Response functions of the unitary Fermi gas from quantum Monte Carlo simulations

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Response functions – definition

Hamitonian defining a system

\[ \hat{H} = \hat{H}_0 + \hat{H}_1 \]

Change of a dynamical variable

\[ \delta \langle \hat{A} \rangle(t) = \langle \hat{A} \rangle(t) - \langle \hat{A} \rangle_0 \]

is given by:

\[ \delta \langle \hat{A} \rangle(t) = \int_{-\infty}^{t} \chi_{AB}(t - t') h(t') \, dt' \]

\[ \chi_{AB}(t - t') = \frac{1}{i\hbar} \theta(t - t') e^{-\varepsilon(t-t')} \langle [\hat{A}(t), \hat{B}(t')] \rangle_0 \]

“Response function” for the observable A with respect to the perturbation B

Time-dependent external perturbation

\[ \hat{H}_1 = h(t) \hat{B} \]

h(t) - “external field”

B – operator of conjugate dynamical variable

Higher orders in h(t) are neglected ⇒ Linear response theory

NOTE!
Generalized susceptibilities

\[ \delta \langle \hat{A} \rangle(t) = \int_{-\infty}^{t} \chi_{AB}(t - t') h(t') \, dt' \]

\[ \delta \langle \hat{A} \rangle(\omega) = \chi_{AB}(\omega) h(\omega) \]

In general operators A and B can have position dependence (example: A,B=n(r) - density operator)

\[ \delta \langle \hat{A}(\vec{q}) \rangle(\omega) = \chi_{AB}(\vec{q}, \omega) h(\vec{q}, \omega) \]

Typically using generalized susceptibilities (complex values) we create new quantities with well defined physical meaning.
Physical system: unitary Fermi gas (unpolarized)

\[ \hat{H}_0 \equiv \sum_{\mathbf{p}, \lambda = \uparrow, \downarrow} \frac{\mathbf{p}^2}{2m} \hat{a}^{\dagger}_\lambda (\mathbf{p}) \hat{a}_\lambda (\mathbf{p}) - g \sum_i \hat{n}_\uparrow (\mathbf{r}_i) \hat{n}_\downarrow (\mathbf{r}_i) \]

UFG: System is dilute but strongly interacting!

\[
\frac{1}{g} = -\frac{m}{4\pi \hbar^2 a} + \frac{k_c m}{2\pi^2 \hbar^2}
\]

\( 0 \leftarrow k_F r_0 \ll 1 \ll k_F a \rightarrow \infty \)

NONPERTURBATIVE REGIME!
Method: Path Integral Monte Carlo

\[ \langle O \rangle_0 = \frac{1}{Z} \text{Tr} \left\{ \hat{O} \exp\left[-\beta(\hat{H}_0 - \mu \hat{N})\right] \right\} \]

\[ Z = \text{Tr} \left\{ \exp\left[-\beta(\hat{H}_0 - \mu \hat{N})\right] \right\} \]

1. The system is placed on a cubic spatial lattice

2. Trotter-Suzuki decomposition to expand imaginary time evolution operator \( \exp\left[-\beta(\hat{H}_0 - \mu \hat{N})\right] \)

3. The interaction is represented by means of a Hubbard-Stratonovich transformation

4. Evaluation of the emerging path-integral via Metropolis importance sampling – **NO SIGN PROBLEM**
\[
\chi_{AB}(t - t') = \frac{1}{i\hbar} \theta(t - t') e^{-\varepsilon(t-t')} \langle[[\hat{A}(t), \hat{B}(t')]]\rangle_0
\]

**PROBLEM:**

\[
\hat{A}(t) = e^{i\hat{H}_0 t/\hbar} \hat{A} e^{-i\hat{H}_0 t/\hbar}
\]

However QMC can be used to compute:

\[
G_{AB}(\tau) = \langle \hat{A}(\tau) \hat{B}(0) \rangle_0 \quad \hat{A}(\tau) = e^{\tau\hat{H}_0} \hat{A} e^{-\tau\hat{H}_0}
\]

“correlators” in imaginary time \( \tau = it \)

In special cases one can easily relate \( G_{AB}(\tau) \) with the response function – static spin susceptibility

\[
\chi_s = \frac{\partial(n_{\uparrow} - n_{\downarrow})}{\partial(\mu_{\uparrow} - \mu_{\downarrow})}
\]

\[
\chi_s = \lim_{q \to 0} \frac{1}{V} \int_0^\beta d\tau \langle \hat{s}_q^z(\tau) \hat{s}_{-q}^z(0) \rangle \quad \hat{s}_q^z = \hat{n}_{q\uparrow} - \hat{n}_{q\downarrow}
\]

Effectively: computation of expectation value of a operator!
Critical temperature from finite size scaling analysis

PSEUDOGAP REGIME

Static spin susceptibility

BCS theory

\[ \chi_s = \partial (n_\uparrow - n_\downarrow) / \partial (\mu_\uparrow - \mu_\downarrow) \]

Analytic continuation

QMC provides:

\[ G_{AB} = \langle \hat{A}(\tau) \hat{B}(0) \rangle_0 \]

"correlators" in imaginary time \( \tau = it \)

Typically:
perform the analytic continuation (numerically 😊)

of the imaginary time correlator to real times/frequencies

\[ G(y) = \int_{-\infty}^{\infty} K(x, y) A(x) dx \]

QMC data (finite set & affected by statistical error)
Kernel -known analytic function
“Response function” unknown

Ill-posed problem & numerically ill-conditioned
ill-posed linear inverse problem

Discretized version:

\[ G_i = \int_{-\infty}^{\infty} K(x, y_i) A(x) dx = \int_{-\infty}^{\infty} K_i^*(x) A(x) dx = (K_i, A) \]

Matrix of dimension \( N_\tau \times \infty \)

By means of SVD decomposition of the kernel functions it can be proved:

\[ A(x) = A_P(x) + A_\perp(x) \]

\[ G_i = (K_i, A) = (K_i, A_P) \]

\[ (K_i, A_\perp) = 0 \]

Data vector \( G_i \) allows only for the reconstruction of \( A_P \)

Infinite number of solutions

Artificial problem:

Data points $G_i$ in the interval $[0, \beta = 10]$ uniformly distributed

SVD solution:

$$A_P(x) = \sum_{i=1}^{M} b_i u_i(x)$$

$$b_i = \frac{\langle \vec{v}_i, \vec{G} \rangle}{\lambda_i}$$
Strategies of solving the problem

\[ A(x) = A_P(x) + A_\perp(x) \]

1. Assume that \( A_P(x) \) is a good approximation of \( A(x) \) [SVD method]

2. Enrich the problem by \textit{a priori} information about the object \( A(x) \) and in this way “fix” the unknown part \( A_\perp(x) \) [MEM]

Types of \textit{a priori} information

Sum rules: \( \int_{-\infty}^{\infty} g_i(x) A(x) dx = c_i \)

Constraints: \( A(x_j) \in [l_j, u_j] \)

Models
(e.g., from approximate theories)

Examples:
\[ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p, \omega) = 1 \]
\[ A(p, \omega) \geq 0. \]
\[ A(p, \omega) = 2\pi |u_p|^2 \delta(\omega - E(p)) + 2\pi |v_p|^2 \delta(\omega + E(p)) \]
Numerically ill-conditioned

SVD solution:  
\[ A_P(x) = \sum_{i=1}^{M} b_i u_i(x) \]

\[ b_i = \frac{(\vec{v}_i, \vec{G})}{\lambda_i} \]

Singular functions
Singular values

Errors \( \Delta \vec{G} \)  \( \Rightarrow \)  \( \Delta b_i = \frac{(\vec{v}_i, \Delta \vec{G})}{\lambda_i} \)

Arrange the set of singular values in descending order:

\[ \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_M \]

\[ \lambda_i \to 0 \quad \Rightarrow \quad \Delta b_i = \frac{(\vec{v}_i, \Delta \vec{G})}{\lambda_i} \to \infty \]

Practically it means that there exist “directions” which are invisible due to statistical uncertainties!

Typically singular values decay exponentially!
Maximum Entropy Method

\[ G_i = \sum_{j=1}^{N} K_{ij} A_j, \quad A_j = A(x_j) \]
\[ \Delta x = x_j - x_{j-1} \]

\[ K_{ij} = K(x_j, y_i) \Delta x \] is a rectangular matrix \( N_T \times N \)

Minimize:

\[ F(\vec{A}) = \frac{1}{2} \chi^2(\vec{A}) - \alpha S(\vec{A}, \vec{M}) \]

\[ \chi^2(\vec{A}) = \sum_{i=1}^{N_T} \left( \frac{G_i^{(QMC)} - G_i(\vec{A})}{\sigma_i} \right)^2 \]

\[ S(\vec{A}, \vec{M}) = \sum_{j=1}^{N} \Delta x \left[ A_j - M_j - A_j \ln \left( \frac{A_j}{M_j} \right) \right] \]

[Statistics]: minimization of \( F(A) \) leads to the most probable solution \( A \) under assumption that the solution is (model) \( M \)-like.
Combining MEM & SVD

Constrained minimization:

\[ F(\vec{A}) = \frac{1}{2} \chi^2(\vec{A}) - \alpha S(\vec{A}, \vec{M}) \]

Constraints:

\[ P[A(x)] = A_{P_{cut}}(x) \]

Greatly improves reconstruction ability

+ sum rules, (asymptotic tails if known)

For UFG: Significant amount of exact results like:
- tail asymptotics [e.g., \( n(p) \sim C/p^4 \) for large \( p \), \( C \) - contact]
- sum rules
  which can be used as a priori information or constraints.
Self-consistent MEM

\[ F(\bar{A}) = \frac{1}{2} \chi^2(\bar{A}) - \alpha S(\bar{A}, \bar{M}) \]

We define a class of models defined by parameters \( \mathcal{M}(x; \vec{f}) \)

\[ \vec{f} = (f_1, \ldots, f_s) \]

Final solution is weakly sensitive with respect initial values of parameters \( f_1, \ldots, f_s \)

Use GenericMEMSolver to solve problem for fixed model

Update model to maximize overlap with solution

Check self-consistency criteria

STOP
Example:

\[ M(\omega; \{c_1, c_2, \mu_1, \mu_2, \sigma_1, \sigma_2\}) = c_1 N(\omega; \mu_1, \sigma_1) + c_2 N(\omega; \mu_2, \sigma_3). \]

The extracted spectral weight function at the unitary regime for the momentum at the vicinity of the Fermi surface at \( T/e_F = 0.12 \)
Resolution limit

Sometimes the method fails.

1. Sharp structure can be overlooked

2. Sharp structure can be reconstructed as wide structure

3. Structures are too close each other

(Sharp structures in response functions are typically associated with well defined quasiparticles)
Spin conductivity

Spin current: \( \dot{j}_s = \dot{j}_{\uparrow} - \dot{j}_{\downarrow} \)

We apply weak external force \( F \) which couples with opposite signs to the two spin populations

Spin conductivity: \( \dot{j}_s = \sigma_s F \)

\( \lambda = \pm 1 \)

spin conductivity is expected to be strongly affected by the presence of the Cooper pairs

QMC provides (for \( q=0 \)):

\[
G^{(jj)}_s(q, \tau) = \frac{1}{V} \langle [\hat{j}^z_{q\uparrow}(\tau) - \hat{j}^z_{q\downarrow}(\tau)][\hat{j}^z_{-q\uparrow}(0) - \hat{j}^z_{-q\downarrow}(0)] \rangle
\]

Analytic continuation:

\[
G^{(jj)}_s(q = 0, \tau) = \frac{1}{\pi} \int_0^{\omega_{\text{max}}} \sigma_s(\omega) \frac{\cosh[\omega(\tau - \beta/2)]}{\sinh(\omega\beta/2)} d\omega
\]

Constraints:

\[
\sigma_s(\omega) \geq 0, \quad \sigma_s(\omega \to \infty) = C/(3\pi\omega^{3/2})
\]

From decay of \( n(p) \sim C/p^4 \)
Theory (lattice)

J. E. Drut, T. A. Lähde, T. Ten

\[
\frac{C}{3\pi \omega^{3/2}}
\]

\[\omega \sim \frac{p^2}{2m}\]

Experiment

J. T. Stewart et al
PRL 104, 235301 (2010)
Spin drag rate

\[ \Gamma_{sd} = \frac{n}{\sigma_s} \]

Enhancement appears consistently with the spin susceptibility suppression.

Shear viscosity

The shear viscosity: determines “friction” force $F$ per unit area $A$ created by a shear flow

$$F = A \eta \frac{\partial v_x}{\partial y}$$

For incompressible fluid or if $\xi = 0$: kinetic energy dissipated per unit time

$$\dot{E}_{\text{kin}} = -\frac{1}{2} \eta \int \left( \frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} \right)^2 \, dV$$

Kinetic theory (Boltzmann equation) prediction:

$$\eta = n \bar{p} l_{\text{mfp}}$$

Expected nearly ideal hydrodynamic behavior
For UFG (small $l_{\text{mfp}}$)

C. Cao, et. al., Science 331, 58 (2011)
**KSS conjecture**

Bound has been proposed on the basis of string theory.

Valid for large class of (string) theories.

Saturated for the case of strongly coupled theory.

Minimum defines a “perfect” fluid.
Shear viscosity from QMC

(Technically very similar to computation of the spin conductivity)
(We compute stress tensor-stress tensor correlator + tail asymptotic
+ sum rule)

G. Wlazłowski, P. Magierski, J.E. Drut,

Problem with averaging procedure of the uniform results
Hydrodynamic description breaks down at the edges.

(\eta/s)_{min} \approx 0.2
Shear viscosity from QMC

C. Chafin and T. Schäfer

Trap averaged of the kinetic theory results
Shear viscosity from QMC

Conservative estimate of upper bound (uncertainties mainly generated by analytic continuation)

Recent simulations

Spectral function (see talk: P. Magierski)

Spectral function $A(p, \omega)$ - defines the spectrum of possible energies $\omega$ for a particle with momentum $p$ in the medium.

\[ G(p, \tau) = \langle \psi^\dagger(p, \tau) \psi(p, 0) \rangle_0 \]

One-body temperature Green's (Matsubara) function

Inverse problem

\[ G(p, \tau) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(p, \omega) \frac{\exp(-\omega\tau)}{1 + \exp(-\omega/\beta)} \]

Constraints:

\[ A(p, \omega) \geq 0, \quad \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p, \omega) = 1, \]

\[ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(p, \omega) \frac{1}{1 + \exp(\omega/\beta)} = n(p), \]

Model:

\[ \mathcal{M}(\omega; \{c_1, c_2, \mu_1, \mu_2, \sigma_1, \sigma_2\}) = c_1 N(\omega; \mu_1, \sigma_1) + c_2 N(\omega; \mu_2, \sigma_3). \]
Spectral function

Huge pairing gap helps!
Lower limit for $T^*$: due to finite resolution of the analytic continuation procedure

P. Magierski, G. Wlazłowski, A. Bulgac
Searching for perfect fluid...

From A. Adams, et al., arXiv:1205.5180

QMC for UFG

Lattice QCD
H.B. Meyer,
PRD 76:101701, 2007

THANK YOU ...