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

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Outline

- Dynamical 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

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

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

Integral Transform 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 → $T(y)$
- Object of interest → $S(x)$

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

PROBLEM

The inverse transform consitutes an Ill-Posed Problem!

Integral Transform for Response Functions

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

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

Integral kernels - Laplace

In QMC methods we routinely use the imaginary-time propagator

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

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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:

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

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!

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 σ_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

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

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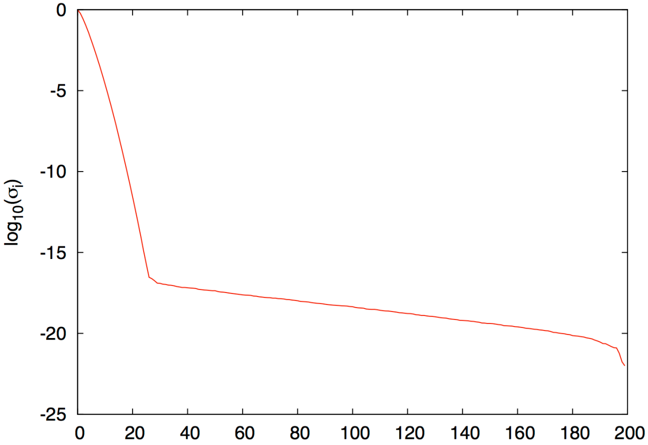
If the matrix K is the result of discretization of a Fredholm Integral equation of the 1st kind the following basic properties holds

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

the decay rate of σ_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]

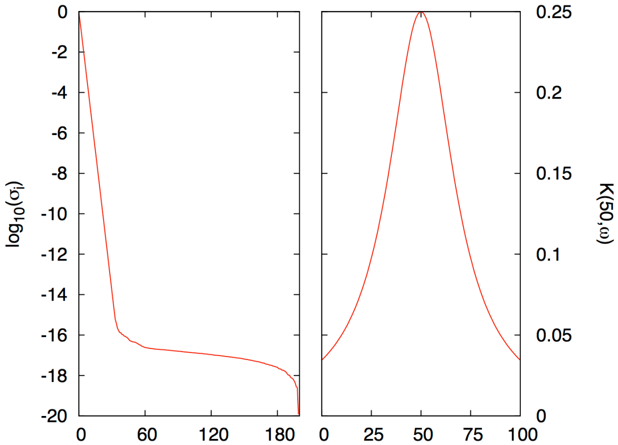
$$K_{Laplace}(\sigma,\omega) = e^{-\sigma\omega}$$

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.

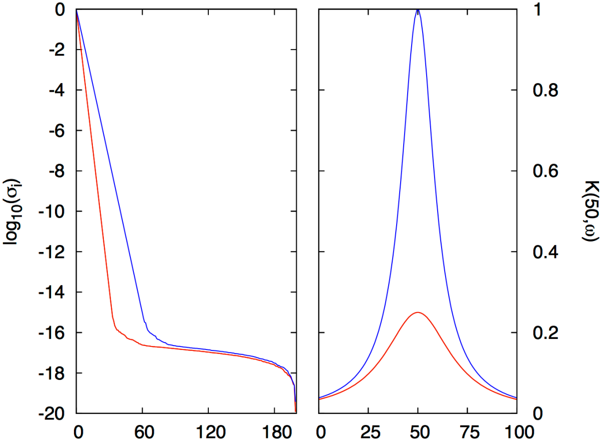
Singular Values and Stability

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



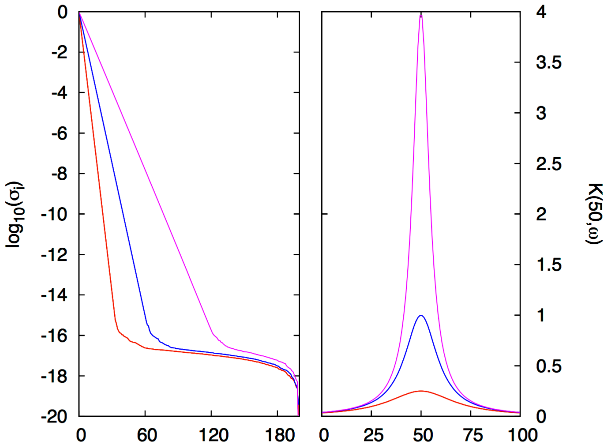
Singular Values and Stability

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



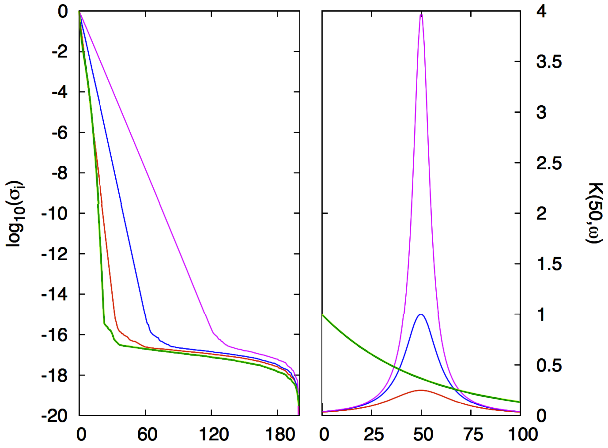
Singular Values and Stability

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



Singular Values and Stability

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

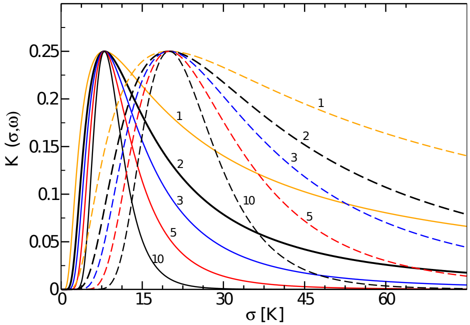


Integral Kernels - Sumudu-like

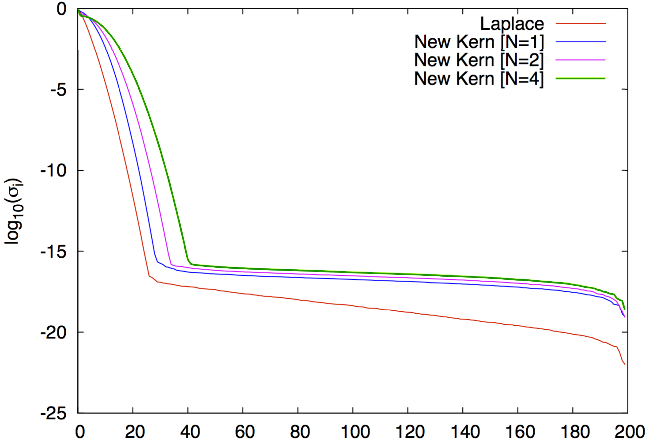
We now want to build an integral kernel which can be calculated in QMC methods and that has the desired form.

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

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



Integral Kernels - New Kernel (SV spectrum)



Application: density response of superfluid He^4

[Alessandro Roggero, FP and G. Orlandini **arXiv:1209.5638**]

- 64 He^4 atoms in a cubic box with Periodic Boundary Conditions
- realistic interaction: *HFDHE*2 pair-potential [Aziz et al. (1979)]
- *Reptation Quantum Monte Carlo* (RQMC) [S.Baroni and S.Moroni (1999)]
- "simple" inversion algorithms (EMML,SMART) [Byrne (1993)]

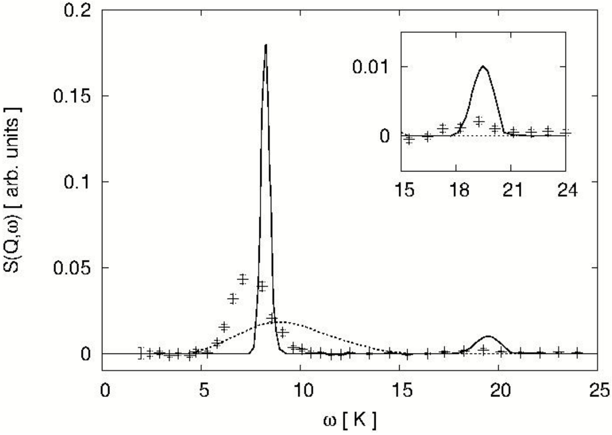
We are interested in the density response of the system, in this case the Response function is the so-called Dynamic Structure Factor

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

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

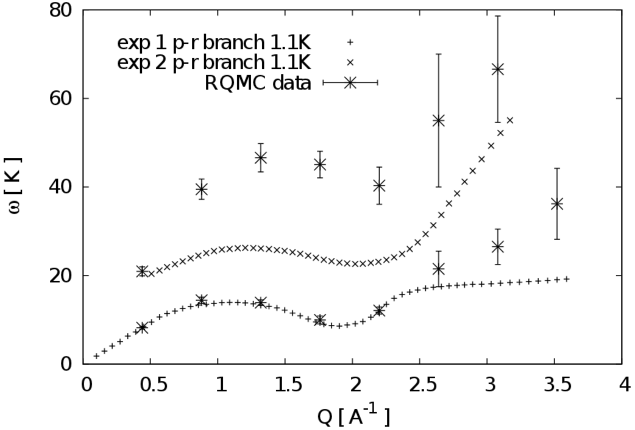
Application: density response of superfluid He^4

Dynamic Structure Factor

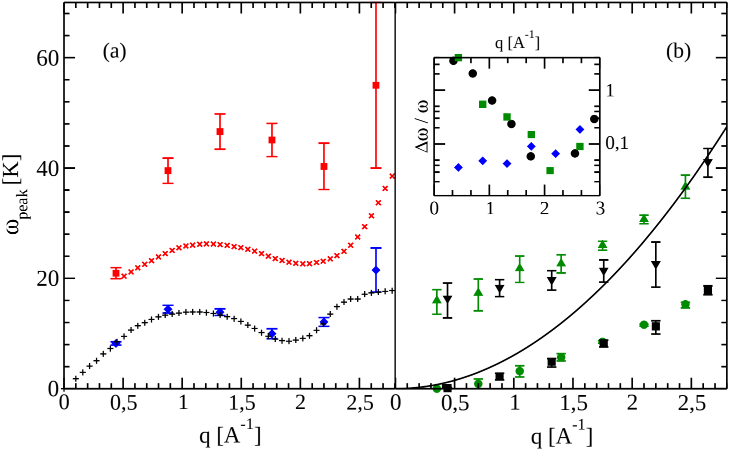


Application: density response of superfluid He^4

Low-Momentum Excitation spectrum



Application: density response of superfluid He^4



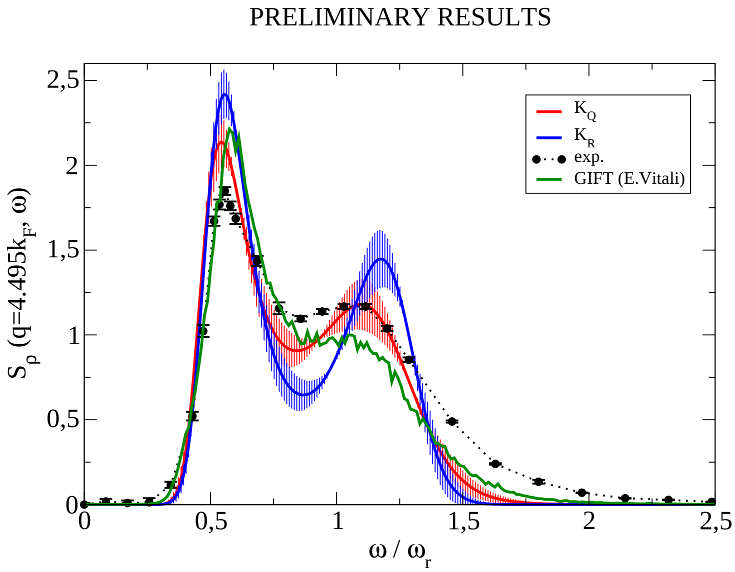
Application: Unitary Fermi Gas

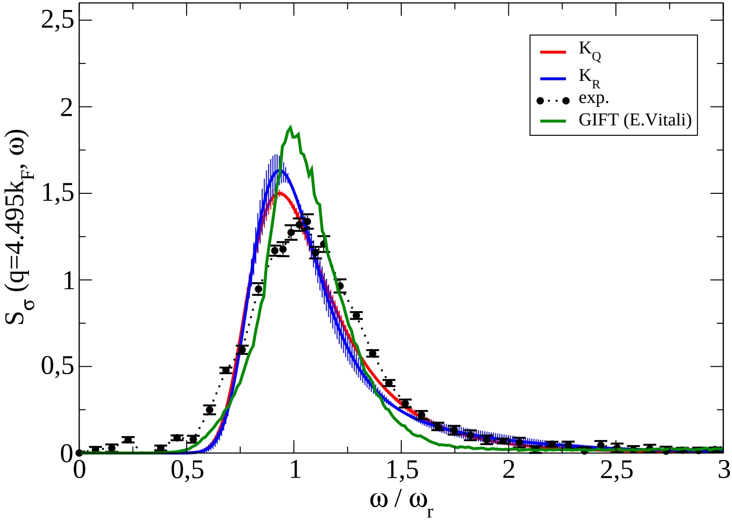
In collaboration with: S. Gandolfi, J. Carlson, E.Vitali

Recent experiments have measured the density–response and the spin–response of a strongly interacting Unitary Fermi Gas at high momentum transfer ($q \approx 4.5 k_f$) [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)

Application: density response of Unitary Fermi Gas





K_Q
K_R
exp.
GIFT (E.Vitali)
S_σ (q=4.495k_F, ω)
ω / ω_r
2,5
2
1,5
1
0,5
0
0,5
1
1,5
2
2,5
3

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
  $\longrightarrow$ try with different Kernels (e.g. Gaussian)
  $\longrightarrow$ use more powerful inversion schemes (e.g. GIFT)

Thanks for your attention