Dynamics of Quantum Many-Body Systems from Monte Carlo simulations

Francesco Pederiva

I.N.F.N. and Physics Department, University of Trento - ITALY

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Collaborators

- Alessandro Roggero (Trento)
- Giuseppina Orlandini (Trento)

Outline

- QMC and Response Functions
- Dynamic Response Functions:
  - Integral transform methods
  - Ill-Posed problems
  - Regularization techniques
- Integral Kernels for Quantum Monte Carlo
  - Laplace Kernel and imaginary-time correlations
  - A better Kernel
- Results
  - Superfluid He^4

QMC and Response functions
A few canonical statements.

Projection QMC methods are acknowledged to give useful and accurate estimates of expectations on the ground state of a given Hamiltonian $\hat{H}$.

Start from a "trial wavefunction" that can be expanded along the basis of eigenstates of $\hat{H}$, applying an imaginary time propagator formally projects the ground state out of the initial state. This is completely general, and does not depend on the representation used (configuration space, momentum space, Fock space, ...).

$$\lim_{\tau\to\infty} e^{-\frac{\tau}{\hbar}(\hat{H}-E_0)}|\Psi_T\rangle = \lim_{\tau\to\infty}\sum_n e^{-\frac{\tau}{\hbar}(E_n-E_0)}|\Phi_n\rangle\langle\Phi_n|\Psi_T\rangle =$$

$$= \langle\Phi_0|\Psi_T\rangle|\Phi_0\rangle$$

QMC and Response functions
A few canonical statements.

It is clear from the previous analysis of imaginary time propagation that the information about excited states must be buried into the filtering process.

How do we extract it?

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How do we extract it?

The good, old answer is **with an inverse Laplace transform!** (See e.g. L-QCD calculations, David Ceperley et al., the ANL/LANL group....). However, everebody knows that this is an **ill posed problem**.

Here we want to analyze the problem a little more closely.

Dynamic Response Function

Spectral representation of DRF

$$\begin{aligned}\mathcal{R}(\omega) &= \sum_\nu |\langle \Psi_\nu | \hat{O} | \Psi_0 \rangle|^2 \delta\left[\omega - (E_\nu - E_0)\right] \\ &= \sum_\nu \langle \Psi_0 | \hat{O}^\dagger | \Psi_\nu \rangle \langle \Psi_\nu | \hat{O} | \Psi_0 \rangle \delta\left(\omega - (E_\nu - E_0)\right) \\ &= \langle \Psi_0 | \hat{O}^\dagger \sum_\nu |\Psi_\nu\rangle\langle\Psi_\nu| \delta\left[\omega - (E_\nu - E_0)\right] \hat{O} | \Psi_0 \rangle \\ &= \langle \Psi_0 | \hat{O}^\dagger \delta\left[\omega - (\hat{H} - E_0)\right] \hat{O} | \Psi_0 \rangle\end{aligned}$$

- $|\Psi_\nu\rangle \longrightarrow$ complete set of Hamiltonian eigenstates
- $\hat{O} \longrightarrow$ excitation operator
- $\omega \longrightarrow$ energy transfer ($\hbar = 1$)

Integral Transform Methods

The response function can be formally written as a ground state expectation:

$$\mathcal{R}(\omega) = \langle \Psi_0 | \hat{O}^\dagger \delta \left[\omega - (\hat{H} - E_0) \right] \hat{O} | \Psi_0 \rangle$$

Since we can't evaluate it directly, one choice is to consider instead an integral transform with some generic kernel K:

$$\begin{aligned} \Phi(\sigma) &= \int K(\sigma, \omega) \mathcal{R}(\omega) d\omega \\ &= \langle \Psi_0 | \hat{O}^\dagger K(\sigma, (\hat{H} - E_0)) \hat{O} | \Psi_0 \rangle \end{aligned}$$

and take the inverse transform to find $\mathcal{R}(\omega)$
$\rightarrow$ **ill-posed problem!**.

Integral Transform methods

Some "obvious" characteristics of a good kernel should be:

- the transform $\Phi(\sigma)$ is easy to calculate
- the inversion of the transform can be made stable
- $K(\sigma,\omega)$ is approximately $\delta(\sigma-\omega)$ (in principle not strictly necessary)

Integral transforms and Ill-posed problems

Ill-Posed Problems [Hadamard]

A problem is called ill-posed when one of the following occours

- the solution does not exist or it is not unique
- the solution does not depend continuosly on the data

An intuitive way to see the problem is to consider
$f_n(y) = \sin(ny)$

$$g(x) = \int_a^b K(x,y)\, f_n(y) dy \xrightarrow{n\to\infty} 0$$

the integration process has a *smoothening effect*.

Integral transforms and Ill-posed problems

Let us consider now the inverse problem. We expect it to behave in the opposite way, i.e. by adding an arbitrary small high frequency perturbation to the input g can lead to an arbitrary high perturbation in the output f

$$g(\sigma) \rightarrow g(\sigma) + g^{HF}(\sigma) \; with \; \|g\| \gg \|g^{HF}\|.$$

$$\|K^{-1} g^{HF}\| \gg \|K^{-1} g\|$$

Singular Value Decomposition (SVD)

We can make a discretization of the Integral transform

$$g(x) = \int_a^b K(x,y) f(y) dy \quad \longrightarrow \quad g_i = \sum_k^N \alpha_k K_{ik} f_k \qquad i \in [1, N]$$

$$g_i \equiv g(x_i) \quad K_{ik} \equiv K(x_i, y_k) \quad f_k \equiv f(y_k)$$

The SVD of the matrix K is a factorization of the form

$$K = U \Sigma V^T \quad \text{with} \quad U, V, \Sigma \in \mathbb{R}^{N x N}$$

with U, V orthogonal and $\Sigma = diag[\sigma_1, \ldots, \sigma_N]$.

The columns $\bar{u}_j$ of U and $\bar{v}_j$ of V can be regarded as orthonormal basis vectors of $\mathbb{R}^N$ and the following holds

$$K \bar{v}_j = \sigma_j \bar{u}_j \quad K^T \bar{u}_j = \sigma_j \bar{v}_j$$

Singular Value Decomposition (SVD) II

In terms of the SVD of the matrix K the direct and inverse problems can be rewritten as

$$\bar{g} = K\bar{f} = \sum_j^N \sigma_j (\bar{v}_j^T \bar{f}) \bar{u}_j \qquad \bar{f} = K^{-1}\bar{g} = \sum_j^N \frac{\bar{u}_j^T \bar{g}}{\sigma_j} \bar{v}_j$$

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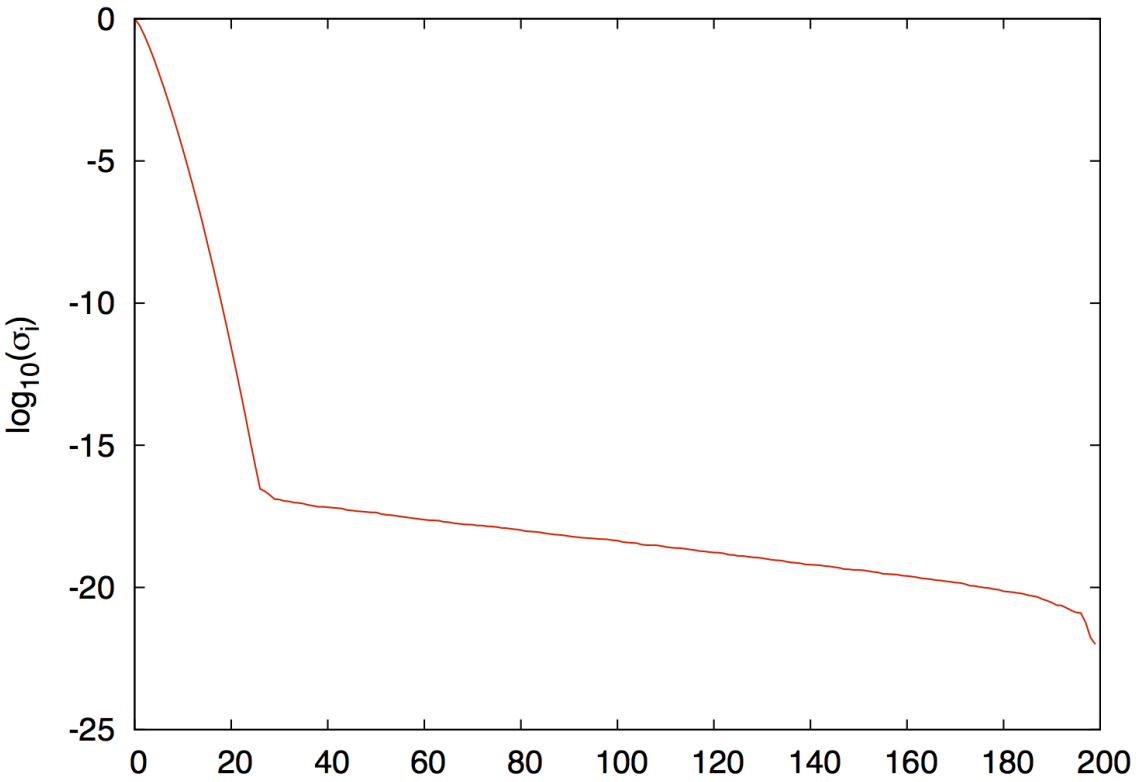
If the matrix K is the result of discretization of a Fredholm Integral equation of the 1st kind the following basic properties holds

- the singular values σ_i decay fast towards zero
- the singular vectors $\bar{u}_i, \bar{v}_i$ have increasing frequencies

We can use the decay rate of singular values to define a sort of *degree of ill – posedness*

Singular Value Spectrum



Regularization techniques

As an escape, it is possible to approximate the original ill-posed problem with a well-posed one, constraining the solution with known features (eg. smoothness, sign, asymptotic behavior...) in this way, (i.e. changing the problem...), the solution is well-defined

In most approaches we have minimization problems of the form

$$\min_{\bar{f}} \; D\left[K\bar{f}, \bar{g}\right] + \alpha L\left[\bar{f}\right]$$

where

- D is a likelihood function (eg. Chi-squared, euclidean norm)
- L is a penalty functional that enforces eg. smoothness
- α is the regularization parameter

Integral kernels - Laplace

Projection QMC methods exploit the long time behavior of the imaginary-time propagator

$$e^{-\tau \hat{H}}|\Phi_0\rangle = \sum_{n=0}^{\infty} e^{-\tau E_n}\langle \Psi_n|\Phi_0\rangle|\Psi_n\rangle \xrightarrow{\tau\to\infty} e^{-\tau E_0}\langle \Psi_0|\Phi_0\rangle|\Psi_0\rangle$$

In this framework it is natural to consider the Laplace kernel:

$$K(\sigma,\omega) = e^{-\sigma\omega}$$

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The transform becomes an imaginary-time correlation function:

$$\Phi(\sigma) = \frac{\langle\Psi_0|\hat{O}^\dagger e^{-\sigma\hat{H}}\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{\langle\Psi_0|\hat{O}^\dagger(0)\hat{O}(\sigma)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}.$$

Singular Values and Stability

In order to understand how bad the Laplace kernel really is. let us compare its SVD spectrum with that of a Lorentz kernel, known to be more stable for inversion.

Laplace kernel [QMC methods]

$$K_{Laplace}(\sigma,\omega) = e^{-\sigma\omega}$$

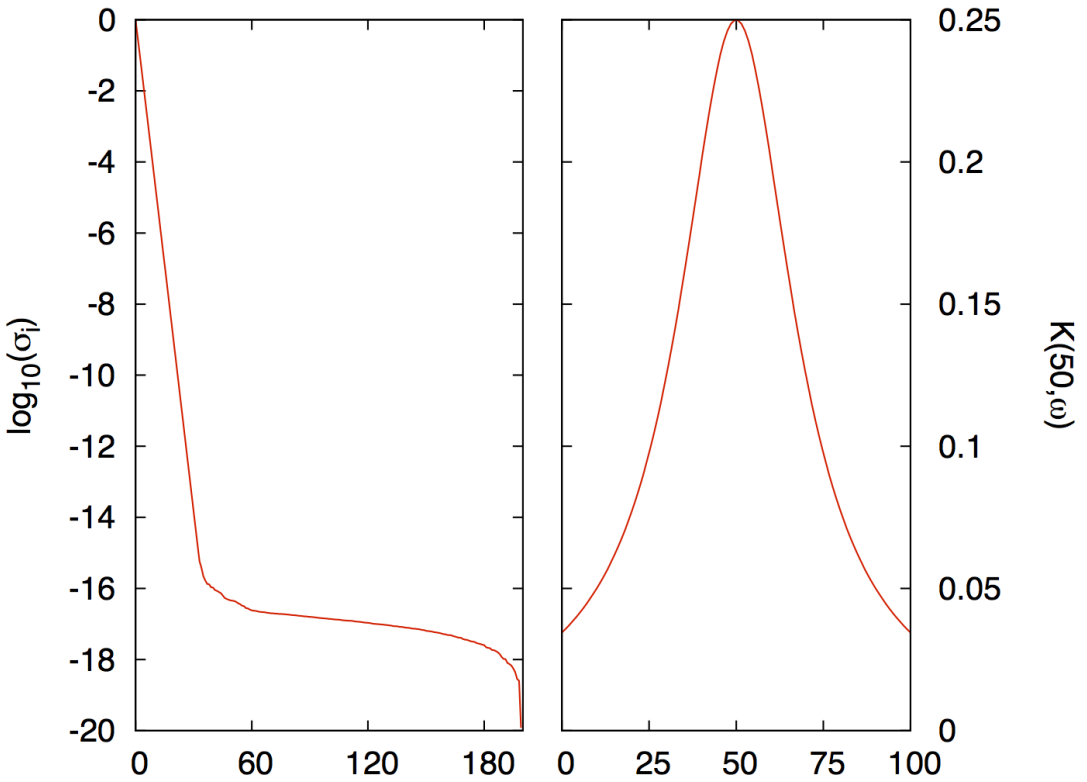
Lorentz kernel [LIT method]

$$K_{Lorentz}(\sigma,\omega) = \frac{\Gamma}{\Gamma^2 + (\sigma-\omega)^2}$$

where the parameter Γ controls the width of the kernel.

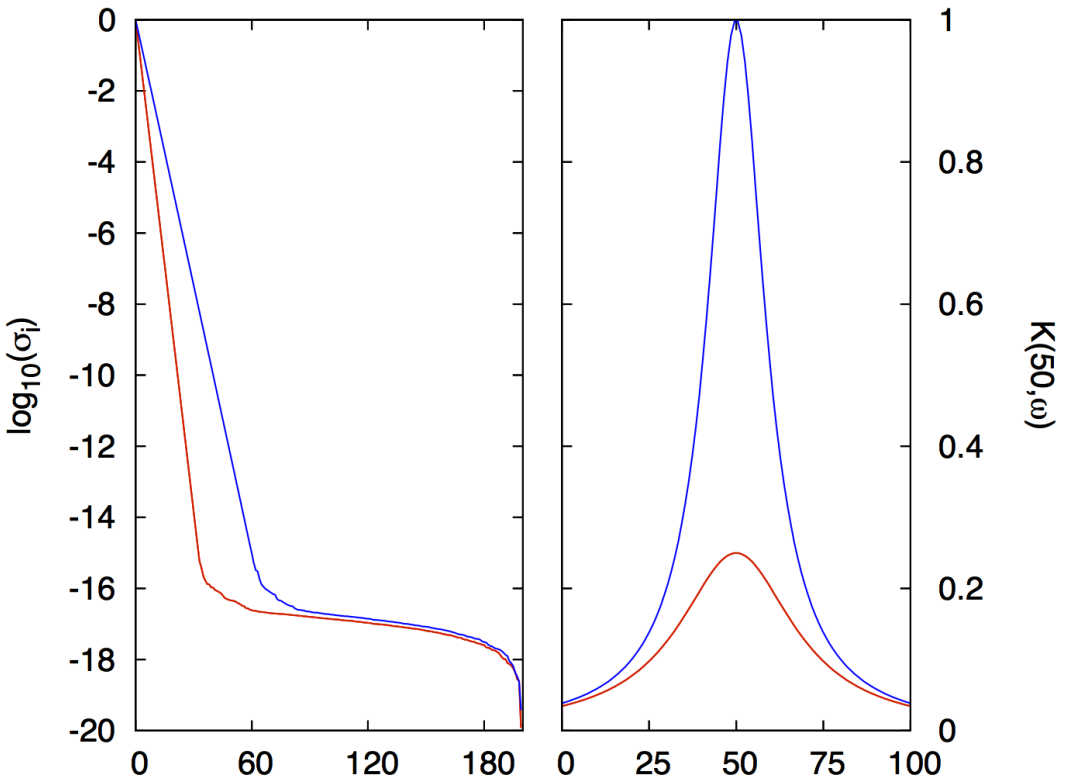
Singular Values and Stability

$K_{Lorentz}\ \{\Gamma = 20\}$



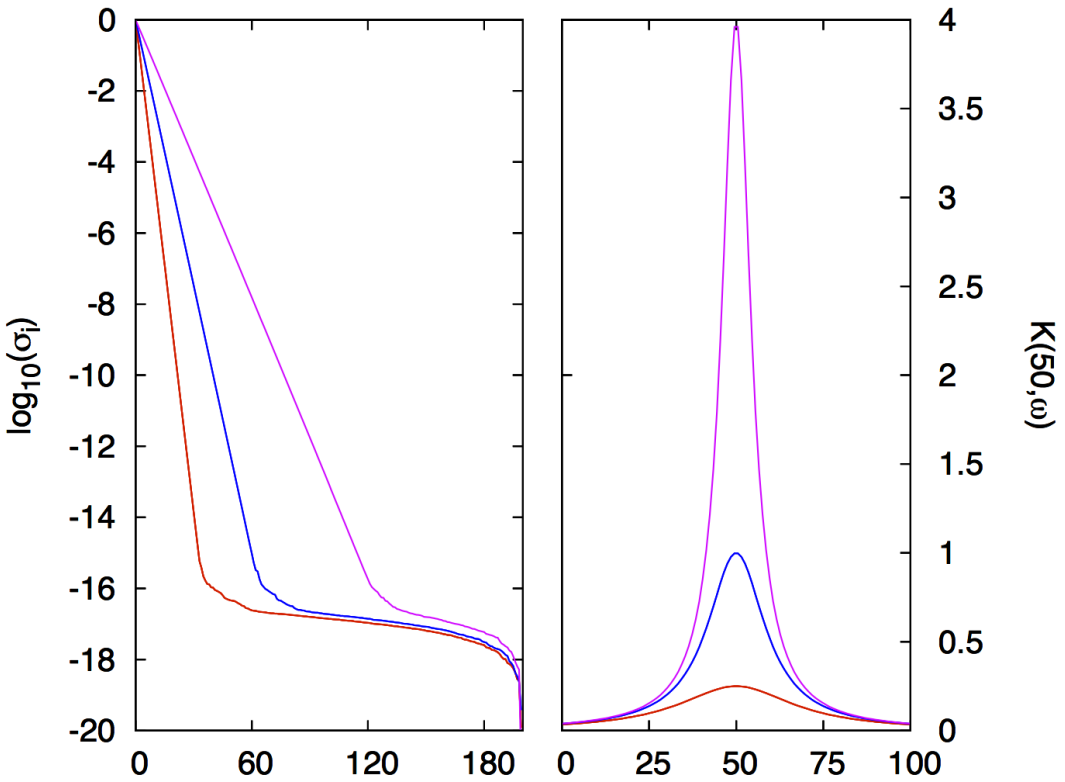
Singular Values and Stability

$$K_{Lorentz}\ \{\Gamma = 20\ ,\ 10\}$$



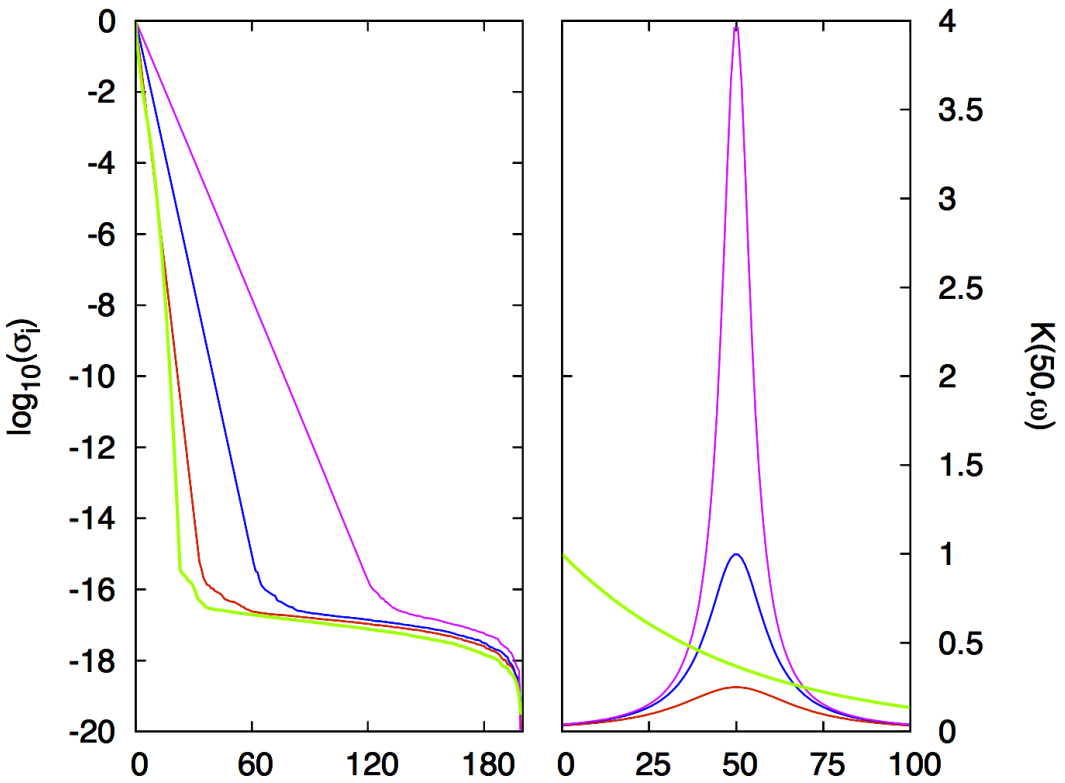
Singular Values and Stability

$$K_{Lorentz}\ \{\Gamma = 20\ ,\ 10\ ,\ 5\}$$



Singular Values and Stability

$K_{Lorentz}$ $\{\Gamma = 20\ ,\ 10\ ,\ 5\}$ $K_{Laplace}$



Integral Kernels - Laplace-like

We now want to build an integral kernel which can be calculated in QMC methods and that has a shape closer to the Lorentz kernel. In general, a better approximation of a Dirac δ function (which has obviously a flat spectrum) seems to be a better guess for the kernel.

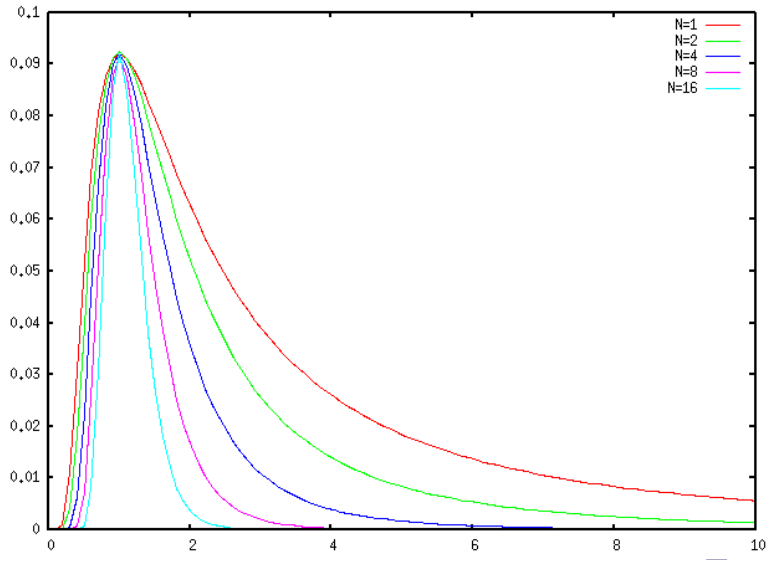
This is an "obvious" statement, but it can be made quantitative by means of the SVD analysis!

Singular Values and Stability

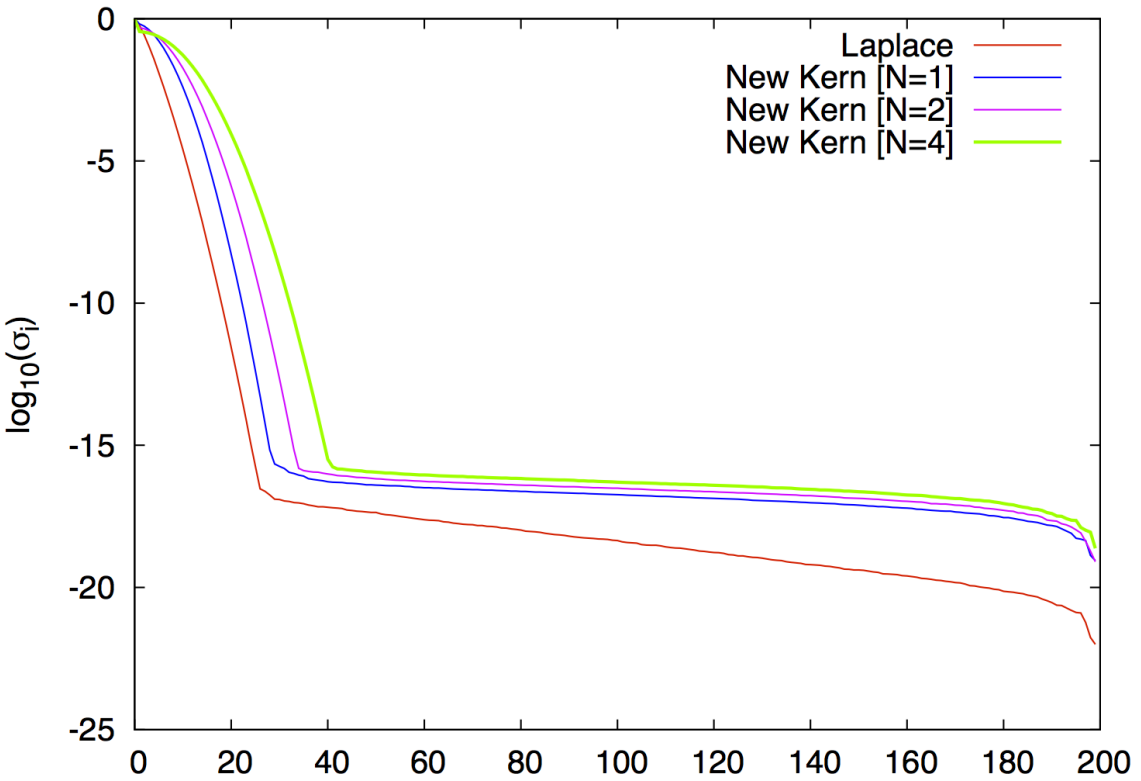
Let us consider the following kernel, that we can easily see as built out of Laplace kernels with different imaginary times (Sumudu Transform):

$$K(\sigma,\omega,N) = \frac{1}{\sigma}\left(2^{-\frac{\omega}{\sigma}} - 2^{-2\frac{\omega}{\sigma}}\right)^N = \sum_{k=0}^{N}\binom{N}{k}(-1)^k e^{-\ln(2)(N+k)\frac{\omega}{\sigma}} \tag{1}$$

As $N \to \infty$ the kernel width becomes smaller.



Integral Kernels - New Kernel (SV spectrum)



Path Integral Methods

How do we calculate imaginary-time correlation function?

Path Integral based methods (VPI,PIGS,RQMC) have access to pure estimators and are naturally suited for imaginary-time properties since we simulate already full imaginary-time paths.

Consider an imaginary-time path of length $2\tau + \beta$ as our "walker" and discretize the path in M time-slices of size $\Delta\tau = (2\tau + \beta)/M$, then:

$$C_O(\beta) = \frac{\langle \Psi_T | e^{-\tau(\hat{H}-E_0)} \hat{O}^\dagger e^{-\beta(\hat{H}-E_0)} \hat{O} e^{-\tau(\hat{H}-E_0)} | \Psi_T \rangle}{\langle \Psi_T | e^{-(2\tau+\beta)(\hat{H}-E_0)} | \Psi_T \rangle}$$

$$\xrightarrow{\tau\to\infty} \frac{\langle \Psi_0 | \hat{O}^\dagger e^{-\beta(\hat{H}-E_0)} \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{\langle \Psi_0 | \hat{O}^\dagger(0) \hat{O}(\beta) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

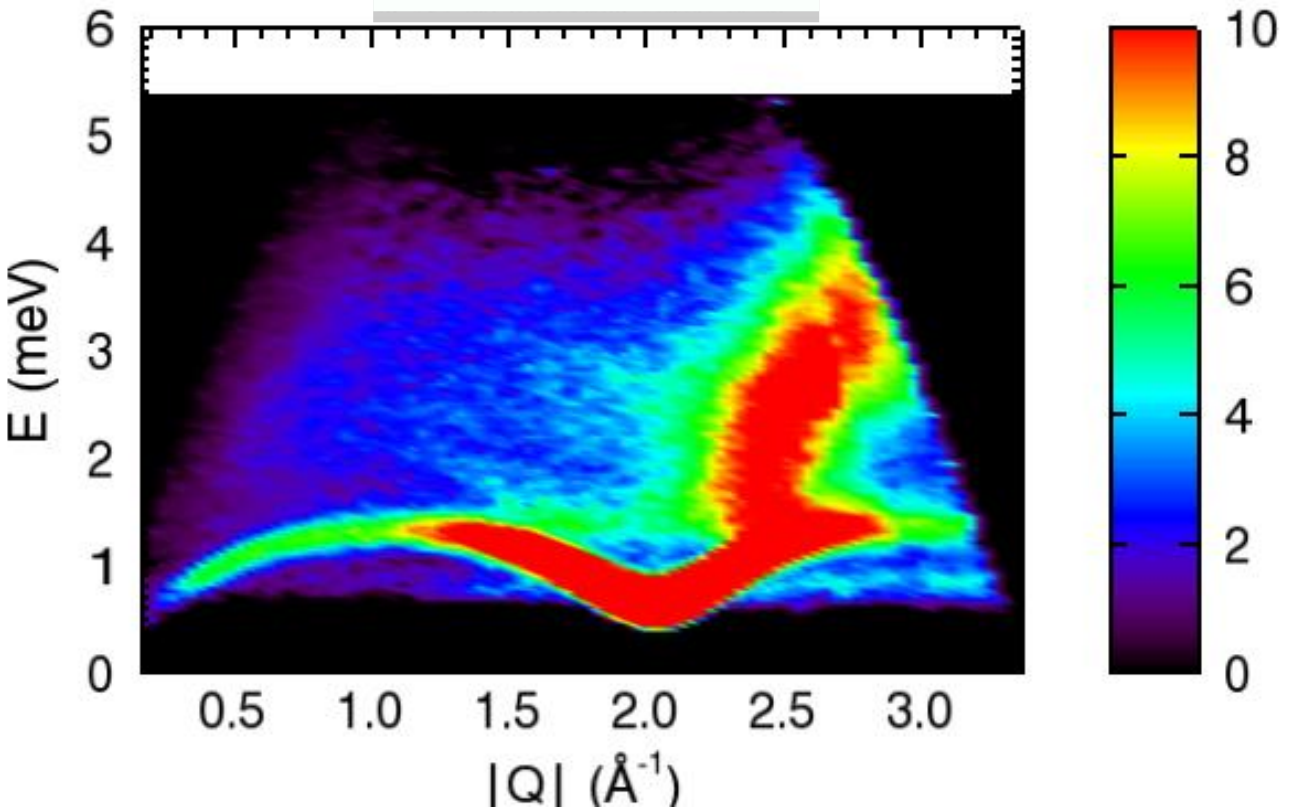
Condensed ^{4}He

Liquid ^{4}He is the "simplest" many-body system on which we can test our kernels.
Quick reminders:

- Liquid ^{4}He becomes superfluid at temperatures < 2.172K
- The interaction is essentially Van der Waals. At saturation the binding energy per atom is 7.12K (1K $= 8.2\times10^{-11}$MeV)

Density response of superfluid He^4

The density response is usually measured by means of neutron scattering.



http://www.cm.ph.bham.ac.uk/group/whoswho/blackburn/blackburn.html

Density response of superfluid He^4

QMC calculation

- 64 He^4 atoms in a cubic box with Periodic Boundary Conditions
- realistic effective interaction: *HFDHE2* pair-potential [Aziz (1979)]. Notice that in condensed ^{4}He 3-body forces would be needed.
- Trial-function with two and three-body correlations
- *Reptation Quantum Monte Carlo* (RQMC) [Baroni (1999)]

Density response of superfluid He^4

Reptation Quantum Monte Carlo is based on a path-integral formulation of the imaginary time propagation, added with importance sampling at every step

$$\phi(X,\tau)\Psi_T(X) = \int dX' G(X,X',\tau)\frac{\Psi_T(X)}{\Psi_T(X')}\Psi_T(X')\phi(X',0)$$

We can split G on short time intervals:

$$G(X,X',\tau) = \int dX''\cdots dX^N G\left(X,X'',\frac{\tau}{N}\right)\ldots G\left(X^N,X',\frac{\tau}{N}\right)$$

Density response of superfluid He^4

The splitted Green's function can be in turn be redefined as a product of importance sampled Green's functions:

$$\tilde{G}(X,X',\tau) \equiv G(X.X',\tau)\frac{\Psi_T(X)}{\Psi_T(X')} =$$

$$= \int dX''\cdots dX^N \tilde{G}\left(X,X'',\frac{\tau}{N}\right)\ldots\tilde{G}\left(X^N,X',\frac{\tau}{N}\right)$$

In the short time approximation, at order $\Delta\tau = \tau/N$(Trotter):

$$\tilde{G}(X,X',\Delta\tau) \sim e^{-\frac{\left(X-\frac{\nabla\Psi_T(X')}{\Psi_T(X')}-X'\right)^2}{2D\Delta\tau}} e^{-\frac{1}{2}\left(\frac{H\Psi_T(X)}{\Psi_T(X')}+\frac{H\Psi_T(X')}{\Psi_T(X)}\right)\Delta\tau}$$

Density response of superfluid ^{4}He

We are therefore lead to sample a *reptile*, i.e. a path $\{X_0 \cdots X_N\}$ in which each time slice is sampled evolving the previous one with a Langevin dynamics:

$$X_{i+1} = X_i + \Delta\tau \frac{H\Psi_T(X_i)}{\Psi_T(X_i)} + \eta(X_i, X_i + 1, \Delta\tau)$$

The reptiles are sampled by randomly choosing one of the two ends, sampling a further point of the path, and destroyng the last point on the oppsite site.
In the middle of the path the points are propagated of an imaginary time $\tau/2$.

ESTIMATORS

Energy:

$$E = \frac{1}{2}\left[E_{loc}(0) + E_{loc}(\tau)\right] \qquad where \quad E_{loc} = \frac{H\Psi_T(X)}{\Psi_T(X)}$$

Other (local):

$$\langle \hat{O} \rangle = \frac{1}{\tau - 2\sigma} \langle \int_{\sigma}^{\tau-\sigma} O(\tau')d\tau' \rangle$$

σ should be large enough to avoid bias from the trial function. The operator averaged at times 0 and τ gives the *mixed estimate* $\langle \Psi_0 | \hat{O} | \Psi_T \rangle$ usually computed in DMC.

An interesting feature of RQMC is the fact that expectations computed at the center of the sample "reptile" are no longer dependent on the importance function.

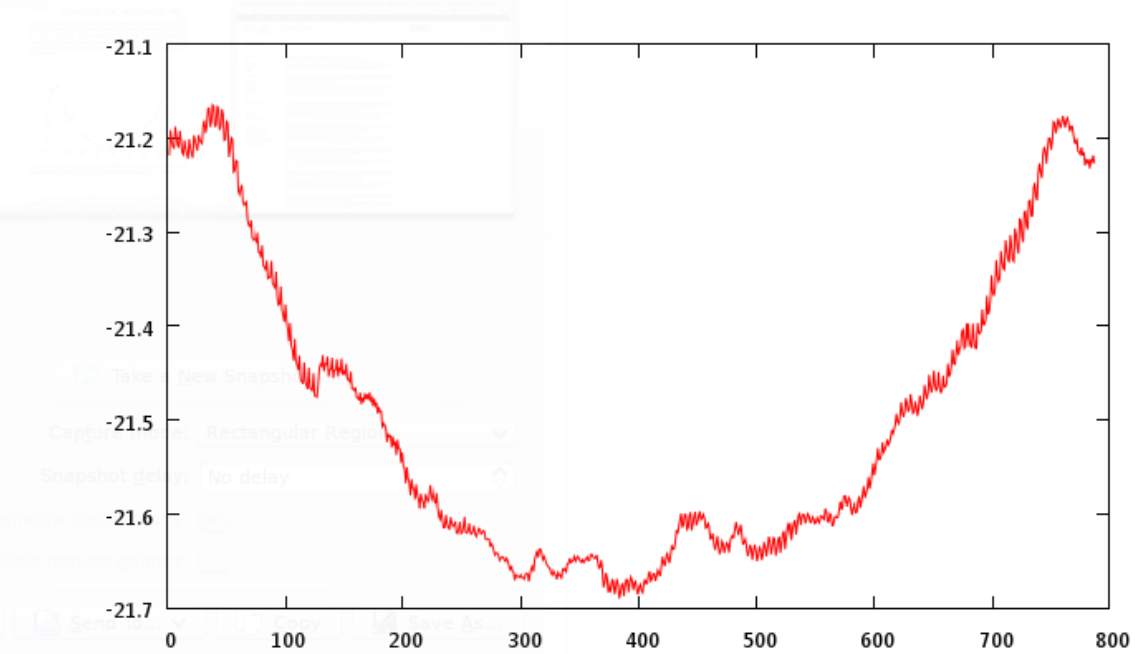


Figure 3.1: Potential energy along an 800 slices-long imaginary-time path obtained with a long run ($\approx 10^7$ samples) and a time step $\epsilon = 0.001K^{-1}$

from A. Roggero M.Sc. thesis

Density response of superfluid ^{4}He

We are interested in the density response of the system, in this case the Response function is the so-called Dynamic Structure Factor

$$S(q,\omega) = \frac{1}{N}\sum_{\nu}|\langle\Psi_\nu|\rho_q|\Psi_0\rangle|^2\delta\left(\omega-(E_\nu-E_0)\right)$$

where ρ_q is the Fourier Transform of the density operator: $\rho_q \equiv \sum_j e^{iqr_k}$.

Density response of superfluid ^{4}He

In RQMC calculations it is possible to compute very efficiently the Laplace transform of the response function. Baroni and Moroni(PRL 82, 4745 (1999)) presented the results of the inversion with ME techniques.

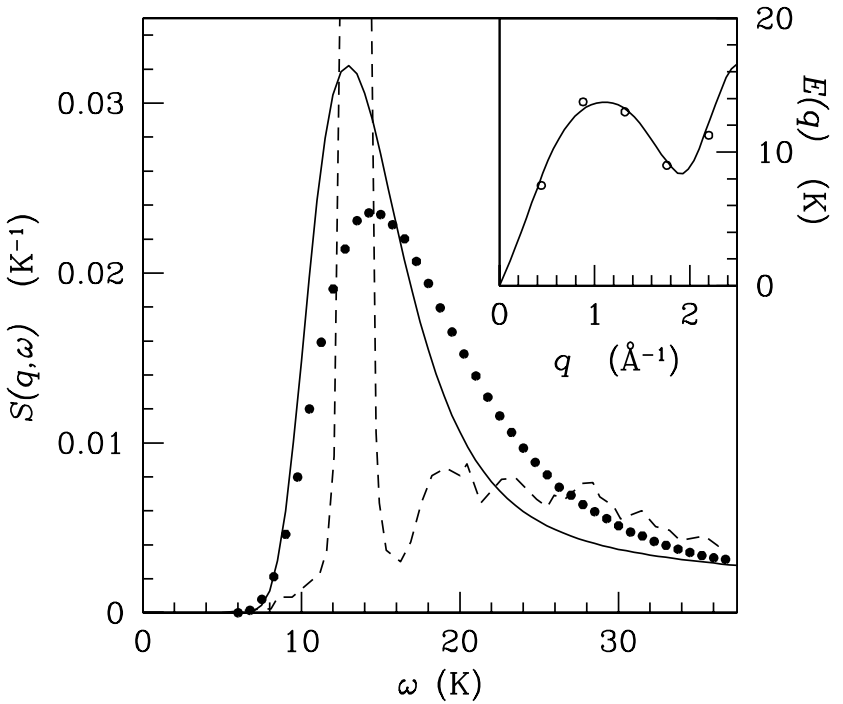
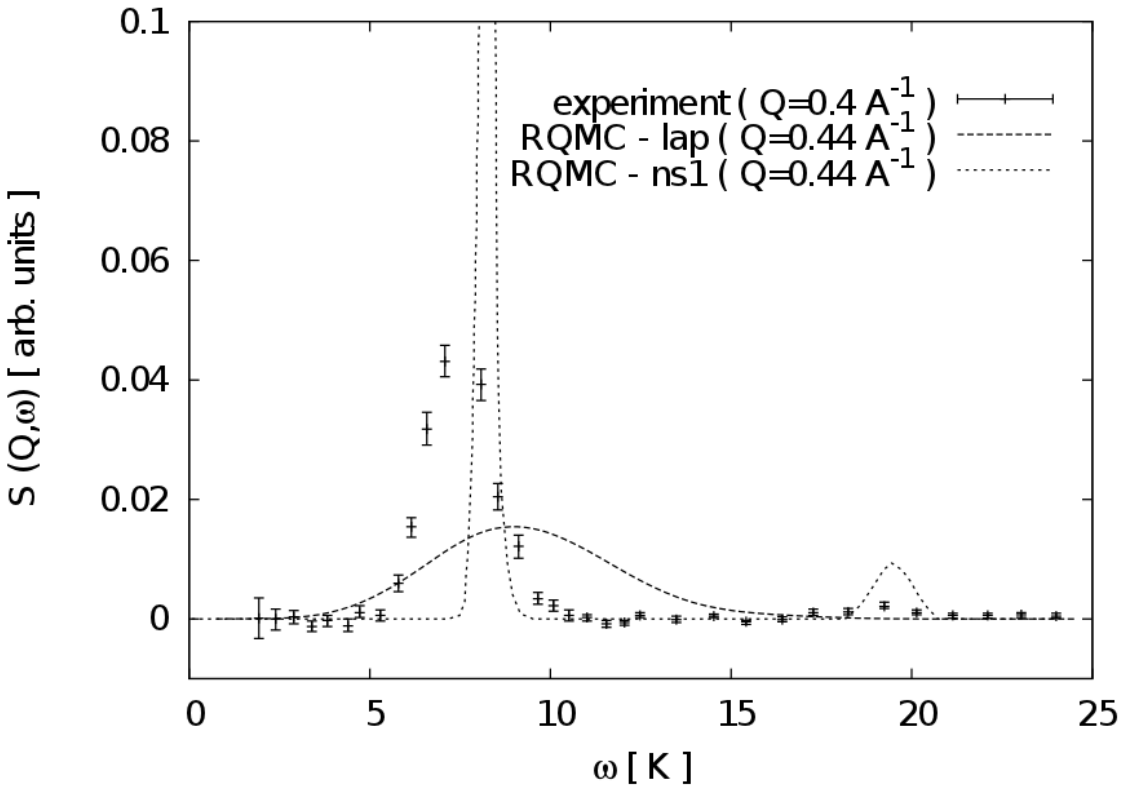


FIG. 3. The ME reconstruction of the dynamical structure factor of ^{4}He at $q = 1.32$ Å^{-1} (solid line). The dotted line is the result of a path integral Monte Carlo calculation [17], and the dashed line is the measured $S(q, \omega)$. The inset compares the positions of the ME peaks at various wave vectors (open circles) with the experimental excitation spectrum.

Density response of superfluid ^{4}He

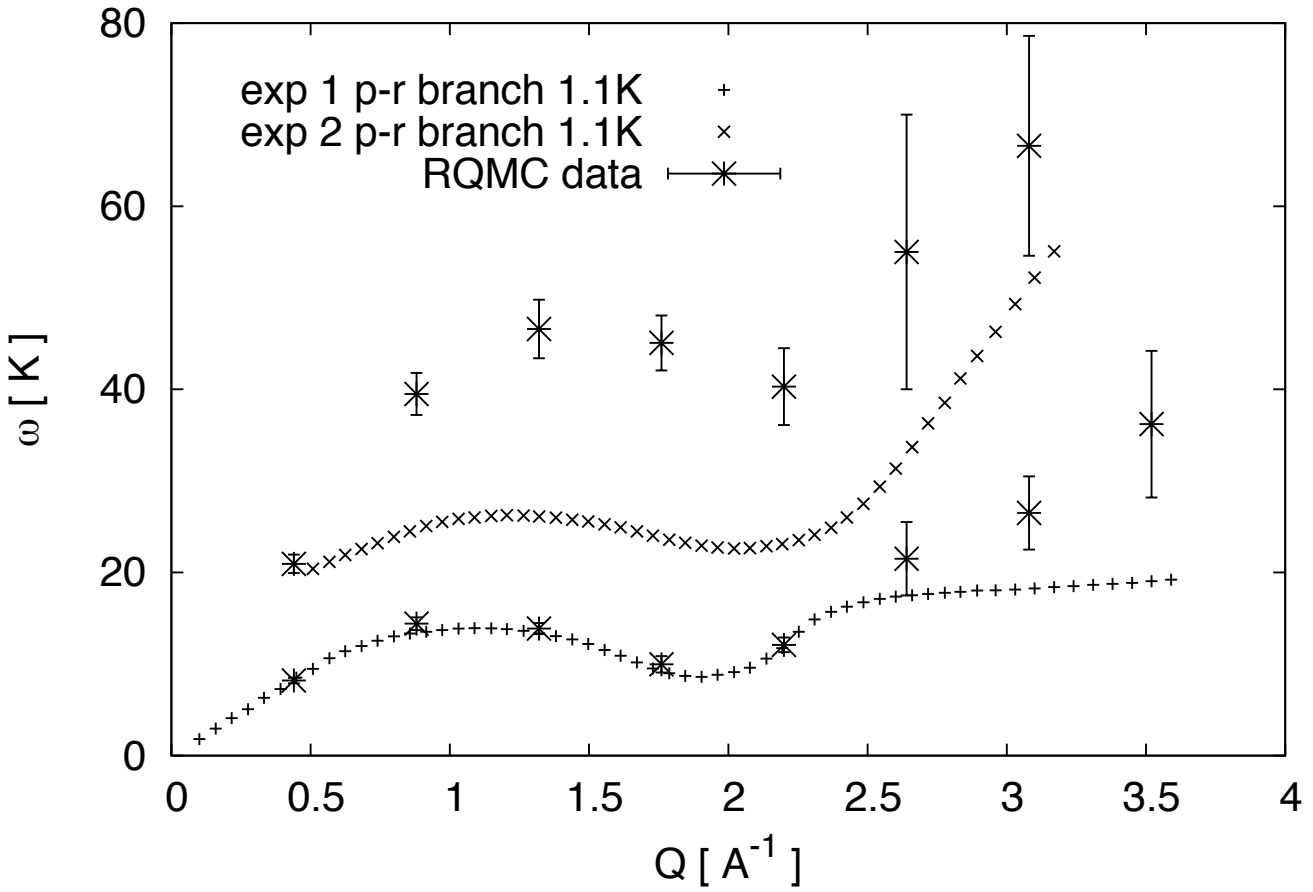
Dynamic Structure Factor



A. Roggero, F. Pederiva, G. Orlandini, arXiv:1209.5638

Density response of superfluid ^{4}He

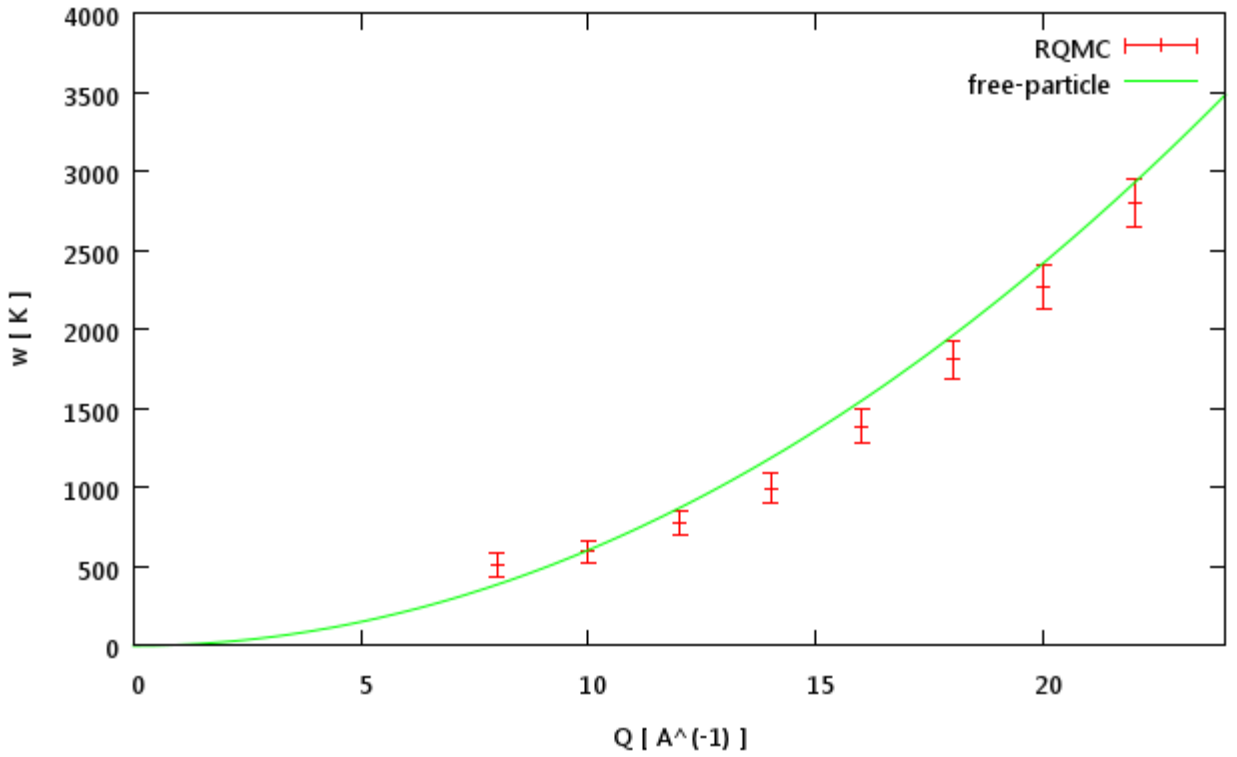
Low-Momentum Excitation spectrum



A. Roggero, F. Pederiva, G. Orlandini, arXiv:1209.5638

Density response of superfluid ^{4}He

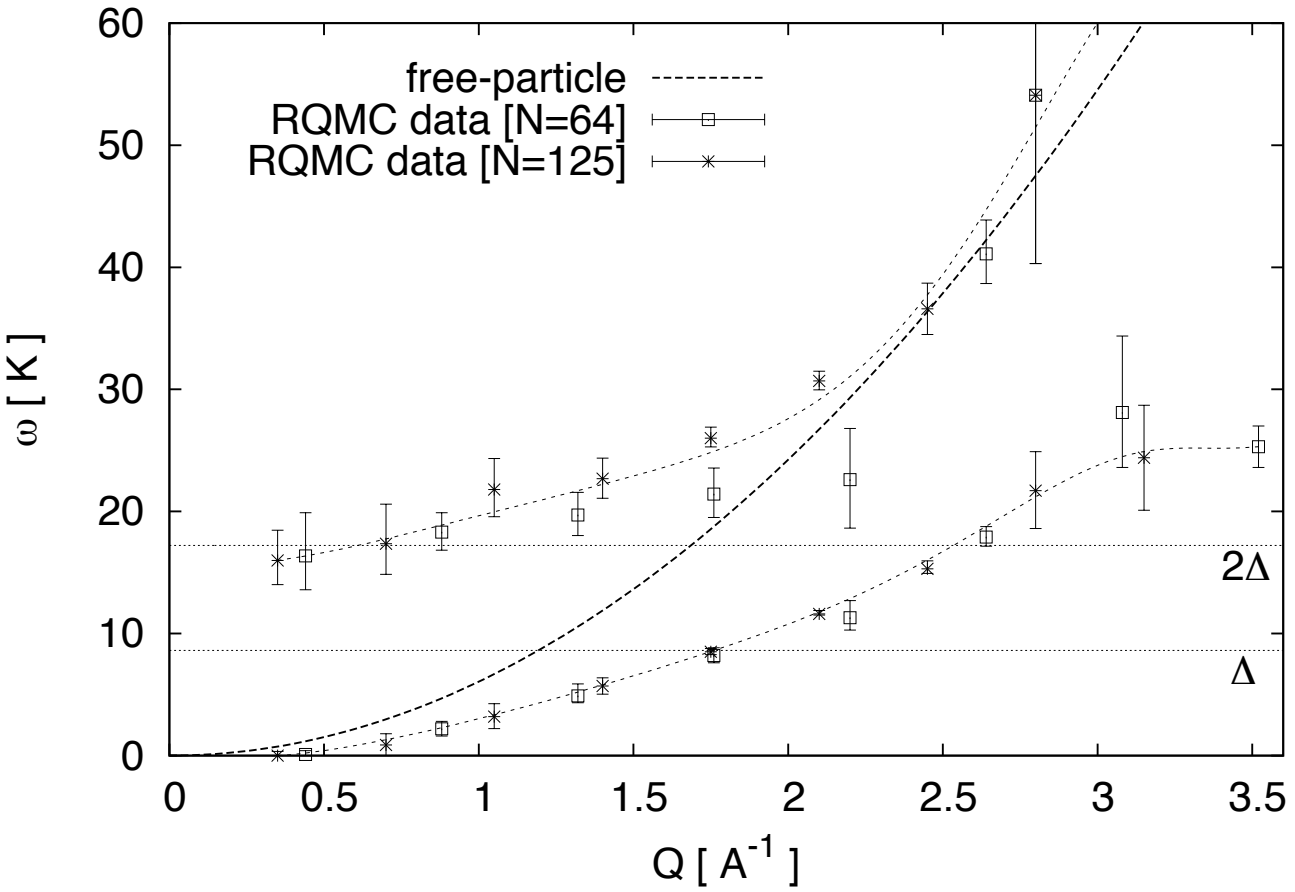
Excitation spectrum in quasi-elastic regime



A. Roggero, M.Sc. thesis

Example: density response of superfluid ^{4}He

Excitation spectrum: incoherent (single particle) part



A. Roggero, F. Pederiva, G. Orlandini, arXiv:1209.5638

Conclusions

Pro

- the only input of the calculation is the interaction potential
- we only need imaginary-time correlation functions

Con

- for high accuracy, extremely long imaginary-time intervals have to be considered
- the inversion procedure still introduces uncontrollable errors