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

A. Roggero, F. Pederiva, G. Orlandini

University of Trento - ITALY

INT - Seattle - 16 Jul, 2013
Outline

- 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
Spectral representation of DRF

\[ \mathcal{R}(\omega) = \sum_{\nu} |\langle \psi_{\nu} | \hat{O} | \psi_0 \rangle|^2 \delta(\omega - (E_{\nu} - E_0)) \]

\[ = \sum_{\nu} \langle \psi_0 | \hat{O}^\dagger | \psi_{\nu} \rangle \langle \psi_{\nu} | \hat{O} | \psi_0 \rangle \delta(\omega - (E_{\nu} - E_0)) \]

\[ = \langle \psi_0 | \hat{O}^\dagger \sum_{\nu} | \psi_{\nu} \rangle \langle \psi_{\nu} | \delta(\omega - (E_{\nu} - E_0)) \hat{O} | \psi_0 \rangle \]

\[ = \langle \psi_0 | \hat{O}^\dagger \delta(\omega - (\hat{H} - E_0)) \hat{O} | \psi_0 \rangle \]

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

The inverse transform constitutes an ill-posed problem!
An Integral Transform maps the original problem in a new domain where it’s simpler to solve it:

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The solution is then mapped back using the inverse transform.

**PROBLEM**

The inverse transform constitutes an Ill-Posed Problem!
\[ R(\omega) = \langle \psi_0 | \hat{O}^\dagger \delta (\omega - (\hat{H} - E_0)) \hat{O} | \psi_0 \rangle \]

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

\[ \Phi(\sigma) = \int K(\sigma, \omega) R(\omega) d\omega \]

\[ = \langle \psi_0 | \hat{O}^\dagger K(\sigma, (\hat{H} - E_0)) \hat{O} | \psi_0 \rangle \]

and take the inverse transform to find \( R(\omega) \) (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

\[ \sum_{n=0}^{\infty} e^{-\tau E_n} \langle \psi_n | \Phi_0 \rangle | \psi_n \rangle \xrightarrow{\tau \to \infty} e^{-\tau E_0} \langle \psi_0 | \Phi_0 \rangle | \psi_0 \rangle \]
Integral kernels - Laplace

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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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Dealing with Ill-Posed problems

Many efforts devoted to performing stable inversions

- 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 smoothened version of the original signal!
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In the limit \( \beta \to 0 \) no inversion needed!!
Singular Value Decomposition (SVD)

\[ g(x) = \int_{a}^{b} K(x, y) f(y) \, dy \quad \rightarrow \quad g_i = \sum_{k}^{N} K_{ik} f_k \quad i \in [1, N] \]

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

The SVD of the matrix \( K \) is a factorization of the form

\[
\begin{bmatrix}
K_{00} & K_{01} & \cdots \\
K_{10} & K_{11} & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix} =
\begin{bmatrix}
U_{00} & U_{01} & \cdots \\
U_{10} & U_{11} & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix} \begin{bmatrix}
\sigma_0 & 0 & \cdots \\
0 & \sigma_1 & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix} \begin{bmatrix}
V_{00} & V_{01} & \cdots \\
V_{10} & V_{11} & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix}^T
\]

where \( \sigma_i \) are called singular–values and \( \vec{u}_j = (U_{0j}, U_{1j}, \ldots) \) and \( \vec{V}_j = (V_{0j}, V_{1j}, \ldots) \) are the (resp. left and right) singular–vectors
In terms of the SVD of the matrix $K$ the direct and inverse problems can be rewritten as

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

$\bar{f} = K^{-1} \bar{g} = \sum_{j}^{N} \frac{1}{\sigma_j} \bar{u}_j^T \bar{g} \bar{v}_j$
In terms of the SVD of the matrix $K$ the direct and inverse problems can be rewritten as

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

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

\[ \log_{10}(\sigma) \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \quad 120 \quad 140 \quad 160 \quad 180 \quad 200 \]

\[ -25 \quad -20 \quad -15 \quad -10 \quad -5 \quad 0 \]
Singular Values and Stability

Lorentz kernel [LIT method]

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

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

$$K_{\text{Lorentz}} \{ \Gamma = 20 \}$$
Singular Values and Stability

\[ K_{Lorentz} \{ \Gamma = 20, 10 \} \]
Singular Values and Stability

\[ K_{Lorentz} \{ \Gamma = 20, 10, 5 \} \]
Singular Values and Stability

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

![Graph showing log10(σ) and K(50, ω) for different values of Γ.](image)
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 \(N \to \infty\) the kernel width becomes smaller and smaller.
Integral Kernels - New Kernel (SV spectrum)

- Laplace
- New Kern [N=1]
- New Kern [N=2]
- New Kern [N=4]
64 $\text{He}^4$ 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: $\rho_q \equiv \sum_j e^{iqr_j}$. 
Application: density response of superfluid $\text{He}^4$

Dynamic Structure Factor

$S(Q,\omega) \text{ [arb. units]}$

$\omega \text{ [K]}$

$0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25$

$0 \quad 0.05 \quad 0.1 \quad 0.15 \quad 0.2$

$0 \quad 0.01 \quad 0$
Application: density response of superfluid $He^4$

Low-Momentum Excitation spectrum

\[ \omega [K] \]

\[ Q [A^{-1}] \]

exp 1 p-r branch 1.1K
exp 2 p-r branch 1.1K
RQMC data
Application: density response of superfluid $^4$He

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

- **density–response** → informations on quasi–elastic response
  - informations on both single–particles and bound molecules (two peaks)

- **spin–response** → informations on single–particles (one peak)
Application: density response of Unitary Fermi Gas

PRELIMINARY RESULTS

\[ S_p (q=4.495k_F, \omega) \]

\[ \omega / \omega_r \]

- \( K_Q \)
- \( K_R \)
- \( \text{exp.} \)
- \( \text{GIFT (E.Vitali)} \)
Application: spin response of Unitary Fermi Gas

\[ S_\sigma(q=4.495k_F, \omega) \]

\[ \frac{\omega}{\omega_r} \]

- Red line: \( K_Q \)
- Blue line: \( K_R \)
- Dotted line: \( \text{exp.} \)
- Green line: GIFT (E. Vitali)

A. Roggero, F. Pederiva, G. Orlandini (University of Trento)
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