Many-Body Wave Functions that Allow Bose Condensation in a Perfect Crystal

Yong-Shi Wu

(in Collaboration with Hui Zhai)

(cond-mat/0501309)

Miniprogram on "Supersolid State of Matter"

KITP, UCSB Feb. 15, 2006

History of Supersolid (The Possibility)

It is also evident from these examples that ODLRO may occurs in a liquid, and it may also occur in a solid. But in a solid the basic group cannot contain particles that are localized, such as the nuclei.

------- C.N. Yang (1962)

Rev. Mod. Phys. 34, 694 (1962)

History of Supersolid (A Mechanism)

Quantum theory of crystal defects

At sufficiently low temperatures localized defects or impurities change into excitations which move freely through the crystal. As a result, ordinary defect diffusion is replaced by a liquid flow consisting of 'defectons' and 'impuritons'.

A crystal of this type is neither a solid body nor a liquid.

Under certain conditions the 'liquid' type of crystal motion possesses 'superfluidity' properties.

------ A.F. Andreev, I.M. Lifshitz, (1969)

Soviet Physics – JETP 56, 2057 (1969)

History of Supersolid (Some Model States)

We shall show-- almost rigorously-- that these model states can *simultaneously exhibit both Bose-Einstein condensation and crystalline ordering. The presence of crystalline order would presumably prevent the appearance of any normal superfluid properties.*

It is now interesting to note that we expect all the model states we have discussed to lead to crystalline order with vacancies present. We may therefore add one finial speculation, namely, that *a quantum crystal can only have a Bose-Einstein condensate if it has a finite fraction of vacancies.*

------- G. V. Chester (1970)

Phys. Rev. A 2, 256 (1970)

History of Supersolid (A Way to Detect)

It is suggested that the property of *nonclassical rotational inertia* possessed by superfluid liquid helium may be shared by some solids.

However, the associated *superfluid fraction* is shown to be *very small (probably < 0.0001)* even at T = 0.

----- A. J. Leggett

Phys. Rev. Lett. 22, 1543 (1970)

Brief Summary:

All agreed vacancies or defects can condense, resulting in supersolid. Many thought vacancies or defects are necessary for supersolid.

Our Theoretical Work:

Show that vacancies or defects are *not necessary for supersolid*, by constructing a class of many-body wave functions for a *perfect crystal (commensurable solid)*, and proving that they possess both *DLRO* (crystalline order) and *ODLRO* (Bose condensation).

Digression: Non-Classical Rotational Inertia

Suppose that we enclose a number N of helium atoms in a crystalline annulus of internal radius R and thickness d, and rotate the enclosing surface about the axis of the cylinders at constant angular velocity ω

$$F(\omega) = F_0 + \tfrac{1}{2} I_0 \omega^2 + \Delta F(\omega)$$

F_0 ↑ Free energy for $\omega = 0$ $\qquad$ I_0 ↑ Classical moment of inertia

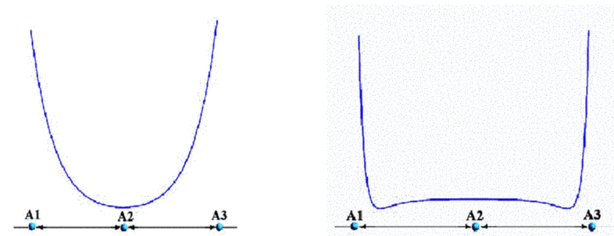
$$\Delta F(\omega) = -\tfrac{1}{2}(\rho_s/\rho) I_0 \omega^2$$

ρ_s/ρ ↑ Superfluid Fraction

The condition for this term nonzero is that the energy of the many body state is sensitive to the twisted phase boundary conditions!

Large Lattice Zero-Point Motion

Total interatomic potential



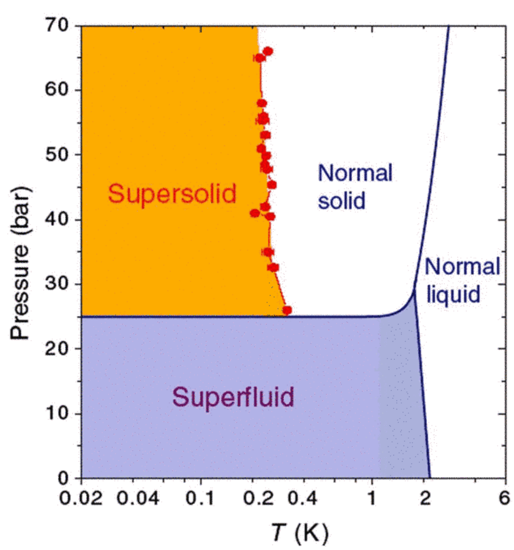
Usual solid (~ quadratic) Solid Helium (Lennard-Jones)

Lindemann ratio: $\gamma = \sqrt{<u^2>}/a \approx 0.28$

Light atomic mass and weak interactions

Large lattice zero-point motion
Very compressible, low density solid
Vacancies easily created and can be very mobile

The Phase Diagram (suggested by experiments)



Motivation for Many-body Wave Function

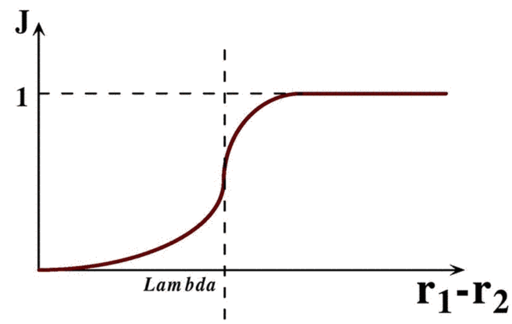
Two-particle case: $\phi(x_1 - a_1)\phi(x_2 - a_2)$

For bosons, the wave function should be symmetric

$$\phi(x_1 - a_1)\phi(x_2 - a_2) + \phi(x_2 - a_1)\phi(x_1 - a_2)$$

Taking the short range repulsion into account: by adding the Jastrow factor

$$[\phi(x_1 - a_1)\phi(x_2 - a_2) + \phi(x_2 - a_1)\phi(x_1 - a_2)]J(x_1 - x_2)$$



Motivation for Many-body Wave Function

Let us formally add two more terms:

$$[\phi(x_1 - a_1)\phi(x_2 - a_2) + \phi(x_2 - a_1)\phi(x_1 - a_2)$$
$$+\phi(x_1 - a_1)\phi(x_2 - a_1) + \phi(x_1 - a_2)\phi(x_2 - a_2)]J(x_1 - x_2)$$

Thanks to the Jastrow factor, this does not change much the wave function and, therefore, the energy. But the nature of the state is changed! And the terms in the bracket becomes a product (simplication!)

$$\prod_{1,2}[\phi(x_i - a_1) + \phi(x_i - a_2)]J(x_1 - x_2)$$

This property can be generalized to a many-body case of a commensurable quantum solid, where the number of atoms precisely equals that of the sites .

Many-body Wave Function

$$\psi = \prod_i f(x_i) \prod_{k<l} J(x_k - x_l)$$

where f(x) is periodic with a crystal symmetry, while $J(x_k - x_l)$ takes care of short-range correlation.

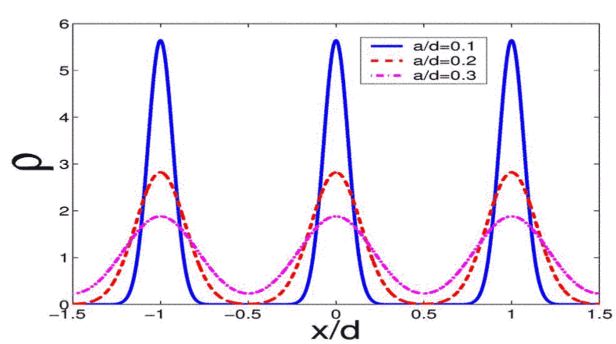
Basic idea: The Jastrow factor has a Bose-Einstein condensation in the zero-momentum state, so by expanding the Jastrow factor in terms of plane waves this wave-function can be rewritten

$$\psi = \prod_i f(x_i) (\sqrt{n_0} + \cdots)$$

Many-body Wave Function

This wave function has a macroscopic occupation on a single particle state with a periodic density modulation.

E.g. for f(x) a sum of Gaussian-like wave packets,



Remark: This many-body state simultaneously exhibits both DLRO and ODLRO.

Proof of Bose Condensation

Theorem (to be proved)

For a many-body wave function of the form

$$\Psi = \prod^{N} f(r_k) \prod J(r_{ij}) = \prod^{N} f(r_k) \prod \exp -u(r_{ij})$$

with the pair potential satisfying

$$\sum_{i=1}^{t} u(r_{is}) \geq -\phi$$

for all $t,\ s,\ r_1, r_2, \cdots$ satisfying

$$\sum_{i<j\leq t} u(r_{ij}) < \infty. \quad ,$$

the one-particle density matrix has a non-vanishing ODLRO:

$$\lim_{|r-r'|\to\infty} \langle r|\rho_1|r'\rangle = n_0 f^*(r) f(r'),$$

where

$$\langle r|\rho_1|r'\rangle = \frac{N}{Q_N}\int \prod_{i=2}^{N} dr_i \Psi^*(r, r_2, \cdots)\Psi(r', r_2, \cdots)$$

with Q_N the normalization constant of Ψ.

Proof of Bose Condensation

Following L. Reatto [Phys. Rev. **183** (1969) 334]

$$n_0 = \lim_{V\to\infty} \frac{1}{V^2}\int dr dr' \frac{\langle r|\rho_1|r'\rangle}{f^*(r)f(r')} = \frac{N}{V}\frac{\zeta_{N+1}}{Q_N},$$

$$\zeta_{N+1} = \int \frac{dr dr'}{f^*(r)f(r')} \prod_{i=2}^{N} dr_i \Psi^*(r, r_2, \cdots)\Psi(r', r_2, \cdots).$$

We have the lower bound $\quad \zeta_{N+1} \geq \frac{e^{-\phi-\Delta}}{\kappa} Q_{N+1},$

Therefore $\quad n_0 \geq \frac{n^2}{z}\frac{e^{-\phi-\Delta}}{\kappa},$

$$(\Delta = \min u(r) \text{ and } \kappa = \max |f(r)|^3)$$

Still need to prove that

$$z = \lim_{V,N\to\infty} \frac{(N+1)Q_N}{Q_{N+1}} \quad \text{is finite.}$$

Proof of Bose Condensation

Q_N can be interpreted as the partition function

$$\int \prod_{i=1}^{N} d\mathbf{r}_i \exp\left\{-\sum_{i<j} u(|\mathbf{r}_i - \mathbf{r}_j|) + 2\sum_i \ln|f(\mathbf{r}_i)|\right\}$$

of a classical statistical system with pair interactions and in a periodic external potential, and with fugacity

$$z = \lim_{V,N\to\infty} \frac{(N+1)Q_N}{Q_{N+1}}.$$

Thus, if

$$n \le n_c \qquad \text{(closely packed density)}$$

Then the thermodynamic limit of the system exists, with a finite fugacity. So finite is

$$n_0 \ge \frac{n^2}{z}\frac{e^{-\phi-\Delta}}{\kappa},$$

Possible Form of the Periodic Part

- **A sum of gaussian-like wave packets for zero-point fluctuations around each site in normal solid helium (Zhai & Wu):**
  Physical meaning: coherent zero-point motions
  or condensation of zero-point motions
  Energetically a little bit higher than normal solid for Helium
  (David Ceperley, unpublished)

✓ **Could some unknown mechanism help to lower the energy?**

- **A sum of deformed wave packets in each cell:**
  (Michael Ma and Fu-Chung Zhang, this workshop)
  Ma and Zhang called the deformed wave packets as excitons
  I call them as condensation of deformed zero-point motions

✓ **If true, a sort of quantum "structural" phase transition?**
(Energetically it seems also disfavorable for Helium.)

◆ **Add vacancies by considering incommensurable solid could help.**

Conclusions

- For *hard-core bosons with short-range repulsion, if "zero-point" fluctuations at different sites become coherent and get condensed,* the quantum boson system at absolute zero can have *macroscopic occupation in a periodic single particle state,* and thus can *possess DLRO and ODLRO simultaneously.*

- The proposed class of many-body wave functions provides a possible mechanism leading to supersolid through *condensation of usual or deformed "zero-point" motions in a commensurable quantum Bose solid.*

- The main objection for this class of wave functions at this moment is *only* that *the energetics* does *not seem right for Helium.*

  Could there be some *unknown mechanism to rescue?*

  Could such wave functions be *realized in some other systems?*