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Microsocopic studies of He-4 solid systems via Path Integral projection methods

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Microscopic studies of ^{4}He solid systems via Path Integral projector methods

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Sede centrale: facciata lungo largo Richini

Sede centrale: cortile del Richini

In collaboration with

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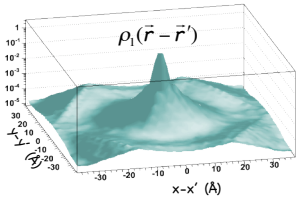

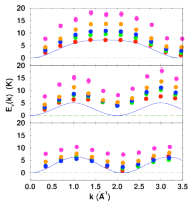

Outline

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Path Integral T=0 K projector methods:

- Study of pure 2D solid ^{4}He:
  - Perfect crystal
  - Crystal with increasing number of vacancies
- 3D: hcp solid ^{4}He
- Dynamics form QMC a genetic algorithm approach
  - Excited states in liquid ^{4}He also with one ^{3}He impurity
  - Excited states in solid ^{4}He also with vacancies and with one ^{3}He impurity
- Conclusions

The Abdus Salam International Centre for Theoretical Physics - Workshop "Supersolid 2008" - 21.08.08

Projector QMC methods: Path Integral Ground State

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

- Aim of projector Quantum Monte Carlo (QMC) methods: evaluate "exact" (within statistical uncertainty) T=0 K, i.e. ground state, averages $\langle \psi_0 | \hat{O} | \psi_0 \rangle$ being ψ_0 the ground state wave function
- How? First ψ_0 is expressed formally as the imaginary time evolution of a trial variational state

$$\psi_0(R) = \lim_{\tau\to\infty} \int dR' \left\langle R \left| e^{-\tau\hat{H}} \right| R' \right\rangle \psi_T(R') \qquad \left(\langle \psi_0 | \psi_T \rangle \neq 0\right)$$

$R \equiv \{\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N\}$ Many-body coordinate

$G(R,R',\tau) = \left\langle R \left| e^{-\tau\hat{H}} \right| R' \right\rangle$ Imaginary-time propagator

- Then one uses the exact property $e^{-\tau\hat{H}} = \left(e^{-\frac{\tau}{P}\hat{H}}\right)^P$ to obtain the Path Integral representation of G(R,R',τ):

$$\psi_0(R) = \lim_{\tau\to\infty} \int dR_1 \cdots dR_P \left\langle R \left| e^{-\frac{\tau}{P}\hat{H}} \right| R_1 \right\rangle \times \cdots \times \left\langle R_{P-1} \left| e^{-\frac{\tau}{P}\hat{H}} \right| R_P \right\rangle \psi_T(R_P)$$

Projector QMC methods: Path Integral Ground State

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

- Approximation 1: finite imaginary time propagation

$$\psi_0(R) \cong \psi_\tau(R) = \int dR_1 \cdots dR_P \left\langle R \left| e^{-\frac{\tau}{P}\hat{H}} \right| R_1 \right\rangle \times \cdots \times \left\langle R_{P-1} \left| e^{-\frac{\tau}{P}\hat{H}} \right| R_P \right\rangle \psi_T(R_P)$$

- Approximation 2: if δτ=τ/M is small, use accurate approximations for the short-time propagator G(R,R',δτ): e.g. Pair-Product (Ceperely, RMP '95)

  this second approximation is exactly the one used in any finite temperature PIMC calculation
- Therefore any PIGS calculation is characterized by two numbers:
  - Value of τ : the total imaginary-time
  - Value of δτ : the "elementary" imaginary-time evolution/projection step

$$\psi_0(R) \xrightarrow[\text{choice of } \tau]{} \psi_\tau(R) \xrightarrow[\text{choice of } \delta\tau]{} \tilde{\psi}_\tau(R)$$

Usually, one first determines how small must be δτ in order to use approximation 2, then increases τ until convergence is reached: if δτ and τ are properly chosen the exact value will be within the statistical uncertainty

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Projector QMC methods: Path Integral Ground State

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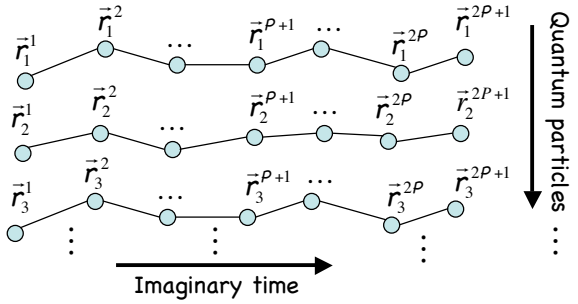
- Classical-Quantum mapping:

$$\frac{\langle\psi_0|\hat{O}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} \cong \int \prod_{i=1}^{2P+1} dR_i \; \hat{O}(R_{P+1}) \frac{\psi_T(R_1)\prod_{j=1}^{2P} G(R_j, R_{j+1}, \frac{\tau}{P})\psi_T(R_{2P+1})}{\langle\tilde{\psi}_\tau|\tilde{\psi}_\tau\rangle}$$

$$p(R_1,\cdots,R_{2P+1})$$

Ground state averages are equivalent to canonical averages of a classical system of special interacting linear polymers:



- P projections: linear polymers with 2P+1 atoms
- Monte Carlo sampling (Metropolis) of 3N·(2P+1) degree of freedom

$\vec{r}_{i=1,N}^{\,l=1,2P+1}$ ← imaginary time; ← particle

Variational theory of a quantum solid

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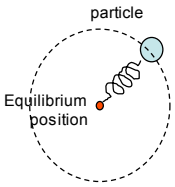
In the framework of variational theory of quantum solids the wave functions fall in two categories:

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

$$\psi_{JN}(\vec{r}_1,..,\vec{r}_N) = \psi_J \times \prod_i^N e^{-C|\vec{r}_i - \vec{R}_i|^2}$$

(Jastrow+Nosanow)



→ Sum over permutation to get Bose Symmetry

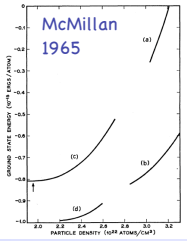
by construction this wave function describes a commensurate solid

2. translational invariant Ψ, first example:

$$\psi_J(\vec{r}_1,..,\vec{r}_N) = \prod_{i<j}^N f(|\vec{r}_i - \vec{r}_j|) \qquad f(r) = e^{-\frac{1}{2}(b/r)^5}$$

(Jastrow)

- b: variational parameter, minimize ⟨H⟩
- at high density Ψ_J describes a solid (spontaneous broken symmetry)



Second example: Shadow Wave Function

Our "exact" tool: Projector QMC from SWF to SPIGS

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- SWF: single (variationally optimized) projection step of a Jastrow wave function

Vitiello, Runge, Kalos, PRL '88

$$\psi_T^{SWF}(R) = \int dS\, F(R,S)\, \psi_T(S)$$

  - Implicit correlations (all orders)
  - Bose symmetry preserved
- SPIGS: "exact" T=0 projector method which starts from a SWF

Galli, Reatto, Mol. Phys. 101, 2003

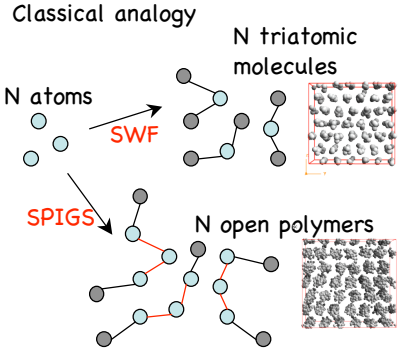
$$\psi_0(R) = \int dR_1 \cdots dR_P dS \left\langle R \middle| e^{-\frac{\tau}{P}\hat{H}} \middle| R_1 \right\rangle \times \cdots$$

$$\cdots \times \left\langle R_{P-1} \middle| e^{-\frac{\tau}{P}\hat{H}} \middle| R_P \right\rangle F(R_P,S)\psi_T(S)$$

  - Notice: unlike PIMC at finite T here no summation over permutation is necessary, this $\Psi_0(R)$ is Bose symmetric if Ψ_T is symmetric

Calculation of $\langle \psi_0 | \hat{O} | \psi_0 \rangle$

Classical analogy



The whole imaginary time evolution is sampled at each MC step

QMC: calculation of the one-body density matrix with SWF and SPIGS

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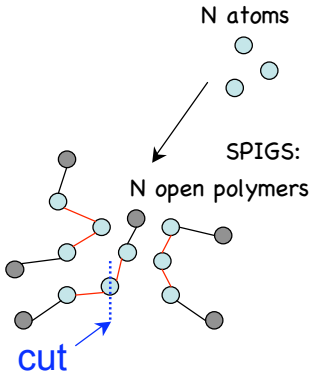
$$\rho_1(\vec{r},\vec{r}') = N \int d\vec{r}_2 \cdots d\vec{r}_N\, \psi_0^*(\vec{r},\vec{r}_2,\cdots,\vec{r}_N)\psi_0(\vec{r}',\vec{r}_2,\cdots,\vec{r}_N)$$

- One of the open polymers is cut and the histogram of the relative distance of the two cut ends is computed
- We have studied commensurate and incommensurate solid ^{4}He with SPIGS: the periodic boundary conditions forces the structure of the solid.
- No "mixed", only pure estimator (exact ground state ρ_1 if τ is large enough!)

Classical analogy:



(S)PIGS: Permutation sampling

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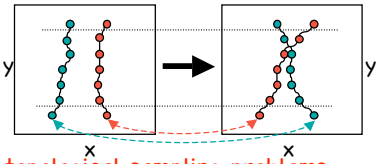
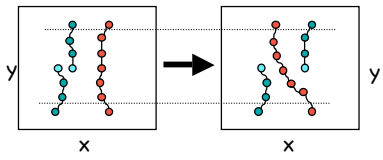
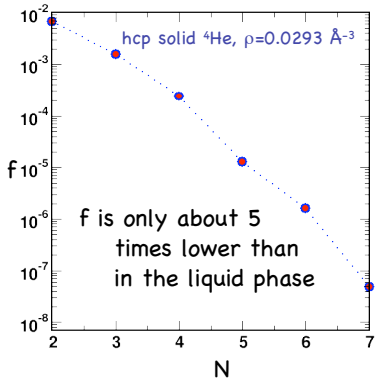
- projection procedure preserves the Bose symmetry if Ψ_T is Bose symmetric



- No topological sampling problems
- It is important for off-diagonal properties in the solid phase
- Sampling scheme: Boninsegni JLTP (2005)
- "swap" moves allowed in off-diagonal calculations: very high acceptance frequency also in the solid phase: about 15%



Off-diagonal calculation: frequency of an accepted permutation cycle with N polymers



Commensurate 2D ⁴He crystal

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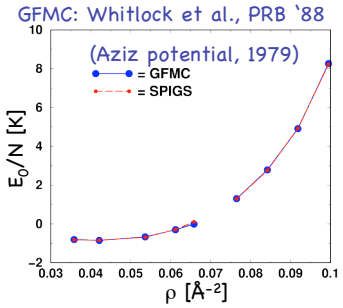
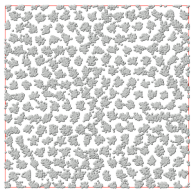
- We have studied pure 2D ⁴He at T=0 K
- Propagator: pair-product with $\delta\tau$=1/40 K^{-1}
- Eq. of state in agreement with previous GFMC calculations

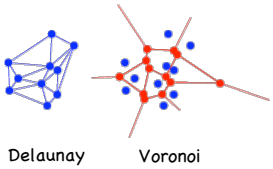
GFMC: Whitlock et al., PRB '88



Example: whole imaginary time evolution: τ=0.8 K^{-1} ⇒ each polymer counts 64 particles well defined crystal

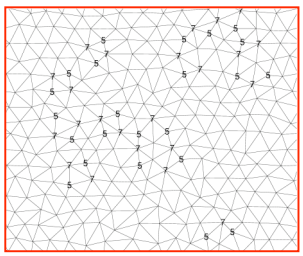


Analysis at a particular (imaginary)time:



Delaunay triangulation — Voronoi diagram

On average, about 18% of the atoms have a wrong (≠6) coordination number



"Exact" ground state methods use a trial function

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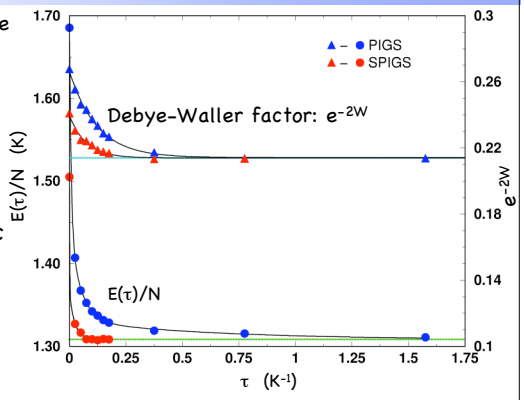
2D solid ^{4}He ρ=0.765 Å^{-2}, triangular lattice

- Is this biasing the results?
- We project on ψ_0 starting from two completely different wave functions:
  - a) a Jastrow-Nosanow :
    - not Bose symmetric
    - not translationally invariant
  - b) a SWF :
    - Bose symmetric
    - translationally invariant



From the τ evolution one can get the overlap $\left|\langle\psi_0|\phi_{trial}\rangle\right|^2$

Overlap per particle: 99.8% for SWF , deviation 0.2%
97.9% for JN , deviation 2.1%

SWF is closer to ψ_0 by one order of magnitude

One-body density matrix

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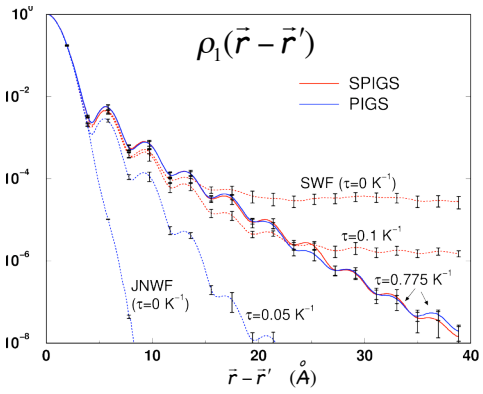
- Calculation of ρ_1 along nearest neighbor direction
- Triangular lattice, N=240
- Convergence of ρ_1 computed with SPIGS and PIGS for increasing projections in imaginary time
- Conclusion: convergence both for diagonal and non diagonal quantities from two radically different wave function
- The 2D commensurate crystal has no BEC
- No size effect (N=180,240,480)
- With PIGS we observe exponential decay up to 60 Å
- No ergodicity problem: study at fixed τ with decreasing $\delta\tau$ (increasing number of particles in the polymers) gives the same results

2D solid ^{4}He ρ=0.0765 Å^{-2}

(Vitali, Rossi, Tramonto, Galli, Reatto: PRB 2008)



Results: full ρ_1 and the momentum distribution

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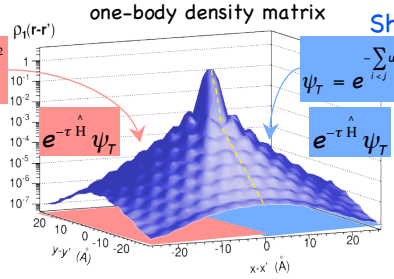
Jastrow-Nosanow:

$$\psi_T = e^{-\sum_{i<j} u(|\vec{r}_i - \vec{r}_j|)} \; e^{-\sum_{i=1}^{N} c|\vec{r}_i - \vec{R}_i|^2}$$

one-body density matrix



Shadow wave function:

$$\psi_T = e^{-\sum_{i<j} u(|\vec{r}_i - \vec{r}_j|)} \int dS \, e^{-\sum_{i=1}^{N} c|\vec{r}_i - \vec{s}_i|^2} \; e^{-\sum_{i<j} v(|\vec{s}_i - \vec{s}_j|)}$$

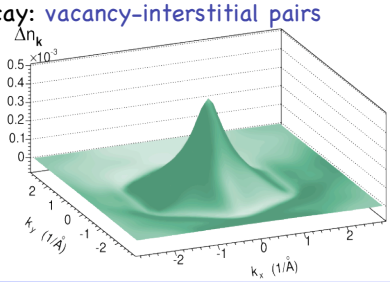
x-x'<0 : PIGS

x-x'>0 : SPIGS

PIGS & SPIGS indistinguishable within statistical uncertainty

We find NO BEC, ρ_1: dominant exponential decay in the large distance range.

Bumps over the exponential decay: vacancy-interstitial pairs



Deviation of the momentum distribution from the Gaussian

There is an excess of particles at low momenta up to k=1.2 Å^{-1}

whereas there is a deficit in the k-space region around k=1.6 Å^{-1}

Question: can we get away from using a trial wave function? Yes!

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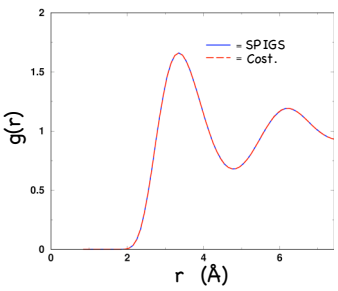
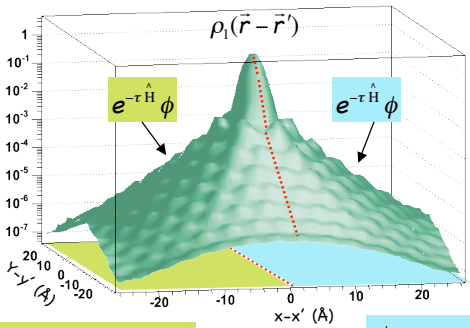
- Path Integral projector methods: the propagator does not depend on ψ_T
- Path integral ground state starting from an ideal gas wave function:

$$\psi_0 = \lim_{\tau \to \infty} e^{-\tau \hat{H}} \phi \qquad \text{when } \phi = \text{constant}$$

- Even in the solid phase we found again convergence of diagonal and off-diagonal properties!

radial distibution function





$\phi \equiv$ Jastrow-Nosanow

$\phi \equiv$ constant

ODLRO- Commensurate state: one-body density matrix SPIGS results

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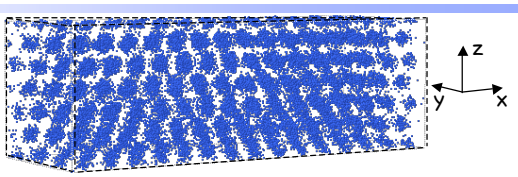
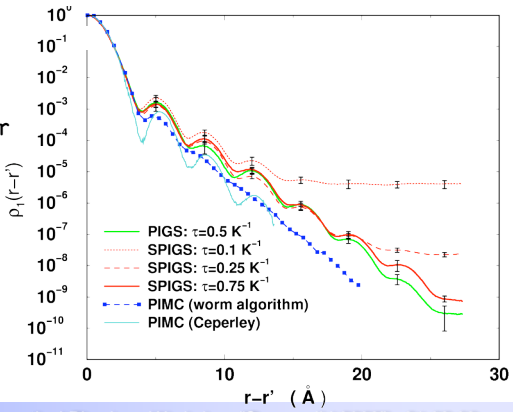
3D hcp solid ^{4}He

- Calculations of the one-body density matrix at T=0 K near melting density ρ=0.0293 Å^{-3}
- N=360
- Propagator: pair-product $\delta\tau$=1/40 K^{-1}
- Sampling along nearest neighbour direction
- Plateau dramatically reduced by the projection procedure
- Exponential decay up to about 27 Å
- Convergence essentially reached between SPIGS and PIGS





Solid ^{4}He: the end of the Andreev-Lifshitz-Chester scenario

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Boninsegni et al. PRL 97, (2006): study of hcp solid ^{4}He

- A uniform dilute gas of vacancies is thermodynamically unstable against separation into a vacancy-rich and a perfectly crystalline vacancy-free phase, which does not melt
- Three vacancies cluster easily and form a tight bound state

---

Recently we have started a systematic study of multiple vacancies in 2D and 3D solid ^{4}He

How can we identify where a vacancy is located?

1. Given a configuration $\{r_j\}$, find the best reference regular lattice $\{R_j\}$ which maximizes a Gaussian local density (In our algorithm the centre of mass is not fixed) $\rho_G = \sum_{j=1}^{N}\sum_{i=1}^{M} e^{-\alpha\left(\tilde{r}_j - \tilde{R}_i^*\right)^2}$
2. Find the vacancies with a coarse-graining procedure which associate particles to the nearest non "occupied" lattice sites
3. In the end vacancies are defined as unoccupied lattice positions

Vacancy-vacancy correlation functions

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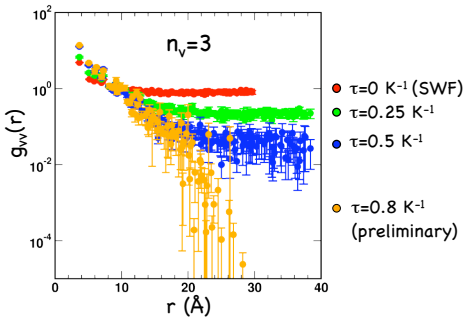
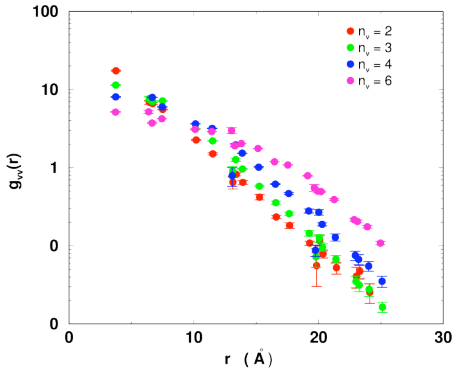
3D hcp solid ^{4}He ρ=0.0293Å^{-3}
(Propagator: pair-product, $\delta\tau$=1/40 K^{-1})
$g_{vv}(r)$ for a crystal with 3 vacancies with increasing projection-time
$g_{vv}(r)$: exponential decay+vanishing plateau with τ
⇒ probable bound state



2D triangular solid ^{4}He ρ=0.0765Å^{-2}
(Propagator: pair-product
τ=0.75 K^{-1} $\delta\tau$=1/40 K^{-1})
$g_{vv}(r)$: exponential decay
⇒ bound state up to 6 vacancies



Putative many vacancy states: do we still have vacancies?

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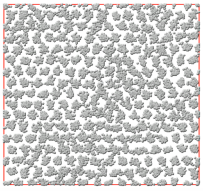
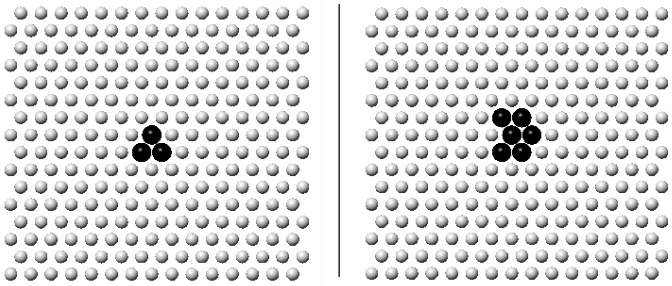
- Vacancies in 2D form a bound state
  (binding energy for 2 vacancies ≈1.5 K)
- Bosons with attractive interaction collapse
- Can vacancies be present in solid ^{4}He at low T?

N-3 Bosons are not equivalent to 3 Bosons
⇒ Why? Many body interactions

2D solid ^{4}He ρ=0.0765 Å^{-2}



Stochastic dynamics of a cluster of vacancies:
first 1000 MC steps;
only the reference lattice is shown (c. of mass is not fixed) and vacancies with black spheres where these are found every 50 MC steps



Many vacancies: two different regimes for 2D triangular crystal

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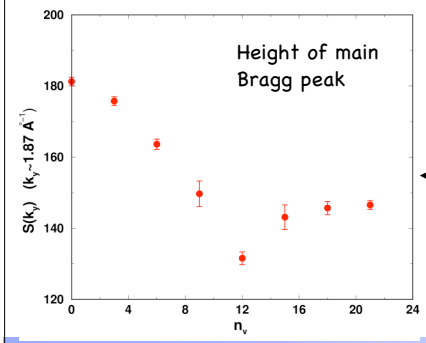
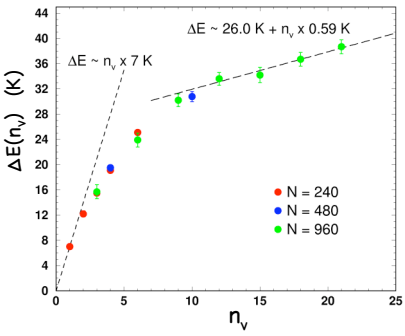
- Regime 1: Up to $n_v \approx 5$

  large energy ≈5 K per vacancy strong depression of cristalline order
- Regime 2: for $n_v \geq 10$

  small energy ≈0.6 K per additional vacancy, small effect on crystalline order





For n_v>12 the crystalline order starts to increase

Formation of linear structures, Line of atoms locally collapse ⇒ edge dislocations

Stochastic dynamics: many vacancies

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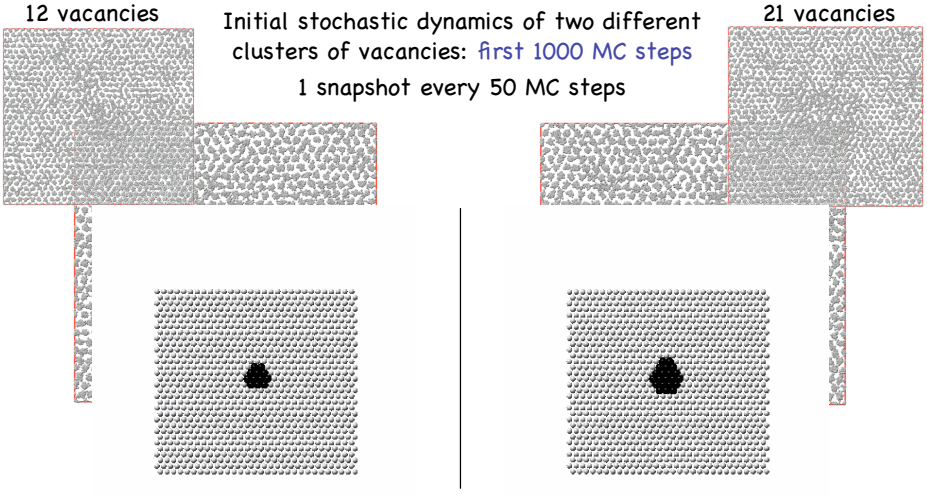
12 vacancies

Initial stochastic dynamics of two different clusters of vacancies: first 1000 MC steps

1 snapshot every 50 MC steps

21 vacancies



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Edge dislocations in 2D solid ^{4}He

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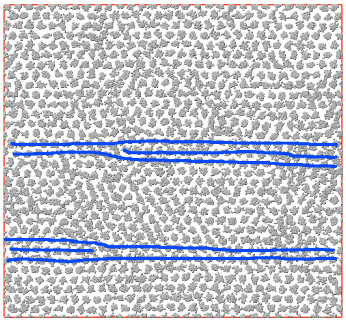
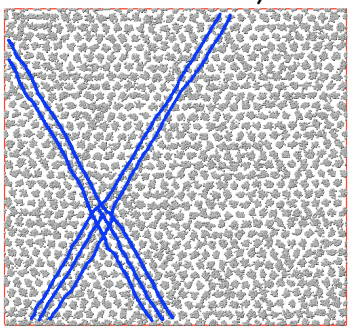
- Many vacancies: linear structures of vacancies are found unstable against the formation of edge dislocations (point like defects in 2D)
- These different kind of defects are found stable and very mobile





- Open question for a similar mechanism in 3D: are clusters of many vacancies unstable against the formations of dislocation loops?
- New 3D simulations under way

Few vacancies and the condensate

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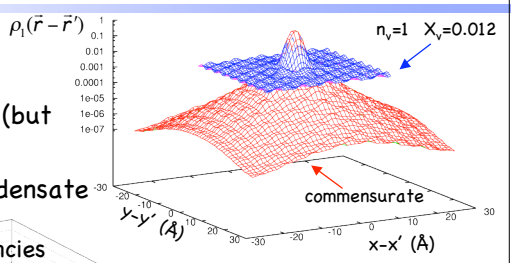
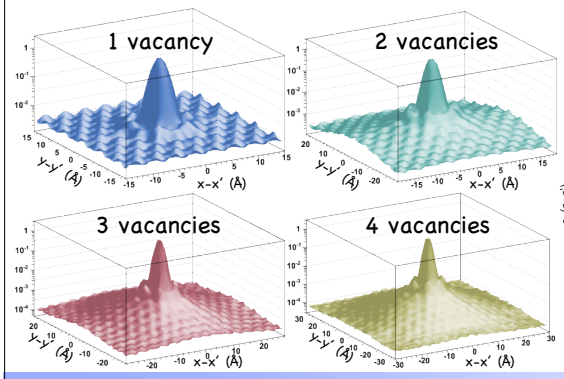
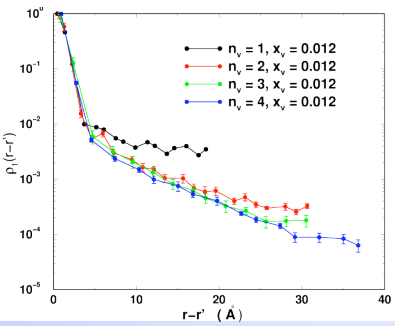
- 2D solid ^{4}He, ρ=0.0765 Å^{-2}

(τ=0.775 K^{-1}, pair-prod. $\delta\tau$=1/40 K^{-1})

- 1 vacancy induces a condensate (but not in the thermodynamic limit)
- Few vacancies suppress the condensate







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Few vacancies and the condensate

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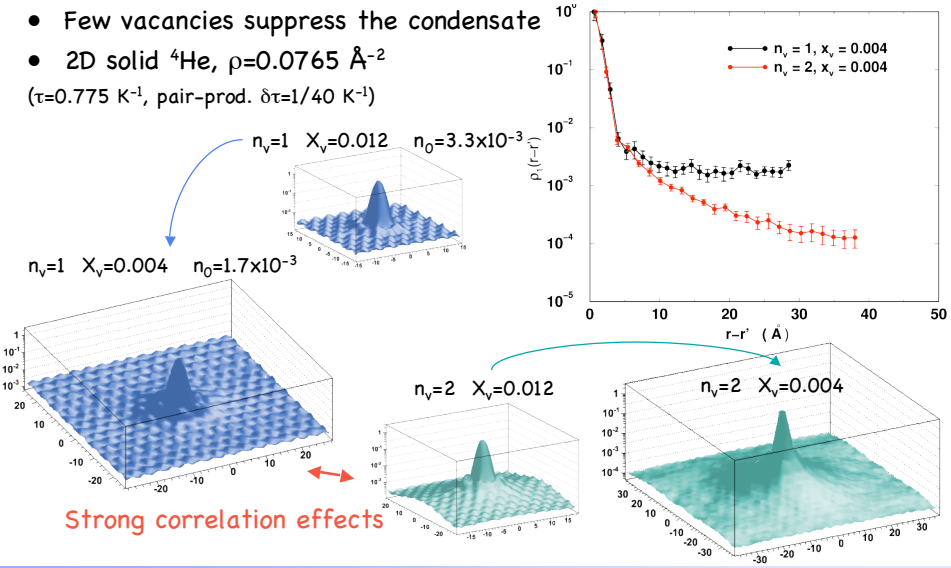
- Few vacancies suppress the condensate
- 2D solid ^{4}He, ρ=0.0765 Å^{-2}

(τ=0.775 K^{-1}, pair-prod. $\delta\tau$=1/40 K^{-1})



Strong correlation effects

Many vacancies (⇒ edge dislocations) and the condensate

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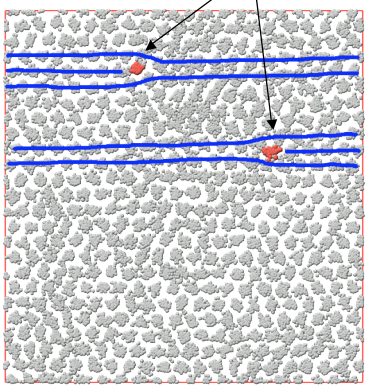
- Dominant contribution to the tail of ρ_1

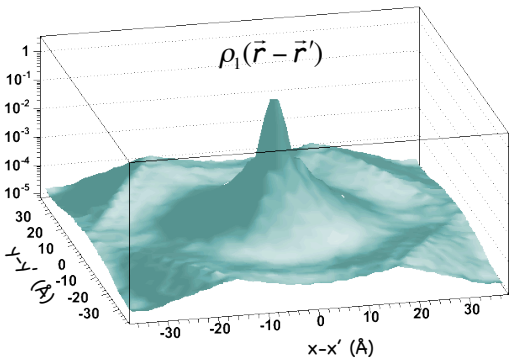
2D solid ^{4}He, ρ=0.0765 Å^{-2}

(τ=0.775 K^{-1}, pair-prod. $\delta\tau$=1/40 K^{-1})

Half polymers in dislocation cores



10 vacancies in a box with 240 lattice sites



transfer a particle from one dislocation to a different dislocation

⇒ Phase correlation transmitted from one dislocation to another

ODLRO & edge dislocations

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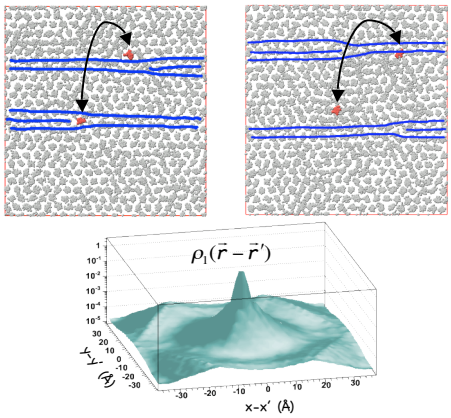
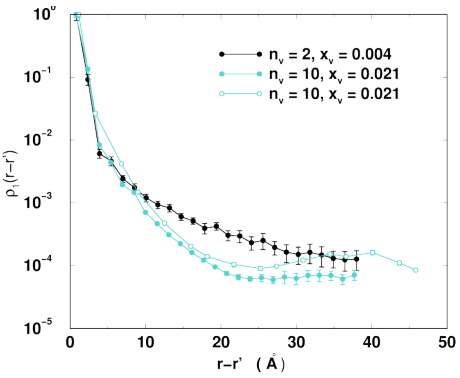
- Off-diagonal long range order (in the plane) induced by the presence of edge dislocations
- Open questions: dependence on concentration of dislocations; relevance in 3D?





Vacancy excitation spectrum: Shadow Wave Function

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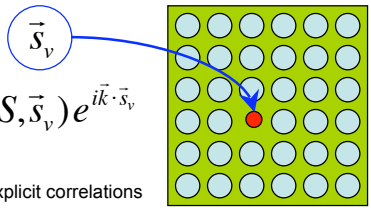
- With the SWF technique we found a way to study the vacancy excitation spectrum (Galli, Reatto, PRL 2003; JLTP 2004):
  - We associated one extra-shadow which localizes in the void of the vacancy in order to study the excitation at finite quasi-momentum

$$\Psi^{SWF}_{\vec{k}}(R) = \int dS\, d\vec{s}_v F(R,S)\Psi_T(S)L(S,\vec{s}_v)e^{i\vec{k}\cdot\vec{s}_v}$$

Shadow-extashadow explicit correlations



  - The inclusion of the extra-shadow improves the variational energy
  - Integration over extra-shadow is a way to change locally the effective many-body correlations around the vacancy

Vacancy excitation spectrum (SWF result)

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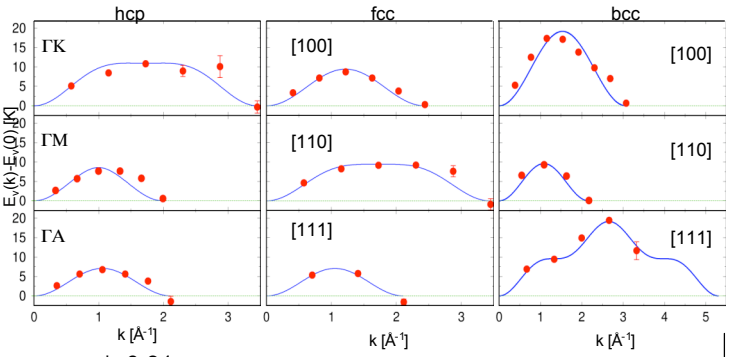
Galli, Reatto, PRL 90, 2003; JLTP 134, 2004



m*=0.31m$_4$
m*=0.39m$_4$ (ΓA)

m*=0.39m$_4$

m*=0.3m$_4$

- Vacancy very mobile, in agreement with recent experiments
  Andreeva et al., JLTP 110, 1998
- Band width decreases at larger density

• SWF result
– n.n. jump model best fit

Near melting density
ρ=0.029 Å^{-3}

residence time (hcp)
$\tau = \frac{\hbar}{\Delta} \cong 0.6 \times 10^{-11}$ sec

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

Dynamics from Quantum Monte Carlo

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- We wish to evaluate the dynamic structure factor of a collection of strongly interacting bosons at T=0 K in order to extract information about the elementary excitations spectrum of the system

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

- The "exact" SPIGS method gives access to the imaginary time evolution of quantum particles at T=0 K :

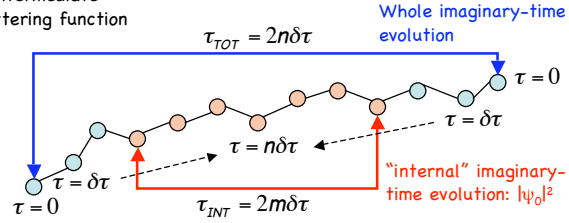
$$\rho_{\vec{q}}(\tau) = \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r}_j(\tau)}$$

Density fluctuation

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

Intermediate scattering function

$$|\psi_0|^2 \cong \langle \psi_\tau | \psi_\tau \rangle \quad \Leftrightarrow$$



Dynamics from QMC

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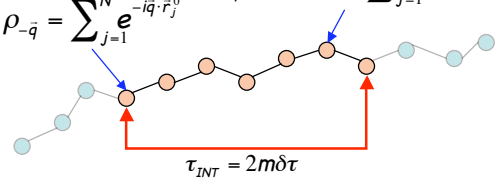
$$F(\vec{q},\tau) = \frac{1}{N}\left\langle \hat{\rho}_{\vec{q}}(\tau)\hat{\rho}_{-\vec{q}}(0)\right\rangle$$

$$\rho_{-\vec{q}} = \sum_{j=1}^{N} e^{-i\vec{q}\cdot\vec{r}_j^{\,0}}$$

$$\rho_{\vec{q}}(\tau = l\delta\tau) = \sum_{j=1}^{N} e^{-i\vec{q}\cdot\vec{r}_j^{\,l}}$$



- Imaginary time formulation of QMC methods makes difficult to study the dynamical properties of a Bose fluid, allowing to evaluate correlation functions in imaginary time, only for a finite set of "instants" (which depends on the time step δτ of the algorithm) with unavoidable statistical errors
- The inversion formula is thus ill-defined: $F(\vec{q},\tau) = \int_0^{+\infty} d\omega\, e^{-\omega\tau} S(\vec{q},\omega)$
- Hence the necessity of recast the problem in the language of probability theory: what is the best prediction of S(q,ω) when our knowledge is limited to the data coming from QMC (with errors) and to a few exact properties (non-negativity and sum rules)?
- No other constraining prior knowledge should be assumed (e.g. Maximum Entropy which it is know to force smoothness of the obtained S(q,ω))

Dynamics from QMC: our statistical framework

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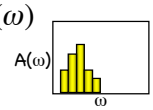
- A functional space of step spectral functions satisfying the constraints of non-negativity and zero-momentum sum rule:

$$A(\omega) = \sum_{i=1}^{N_\omega} a_i \chi_{[\omega_i,\omega_{i+1}]}(\omega)$$

$$\int_0^{+\infty} d\omega\, S(\vec{q},\omega) = \sum_{i=1}^{N_\omega} a_i \Delta\omega = S(\vec{q}) \qquad a_i \in [0,+\infty)$$



- A statistical weight which accounts for the QMC data (and eventually for the f-sum rule) to be maximized:

$$P(A) \propto \exp\left[-\sum_l \alpha_l \left(F_l - \int_0^{+\infty} d\omega\, e^{-\omega l\delta\tau} A(\omega)\right)^2 - \beta\left(|\vec{q}|^2/2m - \int_0^{+\infty} d\omega\,\omega A(\omega)\right)\right]$$

$$\left(\int_0^{+\infty} d\omega\,\omega S(\vec{q},\omega) = |\vec{q}|^2/2m\right)$$

- An "averaging" strategy to take into account the role of the statistical noisy in the QMC data: given the data F_l , new random data are generated as Gaussian random numbers with mean F_l and variance coming from the QMC errors estimation
- An optimization algorithm: we use Genetic Algorithms; several optimizations are performed using such random sets as "input" data; the average of the resuls is taken as the best estimation of S(q,ω)

Dynamics from QMC data: a genetic algorithm approach

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- Typical values: resolution $\Delta\omega \approx 0.25$ K/0.5 K; range in ω [0-200/500] K
  $\Rightarrow$ 400/2000 continuous parameters ($a_{i=1,\ldots,N\omega}$) to be optimized!
- Constraints: non-negativity of a_i , zero-momentum sum rule
- Multi-scope optimization:
  - compatibility with QMC data
  - f-sum rule
- Our optimization technique relies on Genetic Algorithms:
  - An individual (chromosome) is a vector $[a_1 \ldots a_{N\omega}]$ of N_ω real numbers (genes) which take values in the codomains of the step spectral functions
  - The genetic evolution of a starting random population of individuals, aiming towards maxima of the statistical weight P(A), consists of:
    1) "fitness"-based selection (which depends on P(A))
    2) recombination and mutation processes, suitably redistributing the spectral weight to increase the "fitness"
  - Typical values: #individuals ≈5000; #generations ≈ 6000

Dynamics from QMC data: a genetic algorithm approach

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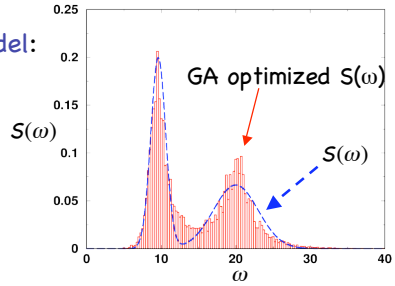
- Naturally, the finite set of available data, the unavoidable statistical errors of QMC data and the highly singular Laplace transform inversion operation induces to think that the number of features we may extract has to be limited
- In order to realize what could be the maximum of information available we devised the test of studying inversion problems such that the analytical solution is know

Results in good agreement with the model:

- Essentially the optimized $S_{GA}(\omega) \neq 0$ only when $S(\omega) \neq 0$
- Slight underestimation of the width of the peaks
- Some overweight between peaks when they are near



$\Rightarrow$ Very promising method to extract at least excitation energies

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Dynamics from QMC: ^{4}He liquid

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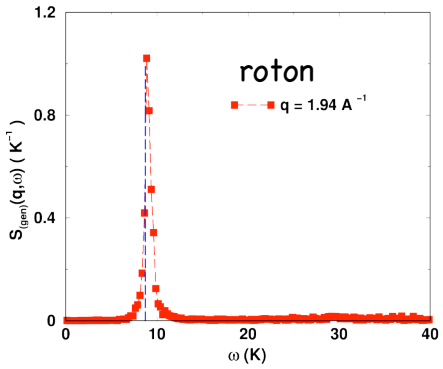
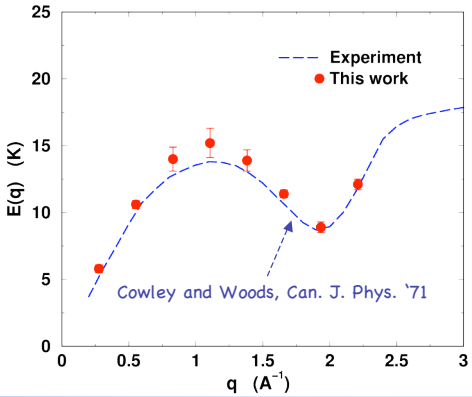
- Our first application: liquid ^{4}He, at equilibrium density ρ=0.0218 Å^{-3} ($N_{^4He}$=256)
- Details: Pair-product propagator $\delta\tau$=1/160 K^{-1}; $\tau_{TOT}\approx$0.6 K^{-1}; $\tau_{INT}\approx$0.2 K^{-1}
- Sharp feature in S(q,ω) indicating the collective excitations
- Good agreement with the experimental excitation spectrum





Dynamics from QMC: ^{4}He liquid + 1 ^{3}He atom

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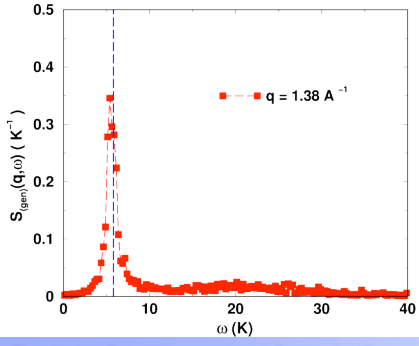
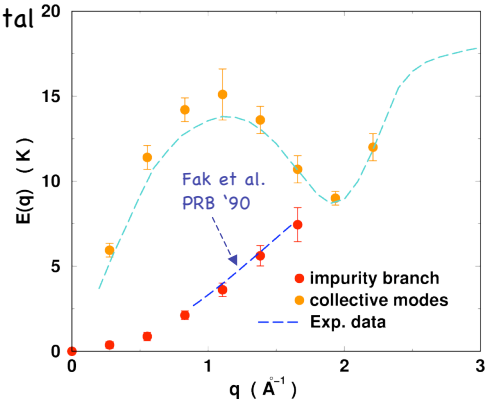
- We have studied also a liquid ^{4}He system at ρ=0.0218 Å^{-3} doped with one ^{3}He impurity ($N_{^4He}$=255)

$$\rho_{\vec{q}}^{(3)}(\tau) = e^{i\vec{q}\cdot\vec{r}_{^3He}(\tau)} \qquad F_{33}(\vec{q},\tau) = \left\langle \hat{\rho}_{\vec{q}}^{(3)}(\tau)\hat{\rho}_{-\vec{q}}^{(3)}(0)\right\rangle$$

- Good agreement with experimental impurity branch





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Dynamics from QMC: solid ^{4}He

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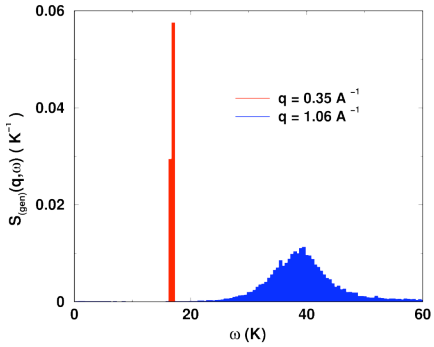
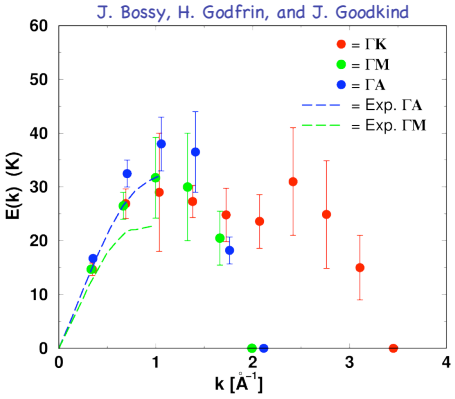
- The same technique can be easily extended to study longitudinal phonons in solid ^{4}He (hcp solid at ρ=0.0293 Å^{-3}; (N_{4He}=180)
- Sharp feature only at small energies where we find good agreement with available experimental data
- Wide peaks at higher energies



Experiments: courtesy of J. Bossy, H. Godfrin, and J. Goodkind



Dynamics from QMC: incommensurate solid ^{4}He (1 vacancy & 1 ^{3}He atom)

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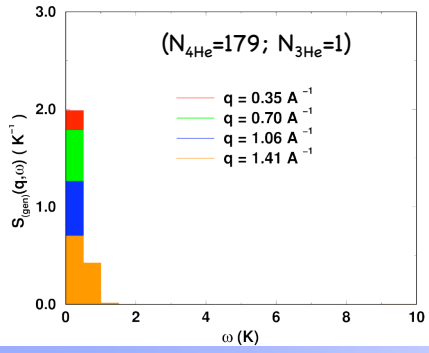
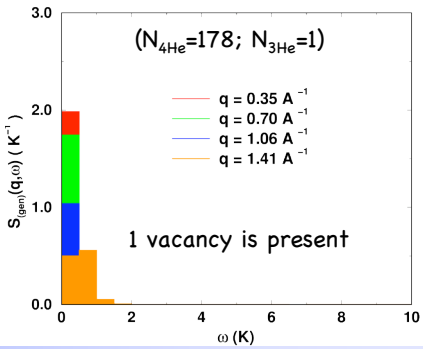
- We have studied also hcp solid at ρ=0.0293 Å^{-3} with one impurity ^{3}He atom with (N_{4He}=178) and without (N_{4He}=179) a vacancy in order to study the dynamics of the impurity induced by the presence of this defect
- Presence of a vacancy: no evident effect on impurity dynamics; ^{3}He atom is essentially fixed on a lattice position





Dynamics from QMC: vacancy excitation spectrum (method)

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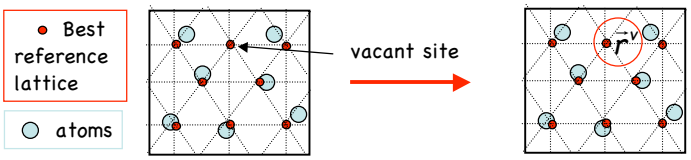
- Once one has an algorithm which is able to find where vacancies are located it is possible to define their coordinates r^v which is a many-body variable because it depends on the positions of all the N ^{4}He atoms



- With these vacancy-variables one can build a density fluctuation and an intermediate scattering function:

$$\rho^v_{\vec{q}}(\tau) = \sum_{j=1}^{N_v} e^{i\vec{q}\cdot\vec{r}^v_j(\tau)} \qquad F_{vv}(\vec{q},\tau) = \frac{1}{N_v}\left\langle \hat{\rho}^v_{\vec{q}}(\tau)\hat{\rho}^v_{-\vec{q}}(0)\right\rangle$$

  which gives information on the imaginary-time evolution of these many-body degrees of freedom

- Excited state properties from $S_{vv}(q,\omega)$

Dynamics from QMC: vacancy excitation spectrum (result 1)

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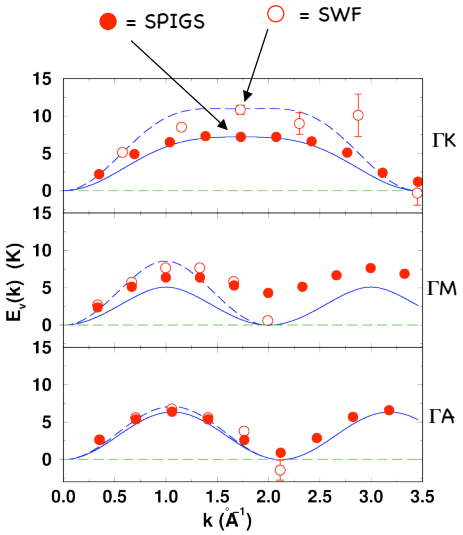
- Excitation spectrum of 1 vacancy in hcp solid ^{4}He at ρ=0.0293 Å^{-3}
- Pair-product propagator:

$\delta\tau$=1/160 K^{-1}; $\tau_{TOT}\approx$0.6 K^{-1}; $\tau_{INT}\approx$0.2 K^{-1}

- Old SWF results: not so different from SPIGS; band-width in SPIGS results is more isotropic
- Tight-binding hopping model analysis of the vacancy spectrum: worse agreement than with SWF
- lower band-width ⇒ higher effective mass:

  $m_v/m_4\approx$0.43(⊥)-0.55
- Evidence of roton-like modes at the reciprocal lattice wave vector



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Dynamics from QMC: vacancy excitation spectrum (result 2)

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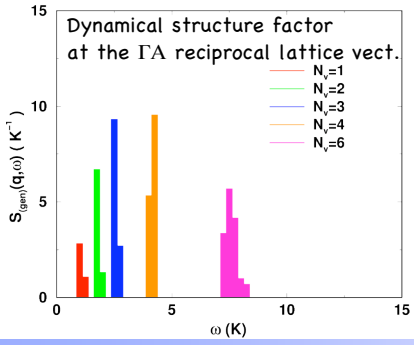
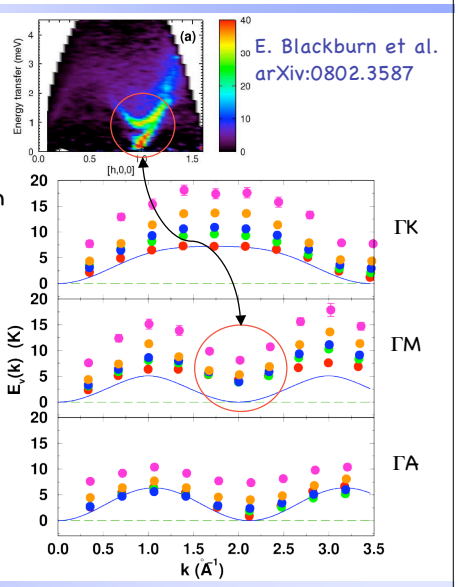
- Excitation spectrum of many (N_v=1-6) vacancies (clusters?)
- Roton-like modes with increasing energy with the number of vacancies
- Open question: connection with recent roton-like modes recently measured with neutron scattering?





E. Blackburn et al. arXiv:0802.3587

Conclusions

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Path Integral projector methods (T=0 K)

a T=0 K simulation method as unbiased as the finite T PIMC

- 2D and 3D Solid ^{4}He: commensurate crystal has NO BEC
- 2D Solid ^{4}He:
  - Few vacancies [1-6] form a bound state
  - More vacancies: formation of linear structures
    ⇒ local collapse of the crystal & formation of edge dislocations
  - Different dislocations induce particle permutations across the system and this induces phase coherence
  - Open question: relevance for the 3D case? (dislocation loops from clusters of vacancies: study underway)
- New method based on Genetic algorithms to obtain dynamics from QMC:
  - Evidence for roton-like vacancy modes in hcp solid ^{4}He