

# Dynamical Structure Factors from Quantum Monte Carlo Calculations of a Proper Integral Transform

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INT - Seattle - 16 Jul, 2013

- Dynamic Response Functions
- Integral transform methods
  - Ill-Posed problems
- Integral Kernels for Quantum Monte Carlo
  - Laplace Kernel and imaginary-time correlations
  - A better Kernel
- Results
  - Superfluid  $He^4$
  - Unitary Fermi Gas

# Dynamic Response Function

Spectral representation of DRF

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

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

# Integral Transform Techniques

An Integral Transform maps the original problem in a new domain where it's simpler to solve it

$$T(y) = \int_x K(x, y) S(x) dx$$

- Accessible object
- Object of interest

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The solution is then mapped back using the *inverse transform*.

## PROBLEM

The inverse transform constitutes an Ill-Posed Problem!

# Integral Transform for Response Functions

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

Consider an IT with generic kernel  $K$   
(Efros,Leidemann,Orlandini-Phys.Lett.B338,130):

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

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

A proper kernel should be one such that:

- the transform  $\Phi(\sigma)$  is easy to calculate
- the inversion of the transform can be made stable

In QMC methods we routinely use the imaginary-time propagator

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

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

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

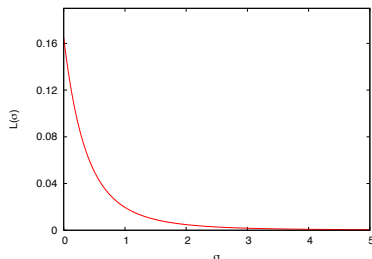
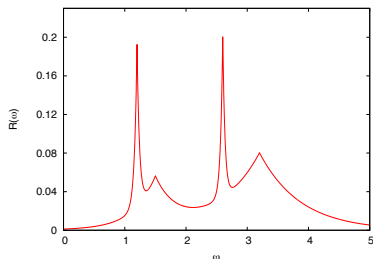
The transform becomes an imaginary-time correlation function:

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



# Integral kernels - Laplace [Toy model]

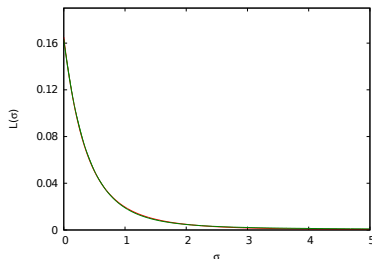
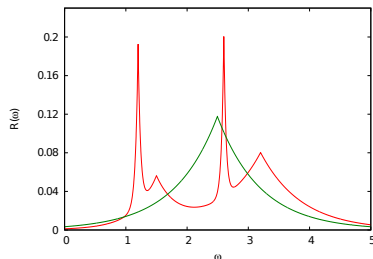
$$L(\sigma) = \int K(\sigma, \omega) R(\omega) d\omega = \int_0^{\infty} e^{-\sigma\omega} R(\omega) d\omega$$



- N.B. : we have access only to a NOISY version of  $L(\sigma)$

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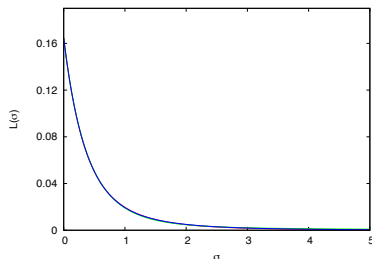
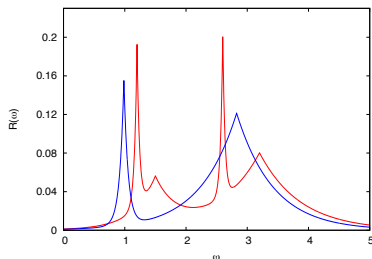
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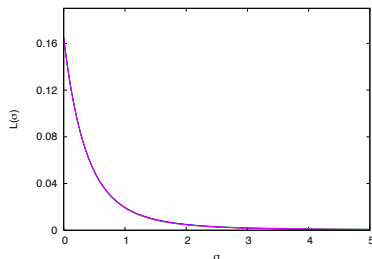
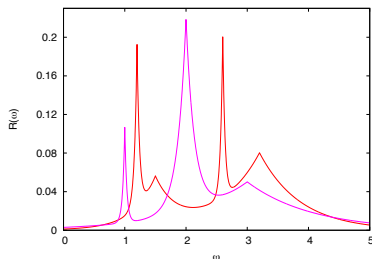
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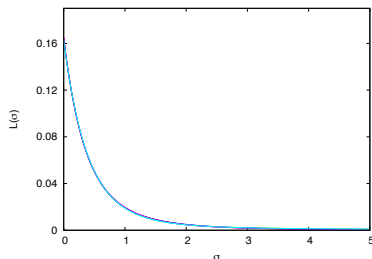
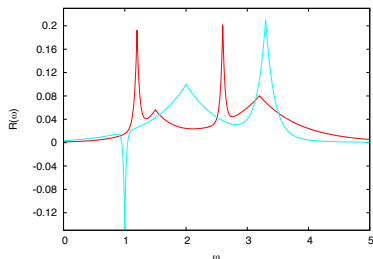
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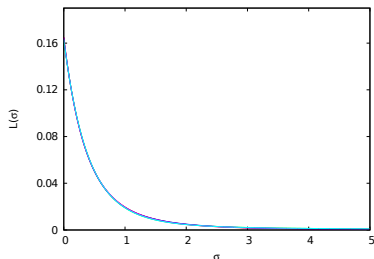
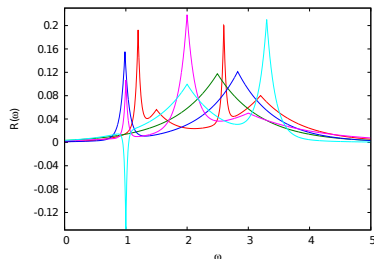
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# Dealing with Ill-Posed problems

Many efforts devoted to performing stable inversions

- Maximum Entropy Method (MEM) [Talbot, J.Inst.Maths.App.23,97]
- Average Spectrum Method (ASM) / Stochastic Analytic Continuation (SAC) [Sandvik,PRB.57,10287]
- Genetic Inversion via Falsification of Theories (GIFT) [Vitali et al,PRB.82,174510]
- ...

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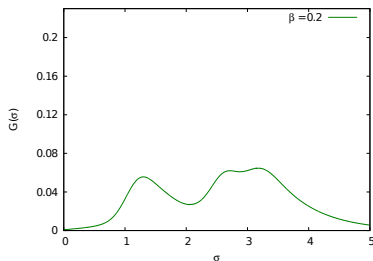
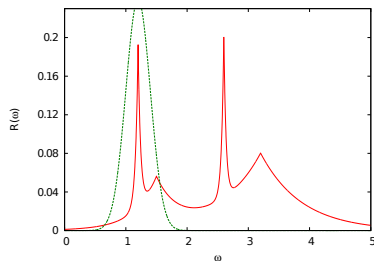
• N.B. : Not much attention devoted to the Kernel function!



# Integral kernels - Gaussian

$$G(\sigma, \beta) = \int K(\sigma, \omega, \beta) R(\omega) d\omega = \int_0^\infty e^{-\frac{(\sigma-\omega)^2}{2\beta}} R(\omega) d\omega$$

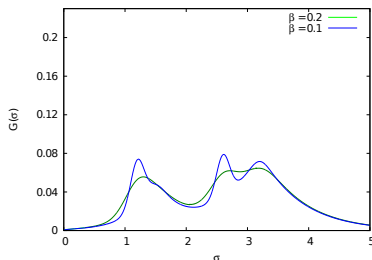
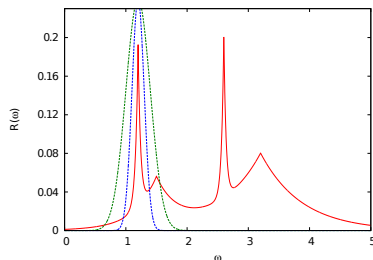
- We have now one more parameter:  $\beta$ . What's its effect?



The transform  $G(\sigma)$  is a smoothed version of the original signal!

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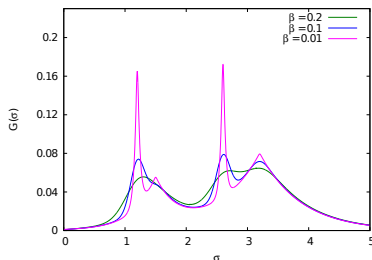
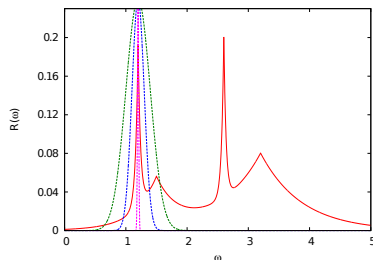
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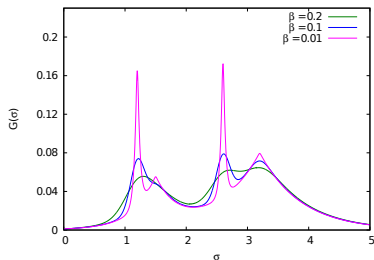
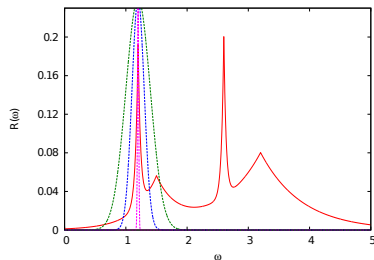
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- We have now one more parameter:  $\beta$ . What's its effect?



In the limit  $\beta \rightarrow 0$  no inversion needed!!

# Singular Value Decomposition (SVD)

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

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

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

$$\begin{bmatrix} K_{00} & K_{01} & \dots \\ K_{10} & K_{11} & \dots \\ \dots & \dots & \dots \end{bmatrix} = \begin{bmatrix} U_{00} & U_{01} & \dots \\ U_{10} & U_{11} & \dots \\ \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} \sigma_0 & 0 & \dots \\ 0 & \sigma_1 & \dots \\ \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} V_{00} & V_{01} & \dots \\ V_{10} & V_{11} & \dots \\ \dots & \dots & \dots \end{bmatrix}^T$$

where  $\sigma_i$  are called *singular-values* and  $\bar{u}_j = (U_{0j}, U_{1j}, \dots)$  and  $\bar{V}_j = (V_{0j}, V_{1j}, \dots)$  are the (resp. left and right) *singular-vectors*

# Singular Value Decomposition (SVD) II

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

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

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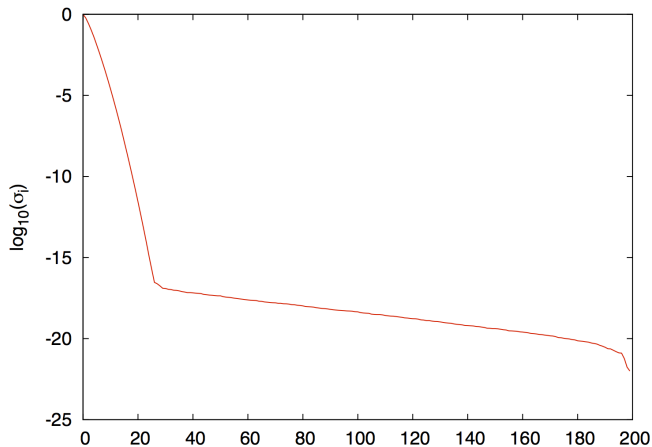
$$\bar{g} = K\bar{f} = \sum_j^N \sigma_j (\bar{v}_j^T \bar{f}) \bar{u}_j \quad \bar{f} = K^{-1}\bar{g} = \sum_j^N \frac{1}{\sigma_j} \bar{u}_j^T \bar{g} \bar{v}_j$$

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  $\sigma_i$  decay fast towards zero
- the singular vectors  $\bar{u}_i, \bar{v}_i$  have increasing frequencies (sign changes)

the decay rate of  $\sigma_i$  is related to a sort of *degree of ill – posedness*

# Singular Value Spectrum





# Singular Values and Stability

Lorentz kernel [LIT method]

(Efros,Leidemann,Orlandini-Phys.Lett.B338,130)

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

Laplace kernel [QMC methods]

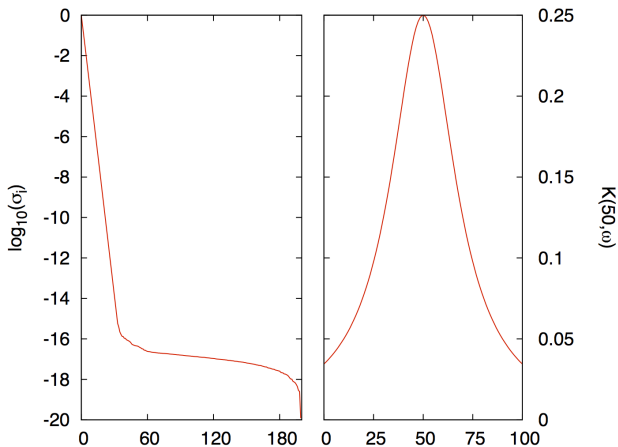
$$K_{Laplace}(\sigma, \omega) = e^{-\sigma\omega}$$

The inversion of the integral transform obtained with the first kernel can be easily made stable while with the second one this is not the case.

We can analyze then the spectrum of singular values to understand why.

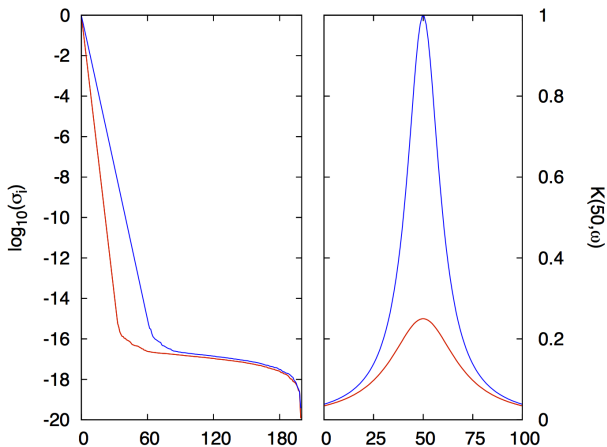
# Singular Values and Stability

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



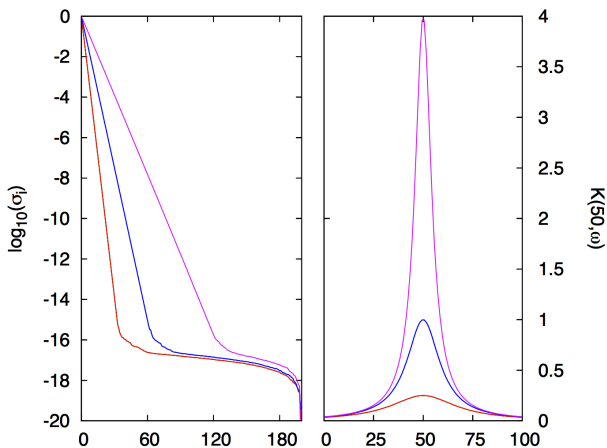
# Singular Values and Stability

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



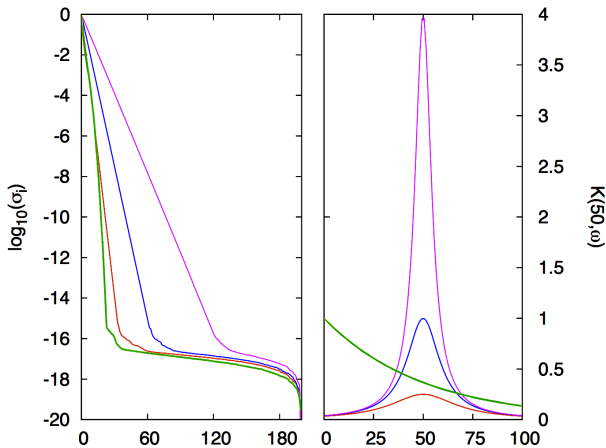
# Singular Values and Stability

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



# Singular Values and Stability

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

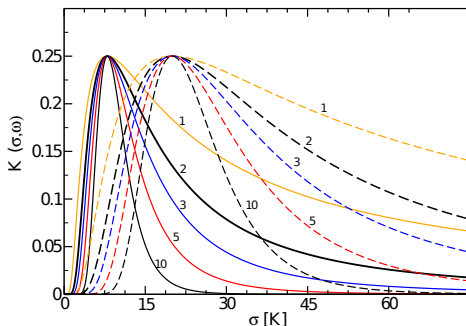


# Integral Kernels - Laplace-like

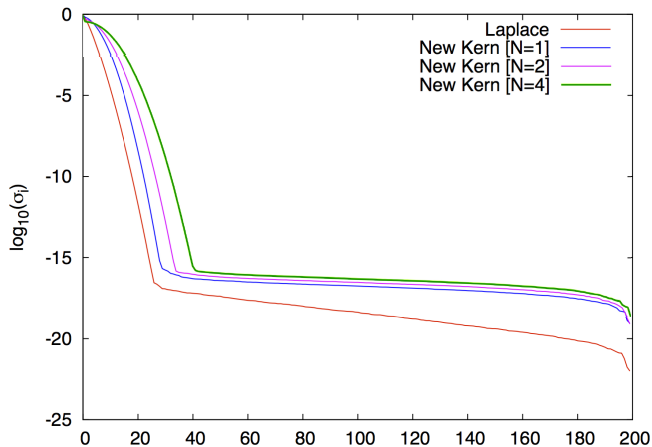
We now want to build an integral kernel which can be calculated in QMC methods and that has the desired form.

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

As  $N \rightarrow \infty$  the kernel width becomes smaller and smaller



# Integral Kernels - New Kernel (SV spectrum)



# Application: density response of superfluid $He^4$

[A. R., F. Pederiva and G. Orlandini **arXiv:1209.5638**]

- 64  $He^4$  atoms in a cubic box with Periodic Boundary Conditions
- realistic interaction: *HFDHE2* pair-potential [ Aziz et al. (1979) ]
- *Reptation Quantum Monte Carlo* (RQMC) [ Baroni et al. (1999) ]
- "simple" inversion algorithms (EMML, SMART) [ Byrne (1993) ]

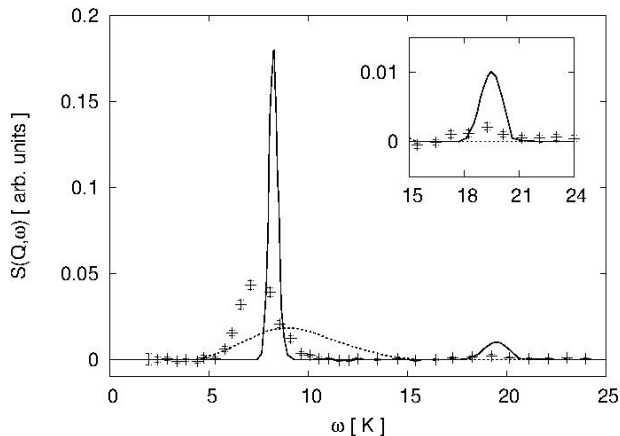
We are interested in the density response of the system, in this case the Response function is the so-called Dynamic Structure Factor

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

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

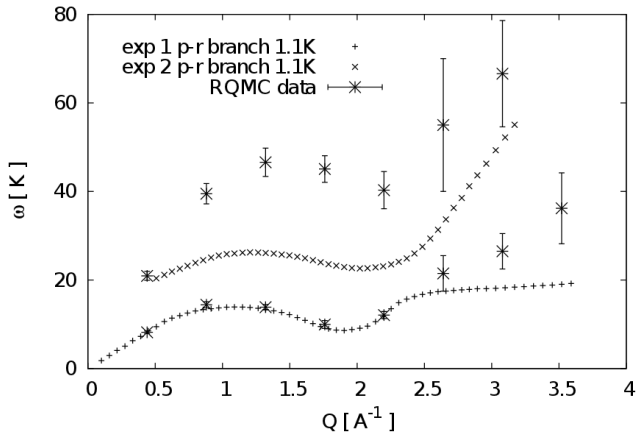


## Dynamic Structure Factor



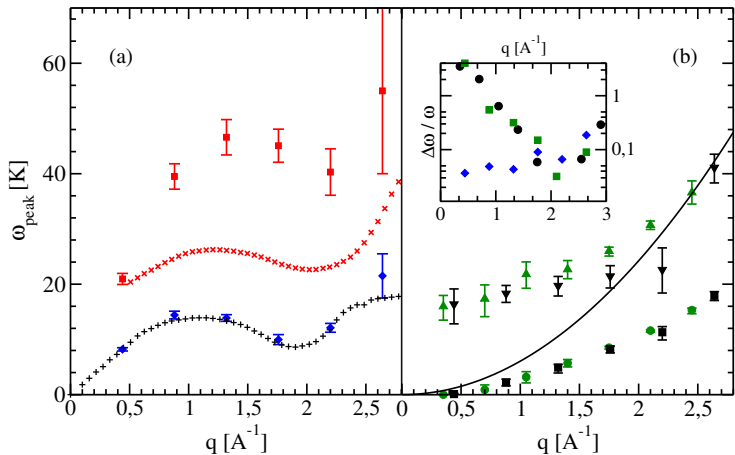
# Application: density response of superfluid $He^4$

## Low-Momentum Excitation spectrum



# Application: density response of superfluid $He^4$

## Incoherent excitation spectrum with widths

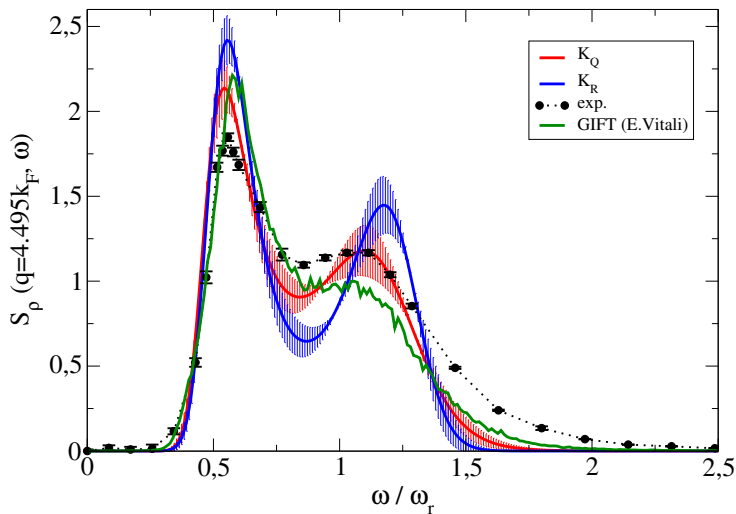


In collaboration with: S. Gandolfi, J. Carlson, E.Vitali

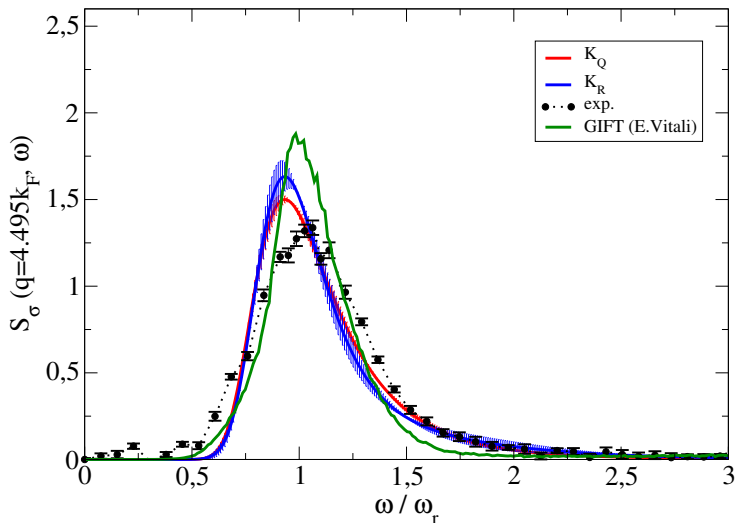
Recent experiments have measured the density–response and the spin–response of a strongly interacting Unitary Fermi Gas at high momentum transfer ( $q \approx 4.5k_f$ ) [Hoinka et al. - PRL.109, 050403 (2012)]:

- density–response  $\longrightarrow$  informations on quasi–elastic response
  - informations on both single–particles and bound molecules (two peaks)
- spin–response  $\longrightarrow$  informations on single–particles (one peak)

## PRELIMINARY RESULTS



# Application: spin response of Unitary Fermi Gas



# Conclusions

## Pro

- may control stability of the inversion by tuning kernel function
- we need just imaginary-time correlation functions

## Con

- for high accuracy, extremely long imaginary-time intervals have to be considered
- the inversion procedure can still introduce uncontrollable errors
  - try with different Kernels ( e.g. Gaussian )
  - use more powerful inversion schemes (e.g. GIFT)

Thanks for your attention