Gross-Pitaevskii Theory of Supersolids

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joint work with Phan Thành Nam (Munich)

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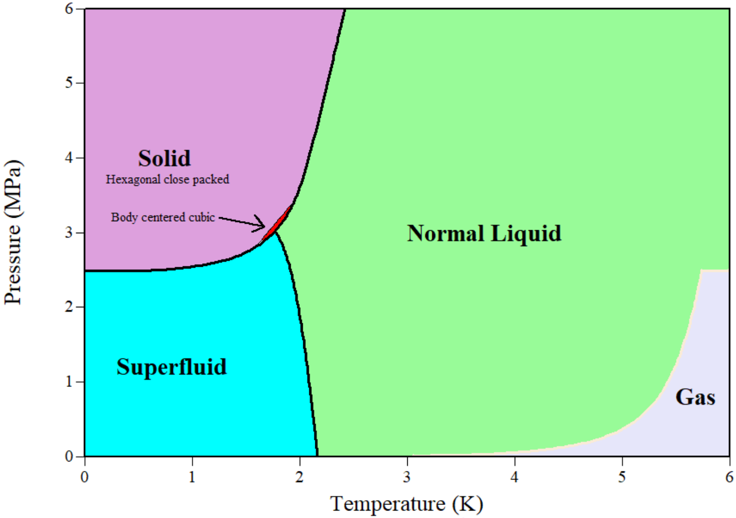
GSSI, L'Aquila, Feb. 2025

Existence of phase transitions for continuous systems

- One of the **most famous open problems in mathematical physics**
- Example of **Helium-4**:



Freezing: "crystallization conjecture"

Conjecture

Any "reasonable" (classical or quantum) infinite interacting system at equilibrium should **break translational symmetry** at low temperature / high pressure.

Blanc, ML, EMS Surv. Math. 2015

- general results only at $T = 0$ in classical case
- interesting links with number theory (Viazovska *et al*)
- no tool to attack this problem for $T > 0$ in full generality
- Gibbs state always unique in finite volume

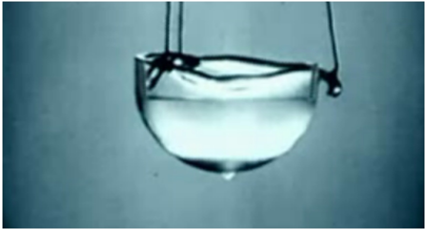
▶ **Main difficulty:** mathematical study of **infinitely many particles**

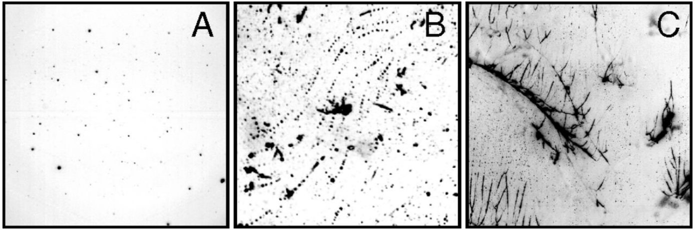
1. notion of **infinite equilibrium state**
2. existence by a thermodynamic limit
3. show that they are **not translation-invariant**, possibly even **periodic**

Superfluidity

At $T \ll 1$, some systems such as Helium-4 exhibit a **quantum phase transition** to a superfluid

- flows with **no viscosity**
- does not react at all to small rotation, large rotation induces **quantized vortices**





Guo *et al*, PNAS 2014

Excitation spectrum (Landau)

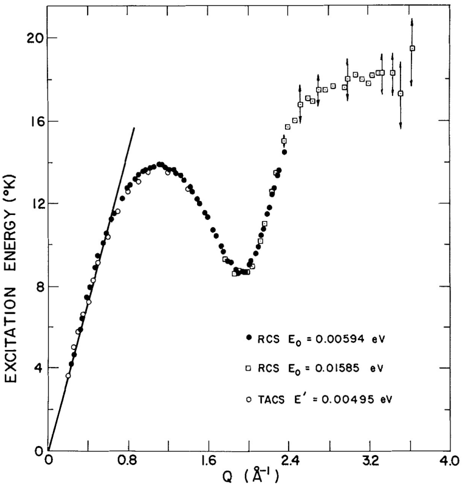


FIG. 7. The experimental results for the energies of the one-phonon excitations at 1.1 °K.

Cowley-Woods, Can. J. Phys. 1971

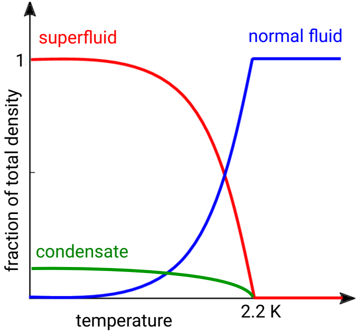
- linear dispersion relation at low momentum
- Perturb Hamiltonian by $v \cdot (-i\nabla)$ and see how system reacts
- Legendre transform $\Rightarrow$ convex hull
- For Helium-4, given by the "roton" part

Bose-Einstein Condensation (BEC)

- **"off-diagonal long range order"**: kernel of the one-particle density matrix satisfies

$$\gamma(x,y)=\left\langle a^\dagger(x)a(y)\right\rangle \underset{|x-y|\to\infty}{\sim} u(x)\overline{u(y)}\neq 0$$

  for some **macroscopic function** $u(x)\neq 0$ called the **condensate wavefunction**
- interpreted as **breaking of particle-number** (for extreme equilibrium states), $u(x)=\left\langle a^\dagger(x)\right\rangle$
- in a fluid $\gamma=g(-i\nabla)$ commutes with translations (Fourier multiplier) hence $u(x)\equiv u_0$ and $\gamma(x,y)=\check{g}(x-y)\to_{|x-y|\to\infty}|u_0|^2>0$. Namely **$g$ contains $|u_0|^2\delta_0$ in momentum space**



In Helium-4:

- BEC appears at same time as superfluidity but only $\approx 10\,\%$ of particles condensed
- superfluid behavior results from complicated correlations between the condensed and non-condensed parts, no simple microscopic model
- in general, BEC can happen without superfluidity (ex: free bosons) and conversely (ex: hard core 1D Bose gas)

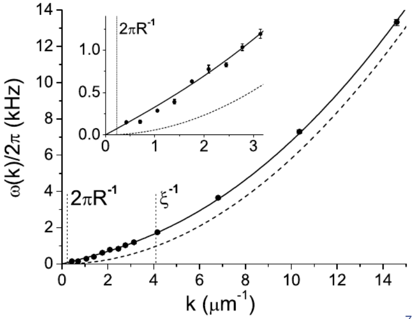
Dilute gases with repulsive interactions (Bogoliubov, 1947)

"It is important to investigate some very simple models of a macroscopic system in order to derive a mechanism capable of explaining an energy spectrum with the above stated properties" (Bogoliubov)

- **positive pair interaction** w (possibly also with $\widehat{w} \geq 0$):
- **complete BEC** in the limit $\rho \to 0$ at $T = 0$
- excitation spectrum given by (a=scattering length of w)

$$\varepsilon(k) = |k|\sqrt{k^2/2 + 4\pi\rho a}$$

- quadratic Hamiltonian in Fock-space describing finite excitations above the condensate
- works also well for **trapped ultra-cold Bose gases**
- important that no bound state can form at $\rho \ll 1$ so that particles become essentially independent
- does not apply to Helium-4, for which w is attractive at large distances (van der Waals) and $\widehat{w}$ has no sign



Condensate of 6×10^7 Rb atoms, Steinhauer-Ozeri-Katz-Davidson, Phys Rev. Lett. 2002

Supersolids

Definition

A **supersolid** is a solid that displays some superfluid properties. Or, simpler, a system with both breaking of translation-invariance and off-diagonal long-range order (BEC):

$$\gamma(x,y) = \left\langle a^\dagger(x) a(y) \right\rangle \underset{|x-y|\to\infty}{\sim} \left\langle a^\dagger(x) \right\rangle \langle a(y) \rangle = u(x)\overline{u(y)}$$

with $u \neq 0$ **not constant** (typically periodic).

Matsuda-Tsuneto (Prog. Theor. Phys. 1970), Chester (Phys. Rev. A 1970)

Supersolid saga

- Penrose-Onsager (1956): cannot exist
- Gross (1957): assumed full BEC and studied the resulting equation for the condensate in a partially attractive w, predicting existence of supersolid phase at high density
- Andreev-Lifshitz (1969): condensation of holes and defects in principle possible in a solid
- Matsuda-Tsuneto (1970): lattice bosons
- Kim-Chan (2004) claimed experimental observation in helium-4 but admitted later in 2012 that was wrong
- supersolidity remains controversial for helium-4 but recent explosion of works for dilute ultra-cold gases with dipolar interactions (2017–)

Unified Theory of Interacting Bosons

EUGENE P. GROSS
Brandeis University, Waltham, Massachusetts
(Received January 25, 1957)

RECENT work has contributed to the understanding of properties of helium II. Yet there is room for a unified theoretical approach to the problem of interacting bosons for both solid and liquid states. In particular the liquid is like the solid as regards cohesive energy and packing. One is interested in computing these from first principles, as well as in the connection between the vibration spectrum of the solid and the excitation spectrum of the liquid, the

$$Ef=-\frac{\hbar^2}{2M}\nabla^2 f+\int V(\mathbf{x}-\mathbf{x}')|f(\mathbf{x}')|^2 d^3x'\cdot f(\mathbf{x}),$$

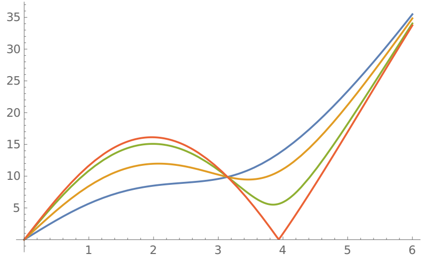
$$\int |f|^2 d^3x = N.$$

We note that there is always a solution of uniform density, namely,

$$f(x)=\left(\frac{N}{L^3}\right)^{\frac{1}{2}},\quad E=\frac{N}{L^3}\int V(\mathbf{x})d^3x.$$

But if $V(\mathbf{x})$ is negative in some region of space, there may be other solutions, such as a periodic solution with E lower than for the uniform solution. In the classical

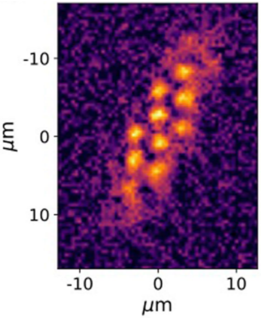
- **full BEC** $\Longrightarrow$ simple PDE for the condensate
  Gross-Pitaevskii equation
  (NB: Pitaevskii 1961 had $w=\delta$!)
- Bogoliubov spectrum with roton-maxon becomes unstable at a certain value of the density
$$\varepsilon(k)=|k|\sqrt{k^2/2+\rho\widehat{w}(k)}$$
- lots of theoretical/numerical works
- application to Helium-4 unclear since not fully condensed



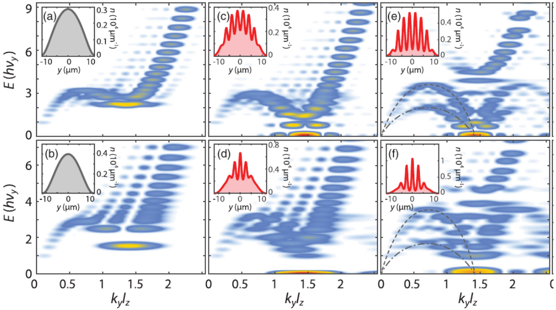
Bogoliubov spectrum for $w(x)=\frac{1}{1+x^6}$ and different values of ρ

Supersolids for trapped ultracold dipolar gases

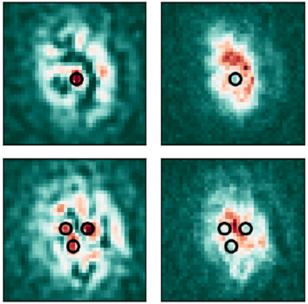
- possibility of tuning the interaction in trapped cold gases
- dipolar interaction scales the same as $\delta \rightsquigarrow$ visible in Bogoliubov dilute regime
- **2017–: 1D supersolids in confined dipolar gases**
  Léonard *et al*, Ketterle *et al*, Modugno *et al*, Pfau *et al*, Ferlaino *et al*
- **2021–: 2D supersolids in confined dipolar gases**, Ferlaino *et al*
- **Nov. 2024:** observation of quantized vortices



Ferlaino *et al* (Nature, 2021)



Ferlaino *et al* (Phys. Rev. Lett., 2019)



Ferlaino *et al* (Nature, 2024)

A roton-maxon of papers

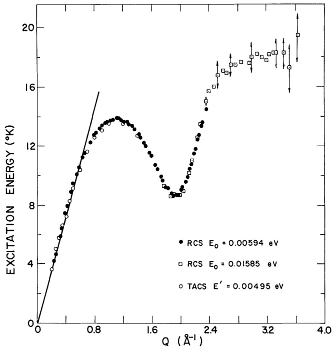
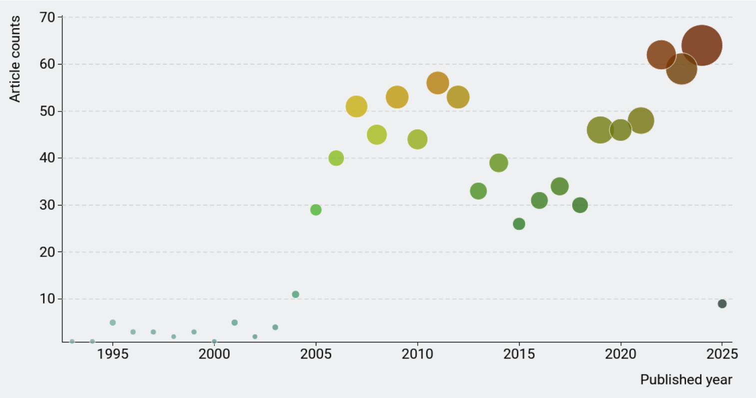


FIG. 7. The experimental results for the energies of the one-phonon excitations at 1.1 °K.



Number of papers per year on arXiv, containing the keyword "supersolid" in their abstract

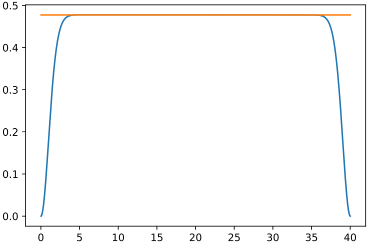
(from ArXiv Analytics)

Goals of the lecture

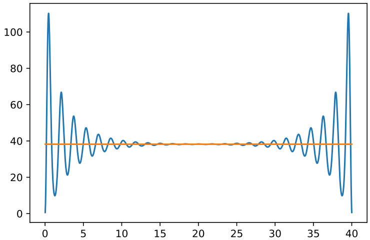
- study the Gross-Pitaevskii equation of Gross 1957 describing a **fully condensed system** with a **general pair interaction potential** w
- proof of the existence of a **unique freezing transition**
- nonlinear PDE for $u \in L^\infty(\mathbb{R}^d)$
- mixture of PDE and statistical mechanics tools
- we assume $w \in L^1(\mathbb{R}^d)$ (no dipolar interaction)
- most previous works were for $w = \delta$
- lots of open problem

THE PHASE TRANSITION

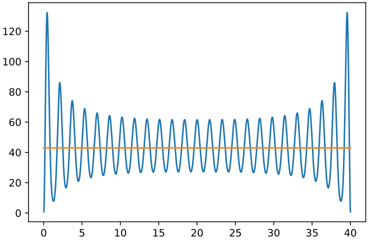
Numerics in 1D



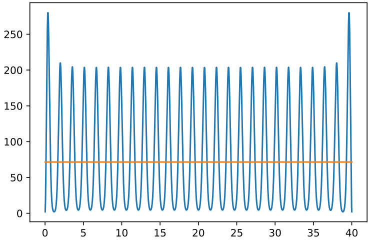
$\mu = 1,\ \rho \approx 0.47$



$\mu = 80,\ \rho \approx 39$



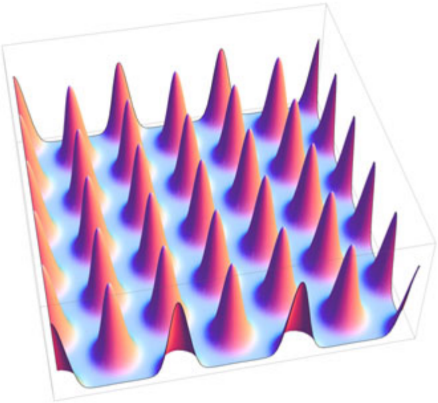
$\mu = 90,\ \rho \approx 44$



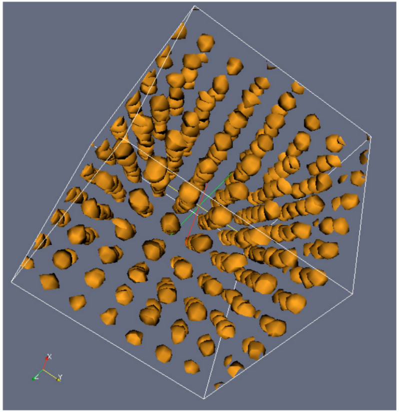
$\mu = 150,\ \rho \approx 77$

- $w(x) = \dfrac{1}{1+x^6}$
- Dirichlet BC
- $\mu_c' \approx 86.5$
- $k_c \approx 3.9$
- period $2\pi/k_c \approx 1.6$
- suggests 2nd order phase transition $\equiv$ bifurcation from $u_{\rm cnst}$ with period $2\pi/k_c$
- scenario predicted by Kirzhnits-Nepomnyashchii (1971)
- numerics by Platt-Baillie-Blakie (Phys. Rev. A, 2024)

Numerics in 2D & 3D



Sepulveda-Josserand-Rica (2010)
Plot of $|u|^2 \rightsquigarrow$ triangular lattice



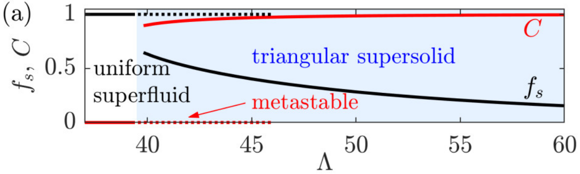
Josserand-Pomeau-Rica (2007)
Contour plot of $\{|u|^2 = c\} \rightsquigarrow$ Hexagonal-Close-Packing

$$w(x) = \alpha \mathbb{1}(|x| \le R)$$

Phase transition in 2D

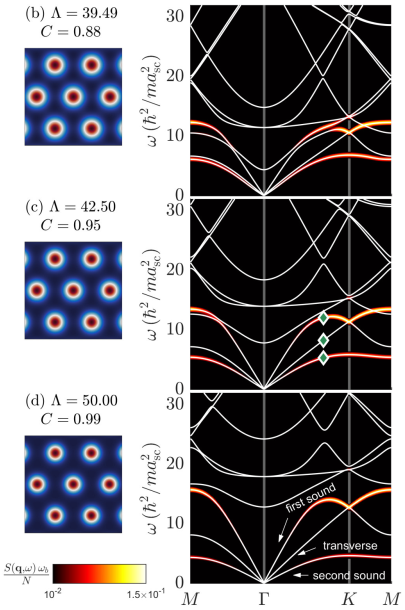
Poli-Baillie-Ferlaino-Blakie (Phys. Rev. A, nov. 2024)

- $w(x) = \alpha \mathbb{1}(|x| \leq R)$ (soft core)
  (ongoing experiments supersolid regime not yet attained)
- found a first order transition to a triangular solid, **before the constant becomes unstable**
- similar results for dipolar interaction



density contrast $C = \frac{\max|u|^2 - \min|u|^2}{\max|u|^2 + \min|u|^2}$

superfluid fraction $f_s = \frac{1}{\rho} \frac{\partial^2}{\partial v_1^2} \mathcal{E}$ in response to perturbation $(-i\nabla + v)^2$



Back to the many-body problem for $w(x) = \alpha \mathbb{1}(|x| \le R)$

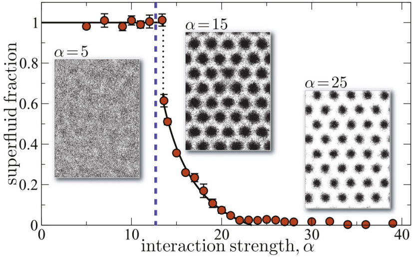


FIG. 1. (Color online) Superfluid fraction of two-dimensional bosons as a function of the dimensionless interaction strength $\alpha = m\rho V_0 R_0^4/\hbar^2$. The points show results of Monte Carlo simulations for 320 particles with a density of $R_0^2\rho = 4.4$, whereas the continuous line is a guide for the eye. The superfluid fraction drops abruptly at $\alpha \approx 13.4$ (dotted line), marking a first-order superfluid-supersolid phase transition, in close agreement with the mean-field prediction of $\alpha = 12.7$ (dashed line). Around $\alpha \approx 22$, the systems enter an insulating phase. The insets show PIMC snapshots for different α, illustrating the particle density profile in the three different phases. We checked that the results do not change for a temperature range of 0.1–0.75 $\hbar^2/mR_0^2$ and particle numbers 160, 320, 640.

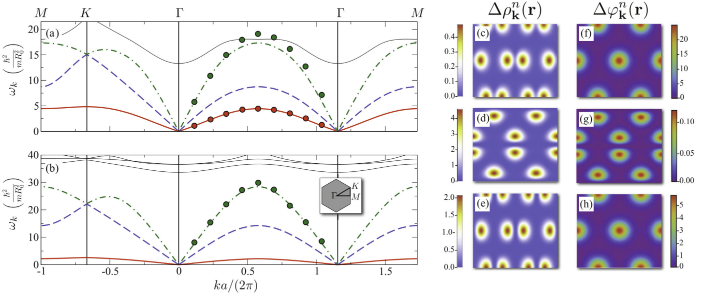


FIG. 3. (Color online) Mean-field spectra (lines) at (a) $\alpha = 16.93$ and (b) $\alpha = 30.62$ obtained from Eqs. (5) along the three symmetry directions of the Brillouin zone [see inset of panel (b)]. The symbols represent the PIMC data of Ref. [25] for longitudinal excitations computed along the direction Γ–M–Γ in the first two Brillouin zones. (c)–(e) Density fluctuations $\Delta\rho_{\mathbf{k}}^n(\mathbf{r}) = |u_{n,\mathbf{k}}(\mathbf{r}) - v_{n,\mathbf{k}}(\mathbf{r})|^2$ and (f)–(h) phase fluctuations $\Delta\varphi_{\mathbf{k}}^n(\mathbf{r}) = |u_{n,\mathbf{k}}(\mathbf{r}) + v_{n,\mathbf{k}}(\mathbf{r})|^2$ computed at $\alpha = 16.93$ and $\mathbf{k} = \vec{\Gamma K}/10$ (directed along the horizontal axis) for the (c), (f) lowest (solid line) band, (d), (g) middle (dashed line) band, and (e), (h) higher (dot-dashed line) gapless band.

Macri-Maucher-Cinti-Pohl (Phys. Rev. A, 2013)