Miniworkshop talk:
Quantum Monte Carlo simulations of low temperature many-body systems

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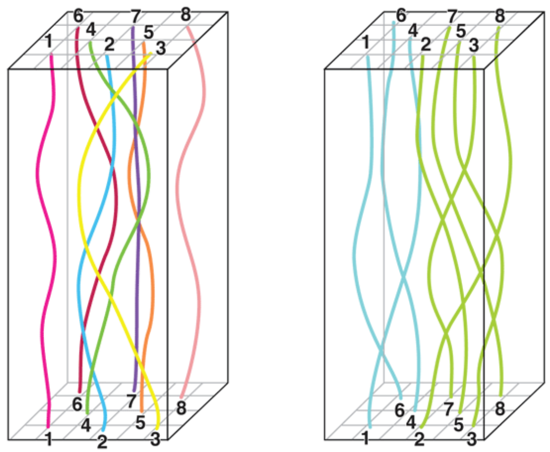
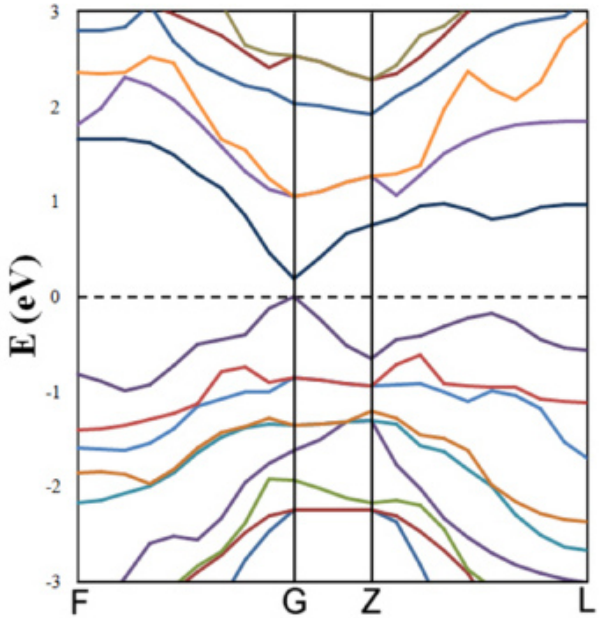


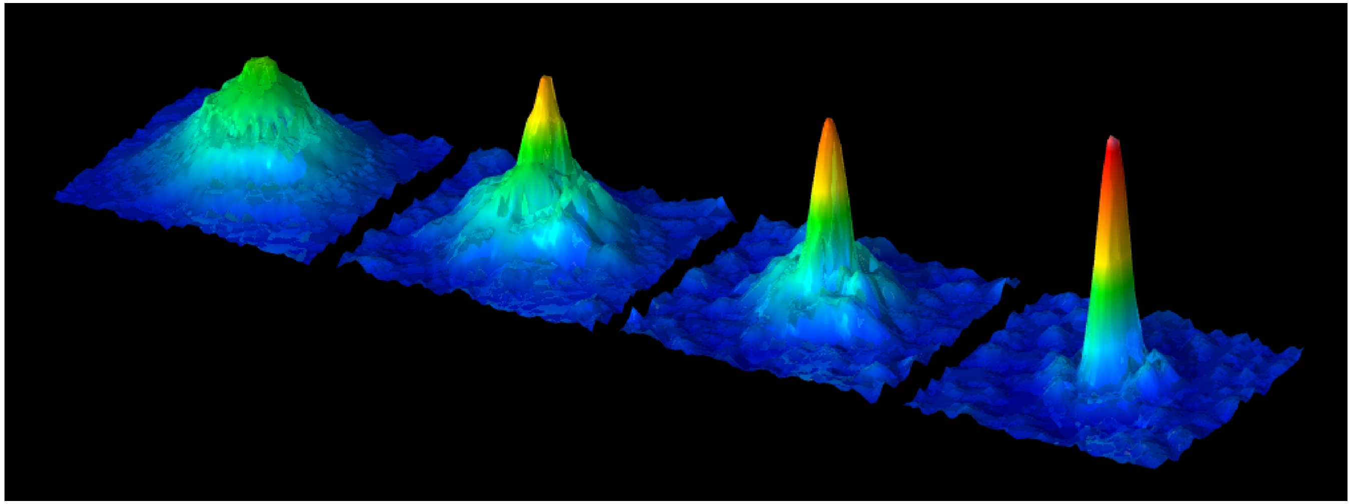
Supervisor: Dott. Davide E. Galli

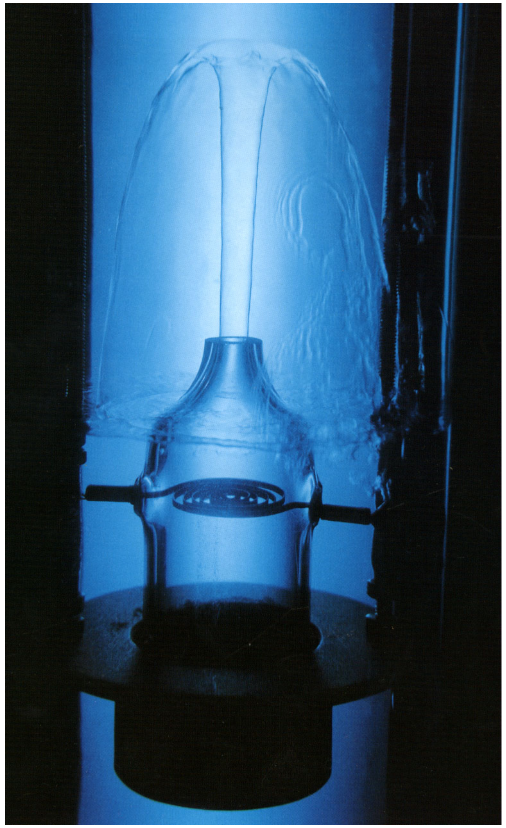
Outline

- Interests in quantum many-body systems
- Three examples of topics of research:
  - The uniqueness of helium
  - Glass transition in supercooled liquids
  - Ultracold gases
- Quantum Monte Carlo methods
  - Dynamic properties: the inversion problem

The quantum many-body problem







Helium

One of the most simple elements: HELIUM

T=4.2 K →

T=2.17 K →

BEC in liquid phase

→ NOT SOLID at low pressure → SOLID only at high pressure

Why?

1. Weak attractive interaction
2. Large zero point motion
3. Bose statistics

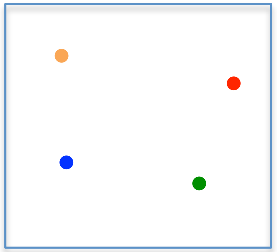
- Quantum Monte Carlo simulations of ^{4}He liquid:

Removing particles exchanges → fictious system of distinguishable atoms → freezes at lower pressure then real system

→ BOSE STATISTICS CONTRIBUTE TO PREVENT THE FREEZING

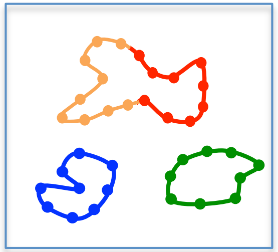
continue **Helium**

Feynman`s path integrals

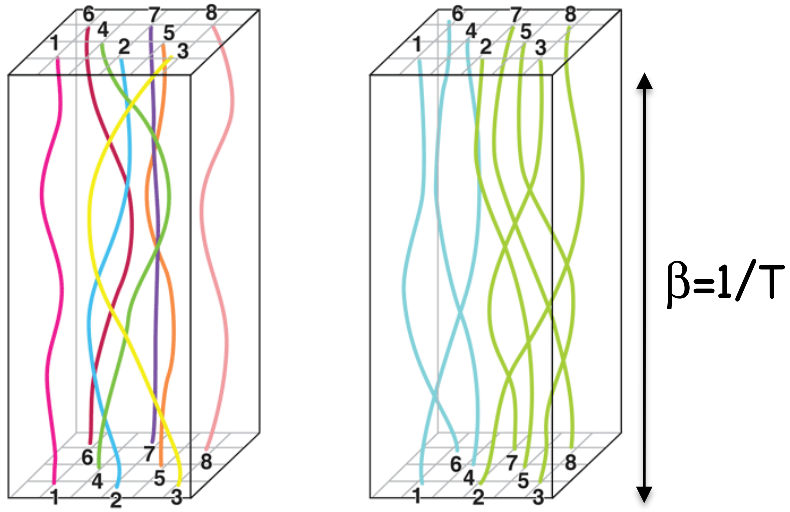


quantum
particles

isomorph
mapping



classical
polymers



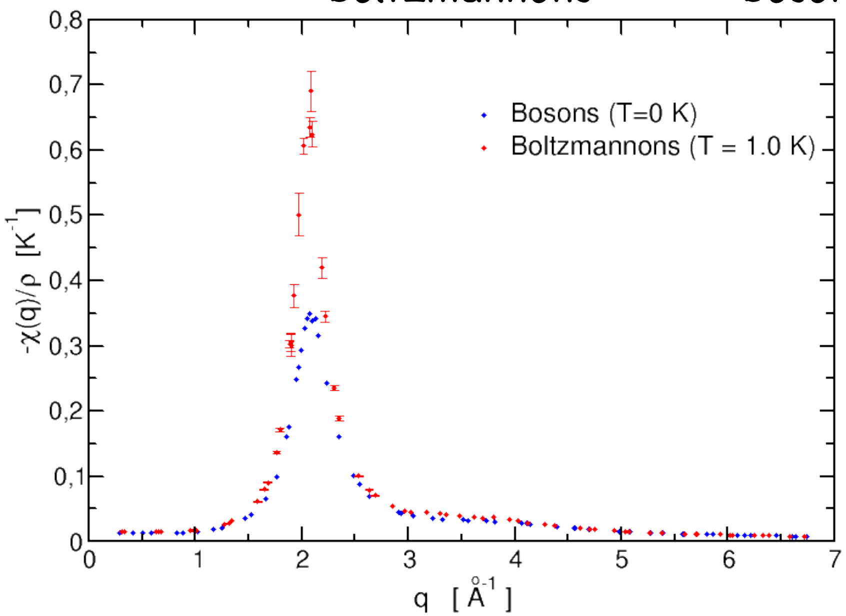
boltzmannons

bosons

Partition function

$$Z = Tr(e^{-\beta \hat{H}})$$

Static density
response function



Glass transition in supercooled liquids

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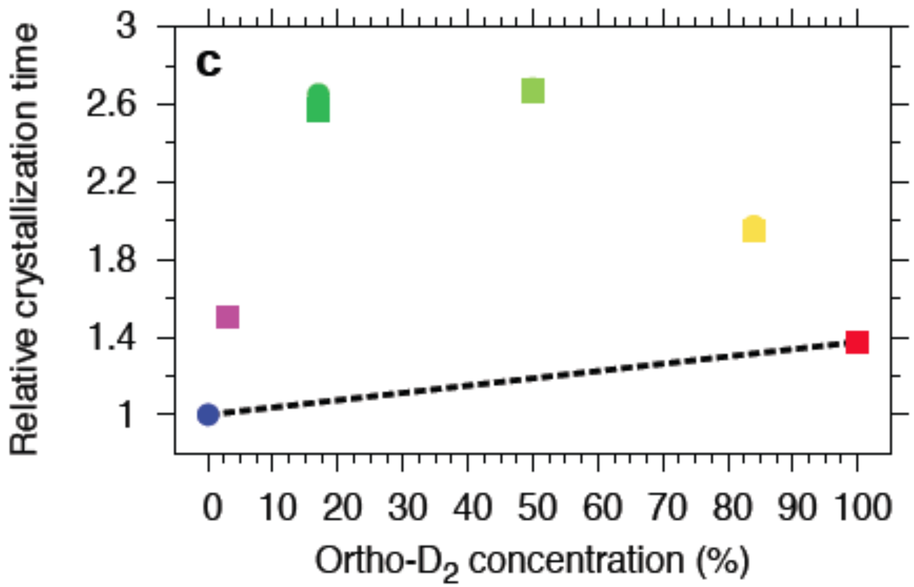
- Supercooled liquids = metastable liquids at $T < T_m$
- Rapid freezing transition of supercooled liquids ⟶ glass-forming
- Simple and common model: binary mixtures of interacting particles
- Idea:

- supercooled liquid mixtures of simple bosonic elements: $p\text{-}H_2$ and $o\text{-}D_2$
- effects of $o\text{-}D_2$ on crystallization of $p\text{-}H_2$



- Large slowing down of crystallization at intermediate concentrations
- Quantum Monte Carlo simulations
- Collaboration with a Frankfurt experimental group

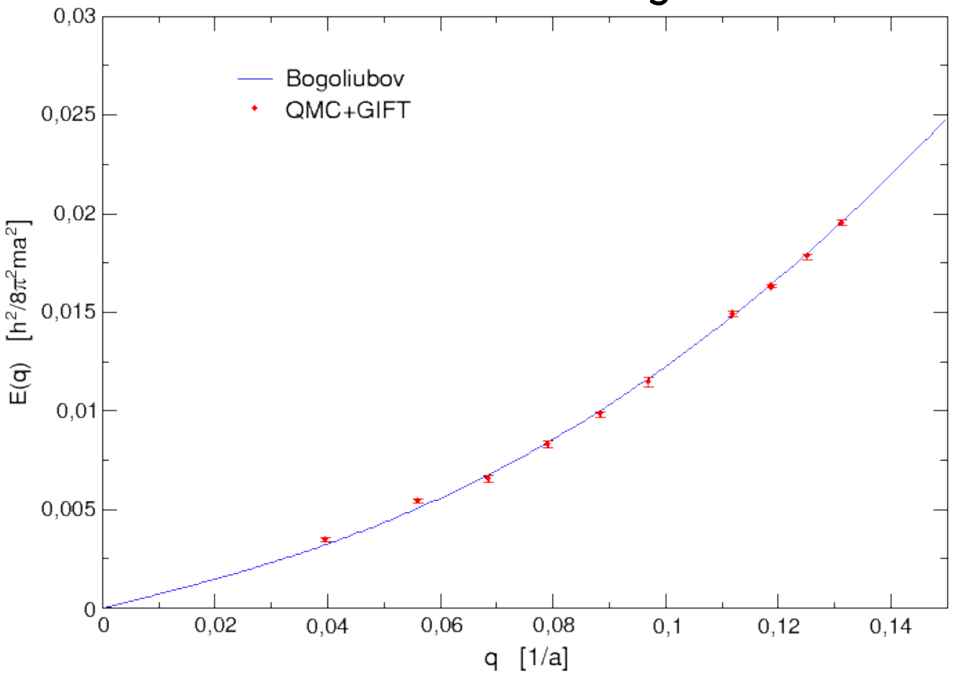
Ultracold gases

- Experimental techniques, through lasers and magnetic fields:
  - magnetic traps
  - optical lattice
  - tuning the strength of interatomic interaction
  - magnetic and electric external fields

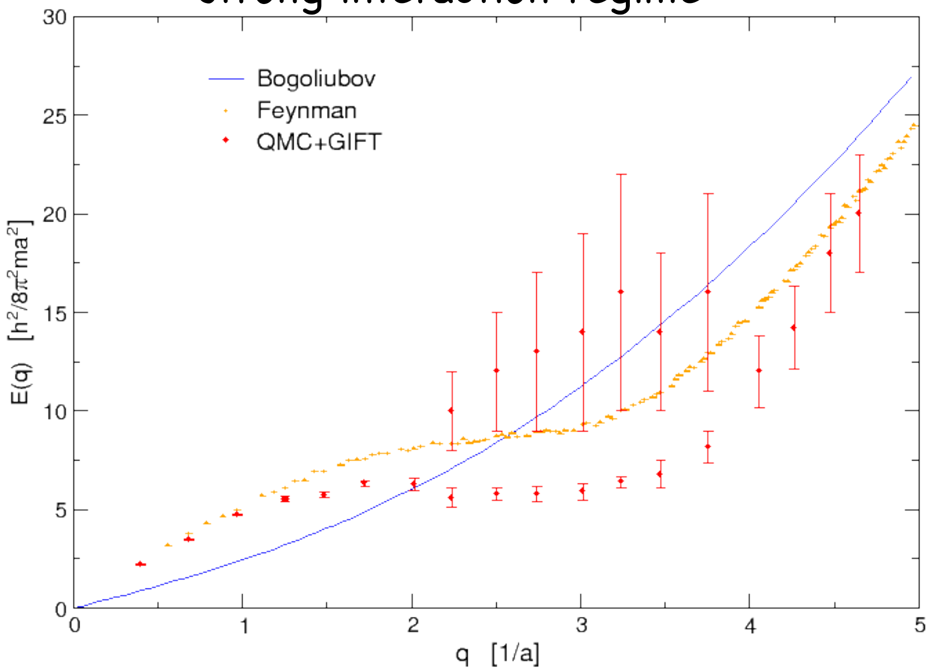
  → tunable many-body Hamiltonian

- Collaboration with a Trento group:
  - hard sphere Bose gas
  - characteristic variable: gas parameter $n\,|a|^3$
  - elementary excitations spectrum
  - second sound

weak interaction regime



strong interaction regime



Quantum Monte Carlo methods 1

- How can I study quantum many-body systems?
- Exact computational methods?
  ⟶ Quantum Monte Carlo methods
- The key ingredient of the exact QMC methods:

real time evolution operator

$$e^{-it\hat{H}}|\psi\rangle = |\psi(t)\rangle$$

$\xrightarrow[\text{Wick rotation}]{it \to \tau}$

imaginary time evolution operator

$$e^{-\tau\hat{H}}$$

In T=0 QMC methods $e^{-\tau\hat{H}}$ projects out a trial state to the ground state

$$e^{-\tau\hat{H}}|\psi_T\rangle \xrightarrow[\tau\to\infty]{} |\psi_0\rangle$$

In T>0 QMC methods $e^{-\tau\hat{H}}$ represents the statistical operator

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z}$$

Quantum Monte Carlo methods 2

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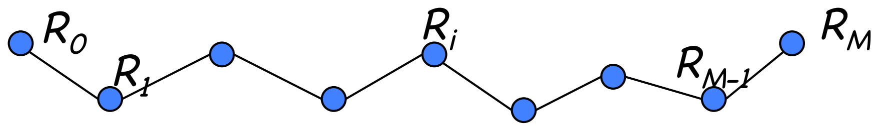
- In both cases we decompose the time evolution operator in many small time steps $\tau = M\delta\tau$

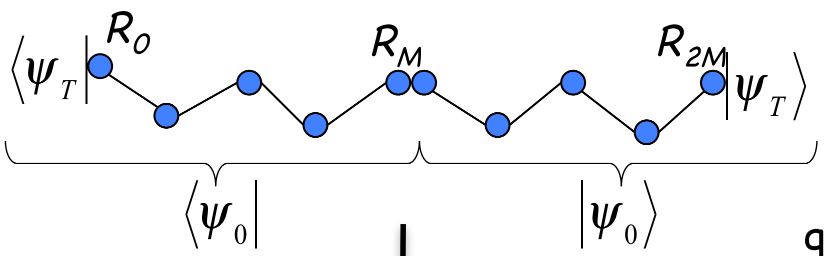
$$e^{-\tau\hat{H}} = \underbrace{e^{-\delta\tau\hat{H}} \ldots e^{-\delta\tau\hat{H}}}_{M \text{ times}} \longrightarrow$$



In spatial coordinate representation

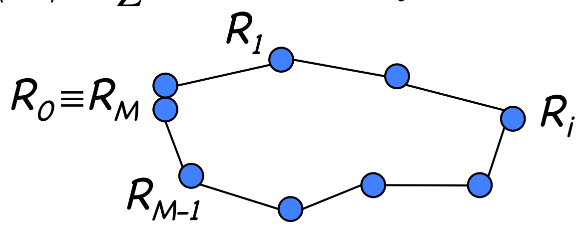
- For T=0 we use the Path Integral ground state method (PIGS):

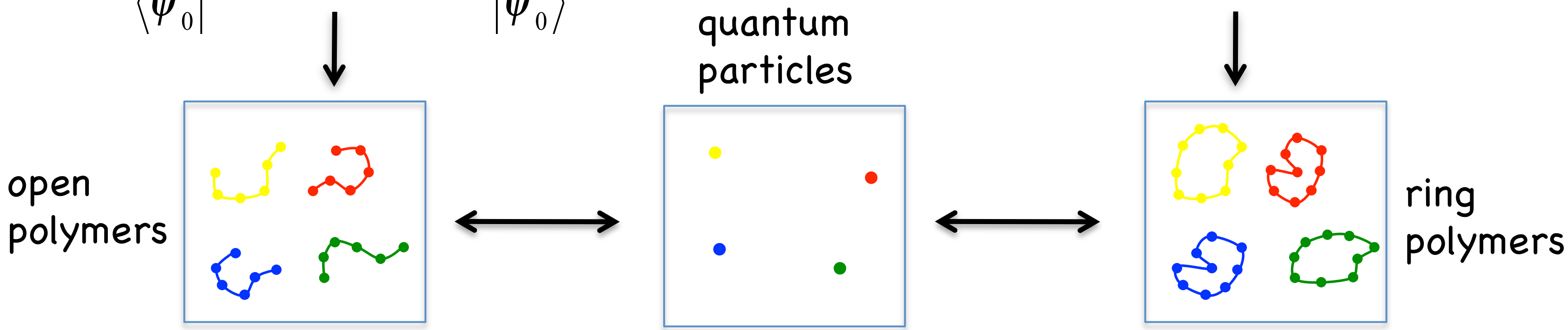
$$\langle \hat{O} \rangle = \langle \psi_0 | \hat{O} | \psi_0 \rangle \cong \langle \psi_T | e^{-\tau\hat{H}} \hat{O} e^{-\tau\hat{H}} | \psi_T \rangle$$



- For T>0 the path integral Monte Carlo method (PIMC):

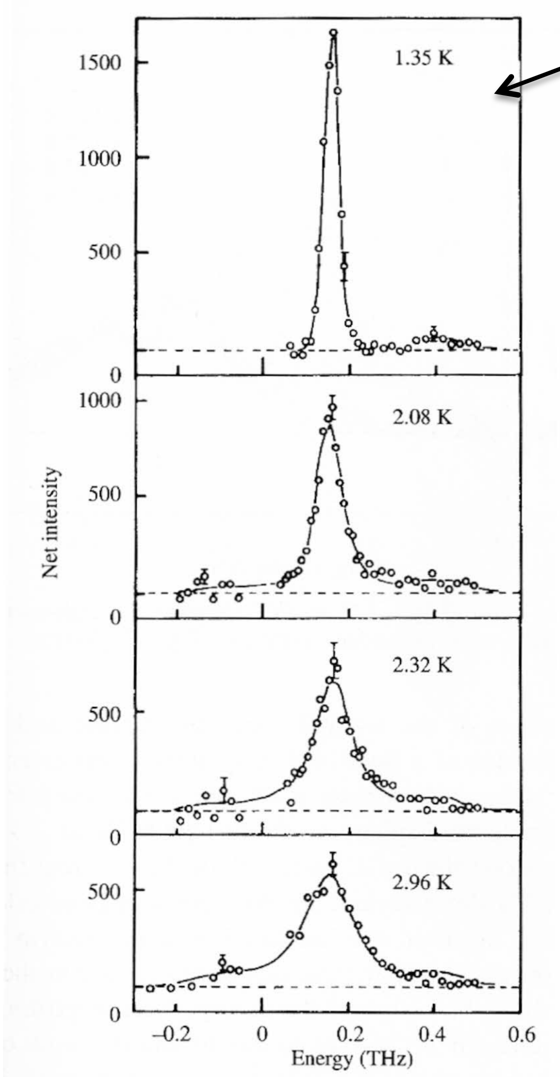
$$\langle \hat{O} \rangle = \frac{1}{Z} Tr(e^{-\beta\hat{H}} \hat{O}) = \int dR \langle R | e^{-\beta\hat{H}} \hat{O} | R \rangle$$





Dynamics properties 1

Neutron scattering mesurements



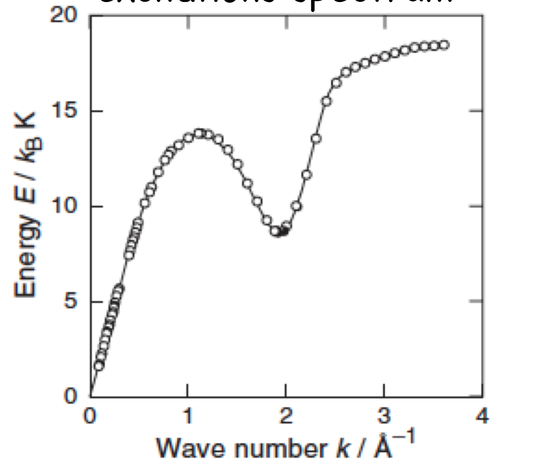
Partial differential cross section

$$\frac{d^2\sigma}{d\Omega d\varepsilon} = N \frac{|\vec{k}|}{|\vec{k}_0|} \frac{b^2}{\hbar} S(\vec{q},\omega)$$

Dynamic structure factor

$$S(\vec{q},\omega) = \frac{1}{2\pi N} \int_{-\infty}^{+\infty} e^{i\omega t} \underbrace{\left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}(0) \right\rangle}_{\text{time correlation function}}$$

Helium elementary excitations spectrum



$$S(\vec{q},\omega) = \frac{1}{N} \sum_{n,m=0}^{\infty} \frac{e^{\beta E_n}}{Z} \left| \left\langle \psi_m \right| \hat{\rho}_{-\vec{q}} \left| \psi_n \right\rangle \right|^2 \delta[\hbar\omega - \underbrace{(E_m - E_n)}_{\text{excitation energies}}] \qquad \hat{\rho}_{\vec{q}} = \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i}$$

- QMC methods ⟶ study dynamic properties
- But we cannot obtain directly $S(\vec{q},\omega)$

⟹ calculate imaginary time correlation functions

Dynamic properties 2

Imaginary time correlation function

Real time correlation function

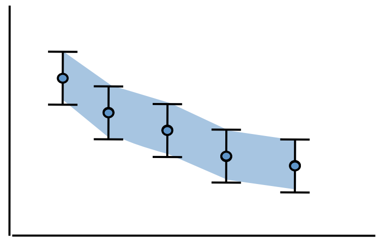
$$F(\vec{q},\tau) \equiv \left\langle \hat{\rho}_{\vec{q}}(\tau)\hat{\rho}(0) \right\rangle \quad \xleftrightarrow[\text{Wick rotation}]{it \to \tau} \quad C(\vec{q},t) \equiv \left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}(0) \right\rangle$$

$$\hat{A}(\tau) = e^{\frac{\tau}{\hbar}\hat{H}}\,\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}}$$

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

Inverse problem **?**

Finite and discrete QMC of $F(\vec{q},\tau)$ + Statistical uncertainty of data



$\Downarrow$

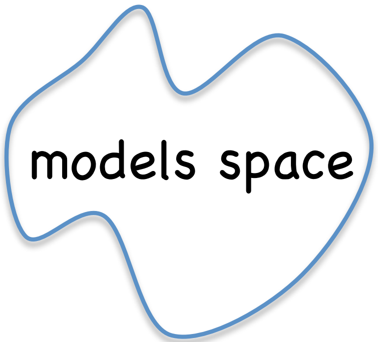
ILL POSED INVERSE PROBLEM

Infinite solutions are compatible with the data

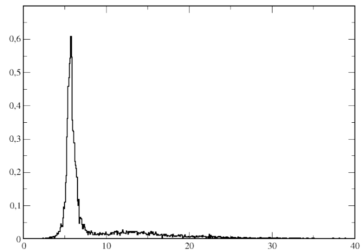
Statistical inversion method

GIFT   Genetic Inversion via Falsification of Theories

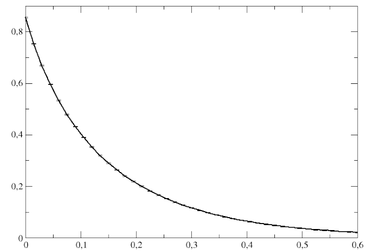
- Scheme of the method:



genetic algorithm →



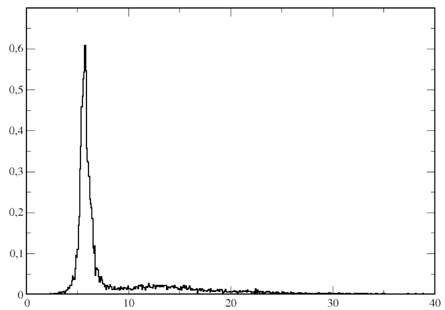
⟷



selection of models compatible with QMC data

→ Extraction of the common features: $\bar{s}(\omega) = \frac{1}{N}\sum_{i=1}^{N} s_i(\omega)$

average on best models



Thank you
for the attention