Quantum Monte Carlo study of the dynamic structure factor of Bose hard-sphere systems

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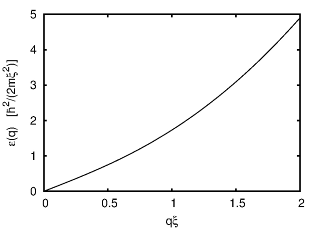
Seattle, 1 July 2013

Motivation

Weakly Interacting regime

- Quasiparticle-like excitations: at $T = 0$, $S(\mathbf{q}, \omega) = S(\mathbf{q})\delta(\omega - \omega_{\mathbf{q}})$
- Bogoliubov spectrum: $\omega_{\mathbf{q}} = \frac{\hbar}{2m\xi^2}\sqrt{(q\xi)^4 + 2(q\xi)^2}$



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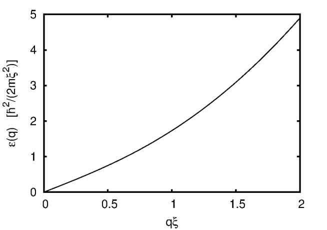
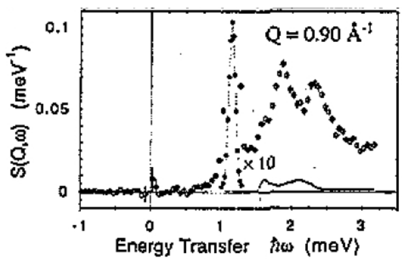


Strongly Interacting regime

Experimental measurements on **superfluid ^{4}He**:

Dynamic structure factor:



from Andersen *et al.*, J. Phys Condensed Matter (1994)

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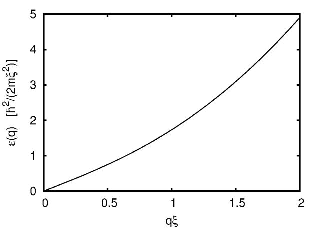

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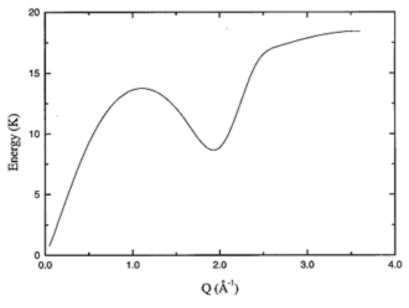

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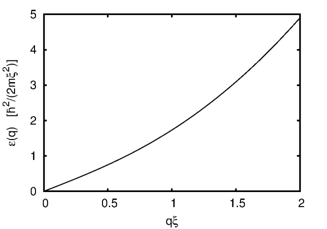

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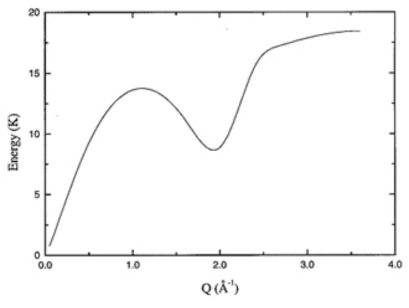

To study the crossover between these regimes, *ab-initio* numerical techniques are needed

Outline

1. Numerical methods
   - Path Integral Ground State
   - Genetic Inversion via Falsification of Theories
2. Results
   - Quantum Hard-Sphere model
   - $S(\mathbf{q}, \omega)$ for the gas phase
   - $S(\mathbf{q}, \omega)$ for the solid phase
3. Conclusions

Path Integral Ground State (PIGS)

Projector methods

$\Psi_0(R_M) = \lim_{\tau\to\infty} \int dR_0\, G(R_M, R_0; \tau)\Psi_T(R_0) \quad \text{if } \langle\Psi_0|\Psi_T\rangle \neq 0$

The imaginary time propagator projects the trial wave function Ψ_T onto the ground state wave function Ψ_0.

$R_i = \{\vec{r}_{i,1}; \vec{r}_{i,2}; \dots; \vec{r}_{i,N}\}$ is a set of coordinates of the N particles

$G(R_M, R_0; \tau) = \langle R_M|e^{-\tau\hat{H}}|R_0\rangle$ is the imaginary time propagator

(notice that $e^{-\tau\hat{H}}$ is the same as $e^{it\hat{H}}$ with $t = i\tau$)

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- The imaginary time propagator is known only for small τ
- Convolution property

$$G(R_3, R_1; \tau) = \int dR_2 \, G\left(R_3, R_2; \frac{\tau}{2}\right) G\left(R_2, R_1; \frac{\tau}{2}\right)$$

Path Integral Ground State (PIGS)

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Path Integral representation of the Ground State wave-function

$\Psi_0(R_M) \simeq \int \prod_{i=1}^{M} dR_i G(R_i, R_{i-1}; \varepsilon)\Psi_T(R_0)$ with $\tau = \varepsilon M$

"Exact" method: by studying the convergence at large M and small ε, we reduce the systematic error within the statistical one.

PIGS: calculation of the physical observables

$$\frac{\langle \Psi_0 | \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \int \prod_{i=1}^{M} dR_i \, O(R_1, \dots, R_M) \underbrace{\frac{\Psi_T(R_{2M}) G(R_i, R_{i-1}; \varepsilon) \Psi_T(R_0)}{\langle \Psi_0 | \Psi_0 \rangle}}_{p(R_1, \dots, R_M)}$$

- Integral suitable for **Monte Carlo** calculations
- Every configuration R_i represents the evolution of the system for a different imaginary time

Choosing $O = \rho_{\mathbf{q}}(R_M)\rho_{-\mathbf{q}}(R_{M+\tau/\varepsilon})$, where $\hat{\rho}_{\mathbf{q}} = \sum_{i=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_i}$ is the density fluctuation operator, we can calculate the density correlation function in imaginary time

$$F(\mathbf{q}, \tau) = \frac{1}{N} \frac{\langle \Psi_0 | e^{\tau \hat{H}} \hat{\rho}_{\mathbf{q}} e^{-\tau \hat{H}} \hat{\rho}_{-\mathbf{q}} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

From imaginary time correlations to real time response

Laplace transform

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

- The inversion of the Laplace transform is an **ill-posed** problem: many very different $S(\mathbf{q},\omega)$ can reproduce similar curves for $F(\mathbf{q},\tau)$.
- **Bayesian approach** (e.g. Maximum Entropy Method, Average Spectrum Method): a prediction for the spectral function $S(\mathbf{q},\omega)$ is inferred estimating the compatibility between a model for $S(\mathbf{q},\omega)$ and the Quantum Monte Carlo data for $F(\mathbf{q},\tau)$

Genetic Inversion via Falsification of Theories (GIFT)

Main features of GIFT algorithm

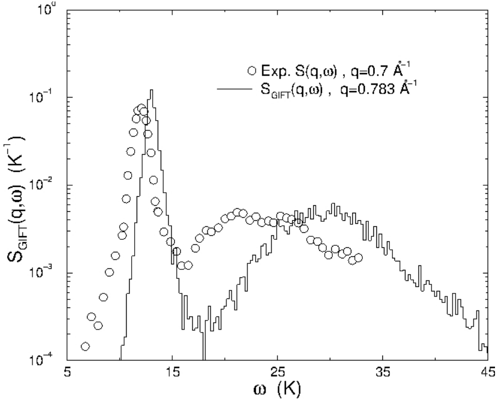
- Space of model $\mathcal{S}$ containing a wide collection of spectral functions $S(\mathbf{q},\omega)$
- Use of **genetic** algorithm to sample the space $\mathcal{S}$
- **Falsification** procedure: we do not search the “best” spectral function but a collection of “good” spectral functions which will be averaged to obtain the final estimation of $S(\mathbf{q},\omega)$

$$\Downarrow$$

Common features shared by the majority of “good” spectral functions will survive to the average procedure and can be ascribed to the true dynamic structure factor.

Genetic Inversion via Falsification of Theories (GIFT)

Dynamic structure factor of superfluid ^{4}He: GIFT vs Experiment



from Vitali *et al.*, Phys Rev B, **82**, 174510 (2010)

The Quantum Hard-Sphere (HS) model

Hamiltonian of the system

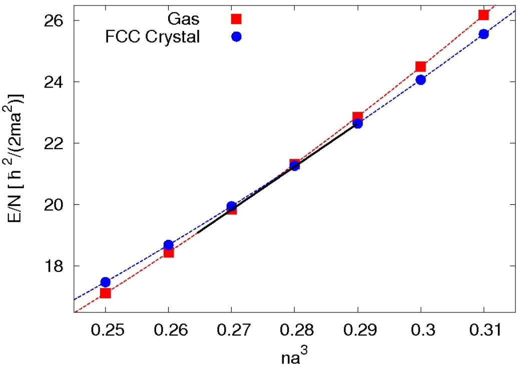
$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} V(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$V(r) = \begin{cases} \infty & (r < a) \\ 0 & (r > a) \end{cases}$$

- Good model both for dilute systems with positive scattering lenght and for dense systems with repulsive hard core dominating over attractive tail
- Cao-Berne approximation for imaginary time propagator
- Different regimes investigated modifying only one parameter (i.e. the reduced density n in units of HS range)

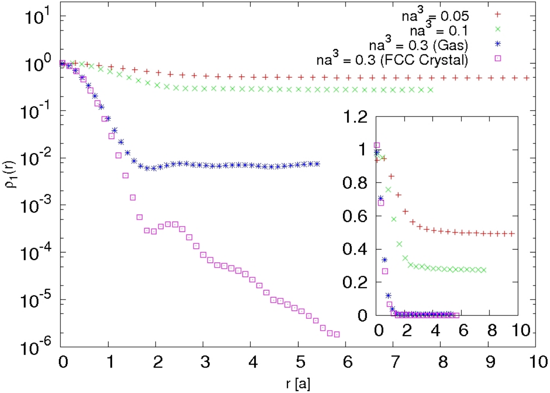
HS model: the gas-solid transition

Equation of state for gas and solid phase:



Freezing density $n_f a^3 = 0.265(1)$
Melting density $n_m a^3 = 0.290(1)$

HS model: the one-body density matrix

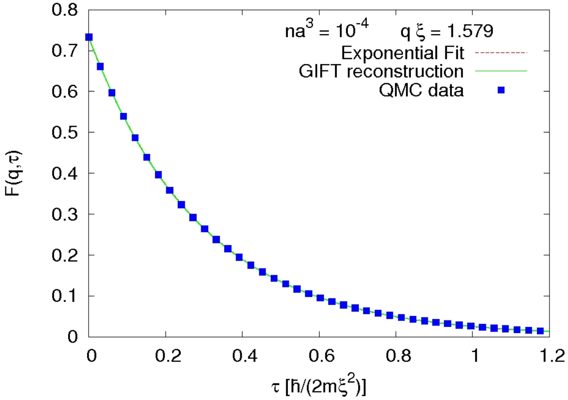


Condensate fraction of the gas:

na^3	n_0
10^{-2}	$(79.0 \pm 0.4)\%$
$5\ 10^{-2}$	$(49.4 \pm 0.1)\%$
10^{-1}	$(27.5 \pm 0.1)\%$
$3\ 10^{-1}$	$(0.695 \pm 0.004)\%$

Above the freezing density, $n_0 > 0$ if the system is in a disordered configuration, $n_0 = 0$ if the system is in a crystalline configuration: analogy with ^{4}He at $T = 0\,K$

Weakly interacting regime: $na^3 = 10^{-4}$



$$S(\mathbf{q},\omega) = S(\mathbf{q})\delta(\omega - \omega_{\mathbf{q}}) \Rightarrow$$
$$F(\mathbf{q},\tau) = S(\mathbf{q})e^{-\tau\omega_{\mathbf{q}}}$$

- PIGS data for $F(\mathbf{q},\tau)$ show an exponential behavior

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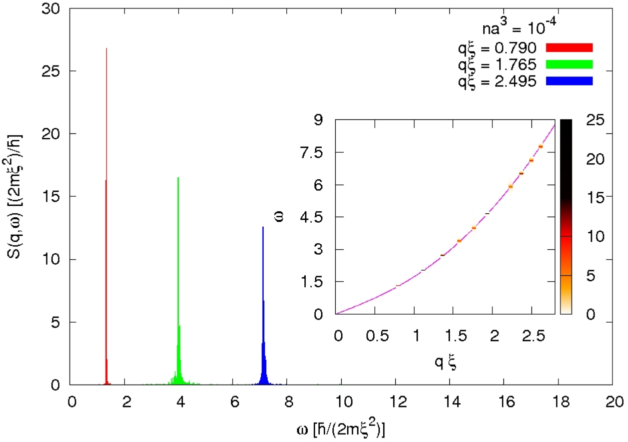
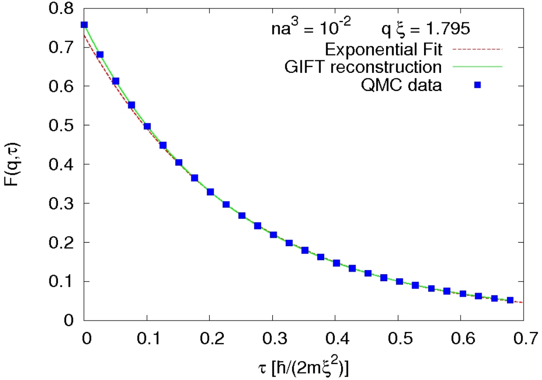


- PIGS data for $F(\mathbf{q}, \tau)$ show an exponential behavior
- $S(\mathbf{q}, \omega)$ shows a narrow peak at the frequncy $\omega_{\mathbf{q}}$ in agreement with Bogoliubov theory

Not so weakly interacting regime: $na^3 = 10^{-2}$



- PIGS data at small τ show deviations from exponential fit

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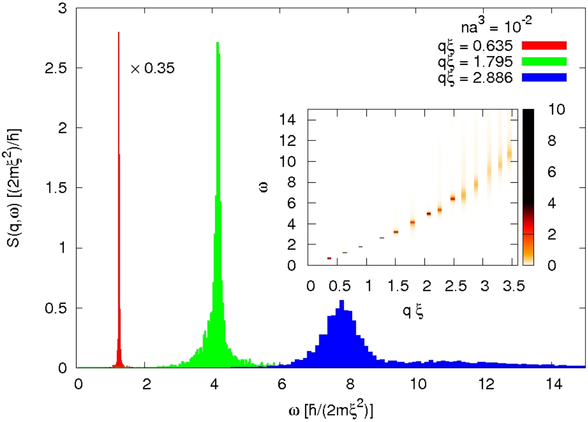

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- As q increases, $S(\mathbf{q},\omega)$ broadens and displays multiphonon contributions

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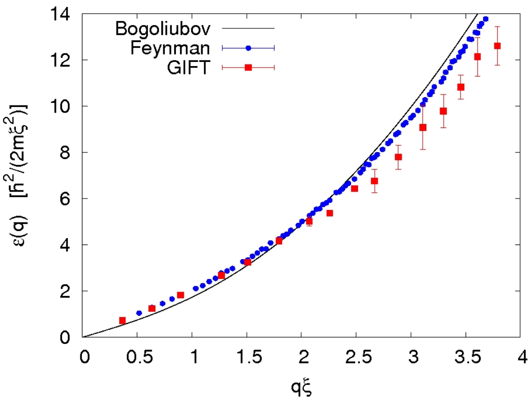
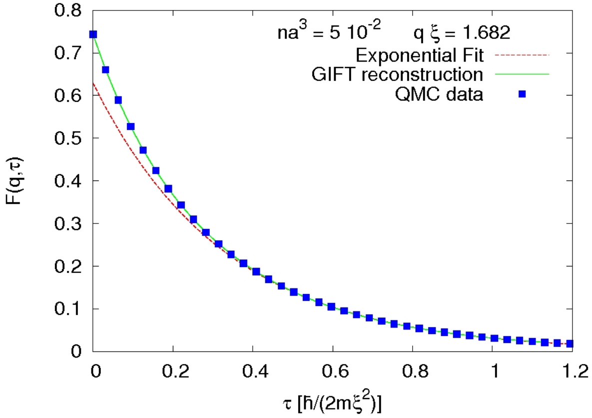


- PIGS data at small τ show deviations from exponential fit
- As q increases, $S(\mathbf{q},\omega)$ broadens and displays multiphonon contributions
- Feynman approximation $\omega_{\mathbf{q}} = \dfrac{\hbar q^2}{2mS(\mathbf{q})}$ works only for small q

The interaction increases : $na^3 = 5 \times 10^{-2}$



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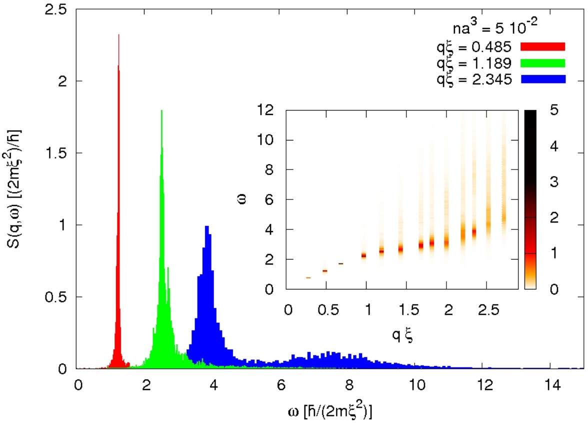
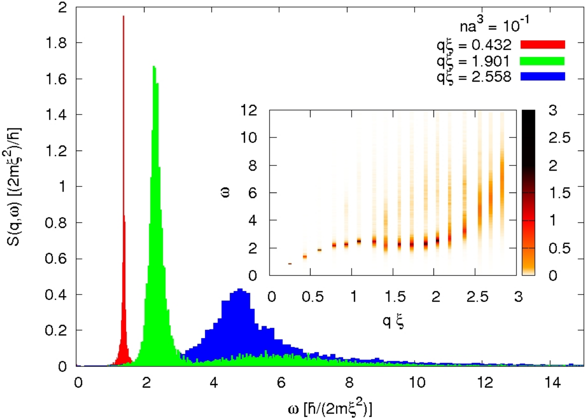


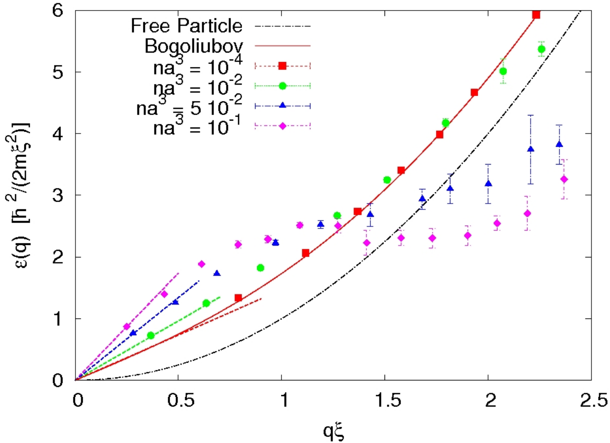
- Exponential fit captures only the tail of $F(\mathbf{q}, \tau)$
- Secondary multiphonon peaks become more evident
- Spectrum of excitations presents a shoulder for $q\xi \sim 1.5 - 2$

The roton appears: $na^3 = 10^{-1}$



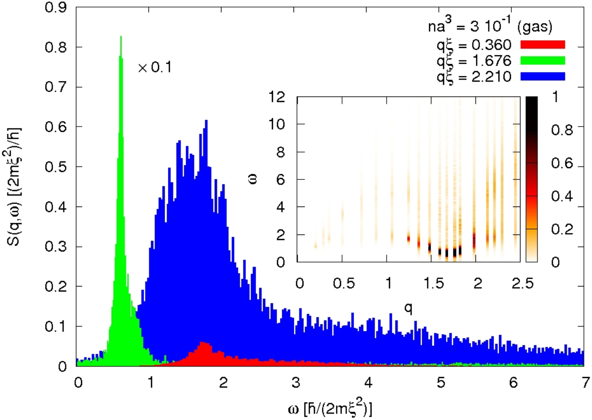
- Spectrum of excitation with a non monotonic behavior: the **roton** appears

The roton appears: $na^3 = 10^{-1}$



At small q, we recover the phonon dispersion $\omega_{\mathbf{q}} = cq$, with c (i.e. speed of sound) obtained from the equation of state of the HS gas (Ref.: Boronat, Casulleras and Giorgini, Physica B (2000))

Above the freezing point: $na^3 = 3 \times 10^{-1}$



- $S(\mathbf{q},\omega)$ presents a narrow peak only for momenta in the region of the roton.

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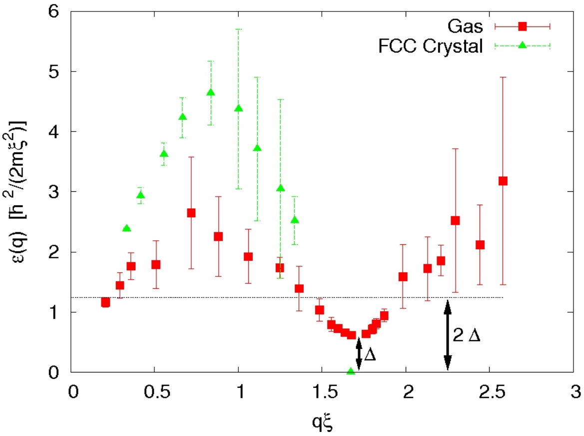

- $S(\mathbf{q}, \omega)$ is broad when the energy of the excitation is higher than 2Δ (with Δ energy of the roton)

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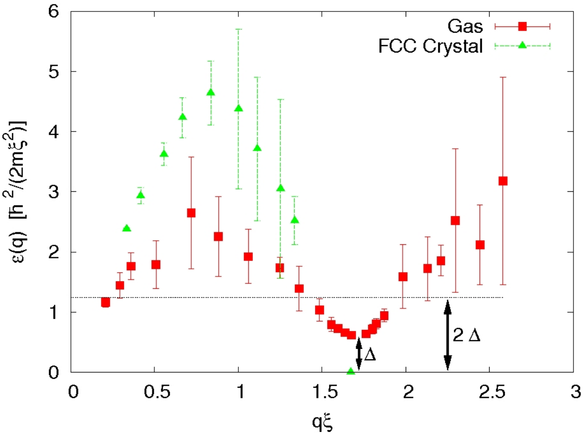

- The momentum of the roton correspond to the smallest vector of the reciprocal lattice of a FCC crystal at the same density

Conclusions

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GIFT algorithm allows us to show the emergence of the multiphonon contribution and the appearance of the roton as the strenght of the interaction increases.

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THANKS FOR YOUR ATTENTION!