Advances in quantum Monte Carlo techniques for non-relativistic many-body systems
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Path Integral Ground State Monte Carlo:

Study of quantum fluids and solids

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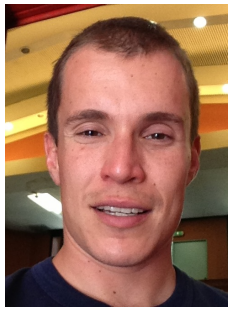

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outline

Prob. #1: exact Ground State of a many-body system

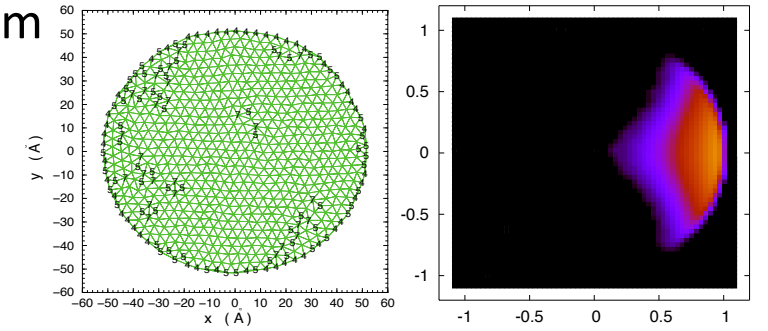
Path Integral Ground State (PIGS) method:

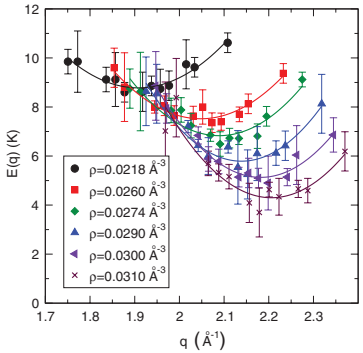
questions & answers

Case #0: 3D bulk ^{4}He

Case #1: 2D bulk solid ^{4}He

Case #2: 2D confined solid ^{4}He



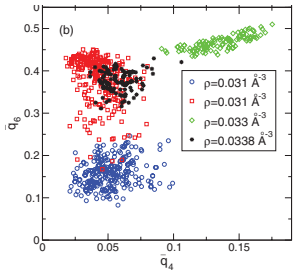


Prob. #2: elementary excitations of a many body system

Genetic Inversion via Falsification of Theories (GIFT) method

Case #3: Overpressurized ^{4}He

excitations in a metastable system

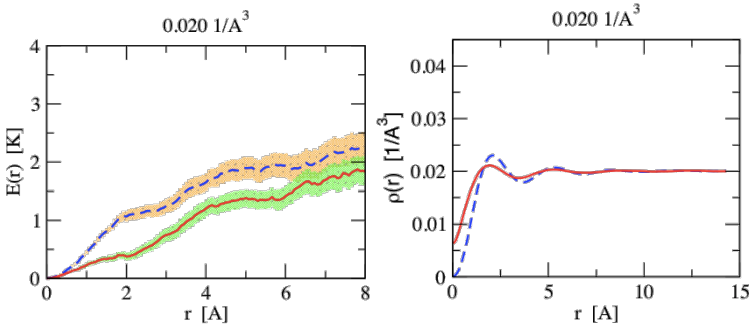


Prob. #3: topological excitations of a many-body system: vortices

Fixed Phase approximation

Case #4: vortex line in liquid and solid ^{4}He

beyond the Onsager-Feynman ansatz



Conclusions

Problem #1: the Ground State

We want to solve the Schrödinger equation for a quantum many-body system of N Bosonic particles described by the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} V(r_{ij})$$

the ground state wave function can be obtained as

$$\psi_0(R) = \lim_{\tau\to\infty} \frac{e^{-\tau\hat{H}}\psi_T}{\langle\psi_0|\psi_T\rangle} \qquad \tau = it/\hbar \quad \text{imaginary time}$$

for any ψ_T provided that $\langle\psi_0|\psi_T\rangle \neq 0$

question $\lim_{\tau\to\infty}$ not reachable in a numerical simulation: how to face with?

An exact approximation of ψ_0: the Path Integral Ground State method

Regardless of a normalization constant, an accurate approximation of the ground state wave function in given by

$$\psi_\tau = \int dR' \; G(R, R'; \tau)\psi_T$$

- the action of $\hat{G} = e^{-\tau \hat{H}}$ exponentially removes from ψ_T any overlap with the excited states during the imaginary time evolution
- The larger is τ the better is ψ_τ
- provide the basis for any zero–temperature Quantum Monte Carlo method

problem

the imaginary time propagator can be accurately written only for small values of τ … but a large τ limit is necessary to ensure the convergence to ψ_0

Two typical exit strategies:

GF- & D-MC

the large τ limit is reached by a recursive procedure: GFMC & DMC

Kalos [PRA 1970]
Reynolds et al. [JCP 1982]

- extremely accurate approximation of $\psi_0\psi_T$
- the trial wave function has a strategic role: involved in each iteration step

Path-Integral Monte Carlo

1. we can use the exact factorization property of the quantum propagator

$$G(R,R';\tau=\tau_1+\tau_2)=\int dR''\ G(R,R'';\tau_1)G(R'',R';\tau_2)$$

to write the large τ propagator as a convolution of small imaginary time propagators (standard path-integral formalism)

2. given $\delta\tau=\frac{\tau}{M}$,the approximated ground state wave function is then

$$\psi_\tau(R_0)=\int\prod_{i=1}^{M}dR_i\left[\prod_{i=0}^{M-1}G(R_i,R_{i+1};\delta\tau)\right]\psi_T(R_M)$$

Sarsa, Schmidt & Magro [JPC 2001]

question

why do we claim this method exact? We are obtaining good (but still) approximations of the ground state wave function...
approx. 1: finite imaginary time τ (M is large but finite)
approx. 2: accuracy of the small imaginary time propagator at the chosen $\delta\tau$

Standard answer: It is possible to reduce all the systematic errors coming from the involved approximations within the unavoidable statistical uncertainty typical of Monte Carlo integration method.
The exact expectation values are exact within their statistical error.

question

even PIGS (as all the zero-temperature QMC methods) relies on a variational wave function (trial wave function)...
Do we have to expect some variational bias in our results?

Standard answer: **In principle NO!** The variational ansatz acts only at the starting point of the imaginary time path, which is governed only by $\hat{G}$.
By choosing properly τ, $\delta\tau$ and M we can reach the true ground state within statistical error

doubt

That's fine! But… **in practice**… can we really reach the exact ground state of a many-body system during a simulation on our pc?

YES, WE CAN!

To convince ourselves we need just a bit more deeper insight in how PIGS works

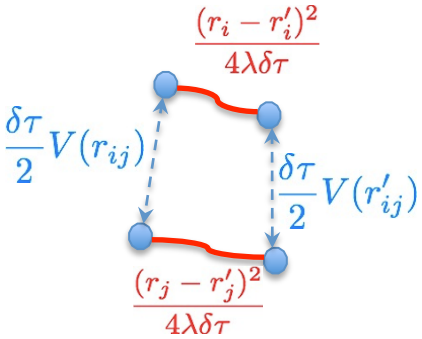
A couple of details:

- projection = elementary imaginary time step obtained by acting with $G(R, R'; \delta\tau)$ the effect will be to increase the overlap with the ground state
- convergence is obtained when adding further projections does not produce any appreciable change in the expectation values (within the statistical error)
- Almost all the most used recipes for $\hat{G}$ factorize it into a kinetic contribution (exactly known) and a contribution that accounts for the interaction (approximated at different extent)

$$G(R, R'; \delta\tau) = G_F(R, R'; \delta\tau) G_I(R, R'; \delta\tau)$$

Exact density matrix of a system of N non interacting particles

Interaction contribution: the explicit form depends on the chosen approximation: the **simplest** is the **primitive approximation**

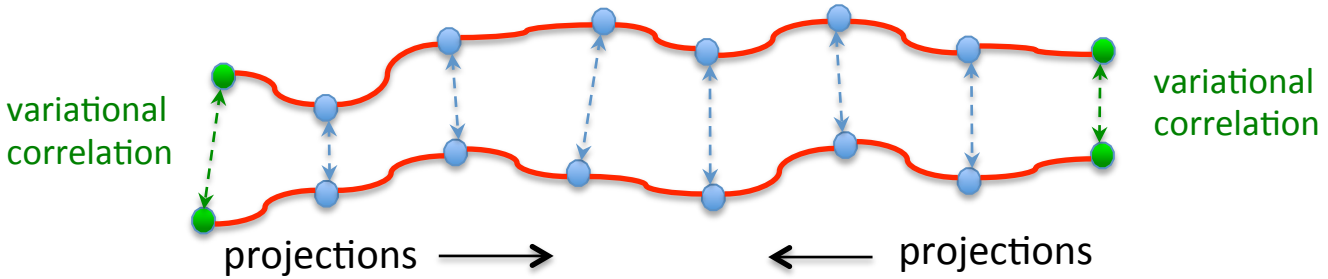


$$= \frac{1}{(4\pi\lambda\delta\tau)^{3N/2}} \prod_{j=1}^{N} e^{-(r_j - r_j')^2/4\lambda\delta\tau} e^{-\frac{\delta\tau}{2}\prod_{i<j} v(r_{ij})} e^{-\frac{\delta\tau}{2}\prod_{i<j} v(r_{ij}')}$$

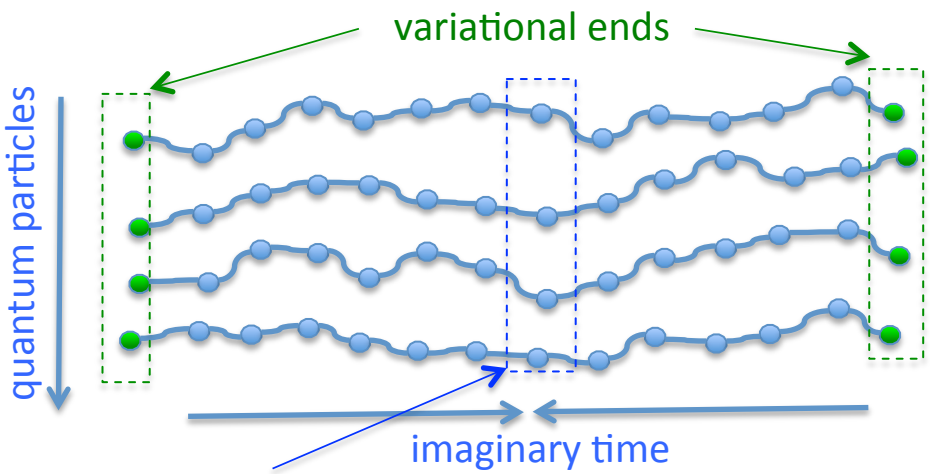
Expectation values & quantum/classical mapping

$$\langle\psi_0|\hat{O}|\psi_0\rangle \simeq \langle\psi_\tau|\hat{O}|\psi_\tau\rangle =$$

$$= \int \prod_{i=1}^{M} dR_i \prod_{j=1}^{M'} dR_j \left[\psi_T(R_{M'}) \prod_{j=1}^{M-1} G(R_j, R_{j+1}; \delta\tau)\right] O(R_0) \left[\prod_{i=1}^{M} G(R_i, R_{i+1}; \delta\tau)\psi_T(R_M)\right]$$



Formal analogy: ground state averages of the quantum system are equivalent to canonical averages of a classical system of special interacting linear polymers



time slice = "picture" of the system at the corresponding imaginary time

polymer = full imaginary path of the quantum particle

the whole imaginary time evolution of the system is sampled at each Monte Carlo step!!!

Beyond primitive

Other approximations for $\hat{G}$:

- Pair-product [Ceperley RMP 1995]
- Suzuki-Chin [Chin PLA 1997]

  even in its pair form (Pair-Suzuki) [Pilati, PhD thesis 2008]
- Multi-product expansion [Zillich, Mayrhofer & Chin JCP 2010]

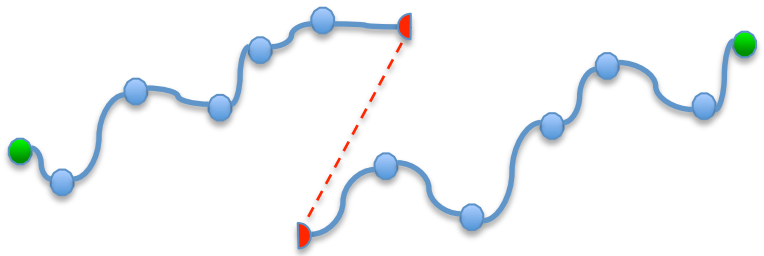
off-diagonal properties

Imaginary time formulation of PIGS prevent direct access to dynamic properties, as for example the superfluid fraction…

- at T=0 K ODLRO is a sufficient condition for NCRI [Leggett Phys.Fen. 1973]
- **ODLRO**: the **one body denisty matrix** ρ_1 has a non zero plateau in the large distance limit (implies **BEC**) [Penrose & Onsager PR 1956]
- ρ_1 is the probability amplitude of destroying a particle in $\vec{r}$ and creating in $\vec{r}'$

$$\rho_1(\vec{r},\vec{r}') = N \int d\vec{r}_2 \ldots \vec{r}_N \; \psi_0(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)\psi_0(\vec{r}',\vec{r}_2,\ldots,\vec{r}_N)$$

In the quantum/classical mapping this corresponds to cut one of the polymers and to histogram the relative distance between the two cut ends (called half polymers)



Let's play with the method!!!

We can consider different trial wave functions and see what happens…

standard variational wave functions

1. Jastrow Wave Function (JWF)

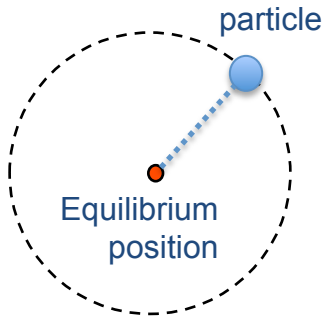
The simplest choice for the wave function of strongly interacting bosons
[Feenberg, Theory of Quantum Fluids, 1969]

$$\psi_J(R) = e^{-\frac{1}{2}\sum_{i<j}\left(\frac{b}{r_{ij}}\right)^m}$$

- Historically one of the first wave functions for ^{4}He [McMillan PR 1965]
- Translational invariant
- ODLRO in any phase (it's a theorem… [Reatto PR 1969])
- It gives also the solid phase, but at the wrong densities…

2. Jastrow-Nosanow Wave Function (JNWF)

$$\psi_{\mathrm{JN}}(R) = e^{-\sum_{i<j}\left(\frac{b}{r_{ij}}\right)^m} \times e^{-c\sum_i(\vec{r}_i-\vec{r}_{0i})^2}$$

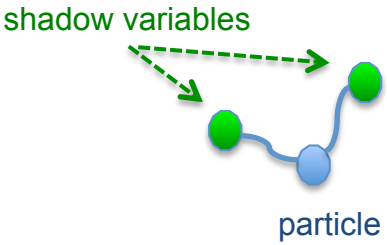


- translational symmetry explicitly broken
- no Bose symmetric (but exchange energy in solid phase is really small… ~10^{-3} K smaller than the typical error-bar…)
- no ODLRO

The best variational wave function for ^{4}He

3. Shadow Wave Function (SWF) [Vitiello, Runge & Kalos PRL 1988]

$$\psi_S(R) = \underbrace{e^{-\sum_{i<j}\left(\frac{b}{r_{ij}}\right)^m}}_{\text{JWF for real coordinates}} \int dS \underbrace{e^{-C\sum_i(\vec{r}_i-\vec{s}_i)^2}}_{\text{Coupling of each real coordinate with its auxiliary one}} \times \underbrace{e^{-\sum_{i<j} v(s_{ij})}}_{\text{JWF for auxiliary coordinates}}$$



- translational invariant (solid phase comes at the right density as a spontaneously broken translational symmetry)
- correlations included at all the order
- Bose symmetric
- ODLRO even in the solid phase (as JWF)

SWF is the best variational description for ^{4}He [Moroni et al. PRB 1998]

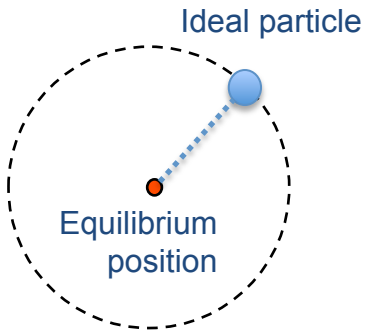
SWF + PIGS = SPIGS [Galli & Reatto MolPhys 2003, JLTP 2004]

"wrong" trial wave functions

we can challenge the convergence ability of PIGS starting from a completely "wrong" description of the system:

4. Gaussian Wave Function (GWF)

$$\psi_G(R) = \prod_{i=1}^{N} e^{-C|\vec{r}_i - \vec{r}_{0i}|^2}$$



- Describes an Einstein crystal
- no Bose-symmetric
- Can it converge to a the correct description of the liquid phase?

5. Constant Wave Function

$$\psi_C(R) = 1$$

- No correlation at all
- Describes an ideal gas
- Can it converge to the correct description of the solid phase?

If we succeed, it will have proved that:

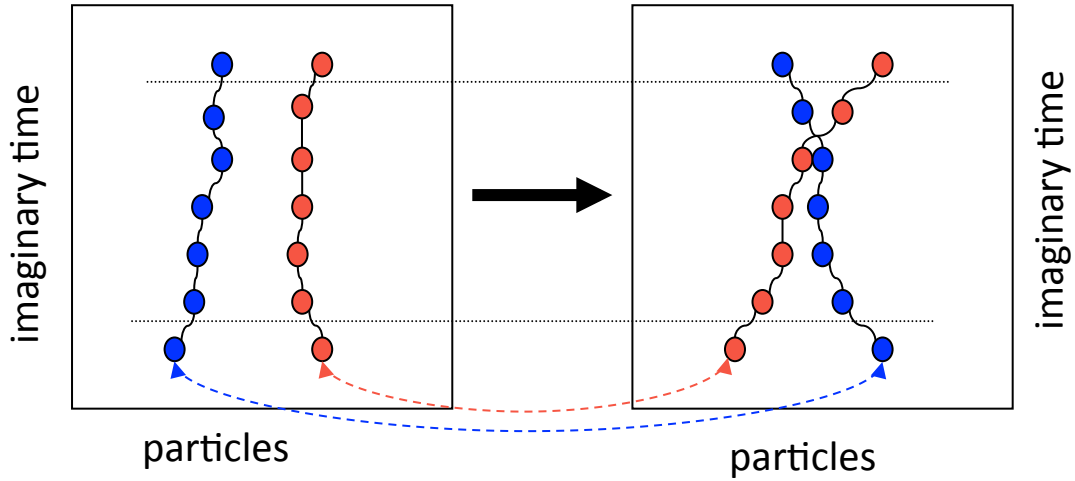
- The projection procedure - removes the overlap with the excited states
  - includes the missing correlations
- we do not need importance sampling with PIGS

… but is better to have it in order to save lifetime

permutation sampling

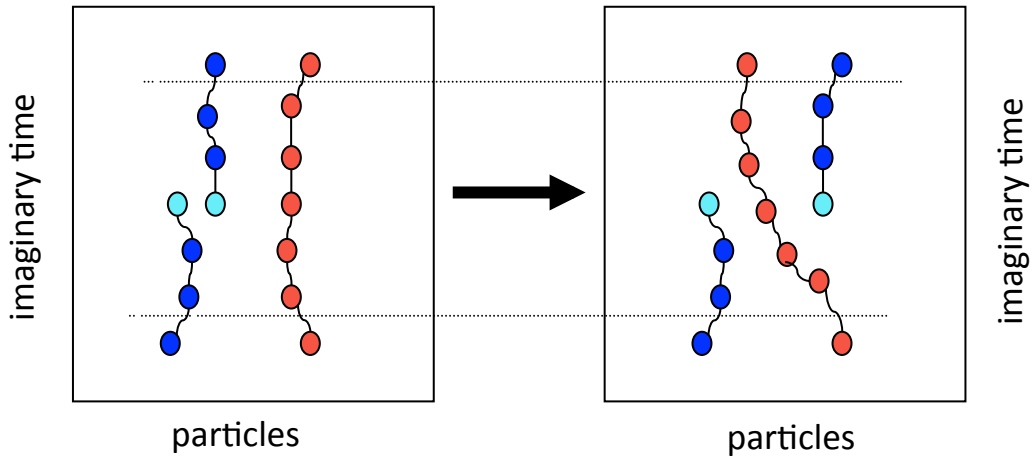
Because of the Bose statistics obeyed by the particles we have to account for permutations in the propagator

- not strictly requested when the initial wave function has the correct symmetry
- permutation circles improve the sampling ergodicity



details on the permutation sampling with PIGS in: Boninsegni JLTP 2005

- swap moves: extremely efficient in the off-diagonal sampling (high acceptance rate)
  [Boninsegni et al PRL 2006; PRE 2007]



- We implement a **canonical worm-algorithm**

For further details go back to Massimo's talk

CASE #0: bulk ^{4}He

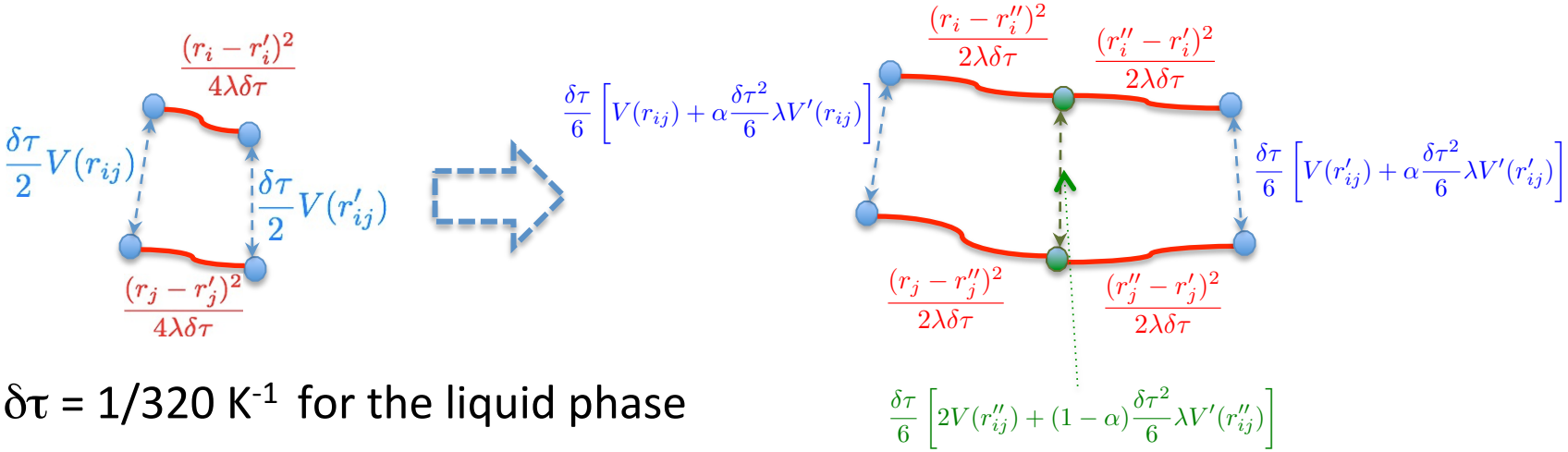
Rossi, Nava, Reatto & Galli JCP 2009

simulation details

- ^{4}He atoms are described as structure-less zero-spin bosons, interacting through a realistic two-body potential (Aziz potential, 1979)
- Periodic boundary conditions (pbc) applied in all the directions
- N = 64 at density ρ = 0.0218 Å^{-3} for the liquid phase

  N = 32 at density ρ = 0.0313 Å^{-3} for the solid phase

  we don't want to solve a real physical problem, we want just to challenge the method
- Pair-Suzuki approximation for the imaginary time propagator $\hat{G}$

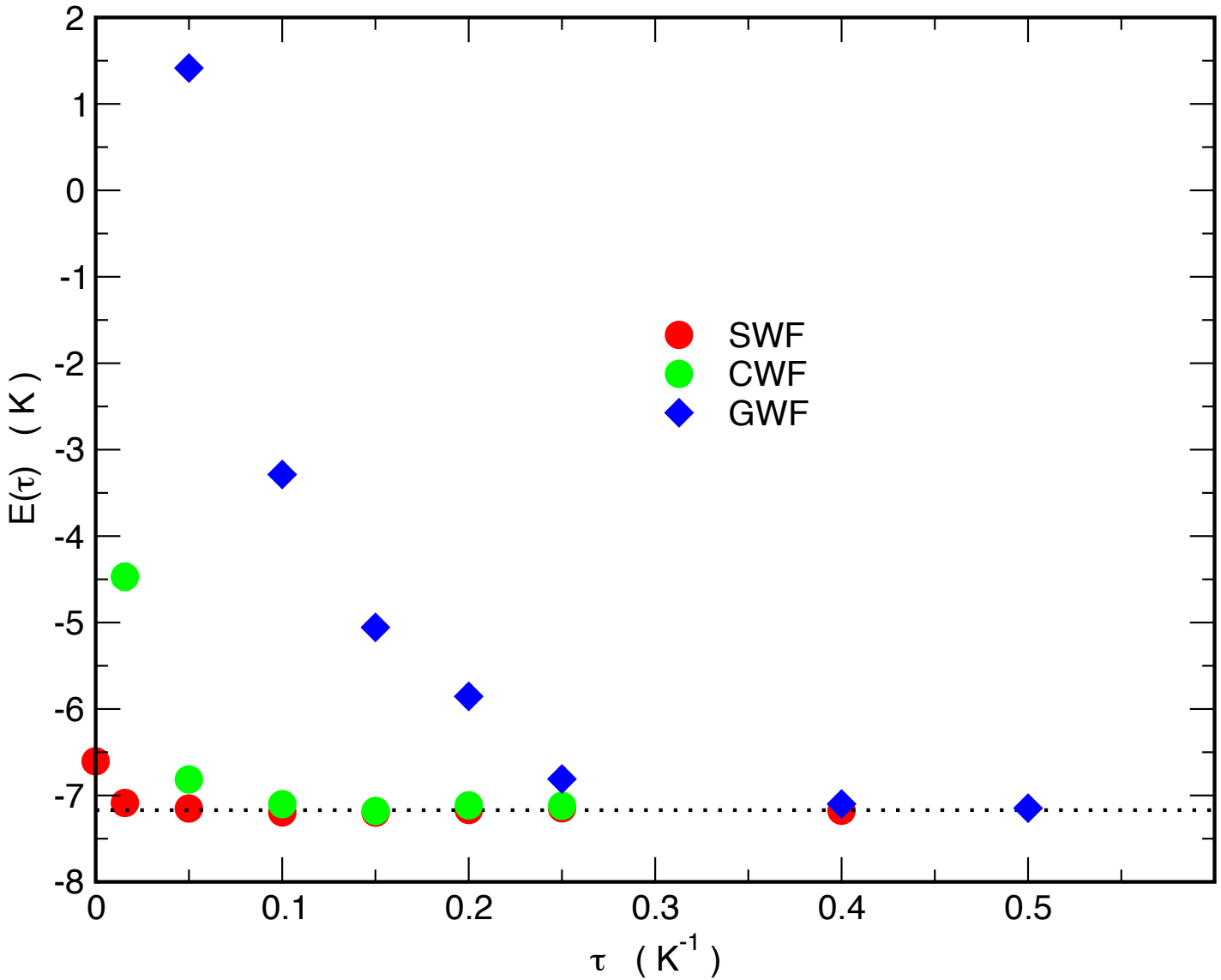


- $\delta\tau$ = 1/320 K^{-1} for the liquid phase

  $\delta\tau$ = 1/480 K^{-1} for the solid phase

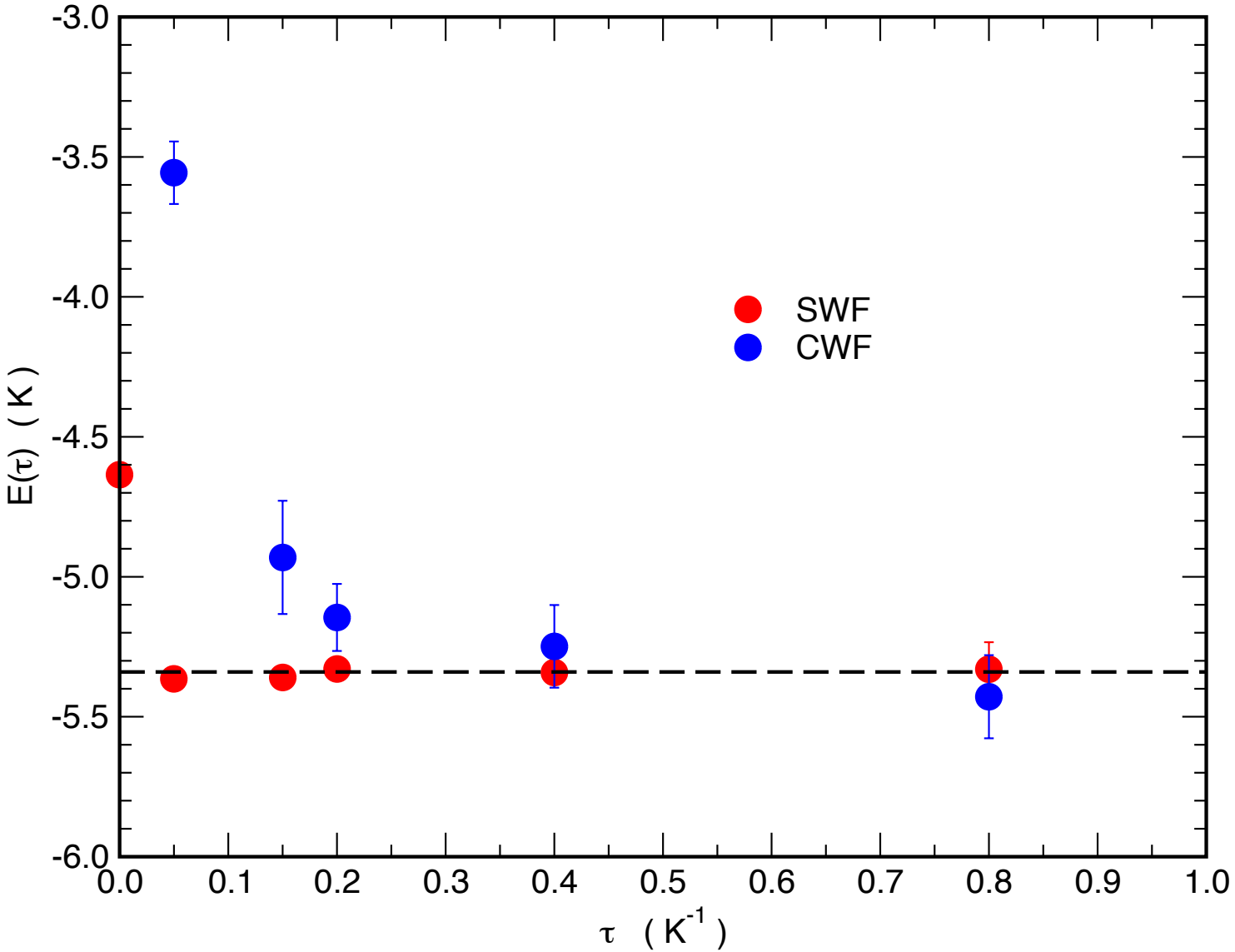
diagonal results: energy per particle

Liquid phase: SWF vs CWF vs GWF



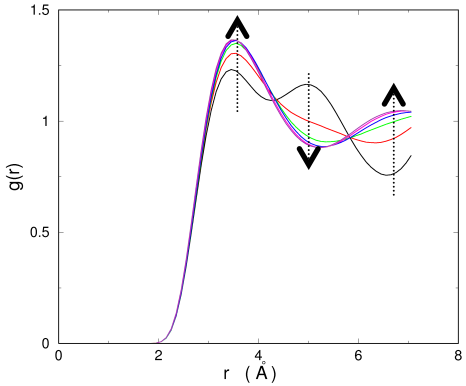
diagonal results: energy per particle

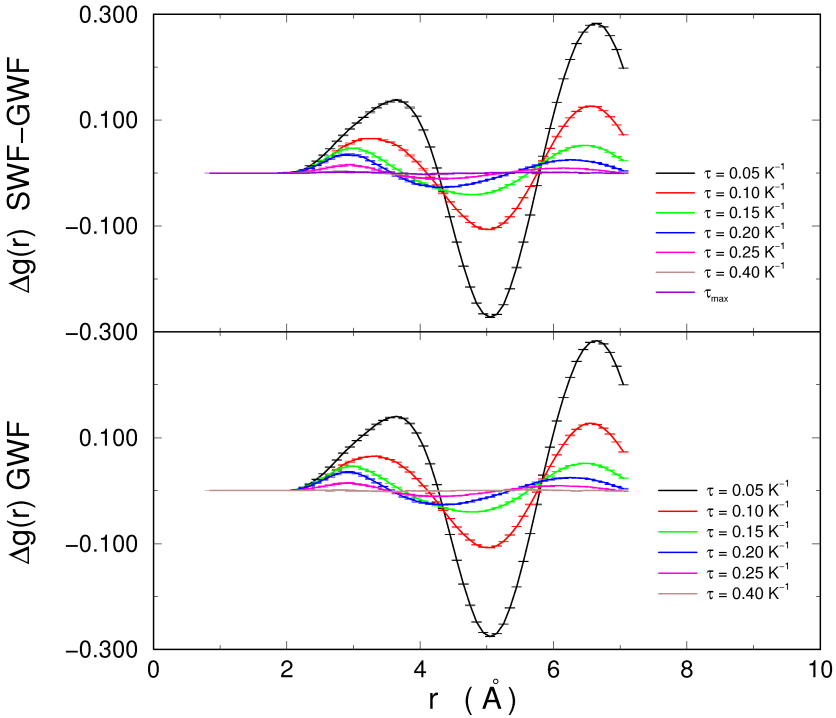
solid phase: SWF vs CWF



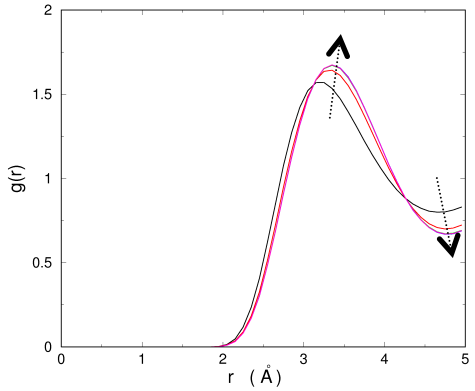
diagonal results: radial distribution function

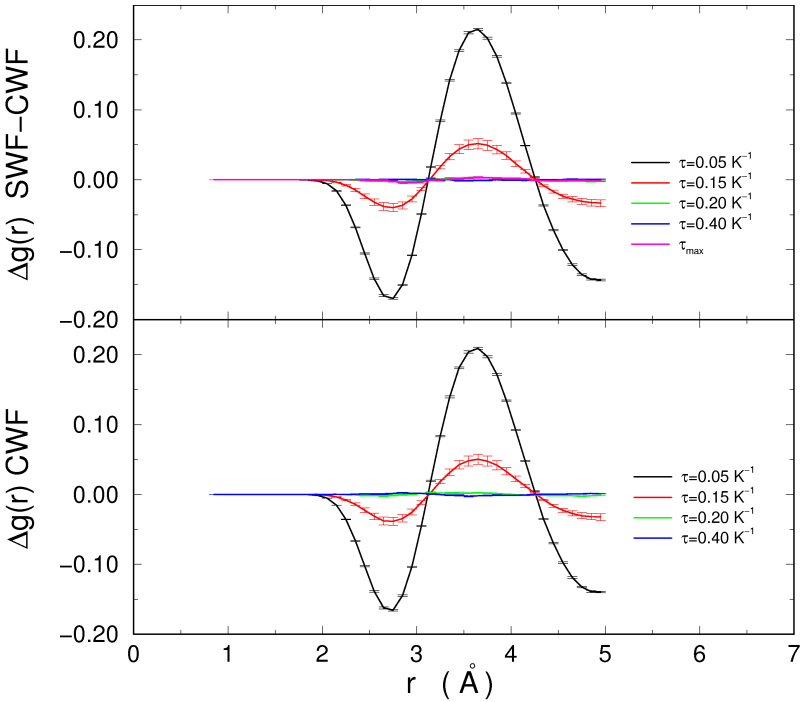
Liquid phase: **GWF**





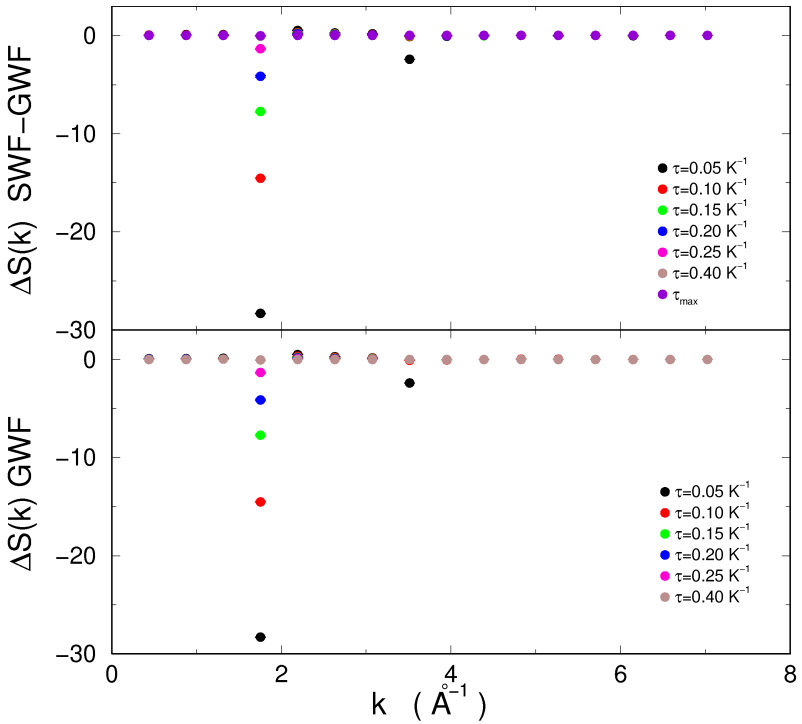
Solid phase: **CWF**





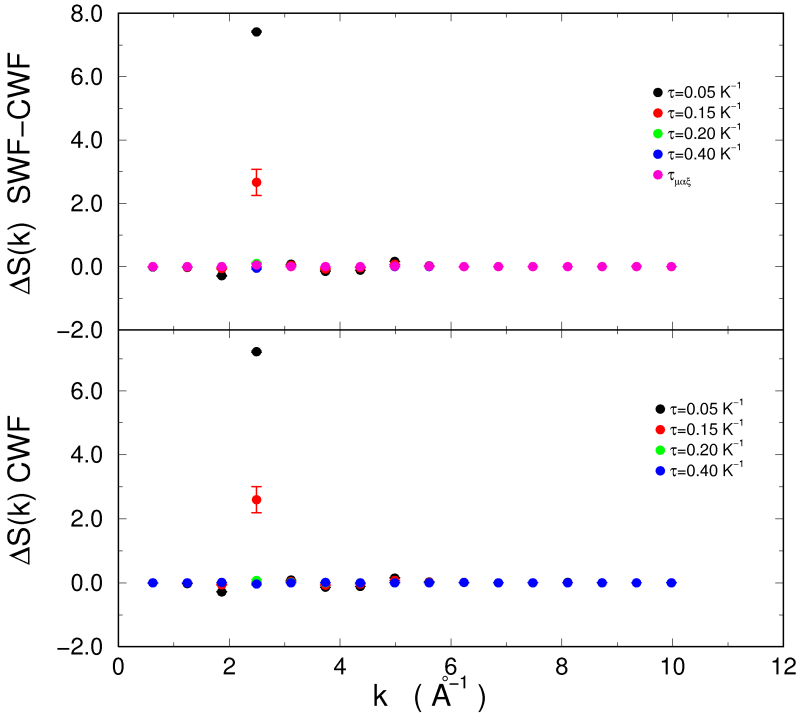
diagonal results: static structure factor

Liquid phase: **GWF**



ψ_G induces Bragg peaks in S(k)
which vanish as τ increases

Solid phase: **CWF**



ψ_C gives a less structured *S(k)* ;
the differences vanish as τ increases

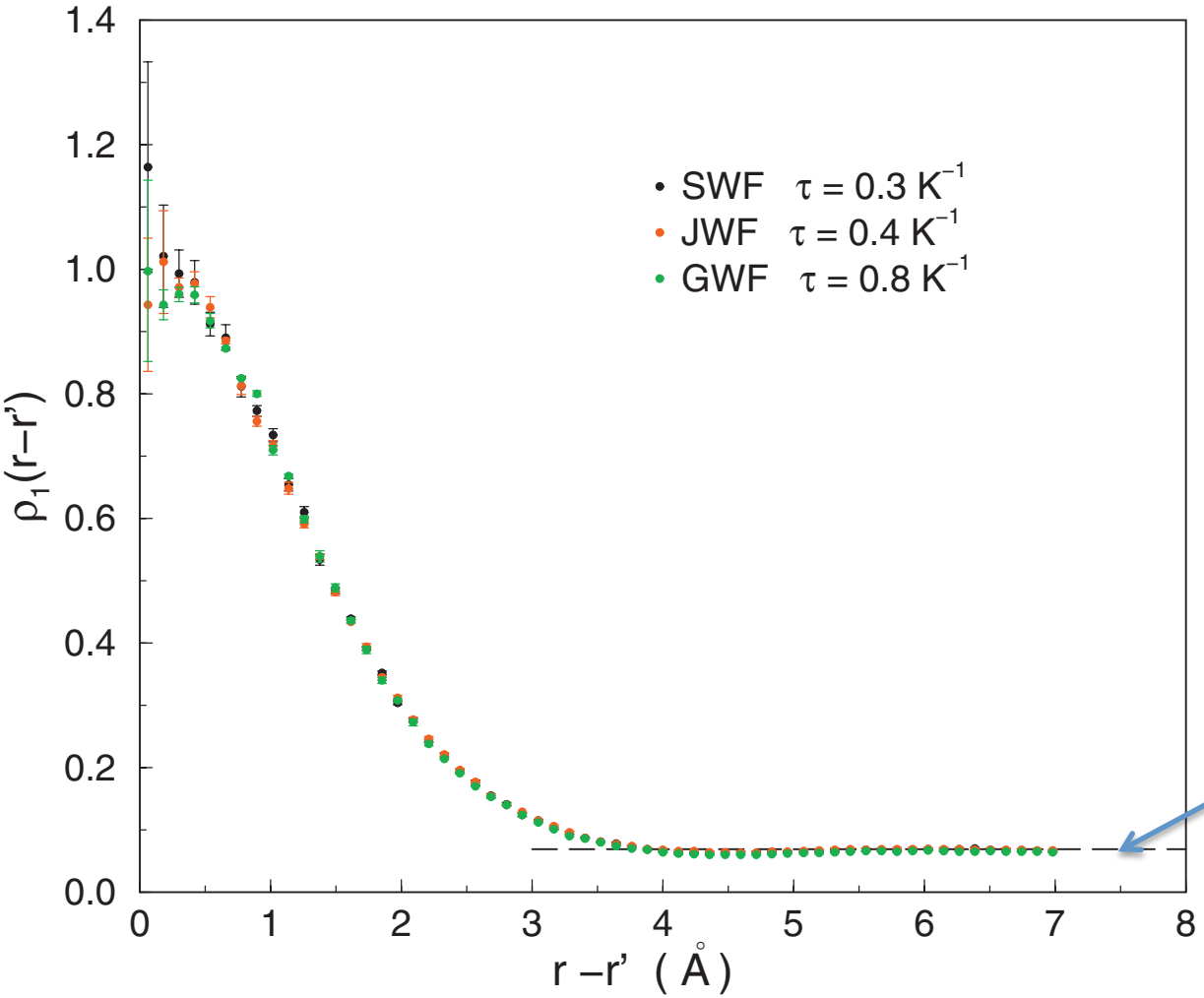
Permutations play a fundamental role

It really works!!! Even without importance sampling!!!

And what about off-diagonal properties?

Liquid phase: **JWF**, **GWF** & **SWF**

$\rho = 0.0218$ Å^{-2} (equilibrium)



$n_0 = 0.069$

in agreement with previous calculations [Moroni & Boninsegni JLTP 2004]

CASE #1: 2D solid ^{4}He

Vitali, Rossi, Tramonto, Galli & Reatto PRB 2008

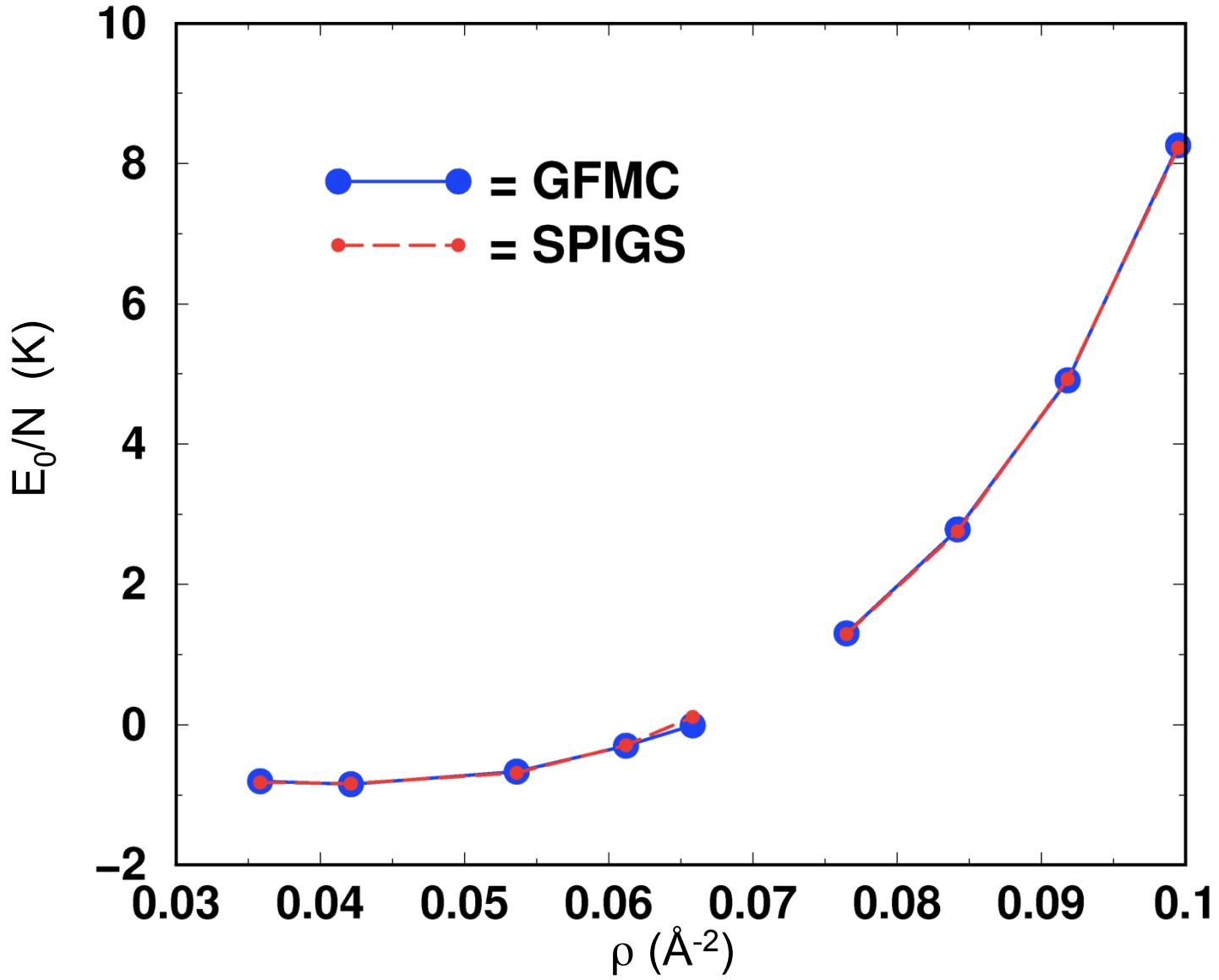
- the reduced dimensionality allows us to study correlations up to larger distances than in 3D (we want also off-diagonal properties…)
- it has been largely studied with other exact methods
- Fluctuations are expected to be stronger in 2D (more stringent test for convergence)
- 2D system is a model that is relevant for adsorbed ^{4}He on a planar substrate like graphite
- could be relevant also for supersolidity

simulation details

- pair-product approximation for $\hat{G}$
- $\delta\tau = 1/40\ K^{-1}$ (compromise between accuracy and computational cost)
- $\tau = 0.775\ K^{-1}$
  (M = 32 => each polymer counts 64 beads)
- simulation box houses exactly a regular triangular lattice and all the sites are occupied by an ^{4}He atom (= perfect crystal)
- N = 224

diagonal results: energy per particle

Equation of state

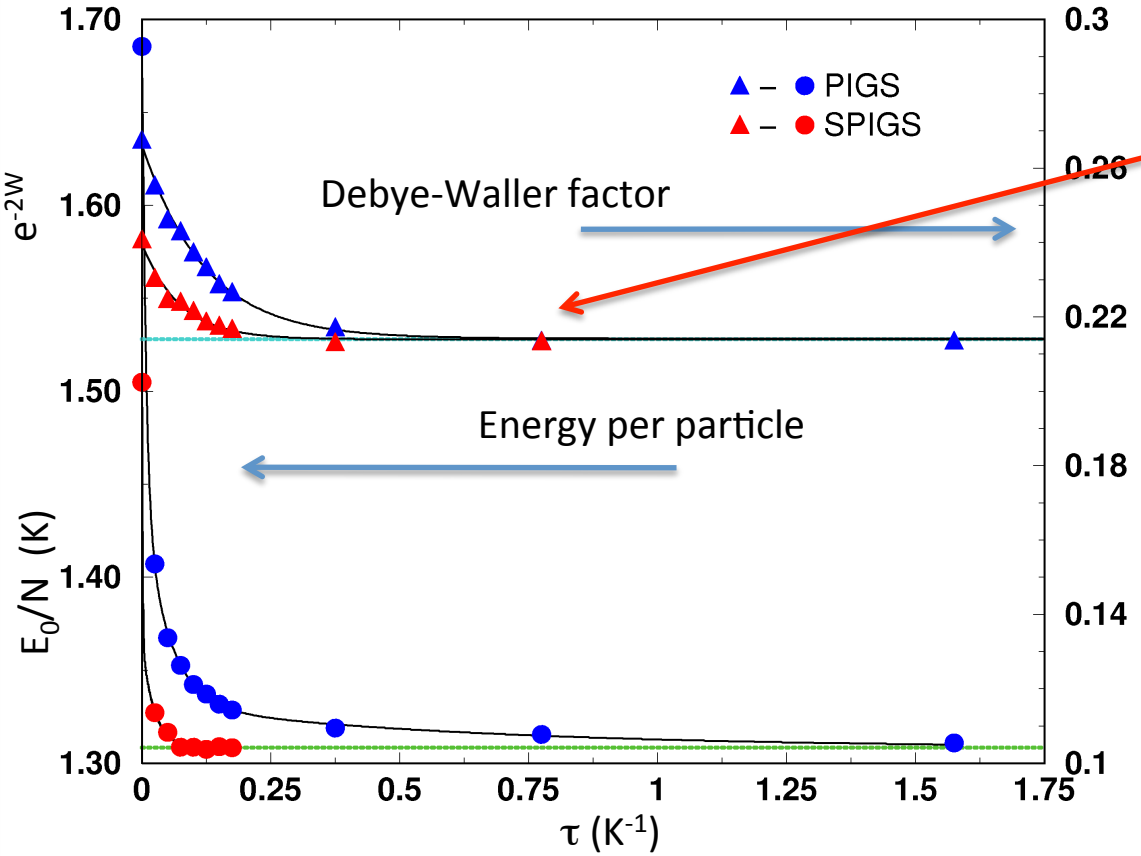


agreement with previous GFMC calculations [Whitlock et al. PRB 1988]

diagonal results: other properties

Solid phase: SWF vs JNWF

ρ = 0.0765 Å^{-2} (just above melting)



each expectation value has its own convergence time!

The "quality" of the trial wave function fixes the number of projections required for convergence

We can get more: from the τ evolution one can get the overlap of the trial wave function with the ground state [Mora & Waintal PRL 2007]

SWF

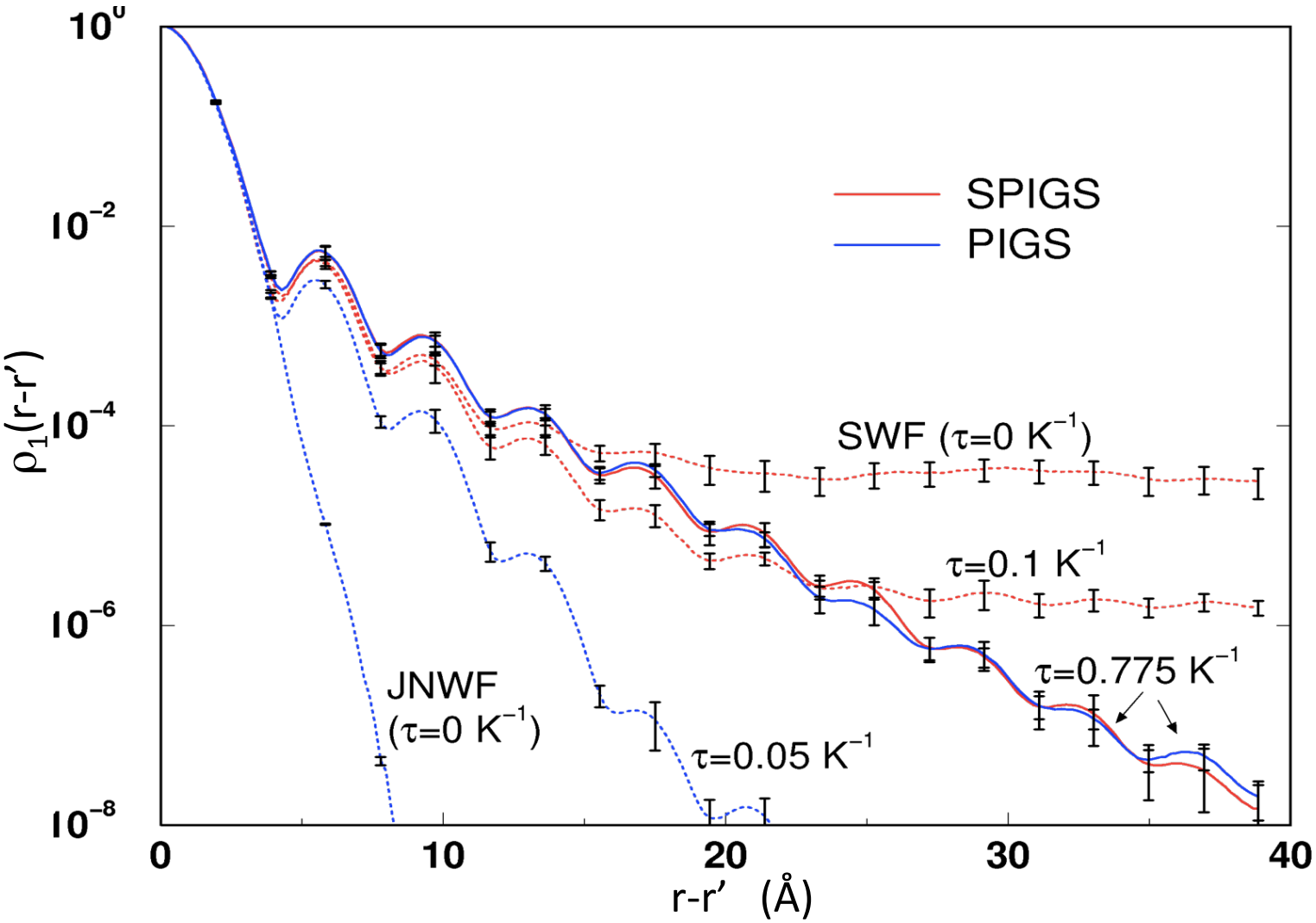
overlap per particle = 99.8%
deviation = 0.2%

JNWF

overlap per particle = 97,9%
deviation = 2.1%

SWF is closer to ψ_0 by one order of magnitude

off-diagonal results



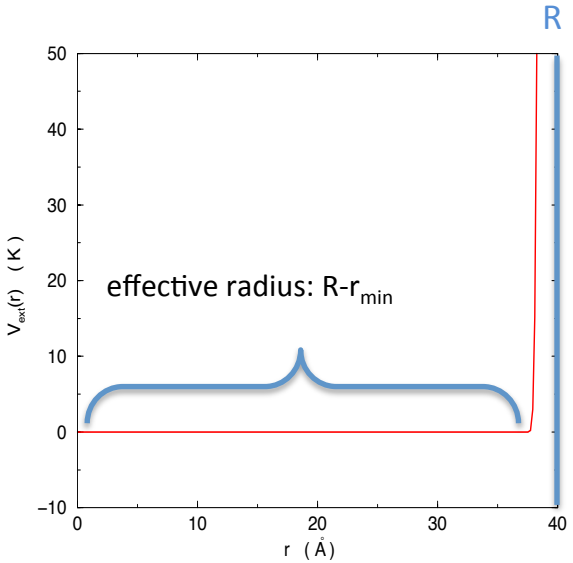
there is **no BEC** in the 2D perfect crystal (it cannot be a supersolid)

Agreement with 3D PIMC (finite temperature) simulations
[Boninsegni et al. PRL 2006, PRE 2006; Clark & Ceperley PRL 2006]

CASE #2: Confined 2D solid ^{4}He

Rossi, Reatto & Galli JLTP 2012

- Defects are able to induce ODLRO in the simulated system [Rossi, Vitali, Galli & Reatto JPCM 2010] but are they present in the macroscopic crystal?
- OPTION 1: study the concentration of defects in the thermodynamic limit. Too large systems (very long and boring simulations)
- OPTION 2: study a crystal in equilibrium with the liquid…
- OPTION 2b: by confining a solid we can create an interfacial region rich of defects, are them injected in the inner crystal?



smooth barrier confining ^{4}He inside a circle of radius R (remove also the stabilizing effect of pbc)

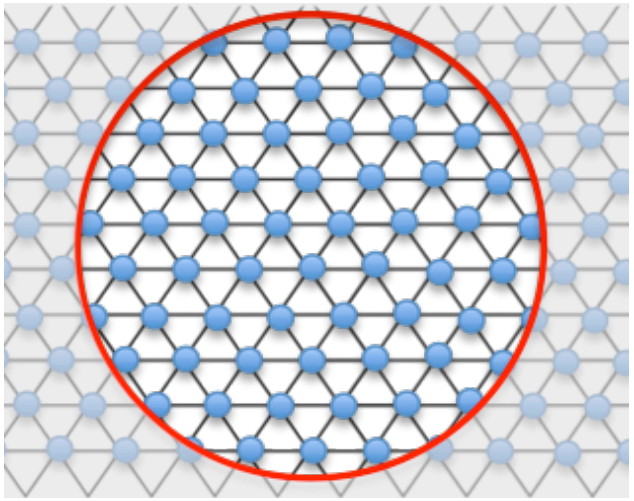
$R-r_{min} < r < R$: integrated and shifted LJ potential (r_{min} is the minimum position of the integrated LJ)

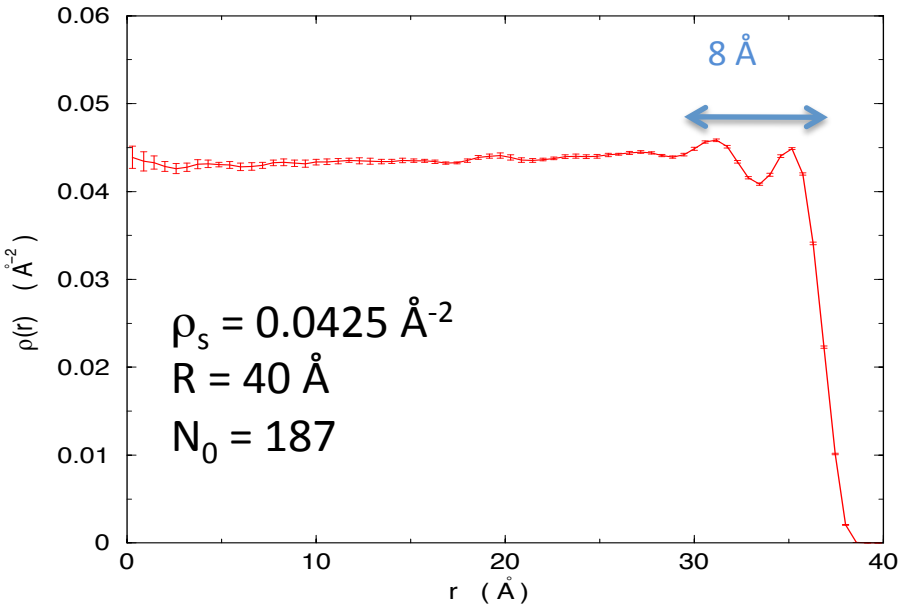
$$V_{LJ}(r) = \frac{3\pi\varepsilon\sigma^6}{8}\rho_{ext}\left[\left(\frac{21\sigma^6}{r^{10}}\right) - \frac{1}{r^4}\right]$$

$0 < r < R-r_{min}$: $V_{ext} = 0$

simulation details

- Pair-Suzuki approximation for $\hat{G}$
- $\delta\tau = 1/320\ K^{-1}$
- $\tau = 0.775\ k^{-1}$ (each polymer contains 250 “real” beads)
- The initial configuration is built starting from a triangular lattice at ρ_s and discarding al the particles that fall out the the disk ($N=N_0$)
- ψ_T = SWF





at low density ρ_s: liquid with small (~10 Å) interfacial layer

Visualization of defects: qualitative analysis

At higher densities the system is solid: $\rho_s = 0.0765$ Å^{-2}

Different R:

R = 44.6 Å	$N_0 = 433$
R = 54.6 Å	$N_0 = 685$
R = 64.6 Å	$N_0 = 931$

We can promote the presence of defects by adding or subtracting particles

N = 671 N = 699

question

How can we visualize defects?

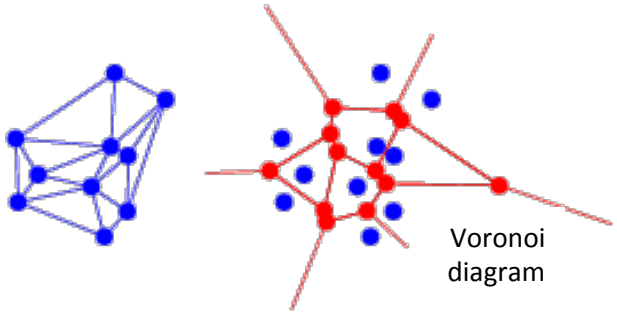
In the regular crystal coordination number is 6, so atoms with coordination different from 6 can be used as an index of disorder

[Krishnamachari & Chester PRB 2000]

Delaunay triangulation:

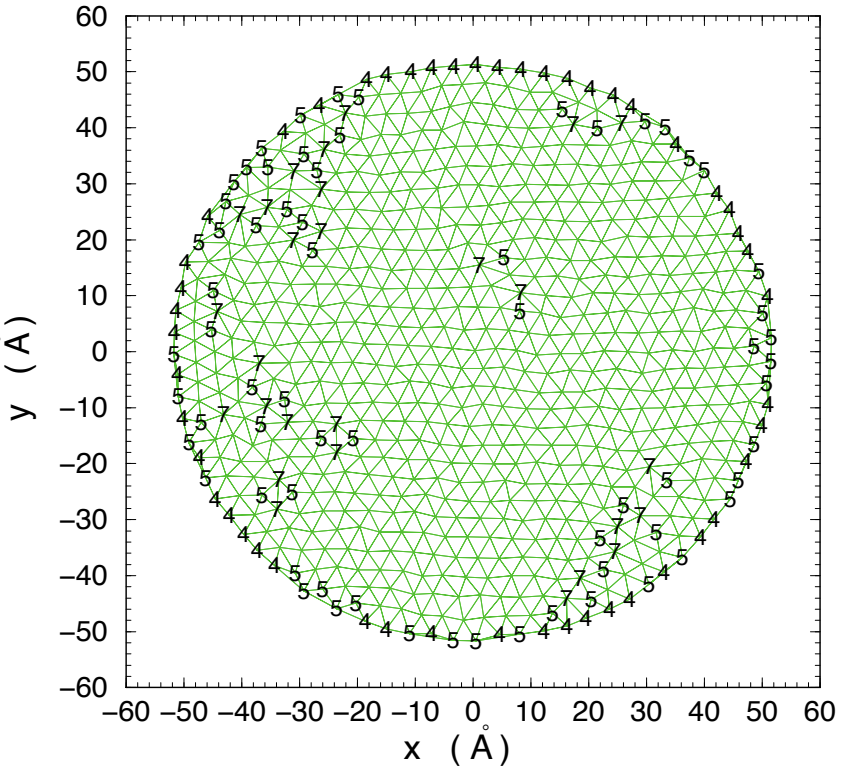
The Delaunay triangulation corresponds to the dual graph of the Voronoi diagram.

The Voronoi cell associated to the site P consists of all the points of the plane closer to *P* than to any other site.



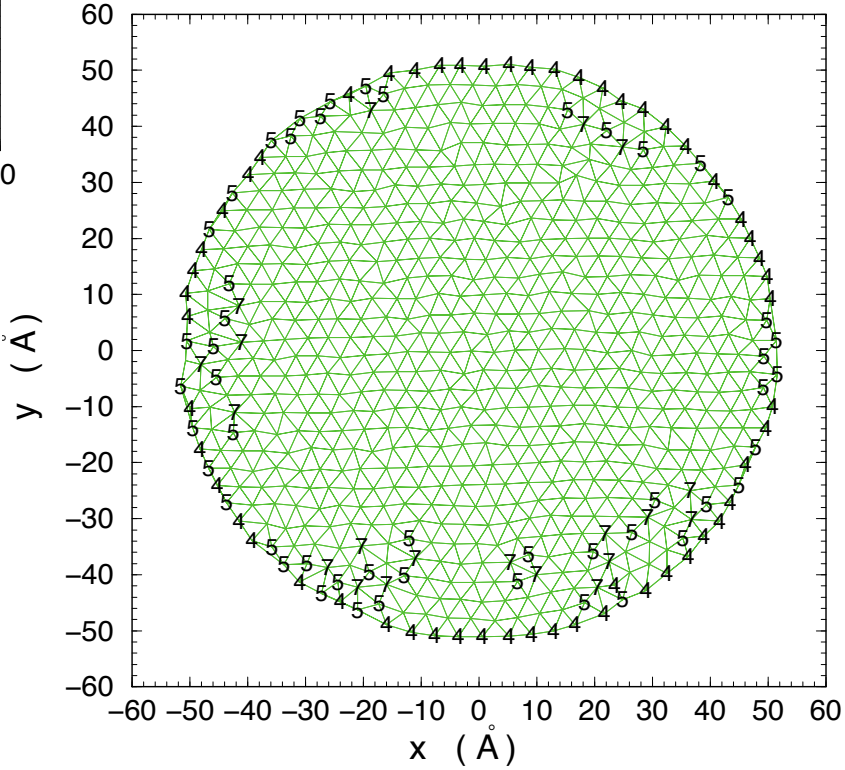
The number of segments ending on a site is equal to the number of first neighbours (coordination number).

Visualization of defects: qualitative analysis



After few MC steps we have defects also in the inner region…

…but after a long equilibration the system reaches equilibrium and we find defects only at the interfacial region



question

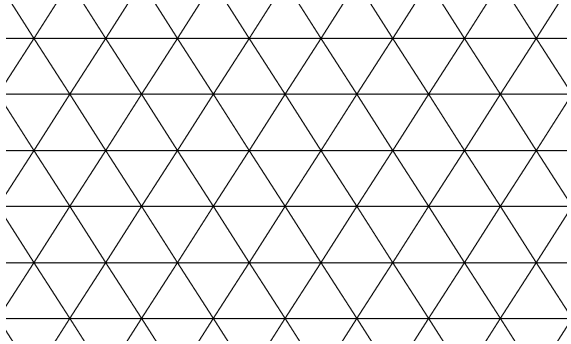
More quantitatively?

The quality of the crystalline order can be quantified via the **orientational order parameter** [McTague, Frenkel & Allen: *Ordering in two dimension*]

$$\Psi_6 = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{1}{n(k)}\sum_{j=1}^{n(k)} e^{i6\theta_{kj}}\right)$$

θ_{kj} : angle between the vector $\vec{r}_k - \vec{r}_j$ and a fixed direction in the plane (x axis)

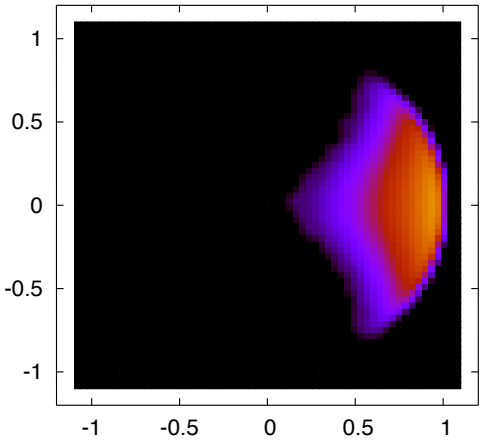
$n(k)$: first neighbors of the k-th particles



for a static perfect triangular lattice

- $|\langle\Psi_6\rangle| = 1$
- the plot of $|\langle\Psi_6\rangle|$ is a single spot on a circumference with unit radius

- because of zero-point motion we expect a broadened spot in solid ^{4}He
- In the limit of a liquid system $|\langle\Psi_6\rangle|$ turns into a distribution centred into the origin



Perfect PCB solid ^{4}He at ρ = 0.079 Å^{-2} (N = 572)

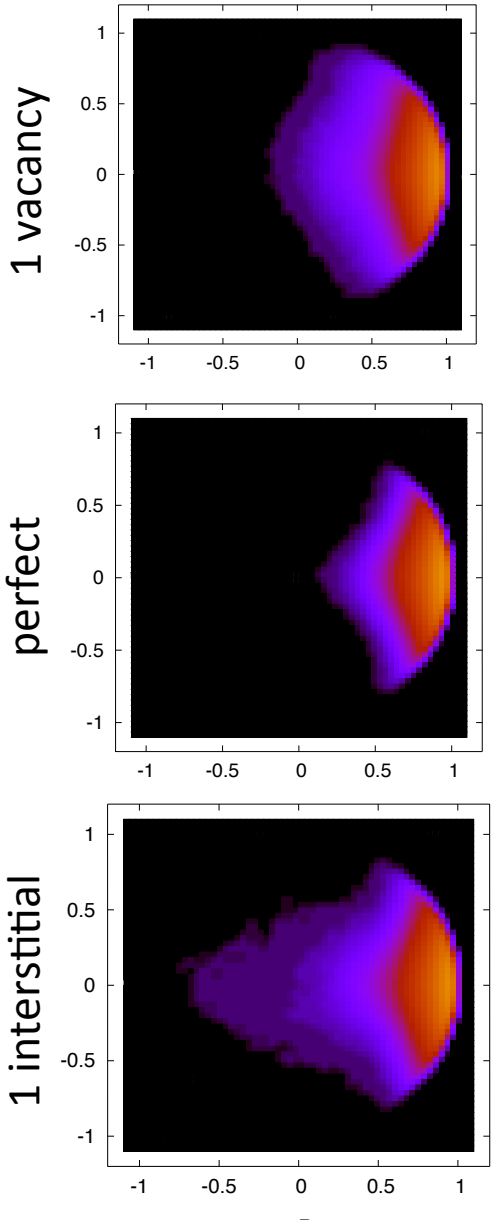
angular order parameter

PCB solid ^{4}He at
$\rho = 0.079$ Å^{-2}

1 vacancy

perfect

1 interstitial



Confined solid ^{4}He with R = 54.6 Å

r < 20 Å

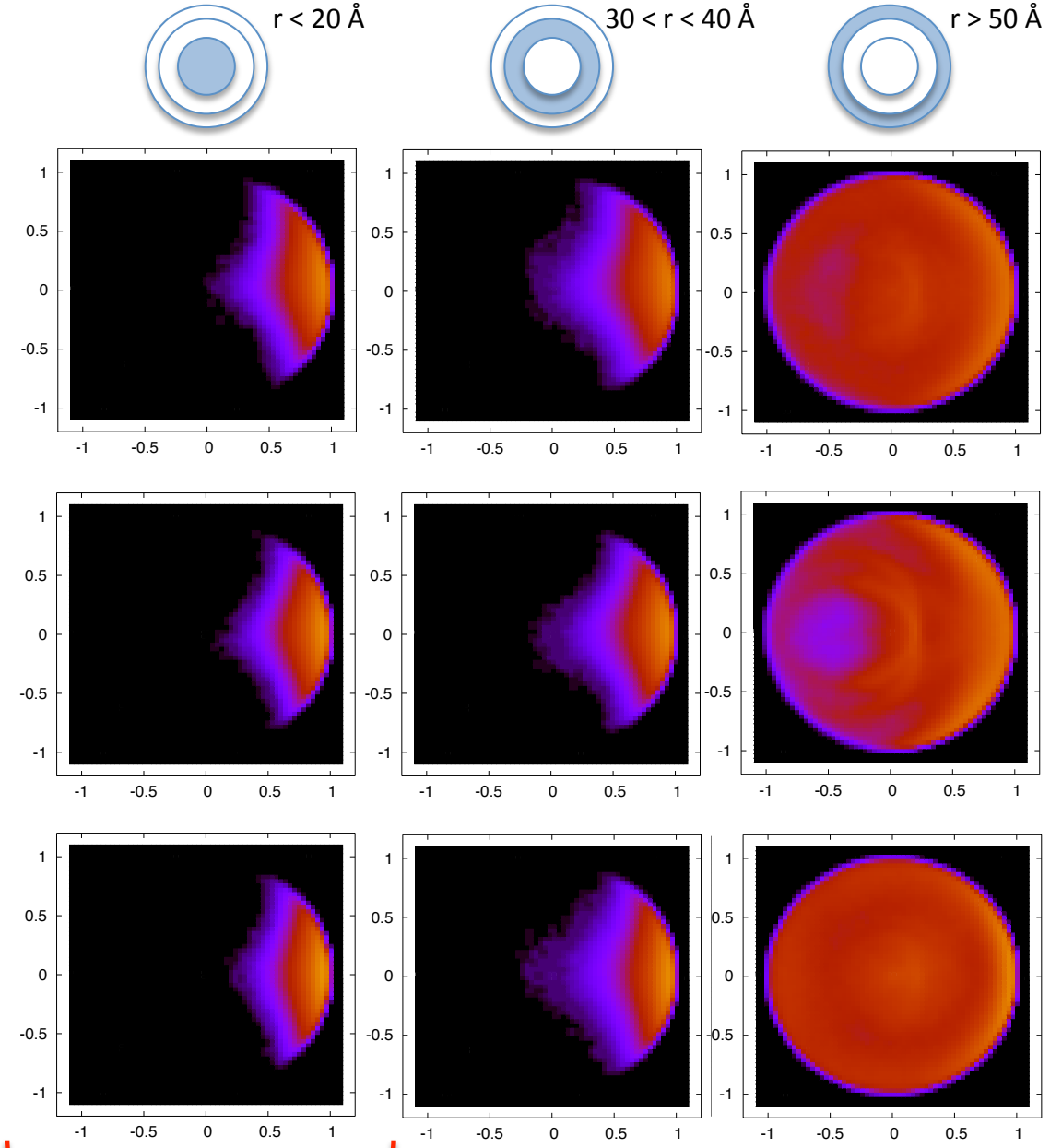
30 < r < 40 Å

r > 50 Å

N = 671

N = 685

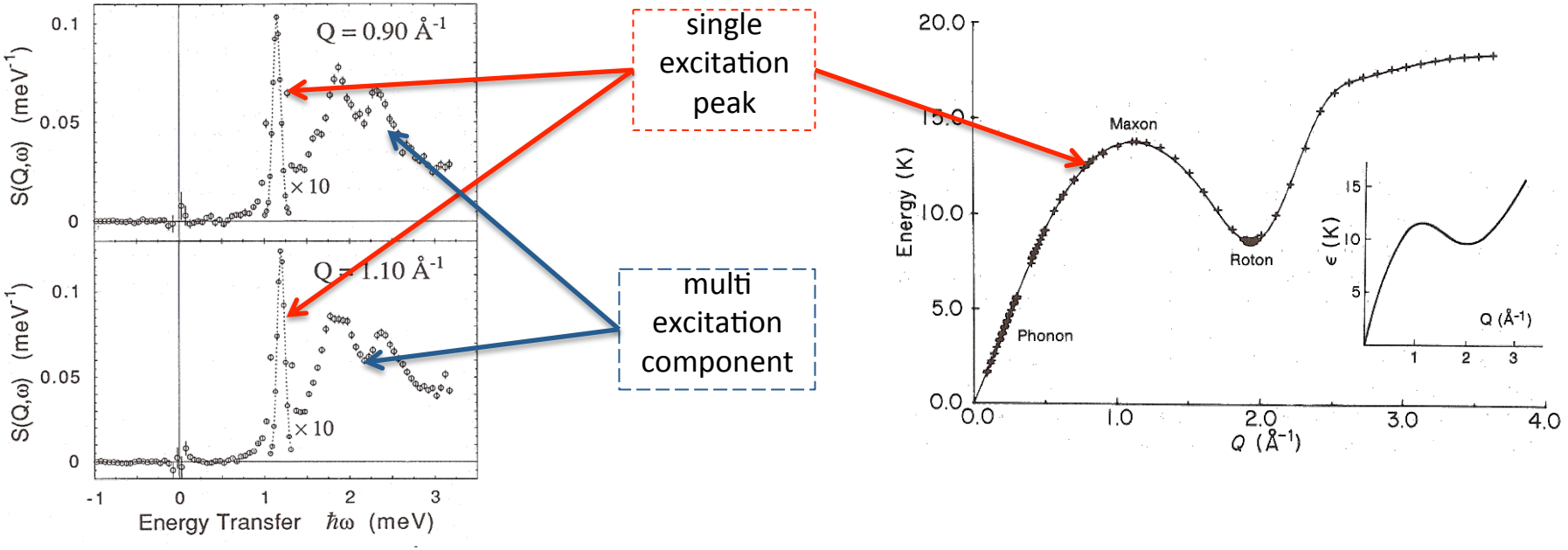
N = 699



Compatible with perfect PBC crystal

Problem #2: elementary excitations

Obtain information on **dynamic properties of the system**: we want to evaluate the **dynamic structure factor *S(q,ω)*** of a collection of strongly interacting bosons to extract information about the **elementary excitation spectrum** of the system



the dynamic structure factor is defined as

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{+\infty} dt\; e^{i\omega t}\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}_{-\vec{q}}(0)\rangle$$

$$\hat{\rho}_{\vec{q}}(t) = \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r}_j(t)}$$

density fluctuation

problem

The imaginary time formulation of PIGS prevent us the access to real time dynamic properties as $\hat{\rho}_{\vec{q}}(t)$

We can work in imaginary time and compute the intermediate scattering function

$$F(\vec{q},\tau) = \frac{1}{N}\langle \hat{\rho}_{\vec{q}}(\tau)\hat{\rho}_{-\vec{q}}(0)\rangle$$

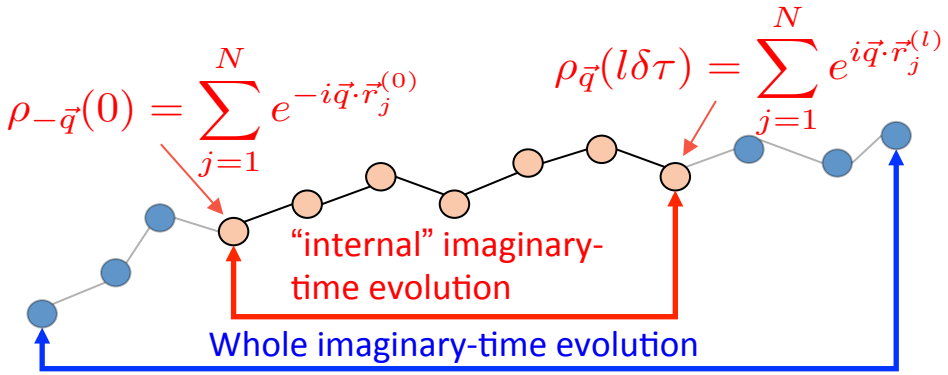
and the dynamic structure factor is obtained **by inverting the Laplace transform**

$$F(\vec{q},\tau) = \int_0^{+\infty} d\omega\ e^{-\omega\tau} S(\vec{q},\omega)$$

Serious problem

The Laplace transform is a smoothing operation, moreover PIGS allows to compute the **exact intermediate scattering function** only over a set of **discrete values of imaginary time**…

$$F(\vec{q},\tau) = F_l(\vec{q}) = \frac{1}{N}\langle \hat{\rho}_{\vec{q}}(l\delta\tau)\hat{\rho}_{-\vec{q}}(0)\rangle$$



… each with its own statistical error…

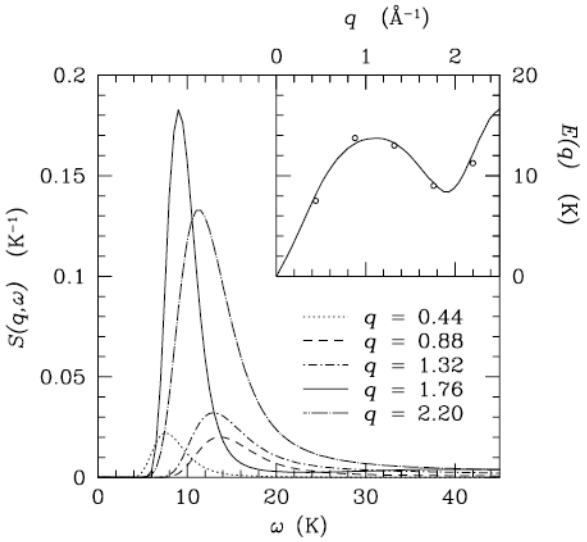
The **inversion** problem is **ill posed !!!**

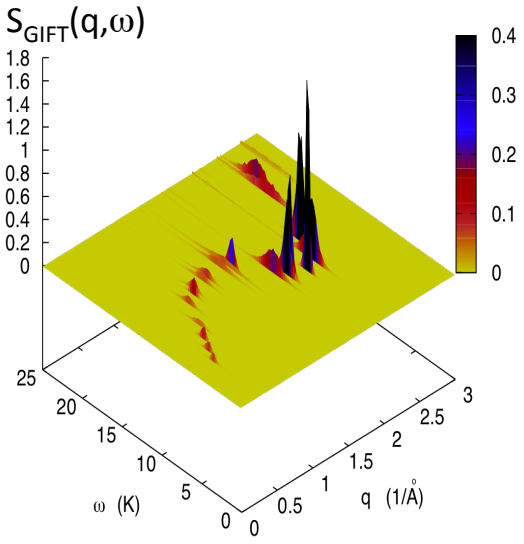
Dynamic from QMC: GIFT

We **must** **relax** on the possibility of obtain **the exact dynamic structure factor**: there are **approximate methods** for **invert** the **intermediate scattering function**

- Maximum entropy method

  qualitative results when applied to liquid ^{4}He [Moroni & Baroni PRL 1999]
- Average spectrum method
- …
- **GIFT** : space model explored with a Genetic Algorithm (non-local stochastic dynamics) & no a-priori constraints





[Vitali, Rossi, Reatto & Galli PRB 2010]

- liquid ^{4}He, at equilibrium density ρ=0.0218 Å^{-3}
- sharp peaks in S(q,ω) indicating energies of elementary excitations
- evidence of a multi-excitation component in S(q,ω) in semi-quantitative agreement with experiments

For more details go back to Ettore's ~~talk~~ discussion

CASE #3: Overpressurized ^{4}He

Rossi, Vitali, Reatto & Galli PRB 2012

- **superfluid – solid transition:** instability of superfluid against density fluctuations with *k* corresponding to the roton excitations [Schneider & Enz PRL 1971]

- Experimental results for excitation in metastable ^{4}He…

  [Chavanne et al PRL 2001; Ishiguro et al JLTP 2007; Pearce et al PRL 2004]

…. But few QMC studies, mainly devoted to off diagonal properties [Moroni & Boninsegni JLTP 2004; Boninsegni et al PRL 2006] & only one study of excitations in overpressurized ^{4}He (with large uncertainties) [Vranjes et al PRL 2005]

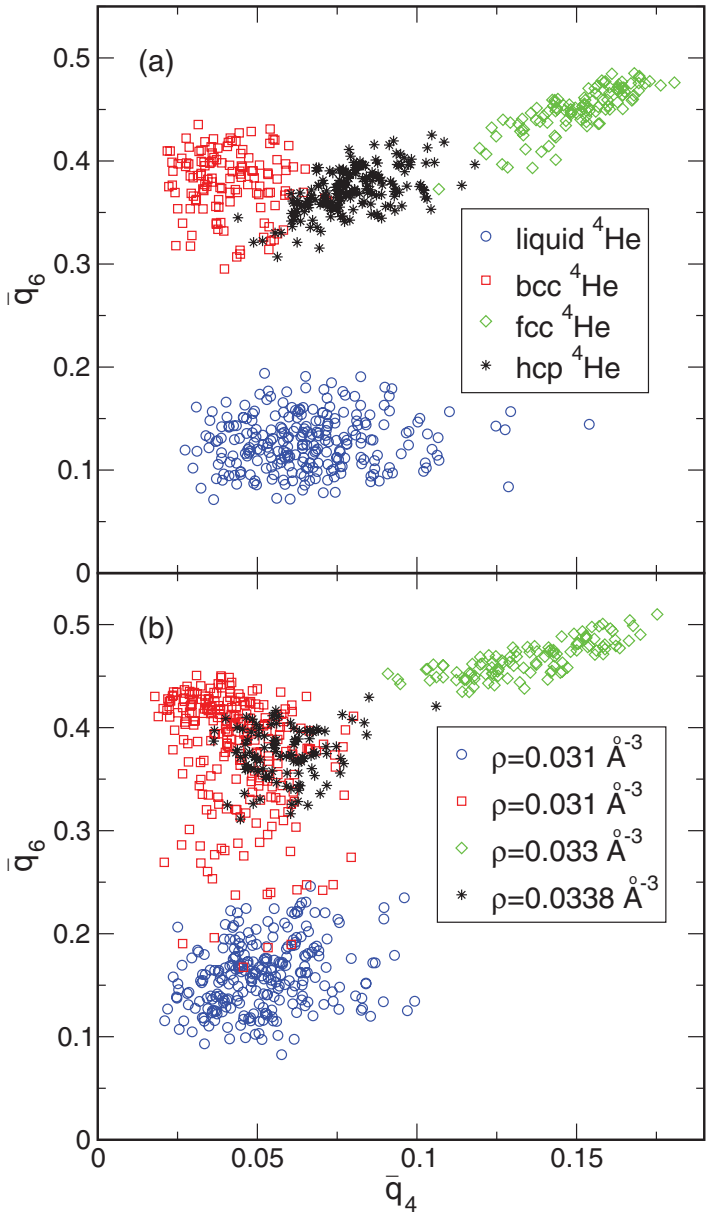
simulation details

- pair-product ($\delta\tau = 1/160$ K^{-1}) & pair-Suzuki ($\delta\tau = 1/320$ K^{-1}) approx. for $\hat{G}$
- $\tau = 0.5$ K^{-1} (very large, but we have to compute $F_l(q)$…)
- two different Aziz potentials [Aziz et al MolPhys 1987, Aziz e al JCP 1979]
- $N = 256$ ^{4}He atoms with pbc
- $0.0200 < \rho < 0.031$ Å^{-3} ($-6 < P < 87$ atm)

  the starting configuration is obtained from an equilibrated configuration at the equilibrium density ($\rho = 0.0218$ Å^{-3}, P = 0 atm) rescaled to match the desired density.
- ψ_T = SWF

liquid until P = 87 atm, for higher pressures (densities) it readily starts a nucleation process

Averaged local bond order parameters



We have monitored the phase of the system via the **averaged local bond order parameters**

[Lechner & Dellago JCP 2008]

Steinhardt parameters

$$\bar{q}_{lm}(i) = \frac{1}{\tilde{N}_b(i)} \sum_{k=0}^{\tilde{N}_b(i)} q_{lm}(k)$$

$$q_{lm}(i) = \frac{1}{N_b(i)} \sum_{j=1}^{N_b(i)} Y_{im}(\vec{r}_{ij})$$

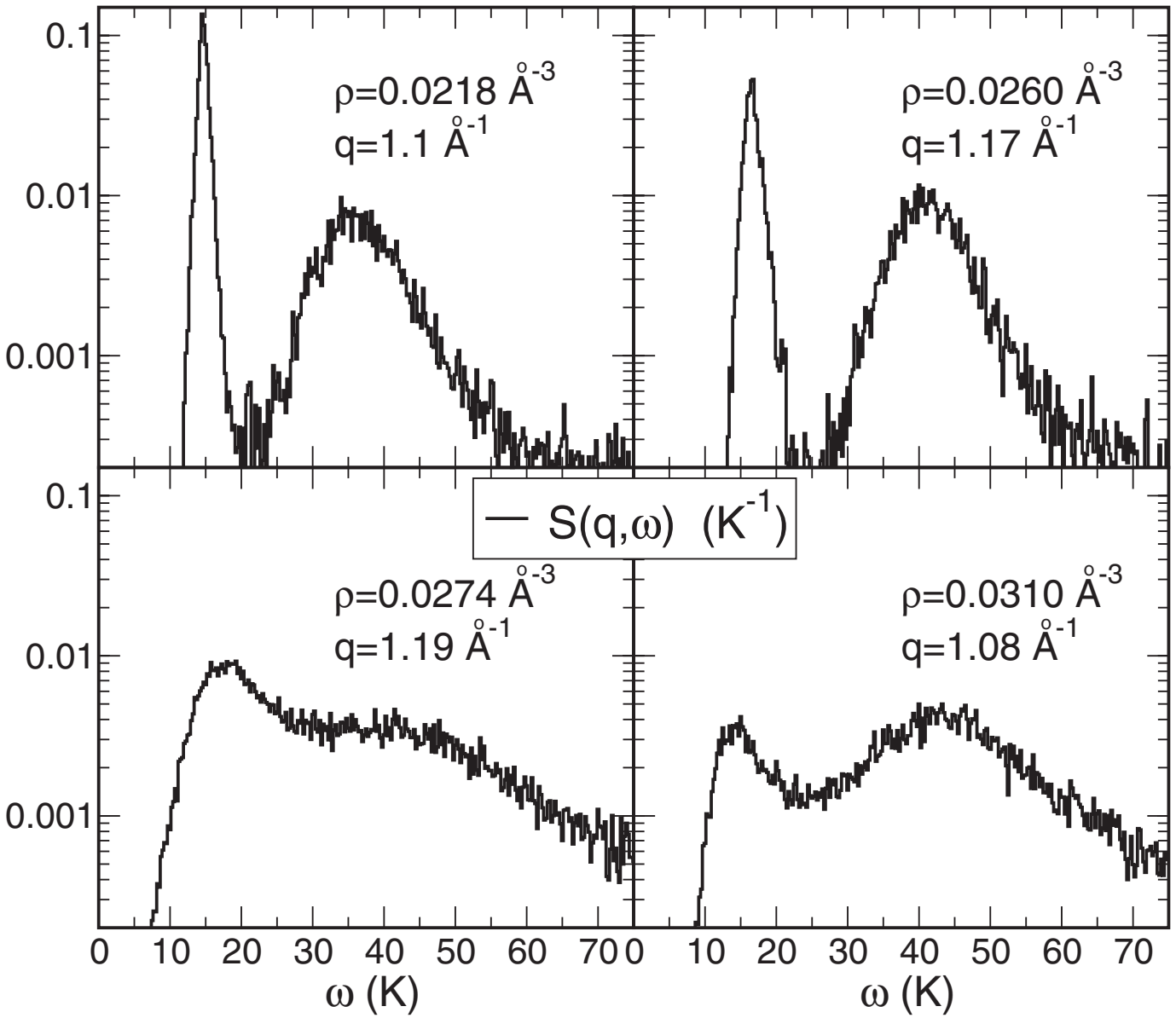
$N_b(i)$: neighbous of the *i*-th particle

$\tilde{N}_b(i)$: $N_b(i)$ + *i* itself

$$\bar{q}_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |\bar{q}_{lm}(i)|^2}$$

For recognize between liquid, bcc, fcc, hcp phase is enough to consider the $\bar{q}_4 - \bar{q}_6$ plane

Results: maxons



The well defined **maxon peak disappears** at densities **above freezing**
(ρ = 0.027 Å^{-3})

Agreement with experiments [Pearce et al PRL 2004]

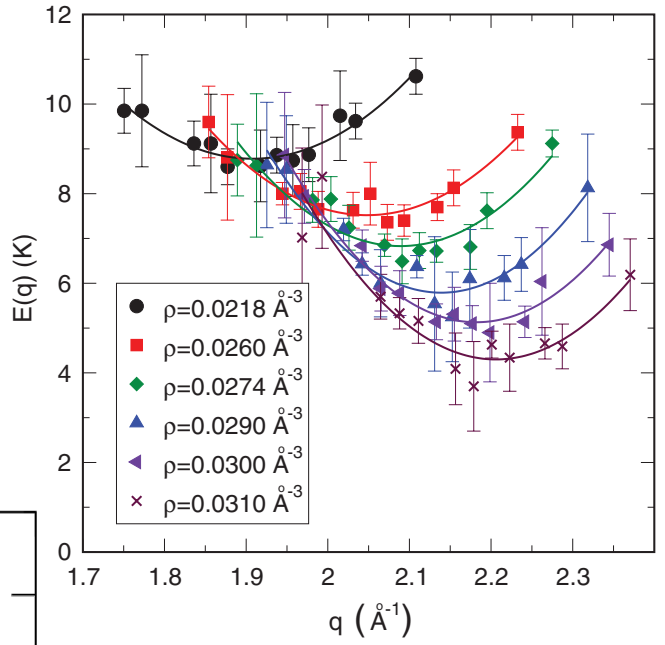
Results: rotons

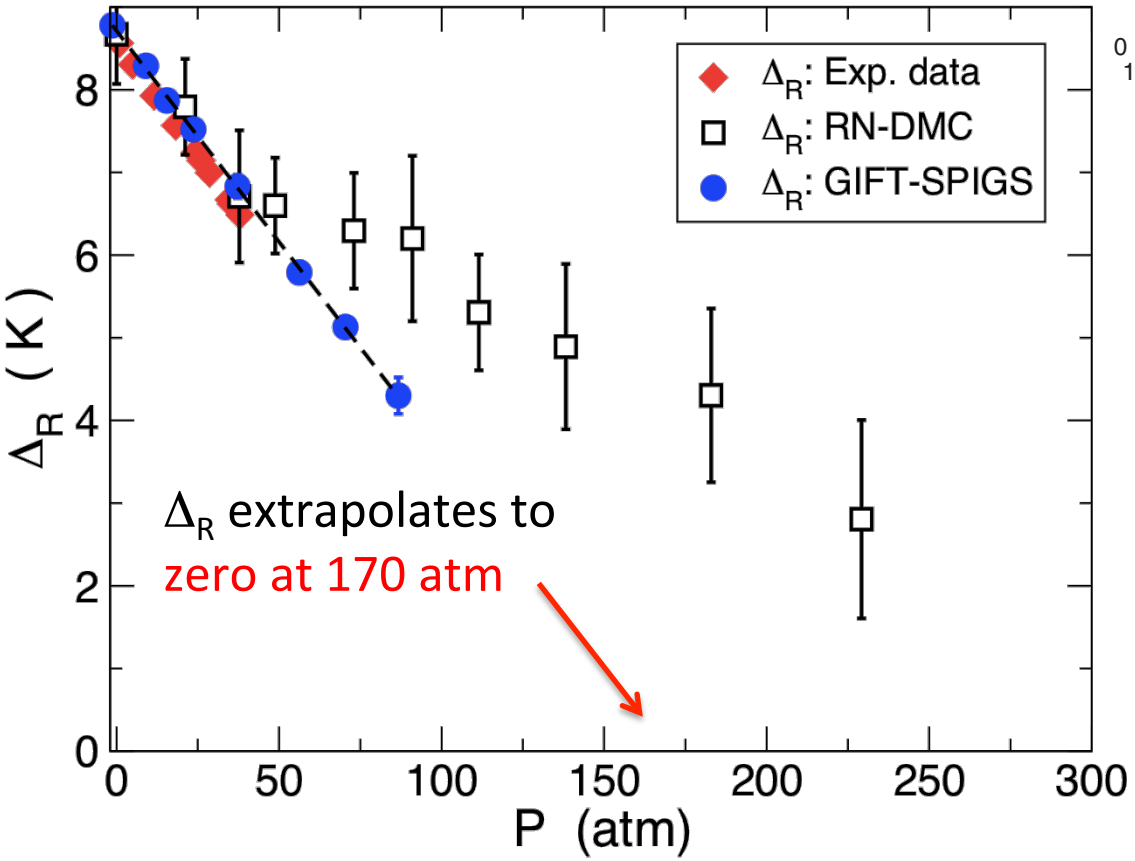
roton minimum decreases with increasing P

- Fitted with Landau formula

$$E(q) = \Delta_R + \frac{\hbar^2}{2\mu_R}(q - q_R)^2$$

- Δ_R has a linear trend with pressure

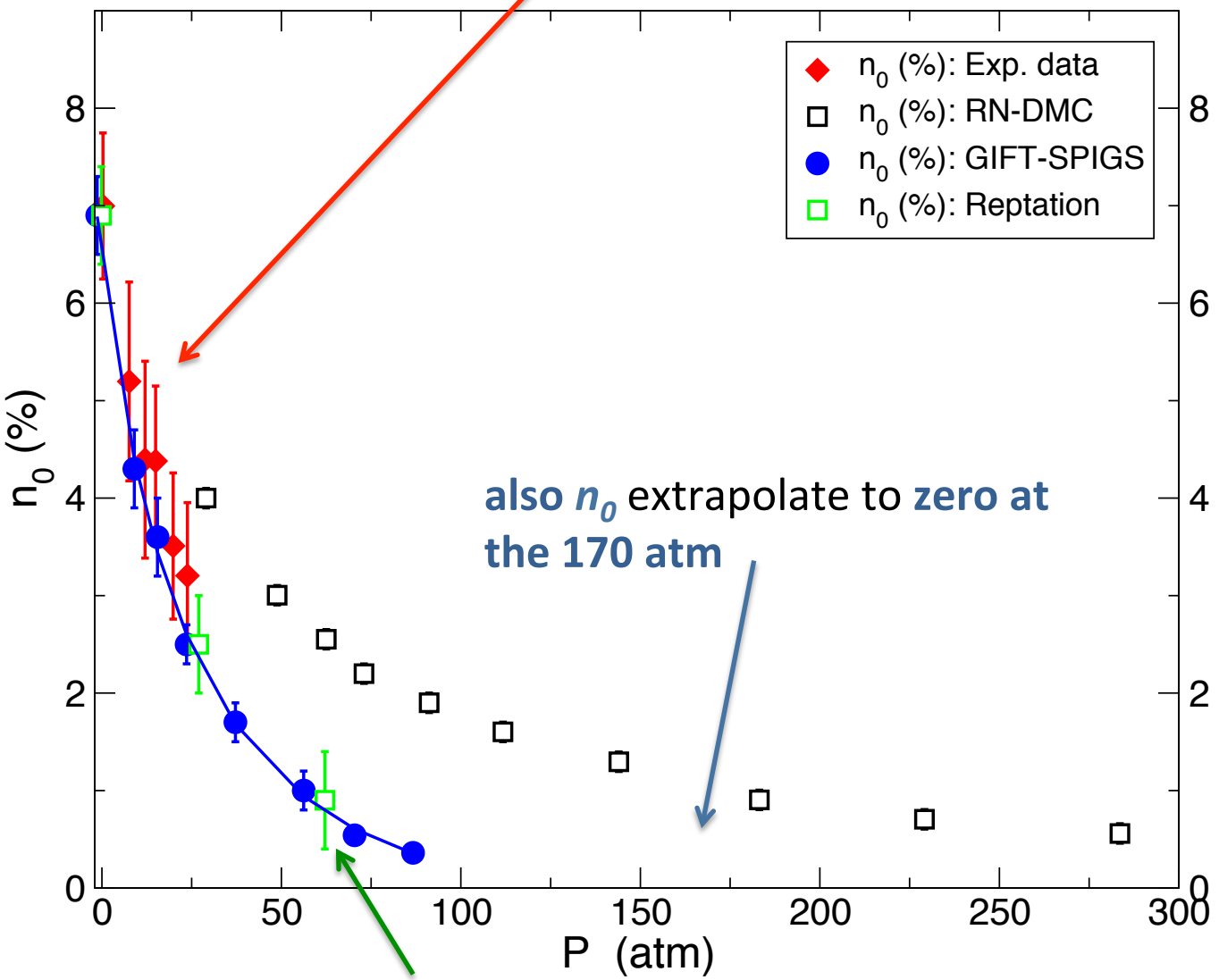




Agreement with experiments

[Pearce et al PRL 2004]

Results: condensate fraction



n_0 in agreement with independent PIGS results

[Moroni & Boninsegni JLTP 2004]

Problem #3: topological excitations

- Class of excitations of fundamental interest in many ordered systems in cond.mat.

- One of the most studied is a **vortex in a Bose superfluid**
  - Intimately related to the superfluidity iteslf (related to critical velocity…)
  - Relevant for **quantum turbulence**
    - Reconnection of vortex lines
    - Pinning of impurities…

question Can we give a microscopic description of a vortex line with PIGS?

The wave function **must be** an **eigenstate** also of the **angular momentum** $\hat{L}_z$

with eigenvalue $\hbar N l$ (l = 1, 2,... quanta of circulation)

We need an explicit **many-body phase Ω(R)** related to the velocity field

$$\vec{v}(R) = \frac{\hbar}{m}\vec{\nabla}\Omega(R)$$

problem If we try to project with PIGS $\psi_T(R) = e^{i\Omega(R)}\,|\psi_T(R)|$ we are led to face very soon sign problems...

We need an exit strategy!

The Madelung transformation $\psi_T(R) = e^{i\Omega(R)} |\psi_T(R)|$

leads to two coupled differential equation equivalent to the Schrödinger one

$$-\hbar \frac{\partial \Omega}{\partial t} = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \left(i\nabla_j^2 \Omega + 2i\vec{\nabla}_j \Omega \cdot \vec{\nabla} \log |\psi_T| \right)$$

$$i\hbar \frac{\partial |\psi_T|}{\partial t} = \hat{H} |\psi_T| + \frac{\hbar^2}{2m} \sum_{j=1}^{N} \left(\vec{\nabla}_j \Omega \right)^2 |\psi_T|$$

Fixed Phase approximation: chose a functional form for Ω, and **solve only** the equation for $|\psi_T|$

- The equation for $|\psi_T|$ is the **Schrödinger equation** for our many body system **with a static external potential**: can be **exactly solved** with PIGS!

Note:

It is an approximation! The result is not exact, since it relies on a variational ansatz on the phase…

- **variational upper bound** for the energy
- lowest energy consistent with the prescribed Ω

…there are other approximations (like Fixed Nodes…) [Giorgini et al PRL 1996]

Simplest choice for Ω: Feynman – Onsager

The simplest choice for the phase Ω that fulfills the prescriptions on the wave functions is the **Feynman – Onsager** one

$$\Omega^{OF}(R) = l \sum_{i=1}^{N} \theta_i$$

l=1,2,... quanta of circulation
θ_i angular polar coordinate of the i-th particle

- introduces the standard centrifugal flow field
- the external static potential potential reads

$$V_e^{OF}(R) = \frac{\hbar^2 l^2}{2m} \sum_{i=1}^{N} \frac{1}{\rho_i^2}$$

ρ_i radial polar coordinate of the i-th particle

note

The OF-phase is largely used not only in QMC studies of vortex lines, but is at the basis also of all the mean field studies (Gross-Pitaevskii, Density Functional...)

[Pitaevskii JETP 1961; Gross NC 1961; Fetter PR 1965; Dalfovo PRB 1992;...]

Simplest choice for the phase: Feynman – Onsager

To avoid energy divergences at the vortex line, Feynman suggested the introduction of a one-body term in the wave function that vanishes as $\rho_i \to 0$, thus, by construction, the OF-phase gives an **hollow vortex core**

Feynman – Onsager prescription for the wave function

$$\psi_T^{OF}(R) = e^{il\sum_{j=1}^{N}\theta_j} \prod_{j=1}^{N} f(\rho_j)\psi_T(R)$$

the same as for ground state studies

$$f(\rho) = 1 - e^{-(\rho/a)^2}$$

Variationally optimized functional form for *f*
a: core parameter

[Chester et al PR 1968]

Used with:

- Variational Monte Carlo (SWF) for a vortex in ^{4}He [Vitiello et al PRB 1996]
- Variational Monte Carlo (JWF) for a vortex in a Bose gas [Nilsen et al PRA 2005]
- Diffusion Monte Carlo (DMC) for a vortex in a ^{4}He droplet [Sola et al PRB 2007]

Can be used also at finite temperature

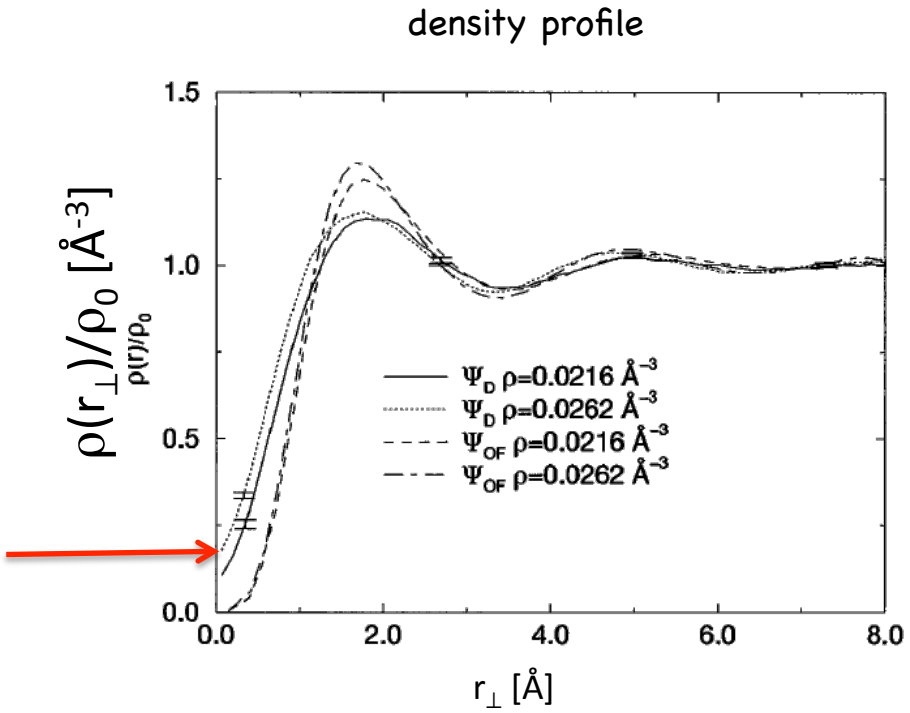
- PIMC for a vortex in a a ^{4}He droplet [Draeger PhD thesis 2001]
- PIMC for a vortex in ^{4}He [Takagi, PhysicaB 2003]

there is a diffuse conviction **that the core of a quantum vortex must be hollow**

question

The empty core is an artifact of the variational ansatz on the phase or is a real feature of a quantum vortex?

With **SWF** it was possible to obtain a **partially filled core** with a (little) **gain in energy**
[Vitiello et al PRB 1996; Sadd et al PRL 79; Sadd et al PRL 1999]



Delocalized vorticity by writing the OF phase on the auxiliary variables

Within the variational point of view this is a **better ansatz**

question

Can we go beyond the OF phase?

Beyond OF: backflow corrections

Ortiz & Ceperly have devised a **scheme to improve** iteratively **the phase** of a many-body wave function: applied to the OF it generates **backflow corrections**

[Ortiz & Ceperley PRL 1995]

$$\psi_T(R)^{BF} = \prod_{j=1}^{N} \left[\frac{\zeta_j + \kappa \sum_{k \neq j} f(r_{jk}, \rho_j, \rho_k)(\zeta_j - \zeta_k)}{\rho_j + a} \right]^l \psi_T(R)$$

the same as for ground state studies

where $\zeta_j = x_j + i y_j$

$f(r_{jk}, \rho_j, \rho_k) = e^{-\left[\alpha r_{jk}^2 + \gamma(\rho_j + \rho_k)^2\right]}$ backflow function

$a, \kappa, \alpha, \gamma$ variational parameters

note

There exist two exact QMC studies with BF wave function

- Green Function Monte Carlo [Ortiz & Ceperley PRL 1995]
- Diffusion Monte Carlo (but with Fixed Node Approx.)

[Giorgini, Boronat, Casulleras PRL 1996}

both for a 2D vortex in ^{4}He

- small gain in energy (few percent)

BUT

- GFMC has a partially filled core, DMC an hollow one **???**

CASE #3: vortex line in ^{4}He

Rossi, Galli, Salvestrini & Reatto, JPCS 2012
Galli, Reatto & Rossi… under progress

- **"Exact"** (for the modulus) **QMC** simulations for vortices in ^{4}He only in 2D (where the vortex is a point defect) with **conflicting results**
- QMC simulation **in 3D only** at a **full variational** level (both on phase and on modulus) with SWF suggesting a partially filled core
- Possible importance of vortices also in the solid phase in connection with supersolidity [Anderson Nature 2007; PRL 2008; Penzev et al PRL 2008]
  No studies of vortices in the solid phase in literature…

simulation details

- ψ_T **= SWF**
- **pair-Suzuki** ($\delta\tau = 1/320$ K^{-1}) & **primitive** ($\delta\tau = 1/$ K^{-1}) approx. for $\hat{G}$
- $\tau = 0.125$ K^{-1}
- Both **OF & BF** phases
- $0.0200 < \rho < 0.03$ Å^{-3} ($-6 < P < 70$ atm)
- $N = 336$ ^{4}He atoms **with…. pbc???**

problem

The external potential is long ranged ($1/r^2$), we cannot resort to standard pbc

… the velocity field will have a sudden jump at the boundary

Possible solutions:

- Confine the system [Ortiz & Ceperley 1995; Vitiello et al 1996; Nielsen et al PRA 2005; Sola et al PRB 2007]
- Simulate a vortex lattice [Sadd et al PRL 1997; PRL 1999]
- Use same tricks on the phase [Giorgini et al PRL 1996]

Our solution: **smooth the flow field**

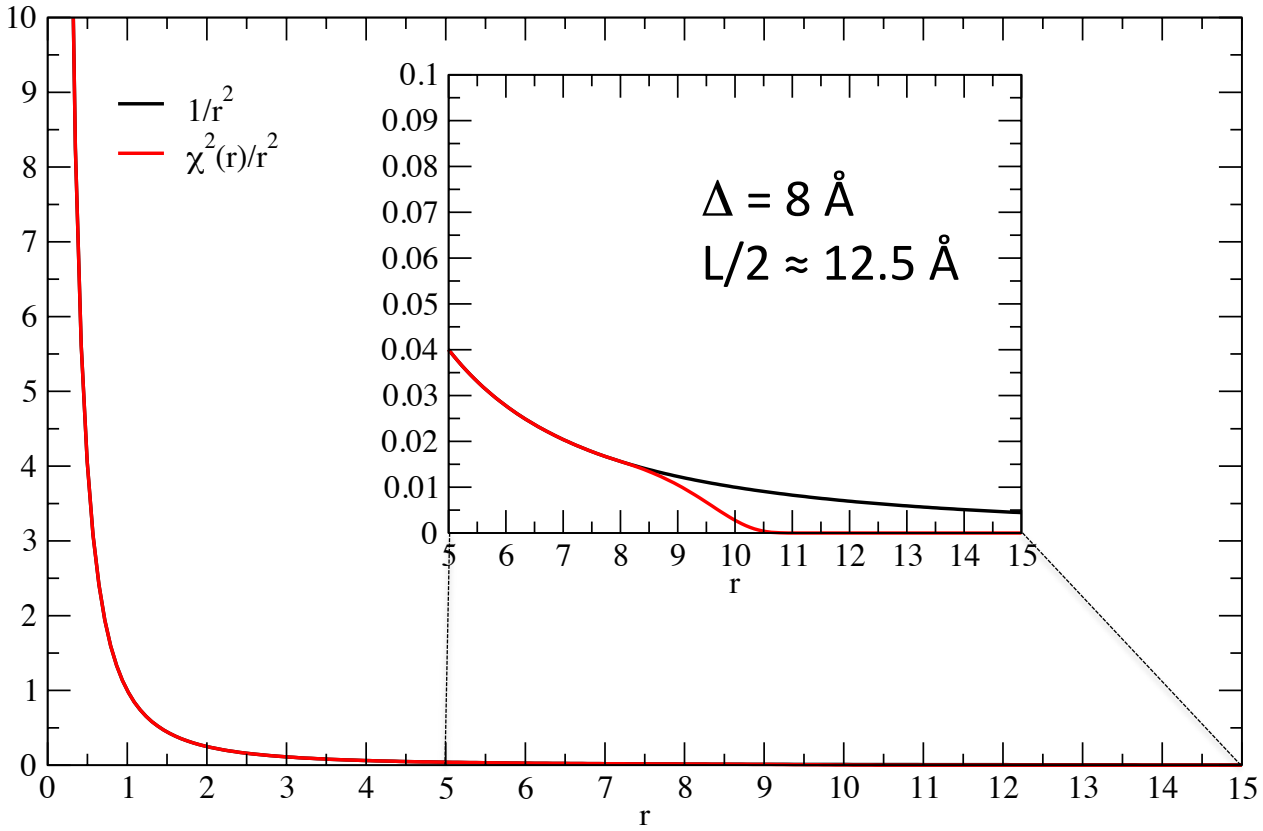
We multiply the leading term 1/r in the phase Ω by the smoothing function

$$\chi(\rho) = \begin{cases} 1 & \rho < \Delta \\ e^{-\left(\frac{\rho-\Delta}{\rho-L/2}\right)^2} & \Delta \leq \rho \leq L/2 \\ 0 & \rho > L/2 \end{cases}$$

L being the side of the simulation box, and Δ = 8 Å

notes

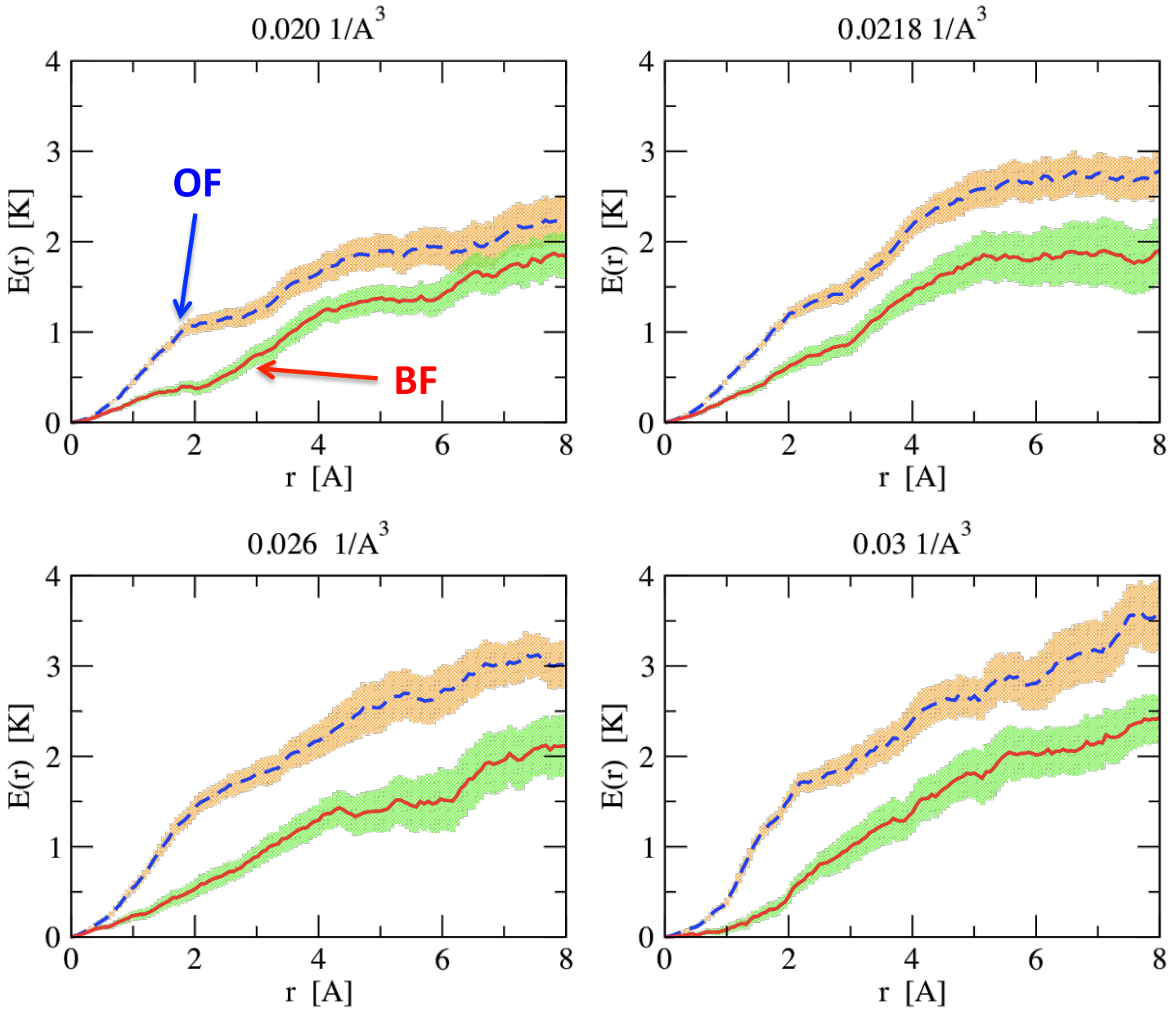
- With this choice our wave function is no more an exact eigenstate of the angular momentum, but it is close to it in the region of interest (around the core)



- As in SWF previous study, we do not have any core parameter at all, we project the same SWF that we usually use in bulk simulations (no extra factor are added).

diagonal results

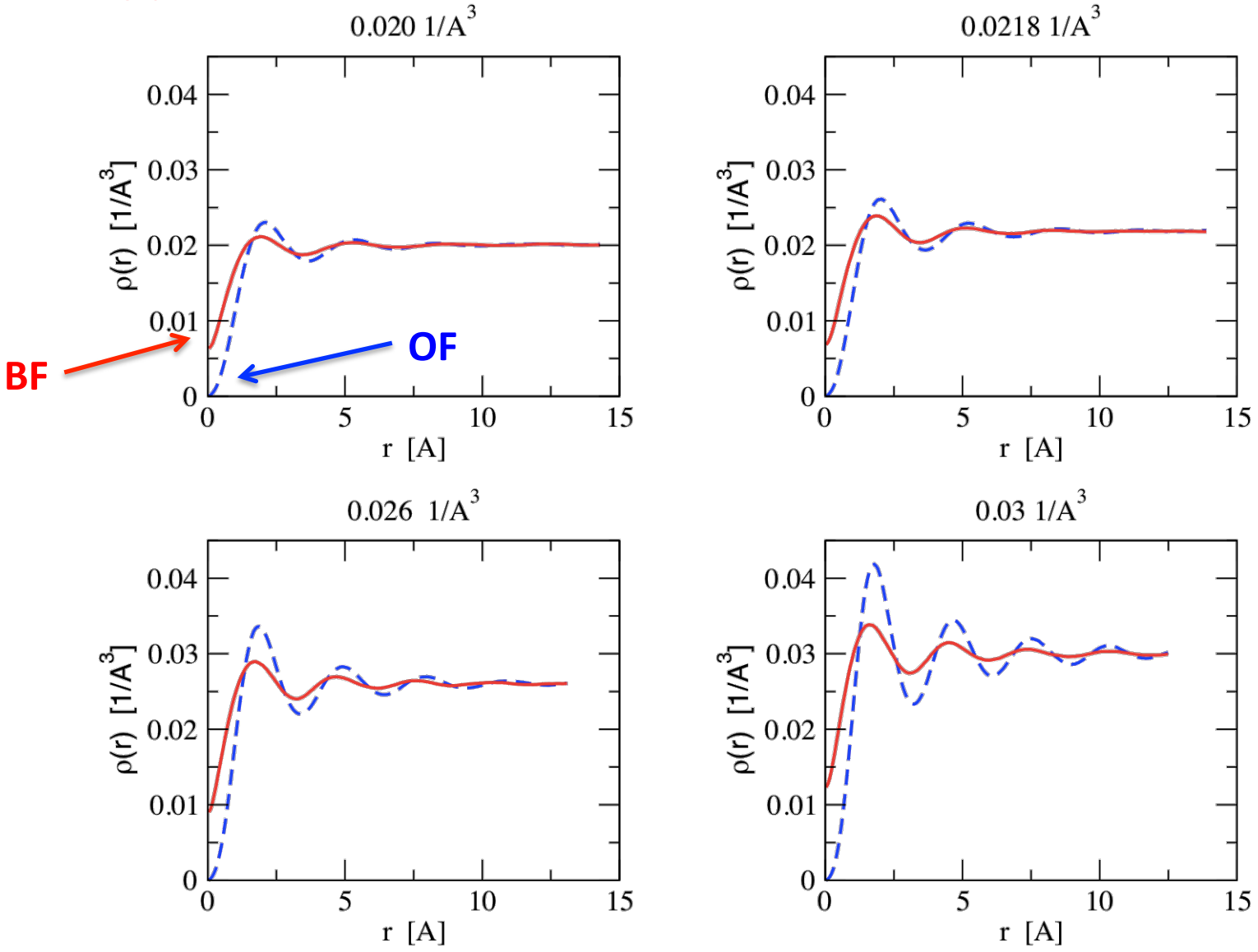
Integrated energy per unit length of a straight vortex line



BF phase is variationally **better**

diagonal results

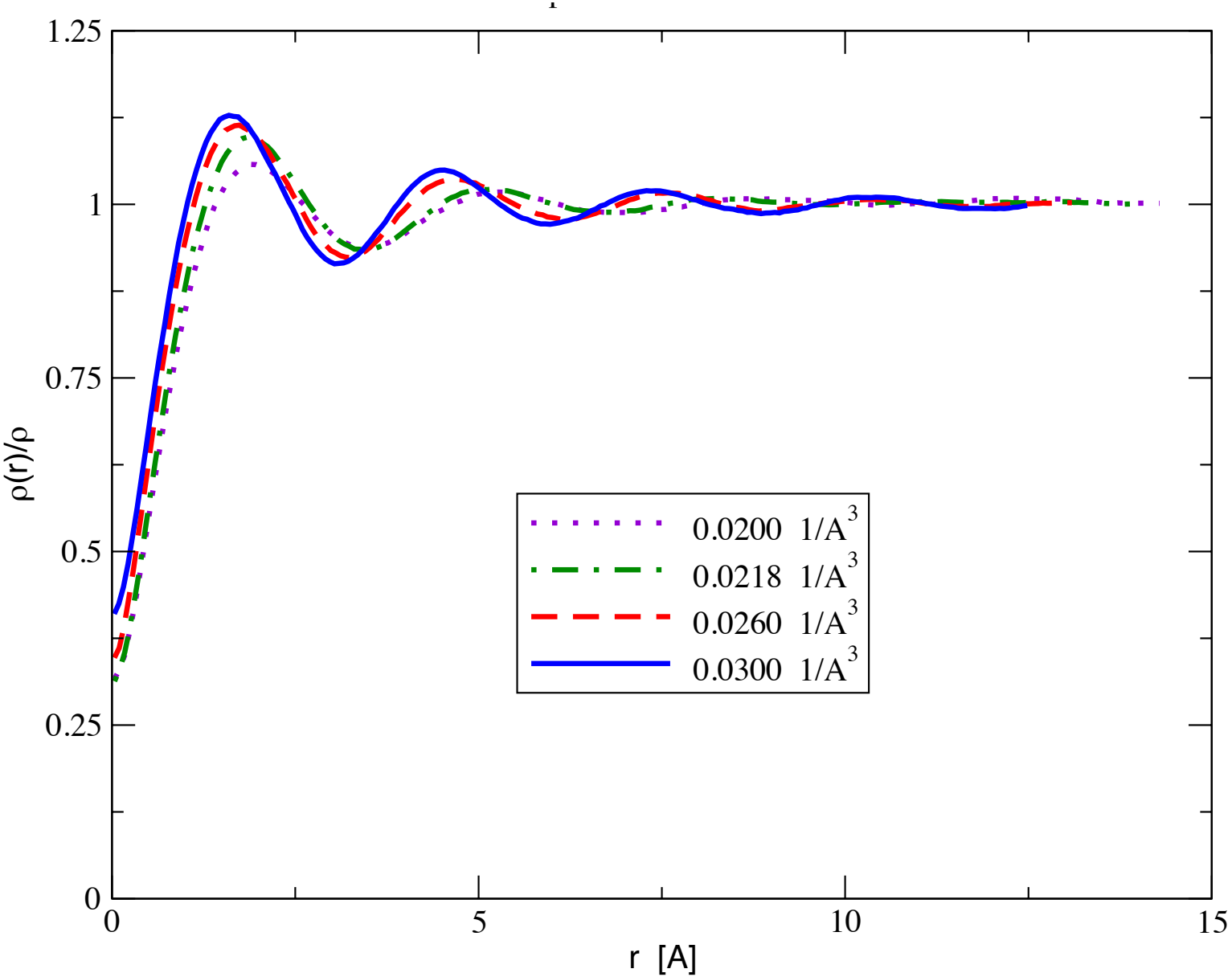
Density profiles



With **BF** the **core** is **no** more **hollow** (as for GFMC in 2D and SWF in 3D)

diagonal results

BF effects are larger at larger densities



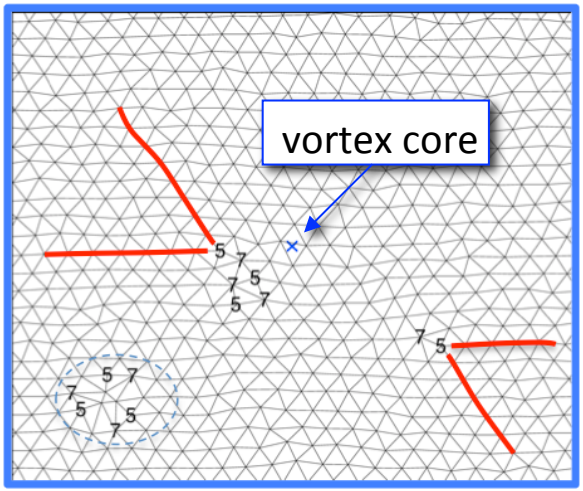
question

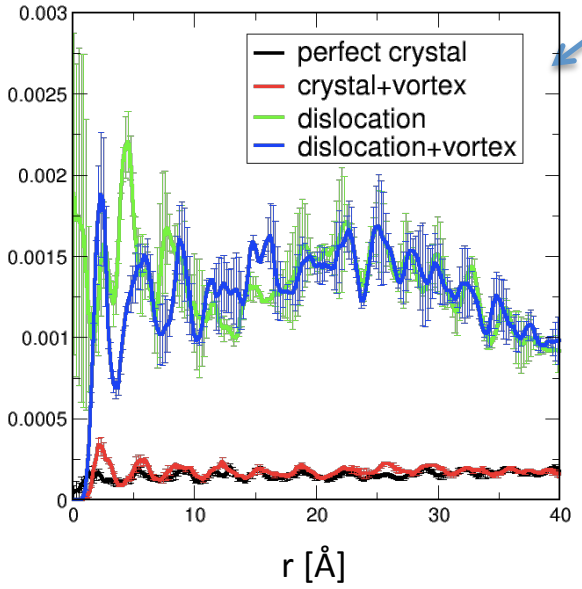
What happens in the solid phase?

Sim. details

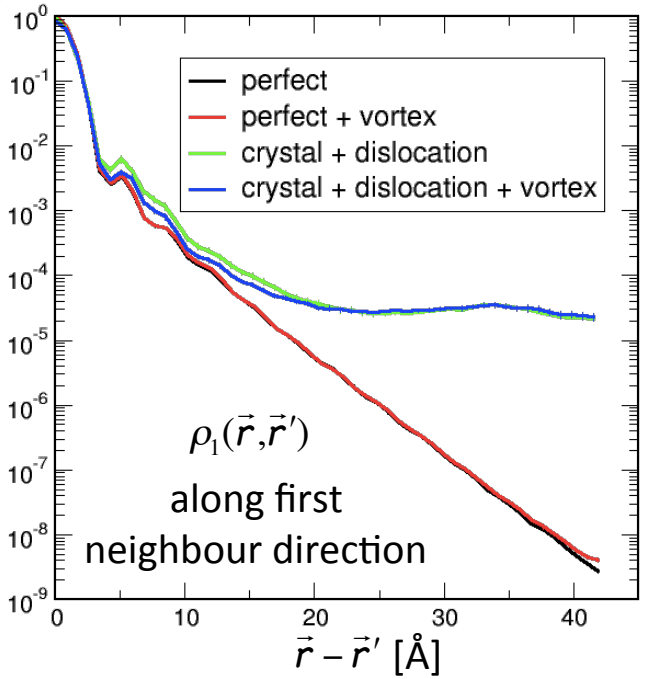
- N = 572
- Δ = 30 Å
- Pair-Suzuki approx. for $\hat{G}$
- τ = 0.83 K^{-1}
- $\delta\tau$ = 1/240 K^{-1}
- density: 0.0765 $Å^{-2}$

Little parenthesis:
Vortex in solid 2D ^{4}He with FO phase ansatz





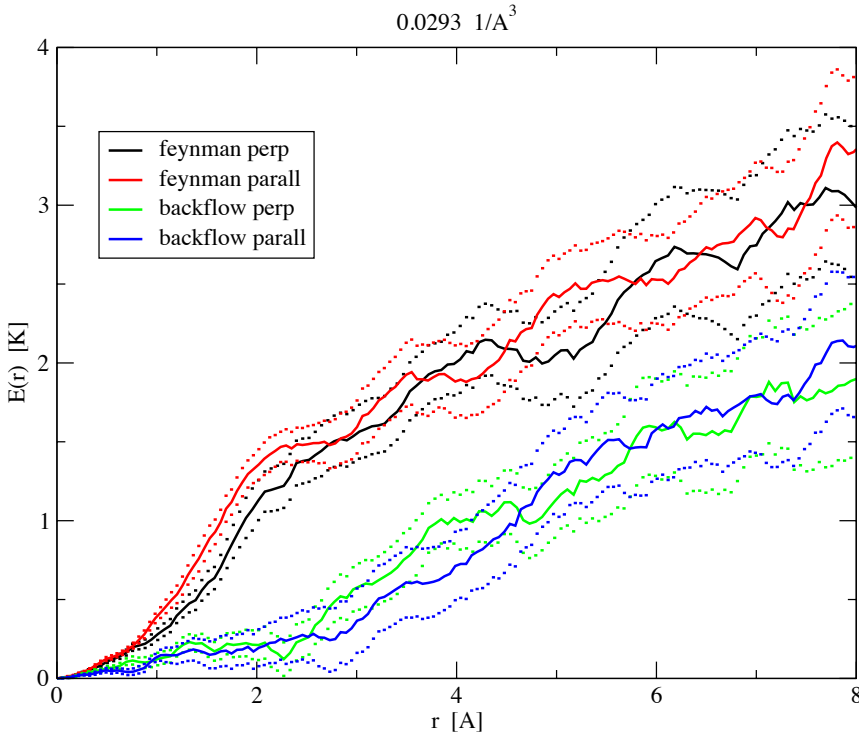
- vortex core found in interstitial position
- vortex does not sensibly affect crystal structure
- true even with defects: no effect on the density of ill-coordinated atoms



- Vortex does not affect either the **off-diagonal** properties

REM: with no BEC we cannot speak about quantized vortices…

Vortex line in 3D solid ^{4}He

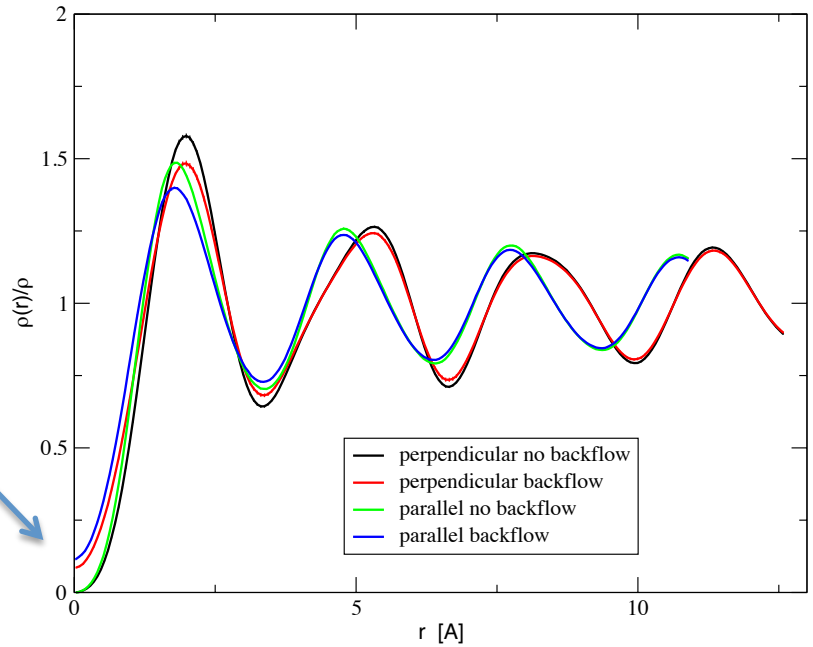


Two different orientations for the vortex line:

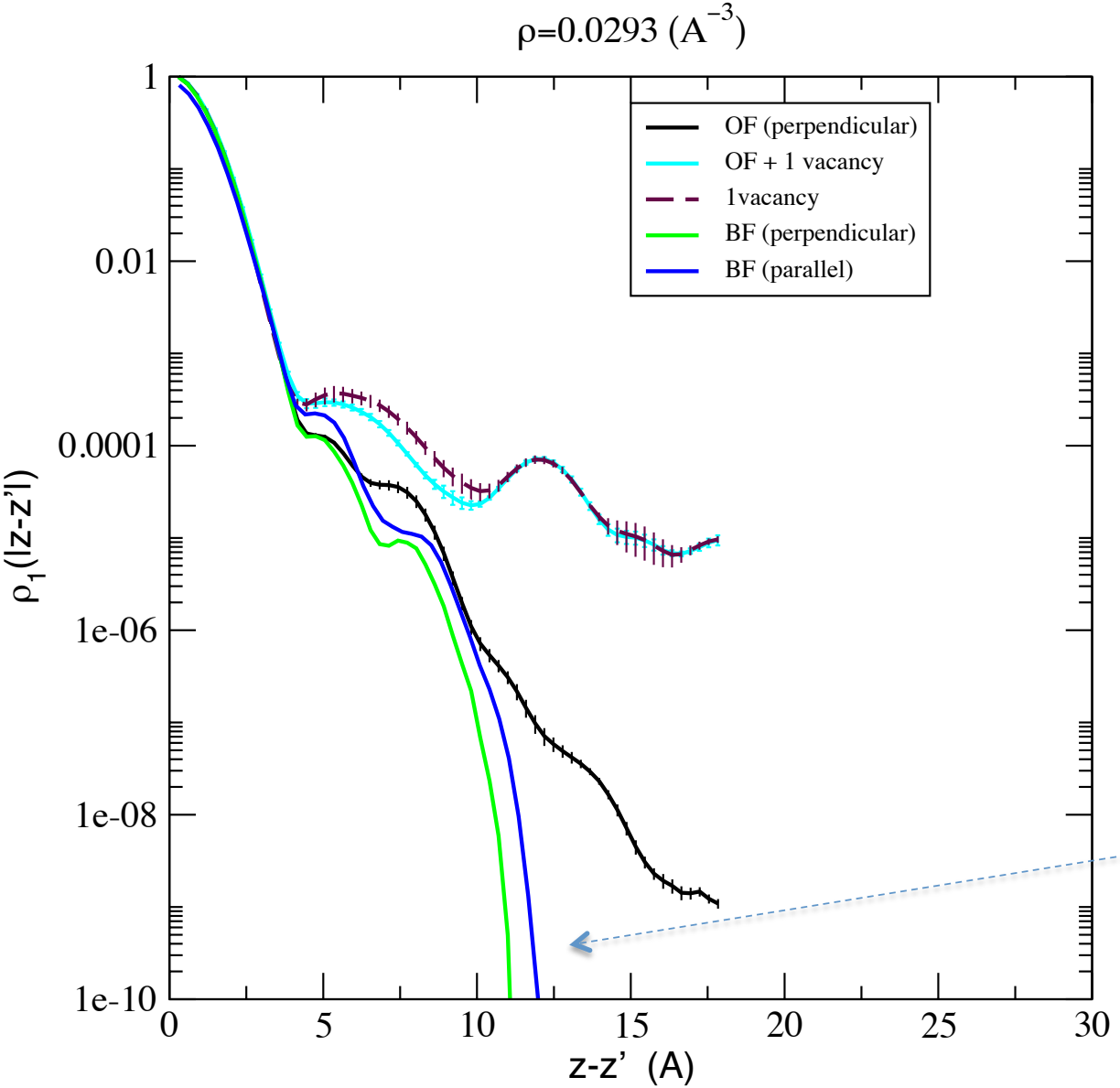
- Perpendicular to the basal plane (c-direction in hcp crystal)
- Parallel to the basal plane

In both the cases **BF** corrections provide a **gain in the energy**

Even in the solid phase the core is not hollow



What about off-diagonal properties?



No BEC !!!

The vortex is not able to induce BEC, thus is **not able to self-sustain** in the solid phase

Not concluded yet…
But these lines come from months of simulations, and we believe that (even going on) no plateau will be reached at all.

Conclusions

- **PIGS** is really **free from** any **variational bias** due to the choice of ψ_T
  - the "only" role of ψ_T is to fix the length of the imaginary time projection
  - **projection** procedure **removes wrong correlations** and **inserts** the **missing ones**
  - each observables has its own convergence time
- **PIGS + GIFT** provide also the **excitation spectrum via the inversion** of imaginary times correlation functions
  - the result is not "The Result" because of the servere ill-posedness of inversion problems
  - good agreement with experimental results
- **PIGS + FA** allow to study **vortices**

2D ^{4}He crystal

- **perfect crystal** can**not** be **superfluid** (no BEC)
- the effect of confinement extends mainly in a layer of width about 15Å
- the inner region displays a crystalline order similar to the bulk crystal with pbc & even if defects are placed in, they are expelled into the interfacial region
- actual simulations put an upper bound of 3 10^{-3} to the concentration of defects in the inner region… larger systems?

overpressurized ^{4}He

- liquid ^{4}He up to 87 atm
  - beyond this pressure the solid nucleates rapidly in system…
- **Maxons disappear** above the freezing density
- **Roton** minumum **decreases** with increasing pressure **with a linear trend**
  - extrapolates to zero at about 170 atm
- The condensate fraction $\mathbf{n_0}$ extrapolates to **zero** at the **same pressure**

Vortex line in ^{4}He

- **Backflow** corrections are a **variationally better ansatz** than the Onsager-Feynman prescription
- The vortex **core** is **not hollow**
- The filling fraction increases with increasing density
- vortex in solid ^{4}He
  - Does not affect structural properties
  - No correlation with defects
  - No BEC induced: such a vortex cannot self-sustain

Thanks for your attention