Quantum Phenomena
at Low Temperatures
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On the supersolid state of ^{4}He

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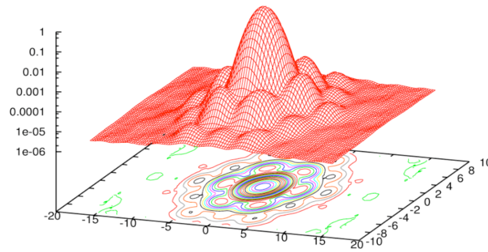
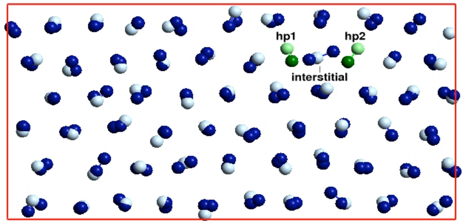
Sede centrale: facciata lungo largo Richini

Sede centrale: cortile del Richini





Outline

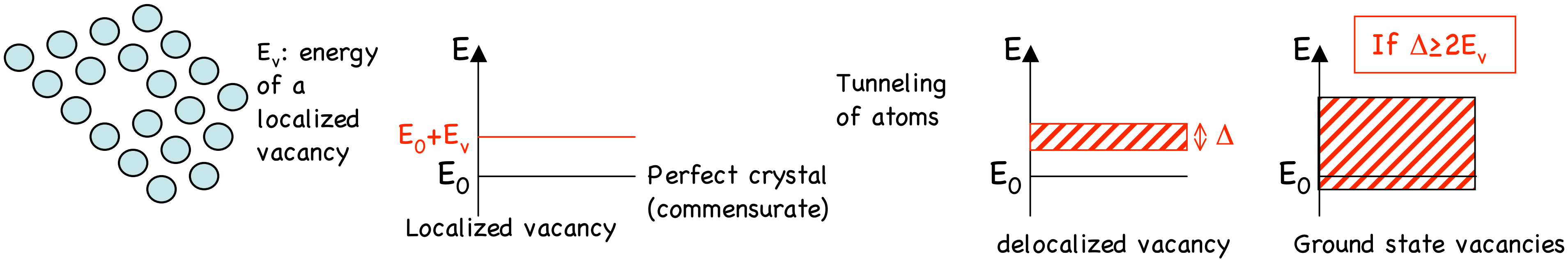
- Introduction: supersolid, experimental results and some basic questions for many body theory
- Some special properties of solid ^{4}He
  - Zero point motion
  - Vacancy-intestitial pairs
  - Vacancy waves
- Theoretical tools
  - Variational Shadow Wave Function (SWF)
  - "exact" Shadow Path Integral Ground State (SPIGS)
- Ground state: commensurate or incommensurate?
  - What is known
- One-body density matrix:
  - Study of ODLRO in a commensurate crystal
    - Variational result (SWF)
    - Exact result (SPIGS)
  - Study of ODLRO in a crystal with vacancies (incommensurate crystal)
    - Variational result (SWF)
    - Exact result (SPIGS)
- Conclusions

SUPERSOLID STATE

A quantum solid (^{4}He) with some sort of superfluid properties like non classical moment of inertia, BEC

Theoretical works ante Kim-Chan experiments (2004)

A. Possible presence of vacancies in the ground state (Andreev and Lifshitz 1969)



B. Model wave functions exist with crystalline order, a finite concentration of vacancies and a finite BEC (Chester 1970, stimulated by proof (Reatto 1969) that a Jastrow wf has BEC)

C. Non classical rotation of a quantum solid;
rigidity of wave function: $\rho_s/\rho > 0$ if local density $\rho(r) > 0$ (Leggett 1970)

D. …work by Saslow, Guyer,…

….

Z. Microscopic computation of the condensate induced by vacancies in solid ^{4}He from variational theory (Galli-Reatto 2001)

Supersolid State

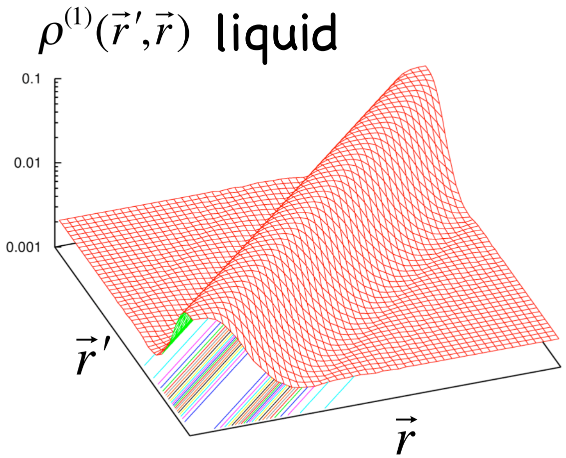
- If Off Diagonal Long Range Order (ODLRO) is present we expect some superfluid phenomena

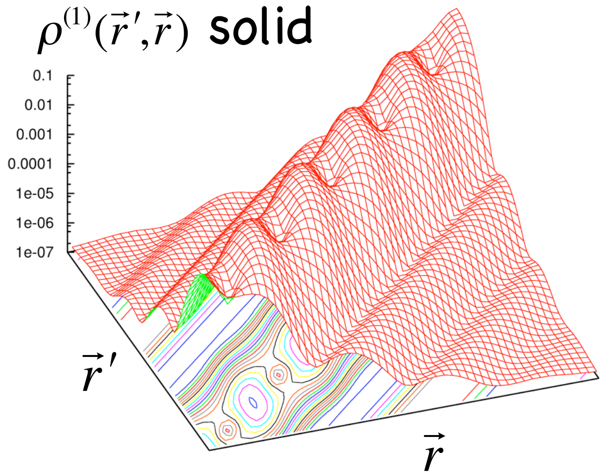
<u>State with LRO+ODLRO</u>

Behavior of the one-body density matrix

$$\rho^{(1)}(\vec{r}\,',\vec{r}) = \left\langle \hat{\Psi}^{+}(\vec{r}\,')\hat{\Psi}(\vec{r}) \right\rangle$$

$\rho^{(1)}(\vec{r},\vec{r})$ = Local density at $\vec{r}$





- No theoretical motivation for why this could not happen (therefore it must happen somewhere)
- There is now solid evidence that Bose Hubbard model on a lattice can show LRO+ODLRO, in ^{4}He however the lattice is self-built by the atoms

Experiments (1)

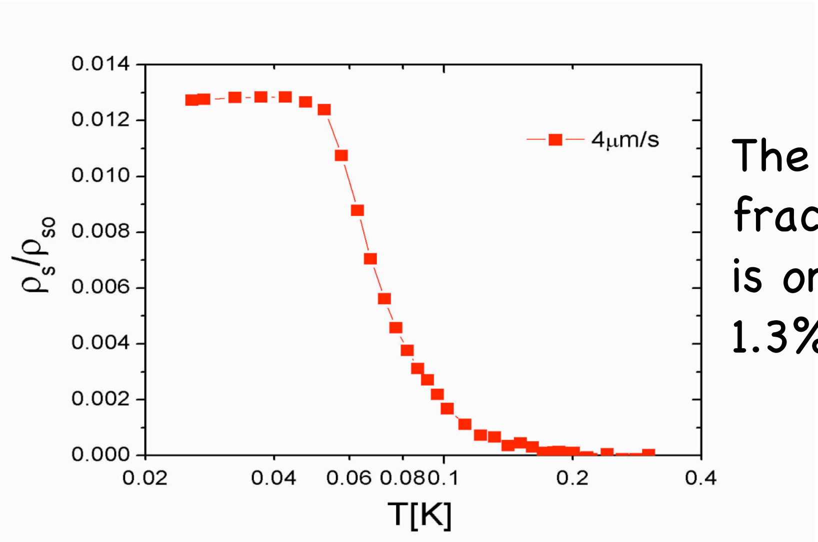
- Experimental search of the supersolid state in the seventies and eighties has been unsuccessful

BREAKTHROUGH

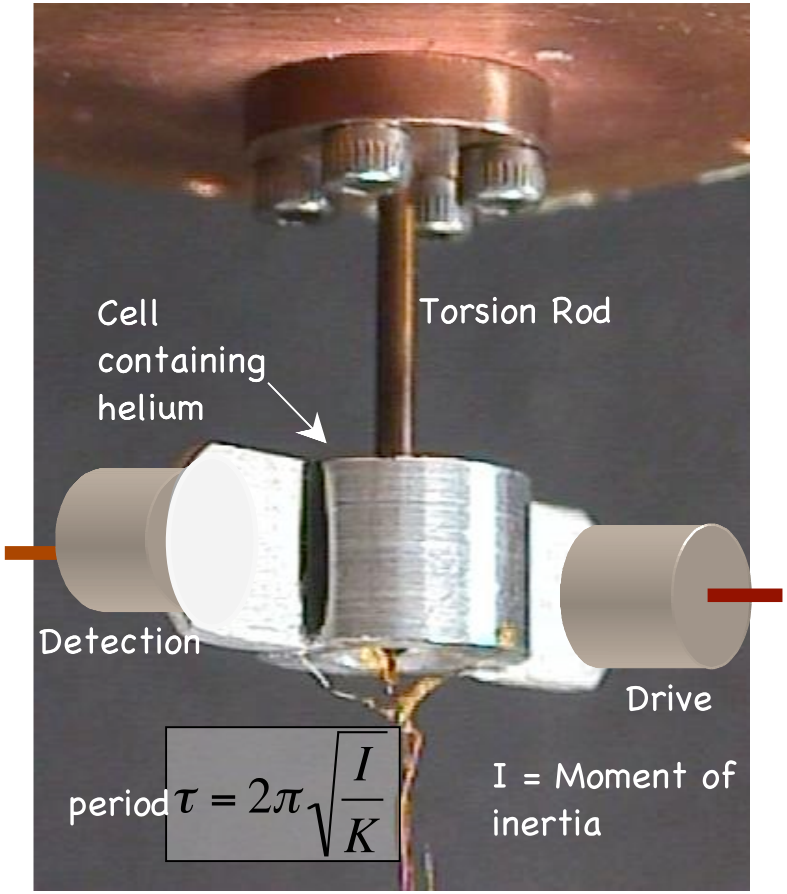
Kim and Chan find non

classical rotational inertia in

- ^{4}He in vycor (Nature, Jan. 2004)
- ^{4}He in porous gold (JLTP, Febr. 2005)
- ^{4}He bulk (Science, Sept. 2004)



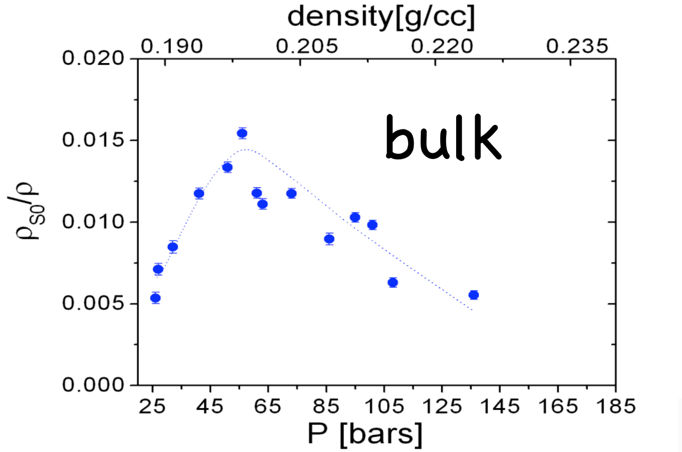
The supersolid fraction
is on the order of 1.3% at lowest T

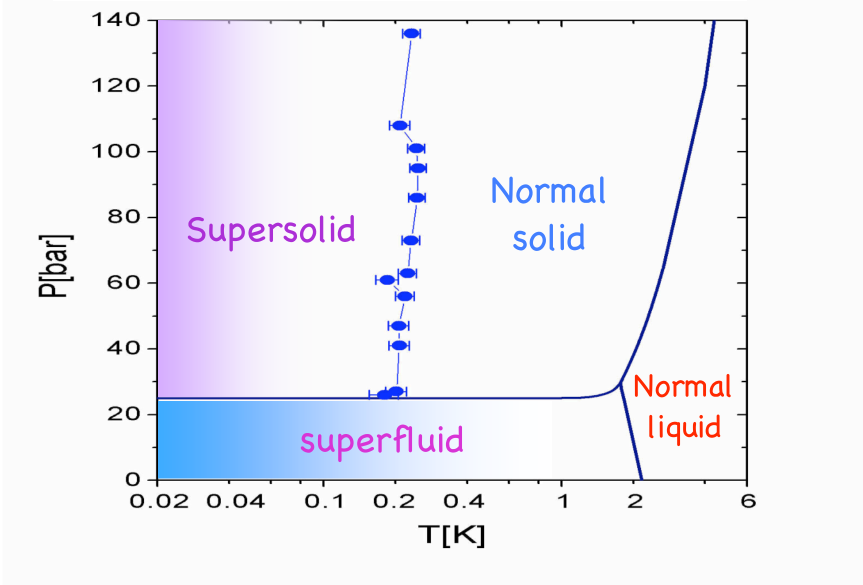


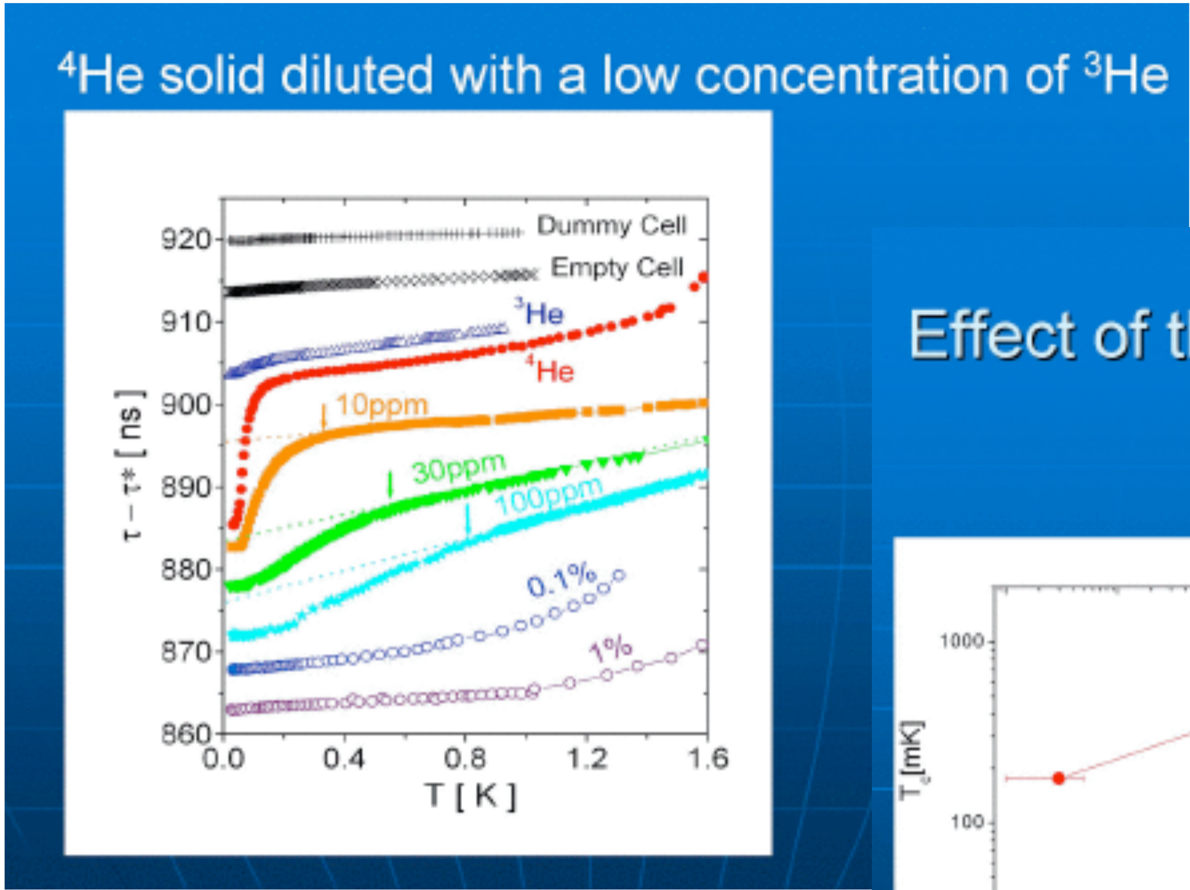
Experiments (2)

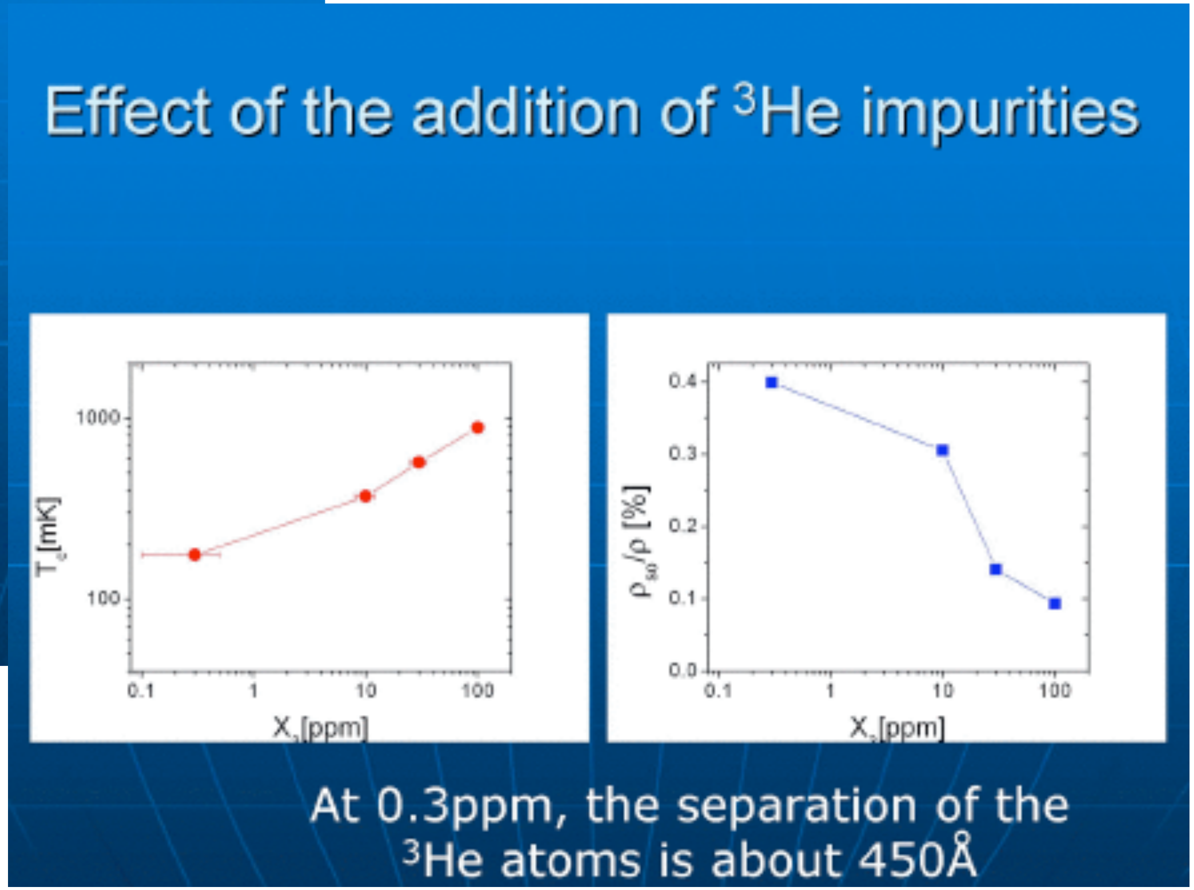
- Superfluidity of bulk crystalline ^4He is the correct explanation?

Beamish and coworkers experiment in vycor (PRL 2005 and 2006) rules out some possible alternative explanations, on the other hand they see no pressure-induced flow in the pores









Latest results from PSU: with X_3=1 ppb ρ_s=0.025%, T_c=80 mK (Baltimore 3/2006)

Supersolid behaviour in torsional oscillator experiments, works in progress reported at "The supersolid state of matter"

Santa Barbara (February 2006)

- Rittner-Reppy (Cornell)
  - They find NCRI, signal goes away after suitable annealing (cross section oscillator is □)
- Shirahama and collaborators (Keio Un.)
  - They find NCRI, ρ_s is one order of magnitude small compared to the PSU results
- Penzyev and Kubota (ISSP, Un. Tokyo)
  - They find NCRI, results comparable with those of PSU

Summary of results from microscopic theories

A. Finite temperature ("exact" results PIMC)

Bulk commensurate solid

1) Superfluid fraction $\rho_s=0$ at $T\geq0.5$ K (Ceperley, Bernu PRL 2004)
2) Condensate fraction $n_0=0$ at $T\geq0.2$ K (Clark, Ceperley PRL 2006; Boninsegni et al. PRL 2006)

Solid ^{4}He in "vycor" (split pore geometry)

$\rho_s\neq0$ at $T\approx0.15$ K due to liquid like monolayer between solid and immobile adsorbed layer (Khairallah, Ceperley PRL 2005)

B. Zero temperature (variational and "exact" results)

Bulk commensurate solid

- Condensate fraction $n_0>0$ variational theory (Galli, Rossi, Reatto PRB 2005)
- Condensate fraction n_0 might be finite exact theory (work in progress)

Incommensurate solid (solid with vacancies)

- Condensate fraction $n_0>0$ variational theory (Galli, Reatto JLTP 2001)
- Condensate fraction $n_0>0$ exact theory (Galli, Reatto PRL 2006)

Solid 4He in "vycor" (cylindrical channel, Ø=26Å)

- Condensate fraction $n_0>0$ variational theory (Rossi, Galli, Reatto PRB 2005)

C. The ground state of bulk solid ^{4}He is commensurate or incommensurate?

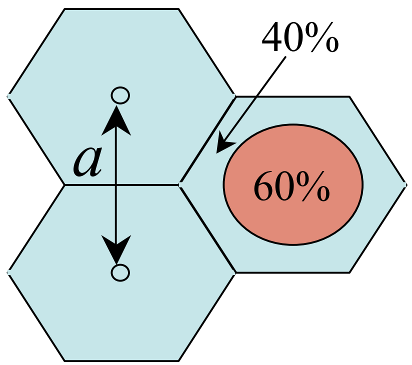
Direct masurements

- Experiment: cannot exclude vacancies below a concentration $X_v\approx0.1\%$ at low T
- Theory: variational theory: $X_v>0$ but X_v not computed yet; exact theory: not know

Solid ^{4}He: some important aspects

- Bragg scattering → translational broken symmetry (LRO)
- Very large Lindeman ratio at low density:

$$\frac{\sqrt{\left\langle \left| \vec{r}_i - \vec{R}_{eq} \right|^2 \right\rangle}}{a} \approx 0.26$$



An atom has a 40% probability to be closer to the border of the Wigner Seitz cell than to the center of the cell

- Solid helium is a very soft solid
- One can grow almost perfect crystals (but it is not easy): large single crystal with very few dislocations

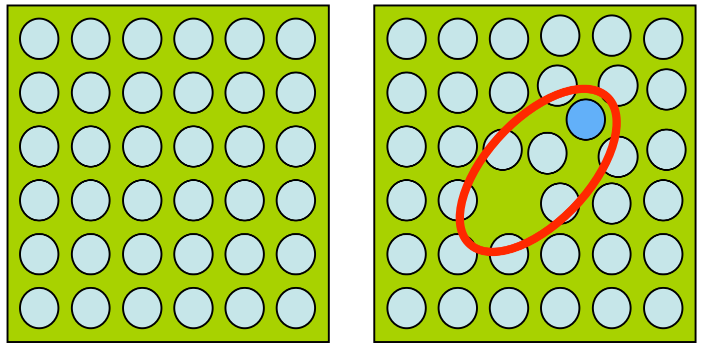
Vacancy-interstitial pairs (VIPs)

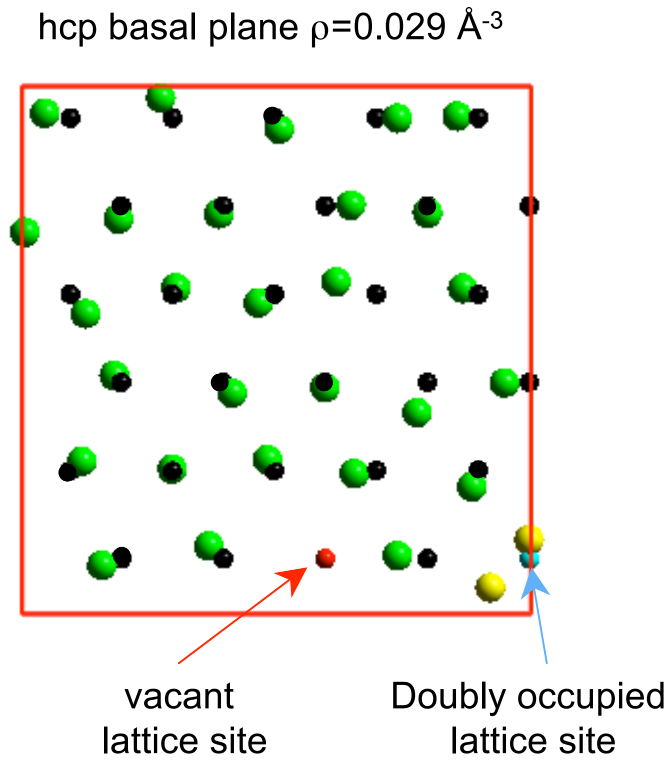
Evidence from theory

- Even in a commensurate state (n° lattice sites = n° atoms) 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 to underline the origin of these zero-point processes.
- Are VIPs unbound?

  Yes for SWF variational theory

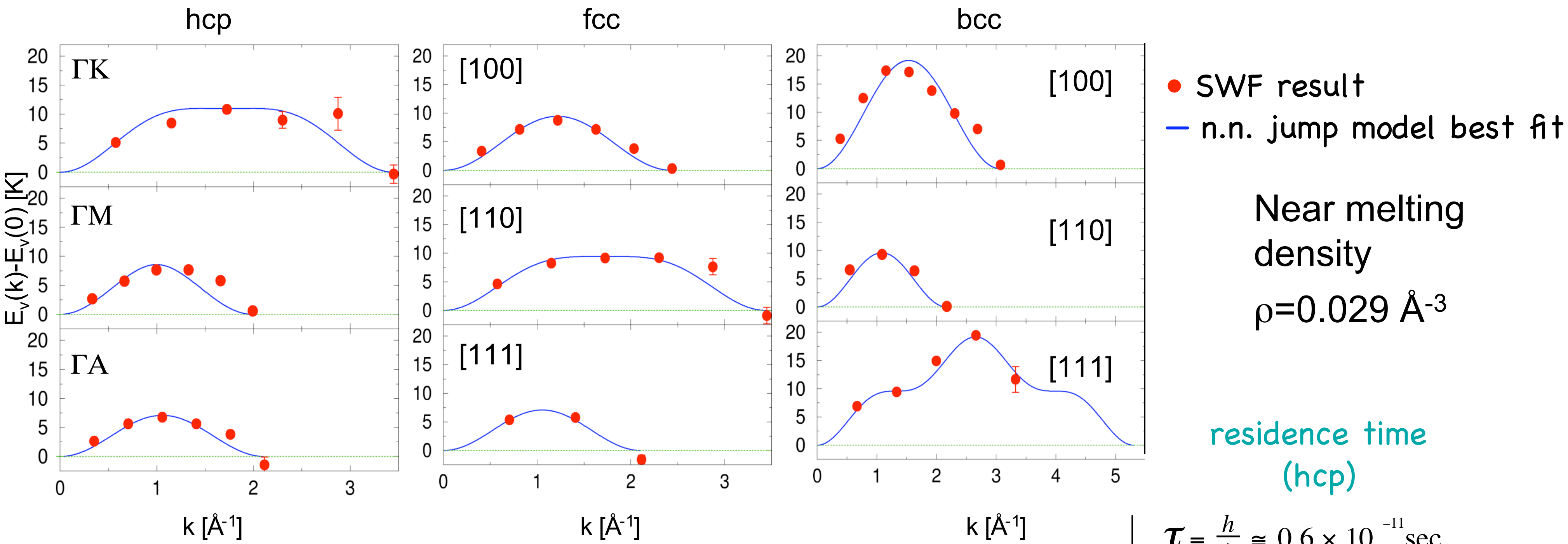
  Not clear yet for exact ground state
- VIP frequency: ≈1 every 2-3x10^3 MC steps with 180 ^{4}He atoms $\Rightarrow X_{vip} \approx 2\times10^{-6}$





vacancy excitation spectrum (SWF result)

Galli, Reatto, Phys.Rev.Lett. 90, 2003;
Galli, Reatto, J.Low Temp.Phys. 134, 2004



$m^*=0.31m_4$
$m^*=0.39m_4$ (ΓA)

$m^*=0.39m_4$

$m^*=0.3m_4$

Near melting density

$\rho=0.029$ Å^{-3}

residence time (hcp)

$$\tau = \frac{h}{\Delta} \cong 0.6 \times 10^{-11} \text{sec}$$

only 4 (and 2 in bcc) time larger than the period of high frequency phonon in the crystal

- Vacancy very mobile, in agreement with recent experiments

Andreeva et al., J.Low Temp.Phys. 110, 1998

- Band width decreases at larger density

Variational theory of a quantum solid

- In the framework of variational theory of quantum solids the wave functions fall in two categories:

1. Ψ has explicit translational broken symmetry, for instance by localizing the atoms around the assumed lattice sites $\{\vec{R}_i\}$

$$\Psi(\vec{r}_1,..,\vec{r}_N) = \Psi_J \times \prod_i^N e^{-C\left|\vec{r}_i - \vec{R}_i\right|^2}$$

(Jastrow+Nosanow)

→ Sum over permutation to get Bose Symmetry

2. translational invariant Ψ, first example:

$$\Psi_J(\vec{r}_1,..,\vec{r}_N) = \prod_{i<j}^N f\left(\left|\vec{r}_i - \vec{r}_j\right|\right)$$

(Jastrow)

Second example: Shadow Wave Function

Our variational tool: Shadow Wave Function

Evolution of Vitiello, Runge and Kalos, Phys. Rev. Lett. 60, 1970 ('88)

Ψ Includes many particle correlations via coupling to subsidiary variables

$$\Psi(R) = \phi_r(R) \times \int dS\, K(R,S) \times \phi_s(S)$$

Direct explicit Jastrow correlations (ϕ_r)

Indirect coupling via subsidiary (shadow) variables ($K(R,S)$, ϕ_s)

Particles coordinates: $R = \{\vec{r}_1, .., \vec{r}_N\}$

Shadow variables: $S = \{\vec{s}_1, .., \vec{s}_N\}$

Jastrow terms: $\phi_r(R),\ \phi_s(S)$

$$K(R,S) = \prod_i^N e^{-C|\vec{r}_i - \vec{s}_i|^2}$$

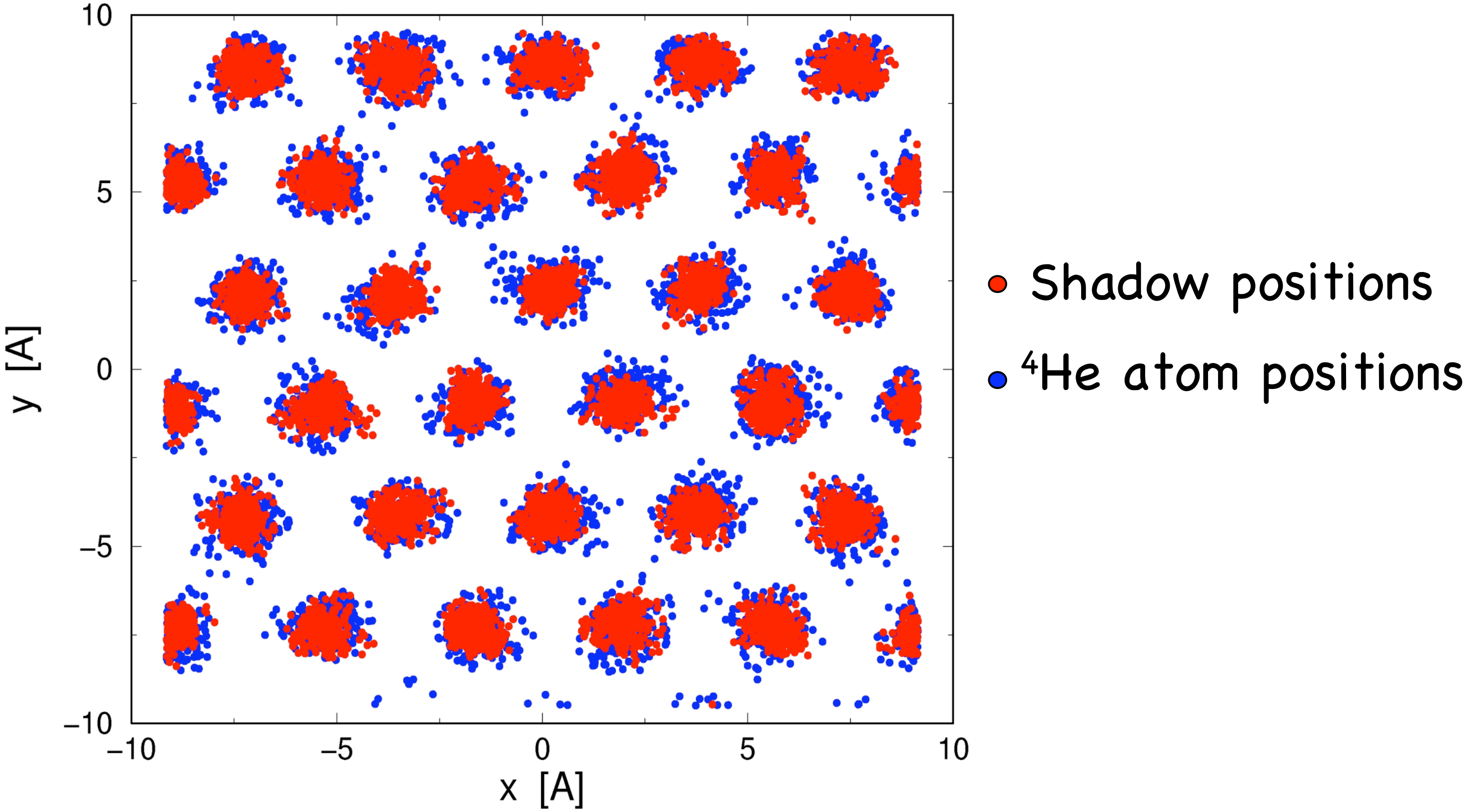
Shadow variables

- Shadow variables are strongly correlated

Spontaneous translational broken symmetry for $\rho>\rho_o$

Crystalline order of ^4He atoms induced by many-body correlations introduced by the shadow variables

SWF simulation of hcp solid ^4He: projection of the coordinates of the real and shadow particles in a basal plane for 100 MC steps



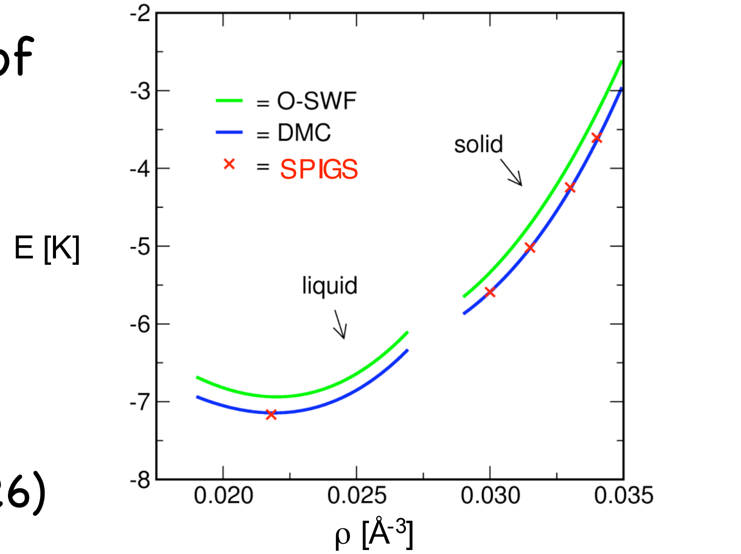
SWF: the solid phase

- Presently (a fully optimized) SWF provides the most accurate variational description of ^{4}He in the liquid and in the solid phase

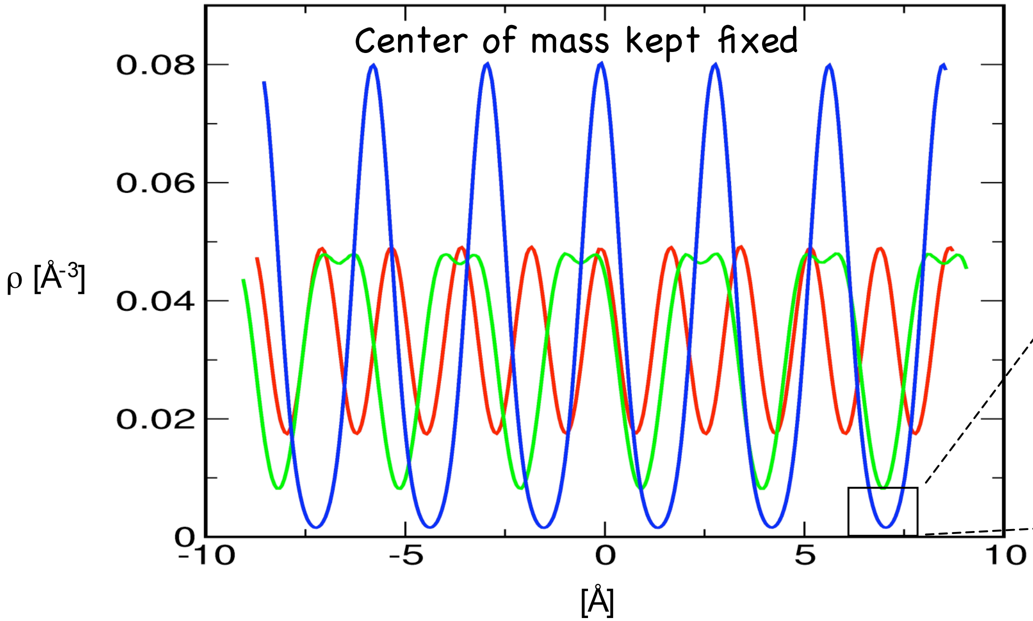
Moroni, Galli, Fantoni, Reatto, Phys.Rev.B58, 1998

- Accurate freezing and melting densities
- Solid phase: spontaneously broken translational symmetry
- Lindeman ratio $\sqrt{|r-R|^2}/a = 0.252$ (exper. 0.26)

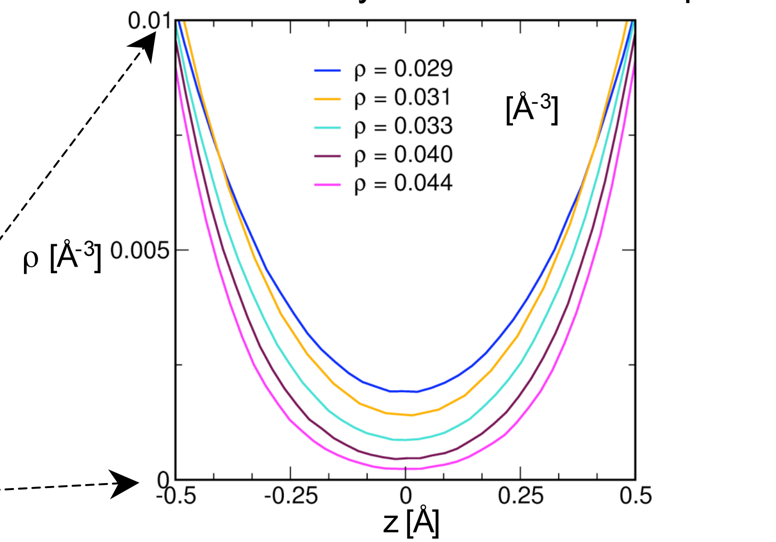
Equation of state (Aziz potential, 1979)



Local density hcp lattice ρ=0.029 Å^{-3}



Local density: direction ⊥ basal plane



Projector QMC methods: Path Integral Ground State

Sarsa, Schmidt, Magro, J.Chem.Phys., 113, 2001

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

$$\Psi_0(R) = \lim_{\tau\to\infty} \int dR' \left\langle R \middle| e^{-\tau\hat{H}} \middle| R' \right\rangle \Psi_T(R') \qquad R \equiv \{\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N\}$$

- Path Integral representation of the propagator:

$$\Psi_0(R) = \lim_{\tau\to\infty} \int dR_1 \cdots dR_M \left\langle R \middle| e^{-\frac{\tau}{M}\hat{H}} \middle| R_1 \right\rangle \times \cdots \times \left\langle R_{M-1} \middle| e^{-\frac{\tau}{M}\hat{H}} \middle| R_M \right\rangle \Psi_T(R_M)$$

- Approximation: finite imaginary time propagation

$$\Psi_0(R) \cong \int dR_1 \cdots dR_N \left\langle R \middle| e^{-\frac{\tau}{M}\hat{H}} \middle| R_1 \right\rangle \times \cdots \times \left\langle R_{M-1} \middle| e^{-\frac{\tau}{M}\hat{H}} \middle| R_M \right\rangle \Psi_T(R_N)$$

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

- With SPIGS: as Ψ_T we use the SWF

Is the ground state of bulk solid ^{4}He commensurate or incommensurate?

- Early theoretical works were based on the assumption of zero-point vacancies (Andreev and Lifshitz, JETP 93 1969; Chester, Phys.Rev.A 2 1970)
- If ground state vacancies are present this will have significant effects on low T behavior of solid ^{4}He

  (phenomenological theory by P.W. Anderson, W.F. Brinkman, D.A. Huse, Science 310 2005)
- Naive answer: it is commensurate because computation of $\langle \Psi_0 | \hat{H} | \Psi_0 \rangle$ for the perfect solid with one vacancy allowed to estimate a vacancy formation energy $\Delta e_v > 0$

Vacancy formation energy Δe_v at melting density (fixed density)

Method	lattice	Δe_v
SPIGS SWF	hcp	15.7±0.8 15.6±0.6

Galli, Reatto
J.Low Temp.Phys. 134 2004.

- This argument is not conclusive: one has deduced Δe_v from computation of the ground state energy of two different systems, Δe_v is a derived quantity as an estimate of the extra energy due to the presence of one additional vacancy

Example of computation of Δe_v

- System 1: commensurate state

  108 atoms in a cubic box of volume V with periodic boundary conditions in which fcc lattice fits exactly

Local density $\rho(\vec{r})$ has 108 maxima

$\Rightarrow$ n° sities = n° atoms

108 108

- System 2: incommensurate state

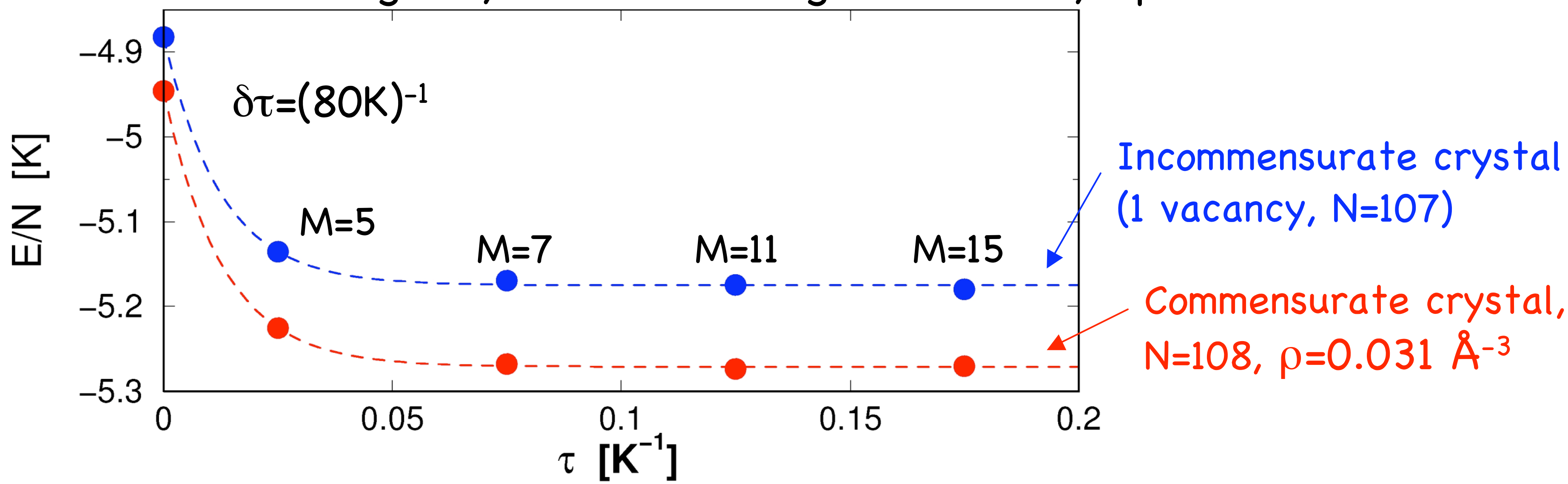
  107 atoms in the same box

Local density $\rho(\vec{r})$ has 108 maxima

$\Rightarrow$ n° sities $\neq$ n° atoms

108 107

Evolution in imaginary time τ starting from a fully optimized SWF



Both wave functions are non negative and represent two ground states: depending on N and box shape the ground state for this small system with pbc is commensurate or incommensurate

Commensurate or incommensurate?

Commensuration effects in small system makes difficult to answer this question, one has to analyze an extended system of $\mathcal{N}$ particles in a volume V so large that boundary conditions have a negligible role

⇒ Similar to what one has to do to treat vacancies in a classical system

Consider translational invariant wave functions

I Example: Jastrow wave function $\Psi_J(\vec{r}_1,..,\vec{r}_{\mathcal{N}}) = \prod_{i<j}^{\mathcal{N}} e^{-\frac{1}{2}u(r_{ij})} / Q_{\mathcal{N}}^{1/2}$

(old argument by Chester)

Normalization constant: $Q_{\mathcal{N}} = \int d\vec{r}_1..d\vec{r}_{\mathcal{N}} \prod_{i<j}^{\mathcal{N}} e^{-u(r_{ij})}$

Ground state averages with $|\Psi_J|^2$ → N classical particles at $\beta^*=1/kT^*$ and with pair potential $v^*(r)$ such that $\beta^* v^*(r)=u(r)$

Normalization constant $Q_{\mathcal{N}}$ → canonical configurational partition function of this classical system

From analysis of $Q_{\mathcal{N}}$ of a classical solid → the lowest free energy corresponds to a state with a finite concentration $\overline{X}_v = (\mathcal{M} - \mathcal{N})/\mathcal{N}$ of vacancies

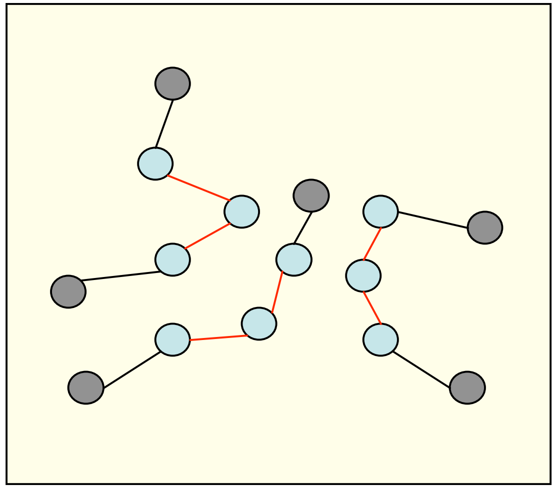
$\mathcal{M}$: n° lattice sites
$\mathcal{N}$: n° particles

Consequence for the quantum system: Ψ_J of an extended system has a finite concentration of vacancies

Commensurate or incommensurate?

Exact ground state averages as given by SPIGS

- Equivalence with a classical system of N open polymers of M beads
- Also here there is a finite concentration $\overline{X}_v(M)$ of vacancies



Therefore SPIGS with a finite number M of projections has a finite $\overline{X}_v(M)$, however $\overline{X}_v(M)$ might vanish in the limit $M \rightarrow \infty$

- At present no computation of $\overline{X}_v(M)$ has been performed

<u>Conclusion</u>: the nature commensurate or incommensurate of bulk solid 4He at T=0 K is undecided from microscopic theory

ODLRO - Commensurate state

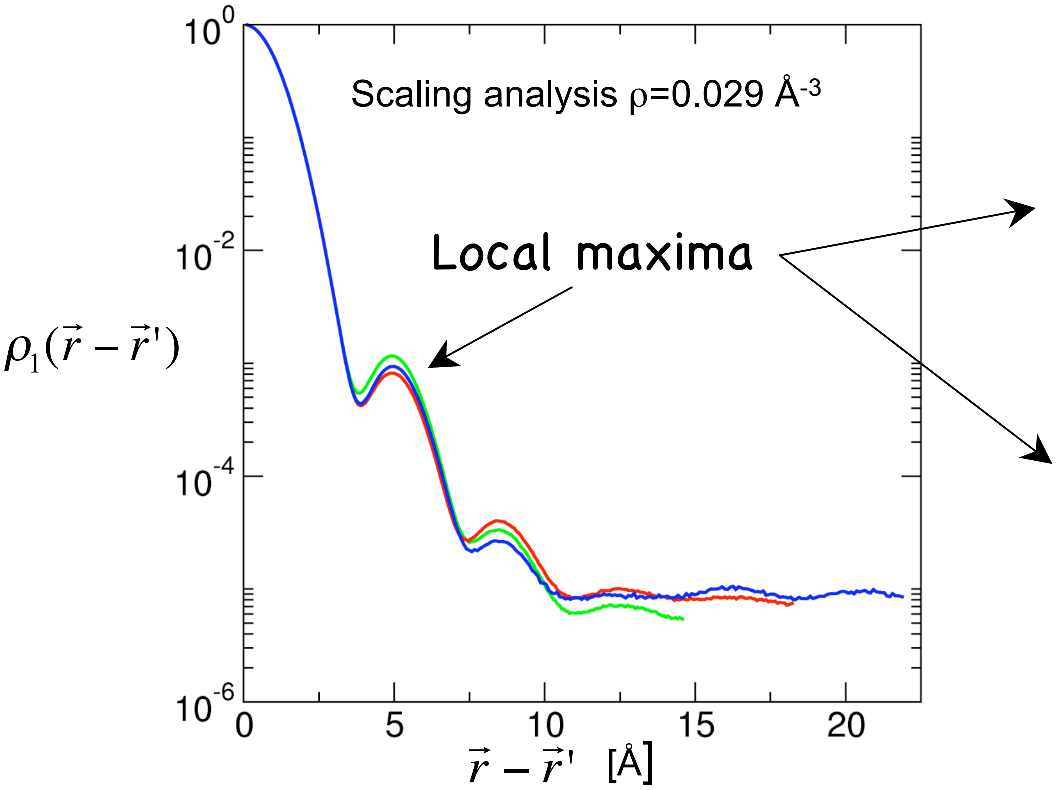
SWF results: ODLRO in commensurate solid ^{4}He

Galli, Rossi, Reatto, Phys.Rev. B 71, 2005

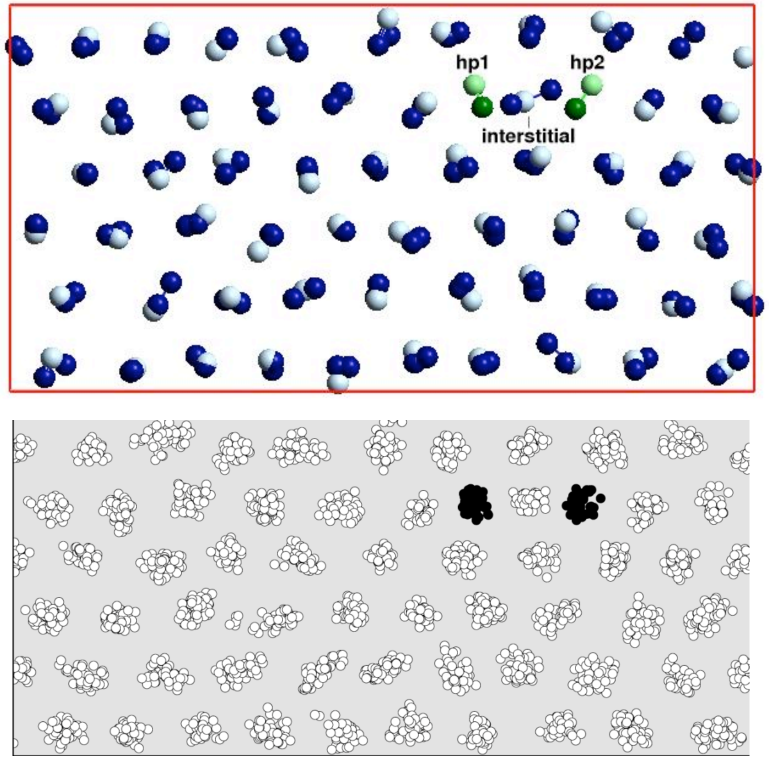
- ODLRO is present: $n_0 \approx 5 \pm 2 \times 10^{-6}$ at melting and for a finite range of densities (up to 54 bars)
- No finite-size effects
- Key process is the presence of VIPs

ODLRO:
microscopic origin

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

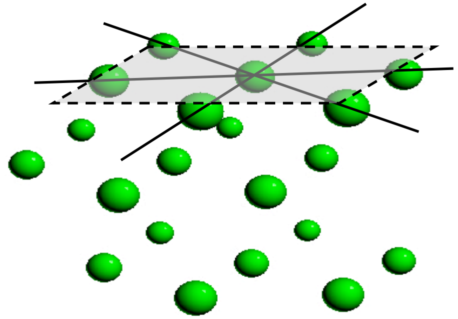


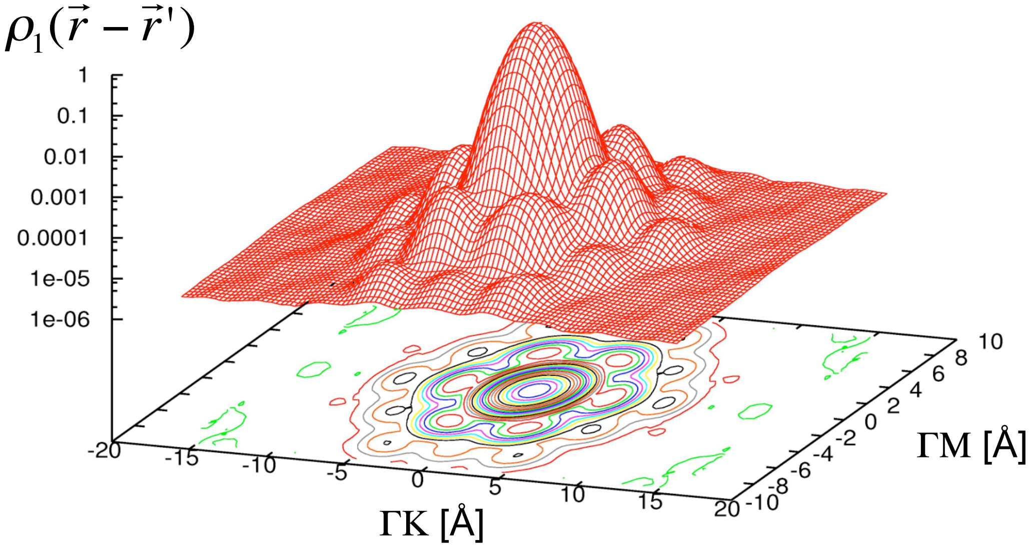
Snapshot of SWF trimers in a basal plane

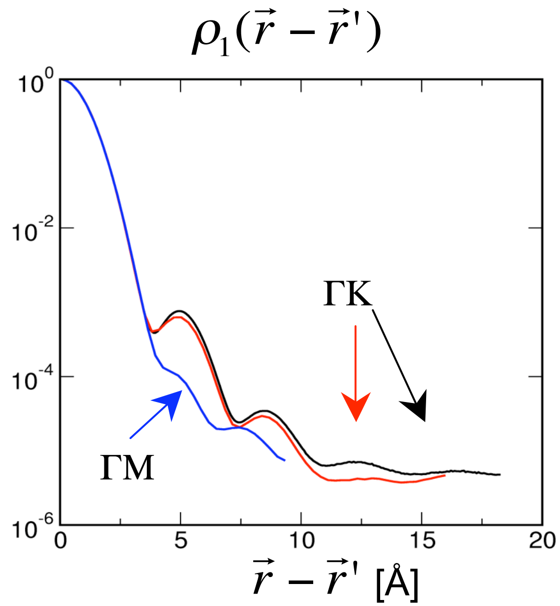


Commensurate crystal
SWF results: ODLRO in a basal plane

- We have computed the one-body density matrix in a basal plane of an hcp solid and along a single axis (n.n. direction)
- ODLRO is present and it is anisotropic only in the middle range 3-14 Å
- Good agreement with the result obtained by sampling in one dimension (n.n. direction)



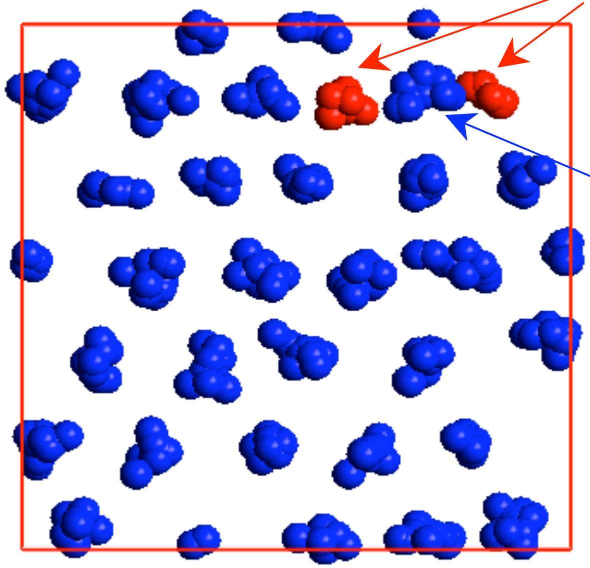


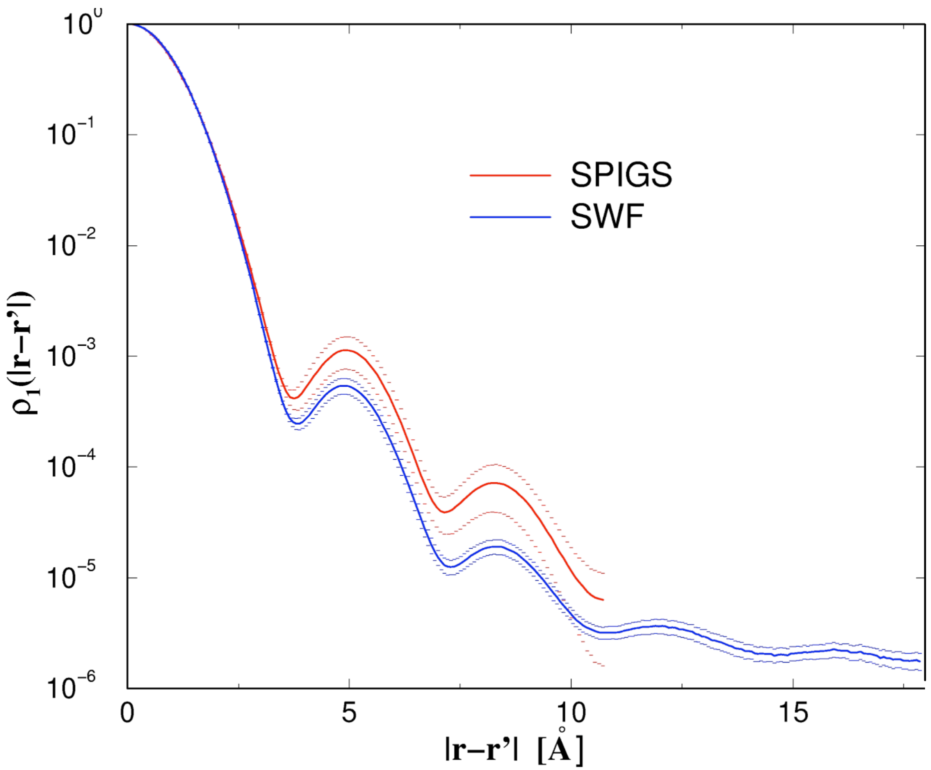


ODLRO - Commensurate state

One-body density matrix: SPIGS results

- Calculations of the one-body density matrix in fcc solid ^{4}He at ρ=0.031 Å^{-3} (this corresponds to pressure p≈54 bars) with SPIGS
- Pair-product approximation: $\delta\tau=(40\ K)^{-1}$; $\tau=0.075\ K^{-1}$ (P=2M+1=7; M=3)
- Oscillations in the tail region are still present (VIPs), the SPIGS result up to 10 Å is above the SWF result
- The system is too small to conclude that ODLRO is present, computation for larger systems is under way





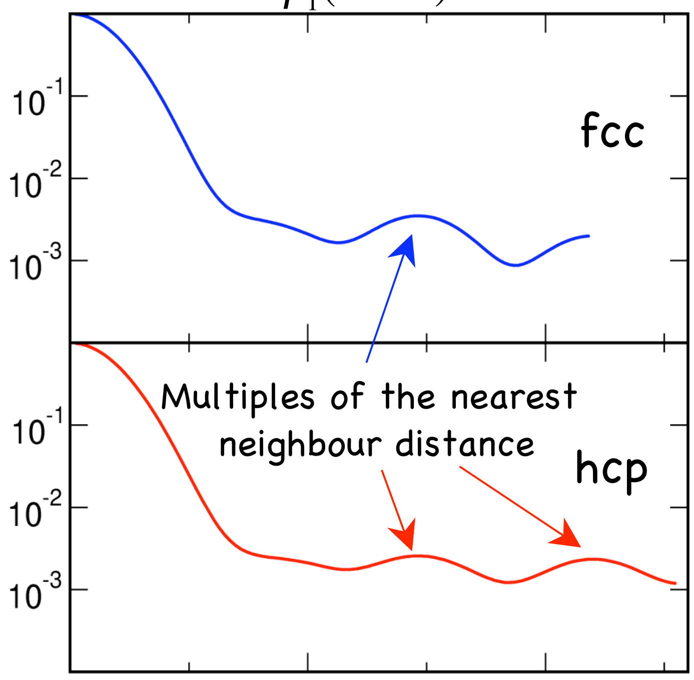
ODLRO - Incommensurate state

Incommensurate solid, SWF results:

(Galli, Reatto, J. Low. Temp. Phys. 124, 2001)

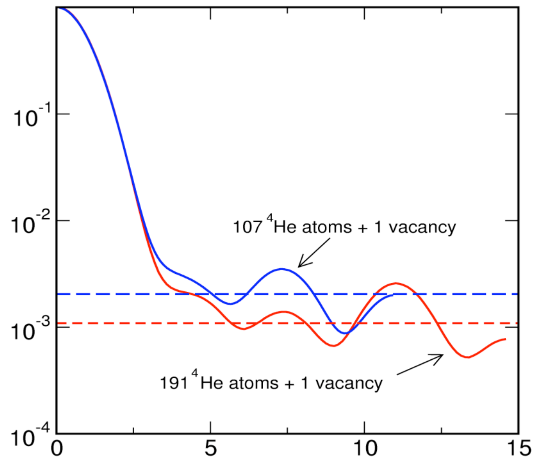
- ODLRO is present in the low density incommensurate solid
- $\rho_1(\vec{r}-\vec{r}\,')$ is Gaussian like only for small distances
- Position of maxima of ρ_1 indicate that ODLRO is vacancy induced in this case

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



$\vec{r}-\vec{r}\,'$ [A]
along nearest neighbours distance

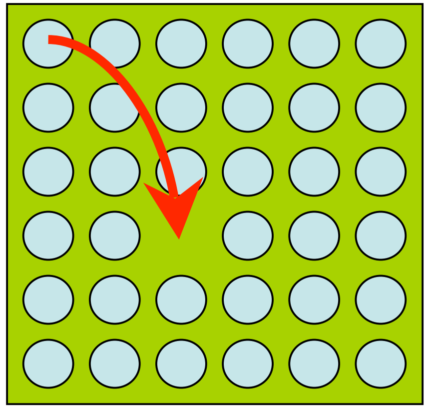
melting density
ρ=0.029 Å^{-3}



$\vec{r}-\vec{r}\,'$ [Å]

ODLRO:
microscopic origin

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



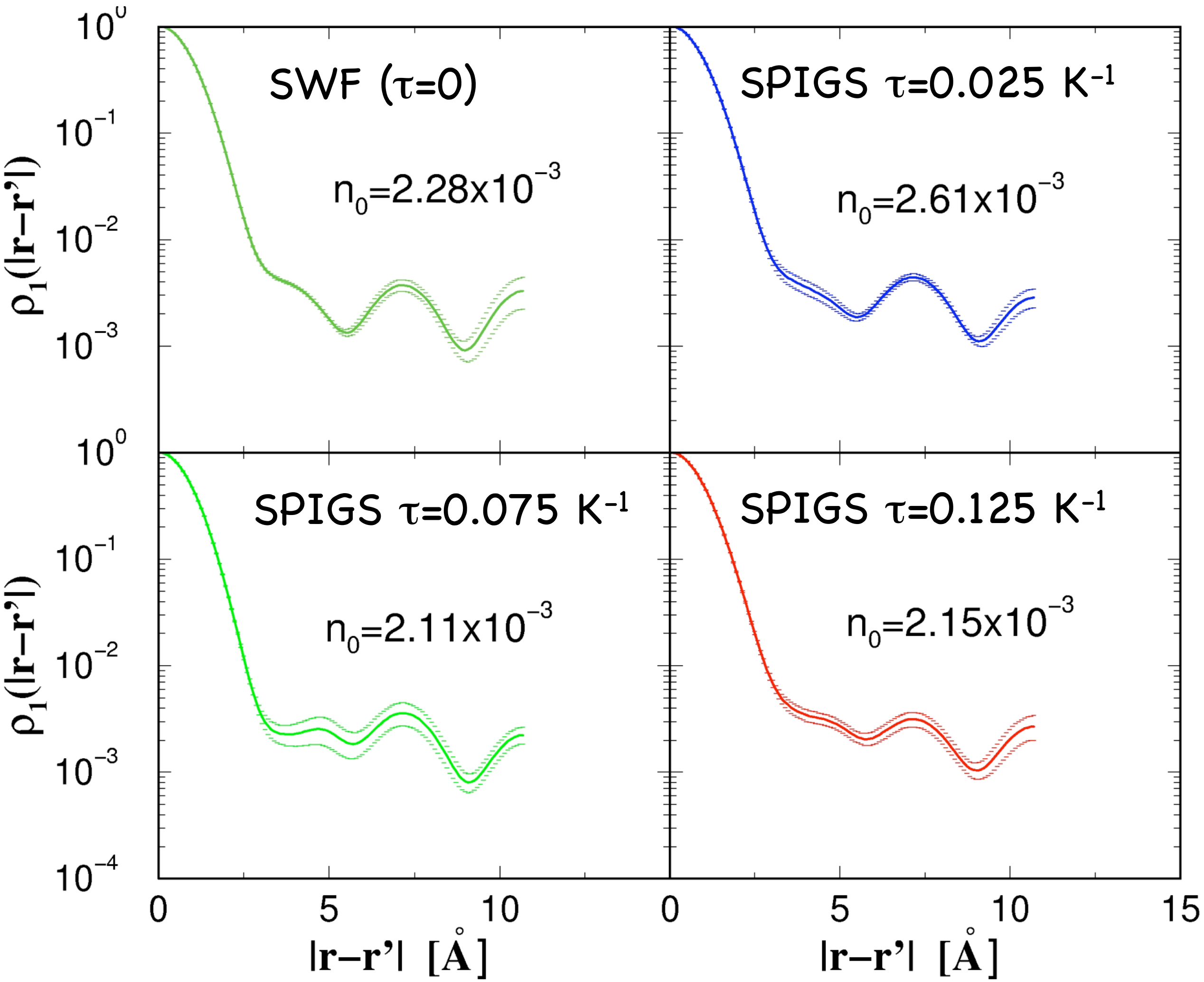
Condensate fraction proportional to the concentration of vacancies

$n_0 = 0.22\ X_v$

at melting density
Similar values in fcc and in hcp

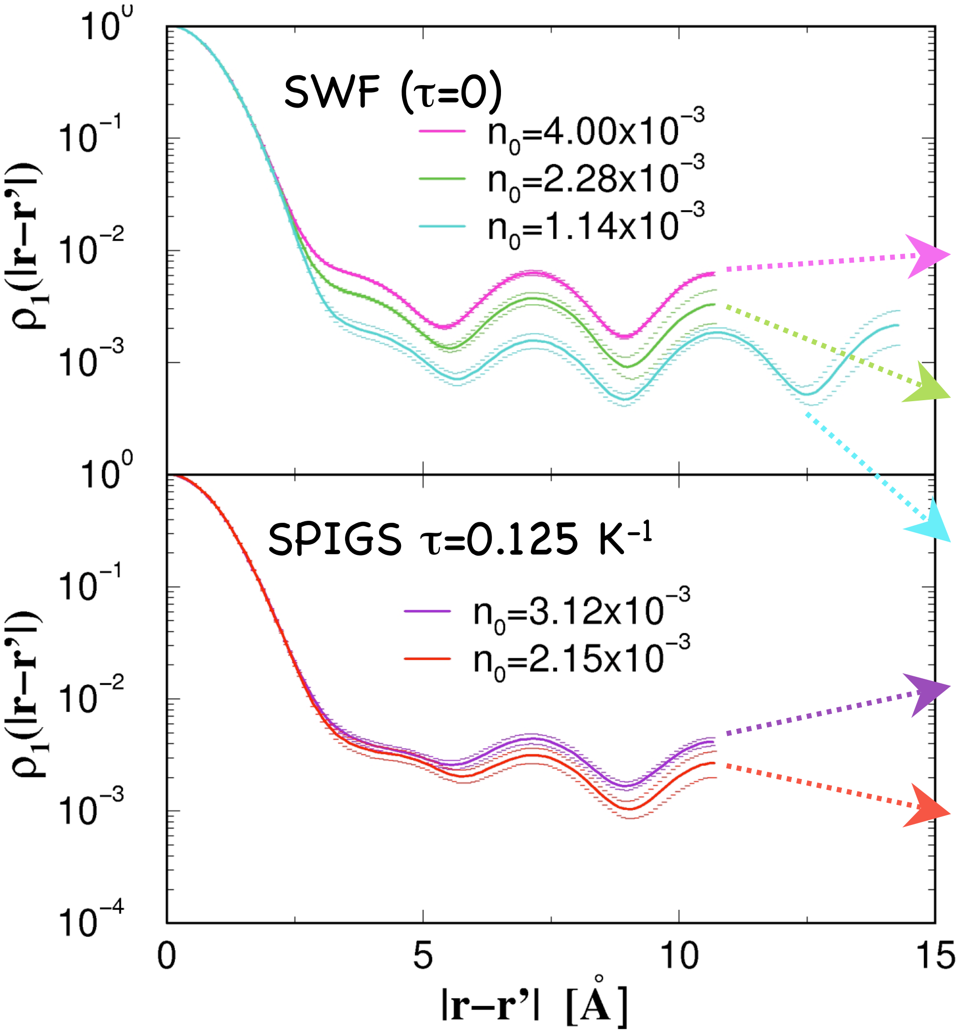
Incommensurate solid, SPIGS results: ODLRO in solid ^{4}He with vacancies

(Galli, Reatto, PRL 2006)



- Sampling along nearest neighbors direction
- fcc $\rho=0.031$ Å^{-3} P=54 bars pair-product approximation $\delta\tau=(40\ K)^{-1}$
- ODLRO is still present with SPIGS

ODLRO - Incommensurate state



n_o sites	n_o atoms
108	106
108	107
192	191
108	106
108	107

Condensate fraction proportional to the concentration X_v of vacancies

$n_0 = 0.23 X_v$ at 54 bars

Vacancies are very efficient in inducing BEC: vacancies as ideal B. gas with effective mass $m^* = 0.35 m_{4He}$

↓

$T_{BEC} \approx 10.8 X_v^{2/3}$

X_v	T_{BEC}
2.3×10^{-3}	200 mK
2.9×10^{-4}	50 mK
2.6×10^{-5}	10 mK
0.8×10^{-6}	1 mK

Conclusions

I have discussed some aspects related to the supersolid state of ^4He at T=0 K

A. Is the ground state of bulk solid ^4He commensurate or incommensurate?

This is still an open question:

- The best variational wave function (SWF) describe an incommensurate state but the equilibrium concentration X_v of ground state vacancies has not yet been computed
- For the exact ground state we do not know if X_v is finite

B. ODLRO-BEC in the commensurate solid

- Variational theory (SWF) gives BEC with $n_o \approx 0.01\%$ at 54 bars
- Exact ground state path integral (SPIGS) result is compatible with similar value of n_o but system size at the moment is too small to be conclusive

C. ODLRO-BEC in the incommensurate solid

- Both variational (SWF) and exact (SPIGS) computations give a finite BEC, n_o scales with concentration X_v of vacancies → at 54 bars the condensate is $\approx 0.23 X_v$

- Vacancies (either equilibrium or non equilibrium) are very efficient to give BEC: estimated T_{BEC} = 200 mK for $X_v = 2 \times 10^{-3}$, T_{BEC} = 10 mK for $X_v = 3 \times 10^{-5}$

Under investigation :

- SPIGS computation for larger system to assess presence of ODLRO-BEC in the commensurate solid
- Determination of the equilibrium concentration of vacancies in the ground state
- Effects on BEC and on vacancies of ^3He impurities