Bose-Einstein condensation
in solid $^4$He

D.E. Galli, L. Reatto and M. Rossi

Dipartimento di Fisica,
Università degli Studi di Milano
Via Celoria, 16 – 20133 Milano, Italy

E-mail: Davide.Galli@unimi.it
$^4\text{He}$: the phase diagram

- Hard-sphere-like pair potential (Lennard-Jones)
- $^4\text{He}$ atoms: Bose-Einstein statistics
- The zero point motion dominates the structure of the phase diagram at low temperatures: macroscopic quantum phenomena

![Phase diagram image](image)
Non Classical Rotational Inertia (NCRI) effects

- **Measurement of superfluidity:** torsional pendulum

\[ \tau = 2\pi \sqrt{\frac{I}{K}} \]

\[ \Delta \tau = 2\pi I_{\text{cylinder}} + I_{\text{normal fluid}} \]

Expected background

Empty cell

Superfluid Decoupling

Drive

Connected Geometry:

Torsion Rod

Cell containing helium

Detection

\( d < \delta \) of normal fluid

liquid helium in annular region between two cylinders

Period shifted due to mass loading
\[ 4^\text{He}: \text{quantum many-body system} \]

Standard many-body wave function: \( \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \)

- **Liquid phase:**
  Jastrow-McMillan (pair correlations)

\[
\psi_{\text{liquid}} = \prod_{i \neq j} e^{-\frac{1}{2} \left( \frac{b}{|\vec{r}_i - \vec{r}_j|} \right)^m}
\]

\[
\begin{array}{c}
\text{i} \quad \text{j} \quad \Rightarrow \quad \psi_{\text{liquid}} \rightarrow 0 \\
\text{i} \quad \text{j} \quad \Rightarrow \quad \psi_{\text{liquid}} \neq 0 \\
\end{array}
\]

- **Solid phase:**
  Jastrow+Nosanow

\[
\psi_{\text{solid}} = \psi_{\text{liquid}} \times \prod_i e^{-C |\vec{r}_i - \vec{R}_i|^2}
\]

\[
\begin{array}{c}
\text{i} \quad \Rightarrow \quad \psi_{\text{solid}} \rightarrow 0 \\
\text{i} \quad \Rightarrow \quad \psi_{\text{solid}} \neq 0 \\
\end{array}
\]
Interacting Bosons: BEC $\equiv$ ODLRO

- The one-body density matrix:

$$\rho_1(\vec{r}, \vec{r}') = N \int d\vec{r}_2 \cdots d\vec{r}_N \Psi^*(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N) \Psi(\vec{r}', \vec{r}_2, \ldots, \vec{r}_N)$$

$$\rho_1(\vec{r}, \vec{r}') = \langle 0 | \hat{\Psi}^+ (\vec{r}) \hat{\Psi} (\vec{r}') | 0 \rangle$$

- Momentum distribution:

$$n(\vec{k}) = V^{-1} \int d\vec{r} \, d\vec{r}' \, \rho_1(\vec{r}, \vec{r}') e^{i\vec{k} \cdot (\vec{r} - \vec{r}')}$$

- **BEC $\iff$ ODLRO**

$$\lim_{|\vec{r} - \vec{r}'| \to \infty} \rho_1(\vec{r}, \vec{r}') = \rho n_0$$

$$n(\vec{k}) = (2\pi)^3 \rho n_0 \delta(\vec{k}) + n'(\vec{k})$$

QMC simulations

In the liquid

Equilibrium density $\rho = 0.0218 \, \text{Å}^{-3}$

$\rho_1(|\vec{r} - \vec{r}'|)$

- SPIGS
- SWF

$\sim 7\%$  $\sim 9\%$
Superfluidity and BEC

- London’s hypothesis (1938):
  “lambda” transition ≡ Bose-Einstein condensation
- ODLRO ⇒ NCRI at T=0 and at T≠0 (3D)


\[
\rho_1(\vec{r}, \vec{r}') = \langle 0 | \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}') | 0 \rangle
\]

ODLRO

\[
\rho_s = \lim_{\omega \to 0} \frac{\rho}{I_{cl}} \frac{\partial^2 E}{\partial \omega^2}
\]

SUPERFLUIDITY

NCRI ≡ \( \rho_s \neq 0 \)

Superfluid component: response to boundary motion
Solid $^4\text{He}$: a quantum solid

- Solid $^4\text{He}$ is a prototype of a quantum solid:
  The zero point motion covers a sizeable fraction of the cell size
- Finite probability of tunneling into neighbors lattice sites, possible new phenomena:
  - Exchange between atoms or more complex phenomena
  - New excitations: Vacancy waves
  - BEC and non classical rotational inertia
A Supersolid Phase in solid $^4$He?

$$\rho_1(\vec{r},\vec{r}') = \langle 0 | \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}') | 0 \rangle$$

No BEC in a perfect solid with localized particles:
Penrose and Onsager, Phys.Rev. 104, 1956

Delocalized particles:
BEC and superfluidity in Quantum Solids with vacancies:
Andreev and Lifshitz, JETP 29, 1969;
Chester, Phys.Rev. A2, 1970

defected ground state?
Still an open experimental and theoretical question.
A Supersolid Phase in solid $^4$He?

- NCRI effects in Quantum Solids; exchanges between atoms are not sufficient for NCRI
  Leggett, *Physica Fennica* 8, 1973

- Vacancies and/or interstitials must be present for NCRI effects

\[ \rho_1(\vec{r},\vec{r}') = \langle 0 | \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}') | 0 \rangle \]

ODLRO needs at least a vacancy-interstitial at arbitrary distance
NCRI effects in solid $^4$He


\[ \tau = 2\pi \sqrt{\frac{I}{K}} \]

The supersolid fraction is on the order of 1.3%
Quantum Monte Carlo calculations;
Computational resources:

- Università degli Studi di Milano

Dipartimento di Fisica
Laboratorio di Calcolo Parallelo e di Simulazioni di Materia Condensata
Cluster LCP: 24 CPU 2.8GHz

Dipartimento di Matematica
Cluster ULISSE: 72 CPU 2.4GHz
Projector QMC methods

• Projector QMC: Ground state as imaginary time evolution of a trial variational state

\[ \Psi_0(R) = \lim_{\tau \to \infty} \int dR' \; G(R,R',\tau) \; \Psi_T(R') \quad R \equiv \{ \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N \} \]

• Path Integral representation of the propagator:

\[ \Psi_0(R) = \lim_{\tau \to \infty} \int dR_1 \cdots dR_N \; G(R,R_1,\tau/N) \times \cdots \times G(R_{N-1},R_N,\tau/N) \; \Psi_T(R_N) \]

• Under control approximation:

\[ \Psi_0(R) \equiv \int dR_1 \cdots dR_N \; \tilde{G}(R,R_1) \times \cdots \times \tilde{G}(R_{N-1},R_N) \; \Psi_T(R_N) \]

Finite imaginary time propagation

Accurate approximation for the short-time propagator, es: Pair-Product (Ceperely, Rev.Mod.Phys. 67, 1995)
Projector QMC: SWF and SPIGS

- **SWF**: single (variationally optimized) projection step of a Jastrow wave function
  
  \[ \Psi_T^{SWF}(R) = \int dS \ F(R,S) \Psi_T(S) \]
  
  - Implicit correlations (all orders)
  - Bose symmetry preserved

- **SPIGS**: “exact” T=0 projector method which starts from a SWF
  
  \[ \Psi_0(R) = \int dR_1 \cdots dR_N dS \ \tilde{G}(R_1, R_2) \times \cdots \]
  
  \[ \cdots \times \tilde{G}(R_{N-1}, R_N) F(R_N, S) \Psi_T(S) \]
  
  - Evolution of the PIGS method

**Calculation of \( \langle \Psi_0 | \hat{O} | \Psi_0 \rangle \)**

Classical analogy

The whole imaginary time evolution is sampled at each MC step
SWF: the solid phase

- Presently (a fully optimized) SWF provides the most accurate variational description of \(^4\)He in the liquid and in the solid phase
  Moroni, Galli, Fantoni, Reatto, Phys Rev B58, 1998
- Accurate freezing and melting densities
- **Solid phase:** spontaneously broken translational symmetry

![Equation of state](image)

Local density hcp lattice \(\rho=0.029\,\text{Å}^{-3}\)

![Local density](image)
SWF & SPIGS description of solid $^4$He

- At all densities the solid described by the SWF technique is more structured: particle are more localized

Near melting density $\rho=0.029 \, \text{Å}^{-3}$

Rigorous upper-bound for the superfluid fraction

$\frac{f_s}{\rho} \leq \left\{ \int d\zeta \rho(\zeta)^{-1} \right\}^{-1}$

Leggett, Phys.Rev.Lett. 25, '70

Galli, Rossi, Reatto, Phys.Rev.B71, 2005

<table>
<thead>
<tr>
<th>P (bar)</th>
<th>SWF</th>
<th>SPIGS</th>
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<tr>
<td>29.3</td>
<td>0.287</td>
<td>0.384</td>
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<td>53.6</td>
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<td>p-H₂</td>
<td>0.028</td>
<td>0.052</td>
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QMC: calculation of the one-body density matrix

\[ \rho_1(\vec{r}, \vec{r}') = N \int dr_2 \cdots dr_N \Psi^*(r, r_2, \ldots, r_N) \Psi(r', r_2, \ldots, r_N) \]

- One of the open polymers is cut and the histogram of the relative distance of the two ends is computed.
- We have studied defected and commensurate solid \(^4\text{He}: the periodic boundary conditions forces the structure of the solid.

Finite concentration of vacancies

Commensurate solid

N triatomic molecules

Classical analogy

N open polymers

SPIGS

SWF

cut
Vacancy-interstitial pairs (VIPS)

- Even by forcing the solid to be commensurate one finds the presence of vacancy-interstitial pairs (VIPS).
- These VIPS are not excitations but simply fluctuations of the lattice; they are part of the large zero-point in the ground state of the solid.
- The term “pairs” is used only to underline the origin of these zero-point processes: via exchange, tunnelling or other processes these VIPS are unbound.
SPIGS: Vacancy-interstitial pairs

- These VIPs are present also in the “exact” sampling of $|\Psi_0|^2$ (SPIGS method); in the examples only the internal atoms of the polymers are shown.
- VIP-frequency: $\approx 1$ every $2-3 \times 10^3$ MC steps with 180 $^4$He atoms $\Rightarrow X_{vip} \approx 2 \times 10^{-6}$
- New excitations? Correlations with $^3$He atoms?
SWF results: ODLRO in solid $^4$He with vacancies


- ODLRO is present in the lowest density defected solid
- Gaussian like only for small distances

$\rho_1(\vec{r} - \vec{r}')$

Near melting density $\rho = 0.029 \, \text{Å}^{-3}$

ODLRO: microscopic origin

$\rho_1(\vec{r}, \vec{r}') = \langle 0 | \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}') | 0 \rangle$

Condensate fraction proportional to the concentration of vacancies

$n_0 \approx 0.3 \times X_v$
SWF results: ODLRO in commensurate solid $^4$He

Galli, Rossi, Reatto, Phys.Rev. B71, 2005

- One-body density matrix along n.n. direction
- ODLRO is present: $n_0 \approx 5 \pm 2 \times 10^{-6}$ at melting and for a finite range of densities (up to 54 bars)
- Local maxima: signature of distorted lattice
- No finite-size effects
- Key process is the presence of VIPs

\[ \rho_1(\vec{r} - \vec{r}') = \langle 0 | \hat{\Psi}^*(\vec{r}) \hat{\Psi}(\vec{r}') | 0 \rangle \]

ODLRO: microscopic origin

Condensate fraction with vacancies comparable when:

\[ X_v \approx 1.5 \times 10^{-5} \]

Runs of the order of $10^8$ MC steps

Scaling analysis $\rho = 0.029 \text{ Å}^{-3}$
VIPs & ODLRO

Galli, Rossi, Reatto, Phys.Rev. B71, 2005

• The tail structure of the one-body density matrix always corresponds to a configuration in which a VIP is involved:

\[
\rho_1(\vec{r}, \vec{r}') = \left| \langle 0 | \hat{\Psi}^+(\vec{r}) \hat{\Psi} (\vec{r}') | 0 \rangle \right|^2
\]

ODLRO: microscopic origin

Stopped wave function (SWF) trimers in a basal plane

Snapshot of SWF trimers in a basal plane

along nearest neighbours distance
**SWF results: ODLRO in a basal plane**

- We have also computed the one-body density matrix along distances which lie in a basal plane of an hcp solid.
- ODLRO is present and it is anisotropic only in the middle range 3-14 Å.
- Good agreement with the result obtained along n.n. direction.

\[ \rho_1(\vec{r} - \vec{r}') \]

\[ \rho_1(\vec{r} - \vec{r}') \]
ODLRO: SPIGS preliminary results

- Calculations of the one-body density matrix in hcp solid \(^4\)He at melting with increasing number of projection steps in imaginary time
- Oscillations in the tail region are still present
- Pair-product approximation: \(\delta \tau = 1/80 \text{ K}^{-1}\)

![Graph showing \(\rho_1(\vec{r} - \vec{r}^\prime)\) with different MC steps and SWF approximation.]

\[\rho_1(\vec{r} - \vec{r}^\prime)\]

- SWF: \(\approx 10^8\) MC steps
- \(N=5; 3\times10^7\) MC steps
- \(N=13; 7\times10^6\) MC steps
Conclusions

• SWF variational results: BEC is present in the defected and in the commensurate solid $^4$He for a finite range of densities

• SWF variational technique is accurate for diagonal properties; off-diagonal quality is under investigation with $T=0$ “exact” SPIGS method

• If SWF off-diagonal results will be confirmed these results could provide the basic explanation of the NCRI effects recently measured by Kim & Chan

• Key processes are the presence of vacancy-interstitial pairs: fluctuations of the lattice due to the large zero point motion... new excitations!