscosity). Can it really exist?
- Numerical simulations give confusing answers. In Helium 4, crystallization occurs too quickly. In binary mixtures, no crystallization but the simulations are heavy and neglected exchange. No clear answer.
- Some lattice modes display a superglass phase. Others do not, but display phase coexistence between superfluid and glass. *But what is the role of the lattice?* Can we have an off-lattice superglass?

A first answer is a proof of principle: we constructed a class of wavefunctions of the Jastrow type that display a superglass phase.

- The condensate wavefunction has strong spatial fluctuations like in the simulation of Boninsegni et al.
- Quantum dynamics is slow as in a glass
- "Almost classical" solid with very small Lindemann ratio and tiny (unobservable, $\sim 10^{-10}$) condensate fraction

[Biroli, Chamon, FZ, PRB 78, 224306 (2008)]

Discussion

- Within the debate on supersolidity in Helium 4 a *superglass* phase was proposed. A new phase of matter displaying at the same time glassiness (slow dynamics) and superfluidity (zero viscosity). Can it really exist?
- Numerical simulations give confusing answers. In Helium 4, crystallization occurs too quickly. In binary mixtures, no crystallization but the simulations are heavy and neglected exchange. No clear answer.
- Some lattice modes display a superglass phase. Others do not, but display phase coexistence between superfluid and glass. *But what is the role of the lattice?* Can we have an off-lattice superglass?

A first answer is a proof of principle: we constructed a class of wavefunctions of the Jastrow type that display a superglass phase.

- The condensate wavefunction has strong spatial fluctuations like in the simulation of Boninsegni et al.
- Quantum dynamics is slow as in a glass
- "Almost classical" solid with very small Lindemann ratio and tiny (unobservable, $\sim 10^{-10}$) condensate fraction

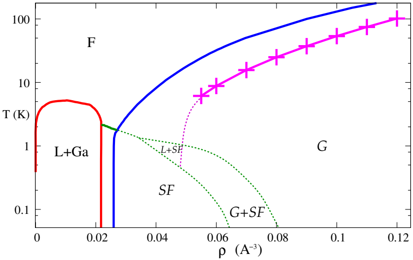
[Biroli, Chamon, FZ, PRB 78, 224306 (2008)]

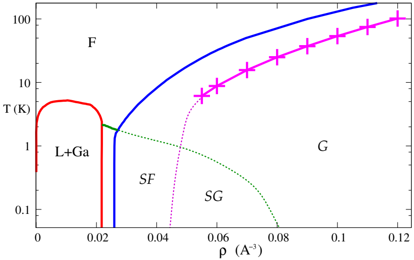
Discussion

Using an approximate semiclassical method, *and neglecting exchange* we were able to compute the glass transition like in Helium 4 at large enough density.

Helium 4 crystallizes quickly, but a suitable binary mixture might remain amorphous for longer times. No concrete proposal yet.

Based on this and on the insight from lattice models, we can conjecture two possible scenarios:





[Biroli, FZ, JLTP 168, 101 (2012)]

Which one is correct, we do not know...
.. new insight might come from the exact solution in $d = \infty$ that we have obtained recently for the classical case.

THANK YOU FOR YOUR ATTENTION!