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

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Response functions – definition

Hamitonian defining a system

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

Time-dependent external perturbarion

$$\hat{H}_1 = h(t)\,\hat{B}$$

h(t) - "external field"

B – operator of conjugate dynamical variable

Change of a dynamical variable

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

is given by:

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

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

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

"**Response function**" for the observable A with respect to the perturbation B

NOTE !

Generalized susceptibilities

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

FT

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

Generalized susceptibilities

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)

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

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

UFG: System is dilute
but strongly interacting!

$$0 \leftarrow k_F r_0 \ll 1 \ll k_F a \rightarrow \infty$$

NONPERTURBATIVE REGIME!

Method: Path Integral Monte Carlo

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

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

1. The system is placed on a cubic spatial lattice

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

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**

needs to be computed

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

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:

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

"correlators" in imaginary time $\tau = it$

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

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

$\hat{s}^z_{\boldsymbol{q}=0}$ commutes with the Hamiltonian

$$\chi_s = \lim_{q\to 0}\frac{1}{V}\int_0^\beta d\tau\langle\hat{s}^z_{\boldsymbol{q}}(\tau)\hat{s}^z_{-\boldsymbol{q}}(0)\rangle$$

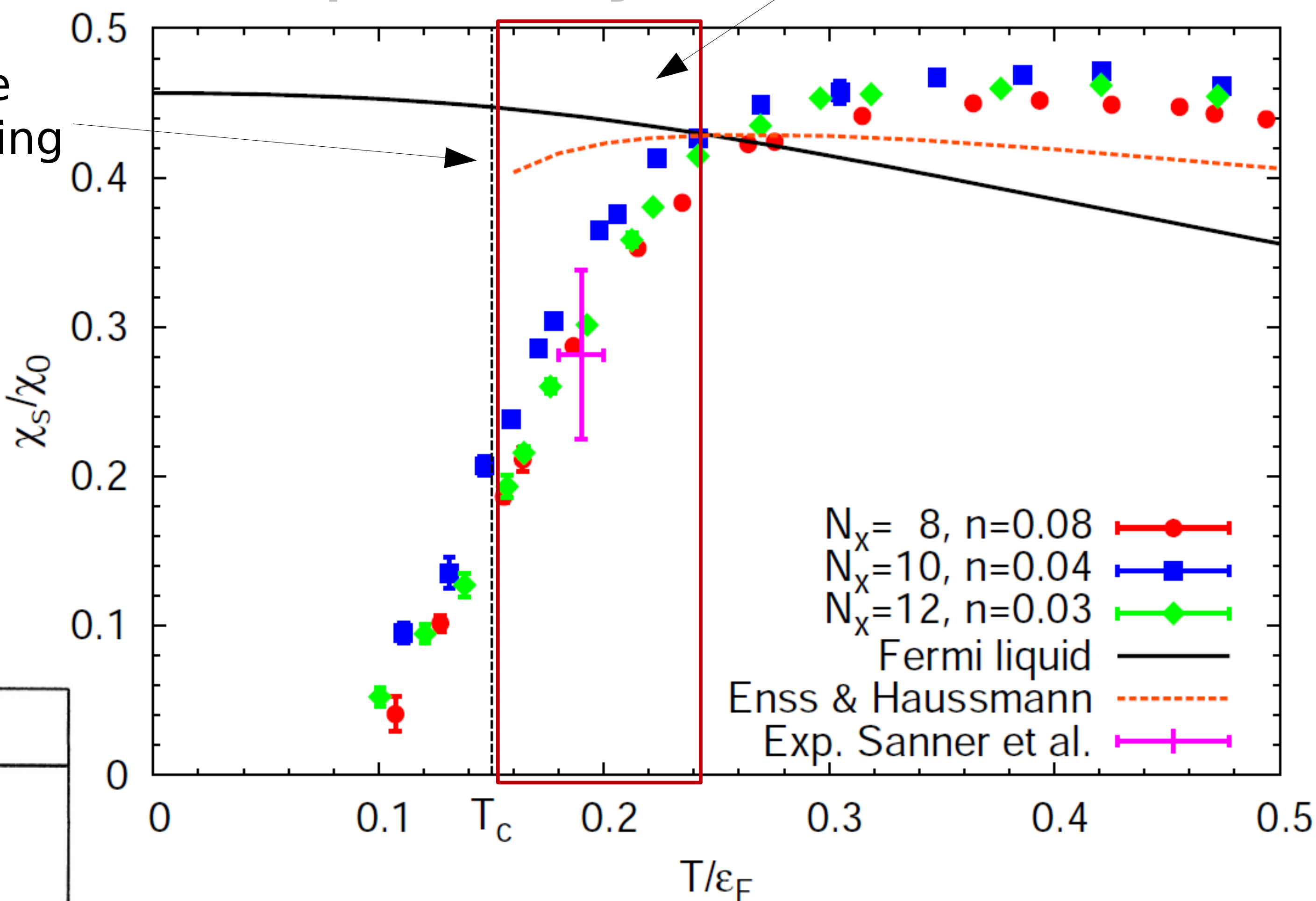
$$\hat{s}^z_{\boldsymbol{q}} = \hat{n}_{\boldsymbol{q}\uparrow} - \hat{n}_{\boldsymbol{q}\downarrow}$$

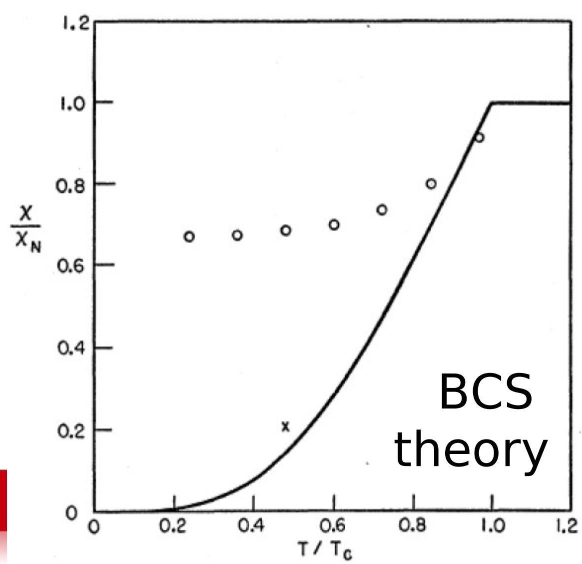
Effectively: computation of expectation value of a operator!

Static spin susceptibility

PSEUDOGAP REGIME

Critical temperature from finite size scaling analysis





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

G. Wlazłowski, P. Magierski, J.E. Drut, A. Bulgac, K.J. Roche,
Phys. Rev. Lett. 110, 090401 (2013)

Analytic continuation

QMC provides:

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

“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:

$$A(x) \;=\; A_P(x) + A_\perp(x)$$

$$G_i = (K_i, A) = (K_i, A_P)$$

Data vector G_i allows only for the reconstruction of A_P

$$(K_i, A_\perp) = 0$$

Infinite number of solutions

For more details see: P. Magierski, G. Wlazłowski, Comput. Phys. Commun. 183 (2012) 2264

$$G(y) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} dx A(x) \frac{\exp(-xy)}{1+\exp(-x\beta)}$$

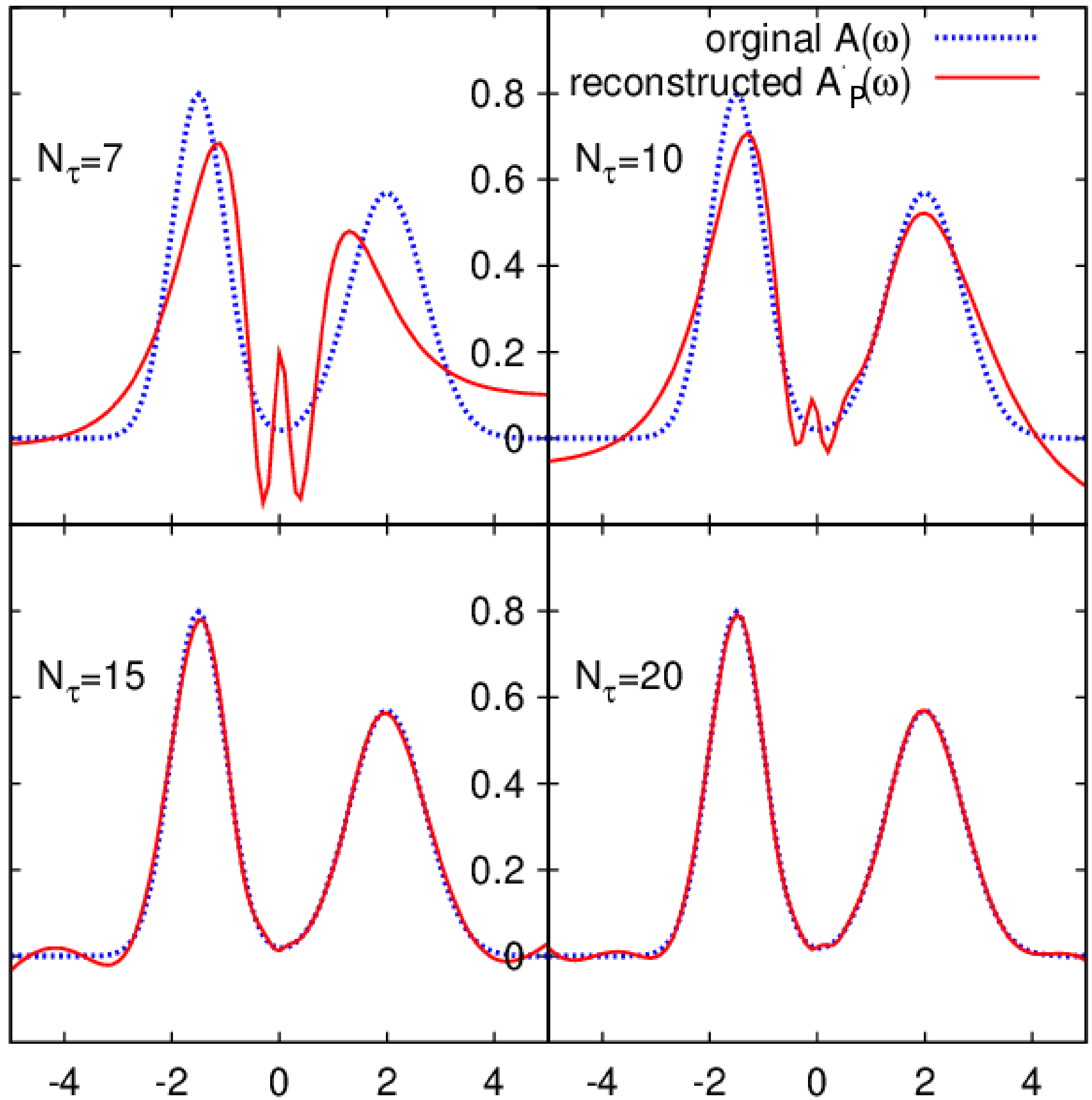
Artificial problem:

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

SVD solution:

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

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



Strategies of solving the problem

$$A(x) = A_P(x) + A_\perp(x)$$

$$G_i = (K_i, A) = (K_i, A_P)$$

$$(K_i, A_\perp) = 0$$

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

2. Enrich the problem by *a priori* information about the object A(x) and in this way "fix" the unknown part $A_\perp(x)$ [MEM]

Types of *a priori* information

Examples:

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

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(\boldsymbol{p}, \omega) = 1$$

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

$$A(\boldsymbol{p}, \omega) \geq 0,$$

Models
(e.g., from approximate theories)

$$A(\boldsymbol{p}, \omega) = 2\pi |u_{\boldsymbol{p}}|^2 \delta(\omega - E(\boldsymbol{p})) + 2\pi |v_{\boldsymbol{p}}|^2 \delta(\omega + E(\boldsymbol{p}))$$

Numerically ill-conditioned

SVD solution: $A_P(x) = \sum_{i=1}^{M} b_i u_i(x)$ $\quad b_i = \frac{(\vec{v}_i, \vec{G})}{\lambda_i}$

Singular vectors *Singular functions* *Singular values*

are known exactly since they are fully determined by the kernel functions

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

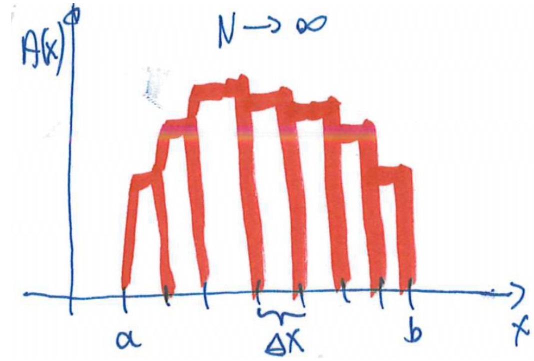
Arrange the set of singular values in descending order: $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_M$

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

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

Typically singular values decay exponentially!

Maximum Entropy Method



$$G_i = \sum_{j=1}^{N} K_{ij} A_j, \qquad A_j = A(x_j)$$

$$\Delta x = x_j - x_{j-1}$$

$K_{ij} = K(x_j, y_i)\Delta x$ is a rectangular matrix $N_\tau \times N$

Minimize: $$F(\vec{A}) = \frac{1}{2}\chi^2(\vec{A}) - \alpha S(\vec{A}, \vec{\mathcal{M}})$$

a priori model

“Penalty term”
Maximal value (zero)
if A(x)=M(x)
otherwise negative

$$\chi^2(\vec{A}) = \sum_{i=1}^{N_\tau} \left(\frac{G_i^{(QMC)} - G_i(\vec{A})}{\sigma_i} \right)^2$$

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

[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:

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

P[...] - projection operator onto SVD subspace

+ sum rules, (asymptotic tails if known)

Greatly improves reconstruction ability

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.

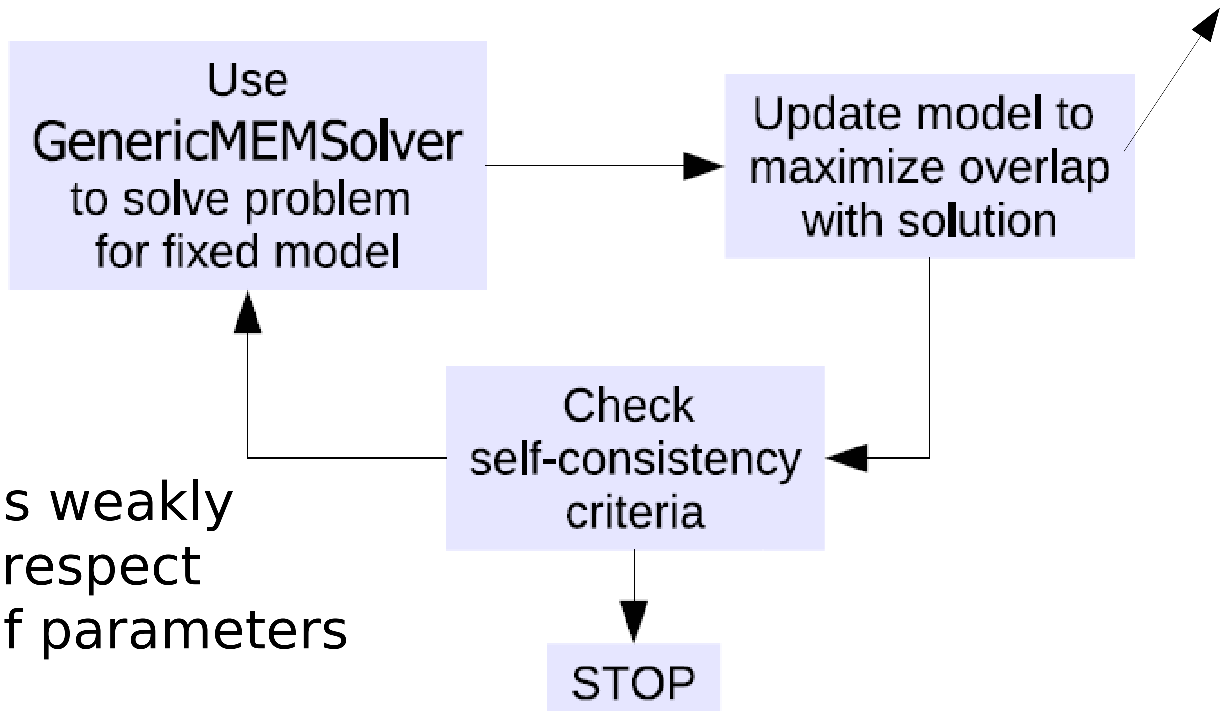
Self-consistent MEM

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

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

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

$$O(\vec{f}) = \frac{\left(\sum_{i=1}^{N} A_i \mathcal{M}_i(\vec{f})\right)^2}{\sum_{i=1}^{N} A_i^2 \sum_{i=1}^{N} \mathcal{M}_i^2(\vec{f})}$$

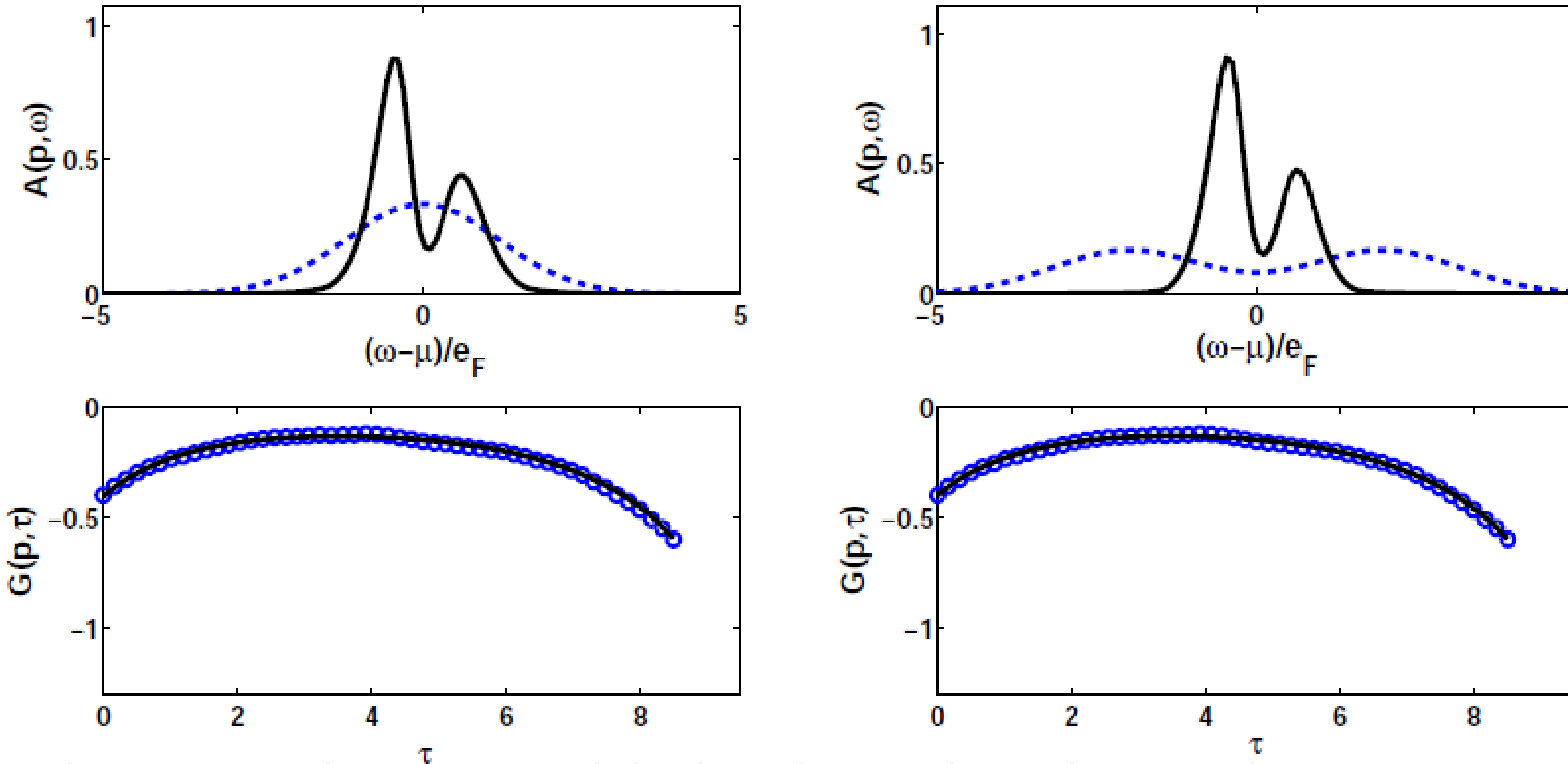


Final solution is weakly sensitive with respect initial values of parameters $f_1, \ldots, f_s$

Example:

Gaussian function

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

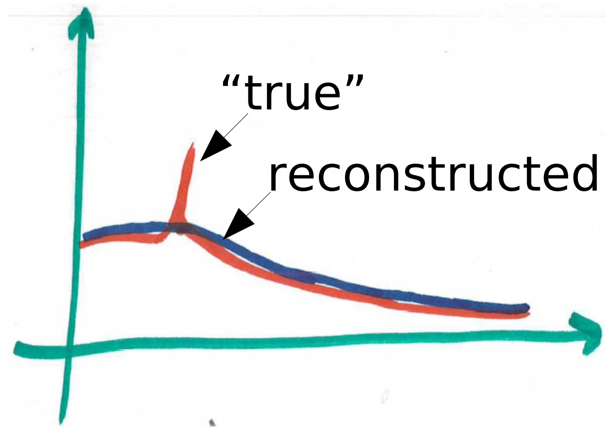


The extracted spectral weight function at the unitary regime for the momentum at the vicinity of the Fermi surface at $T/e_F = 0.12$

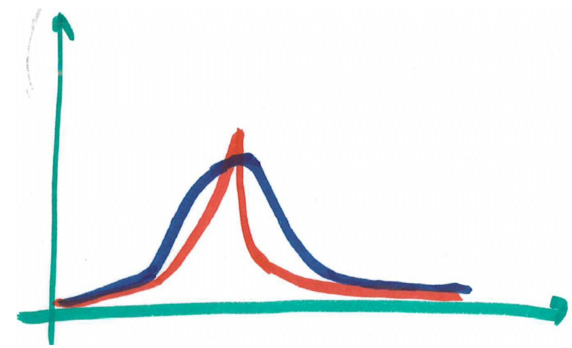
Resolution limit

Sometimes the method fails.

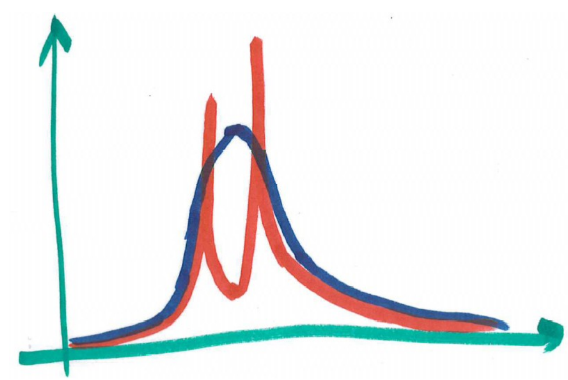
1. Sharp structure can be overlooked



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: $\boldsymbol{j}_s = \boldsymbol{j}_\uparrow - \boldsymbol{j}_\downarrow$

$$\boldsymbol{F}_\lambda = \lambda \boldsymbol{F}$$
$$\lambda = \pm 1$$

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

Spin conductivity: $\boldsymbol{j}_s = \sigma_s \boldsymbol{F}$

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

QMC provides (for q=0):

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

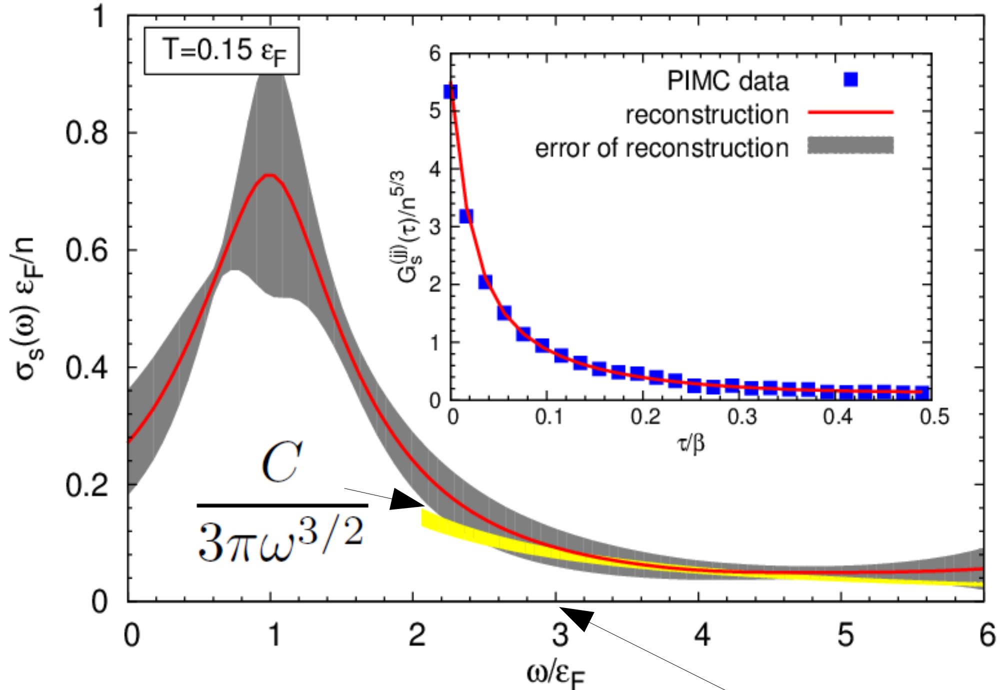
Analytic continuation:

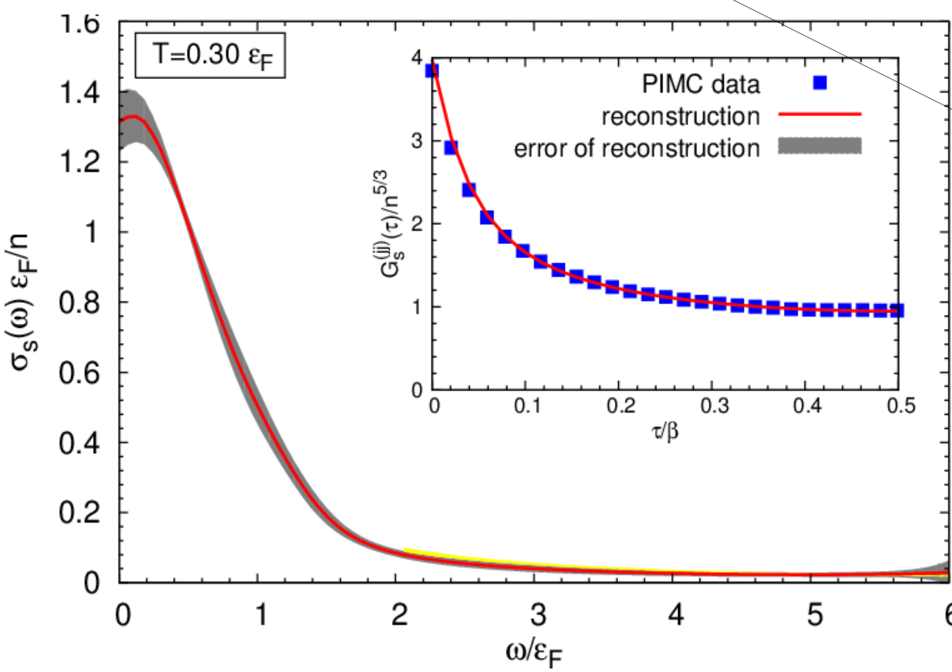
$$G_s^{(jj)}(\boldsymbol{q}=0,\tau) = \frac{1}{\pi}\int_0^{\omega_{\max}} \sigma_s(\omega)\,\omega\frac{\cosh[\omega(\tau-\beta/2)]}{\sinh(\omega\beta/2)}d\omega$$

Constraints:

$$\sigma_s(\omega) \geqslant 0, \quad \sigma_s(\omega\to\infty) = C/(3\pi\omega^{3/2})$$

From decay of n(p)~C/p[4]

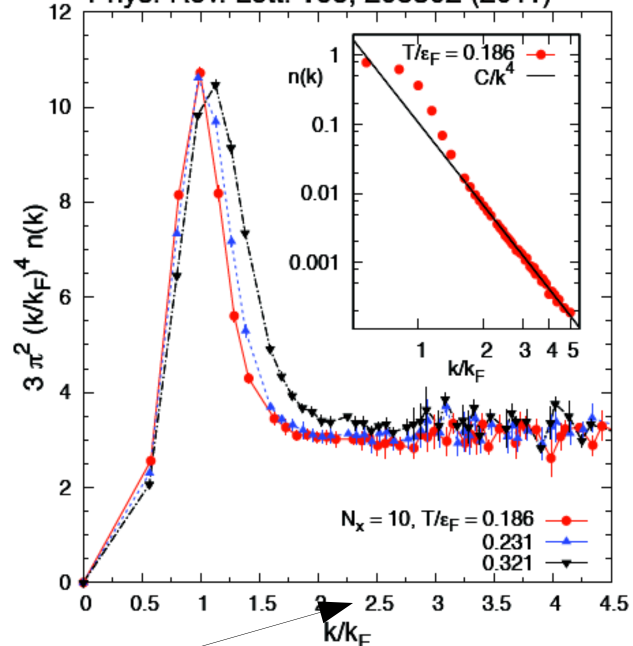




$$\omega \sim \frac{p^2}{2m}$$

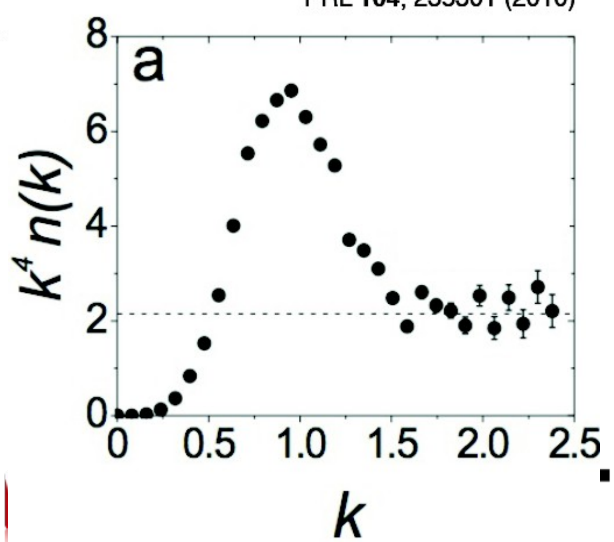
Theory (lattice)

J. E. Drut, T. A. Lähde, T. Ten
Phys. Rev. Lett. **106**, 205302 (2011)



Experiment

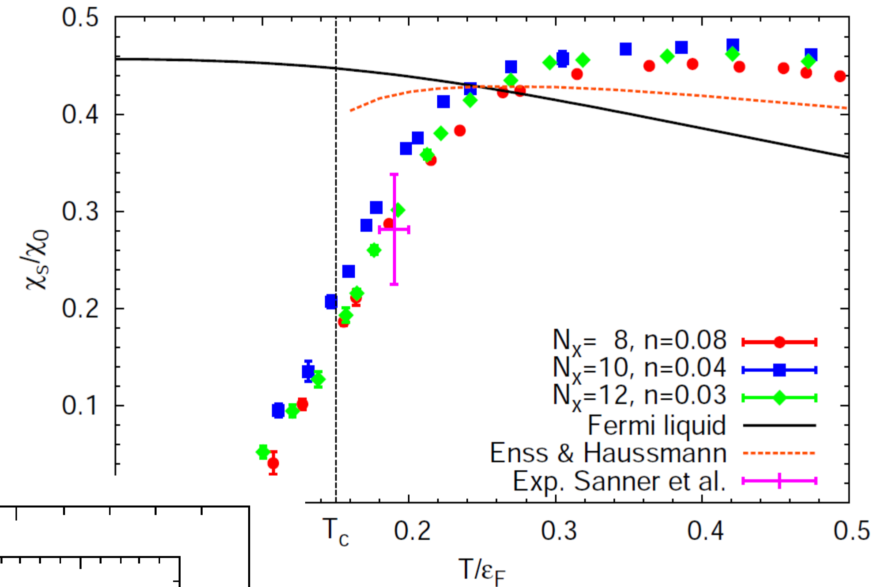
J. T. Stewart et al
PRL **104**, 235301 (2010)

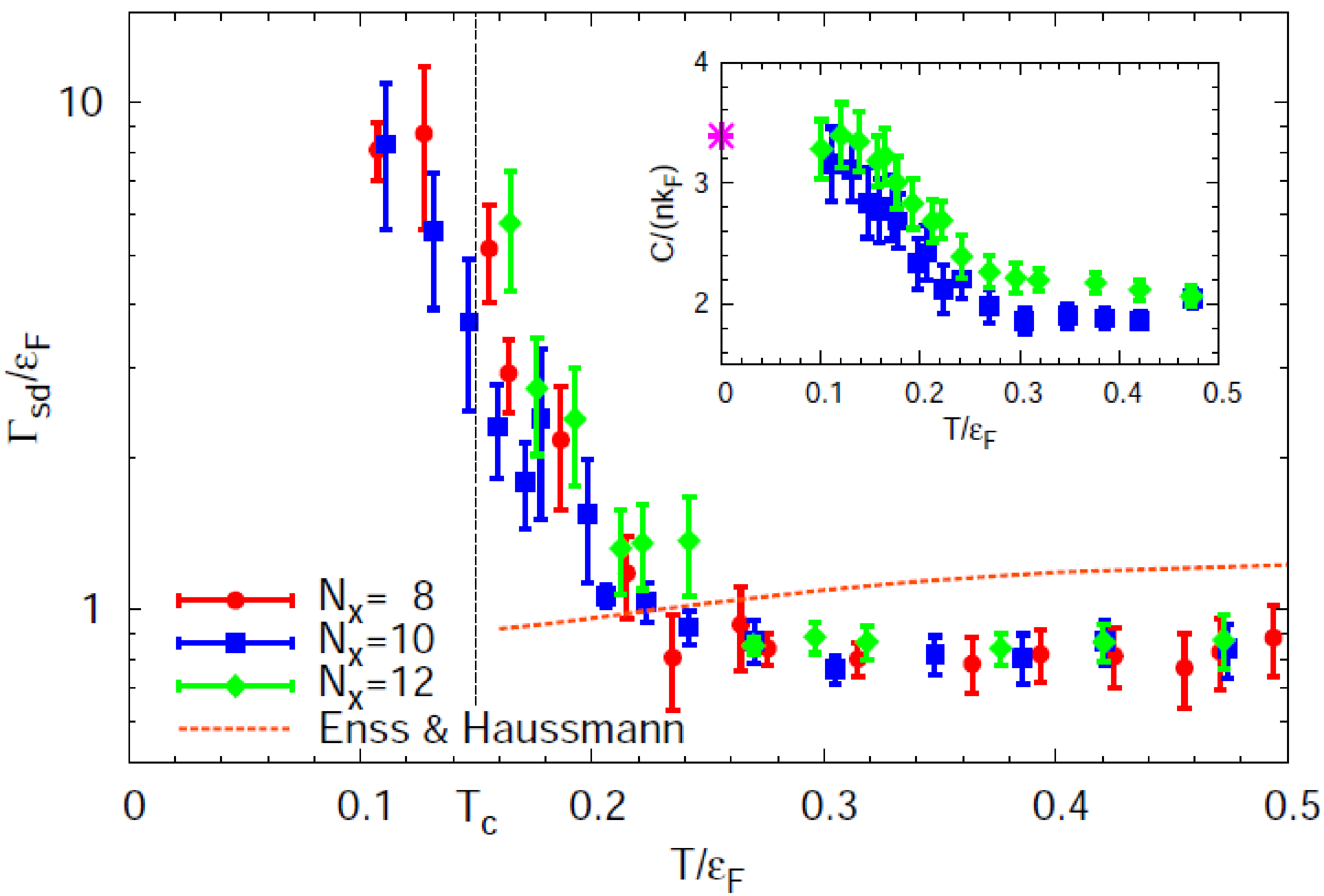


Spin drag rate

$$\Gamma_{sd} = n/\sigma_s$$

Enhancement appears consistently with the spin susceptibility suppression





G. Wlazłowski, P. Magierski, J.E. Drut, A. Bulgac, K.J. Roche, PRL 110, 090401 (2013)

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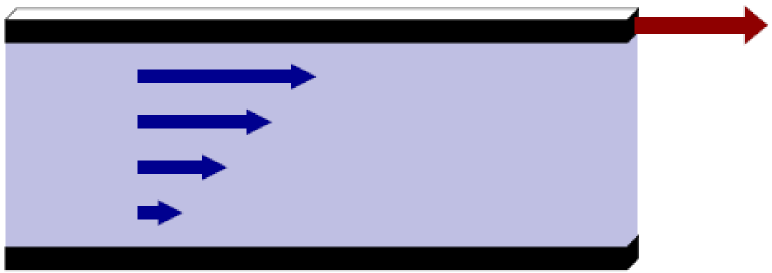
Shear viscosity

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

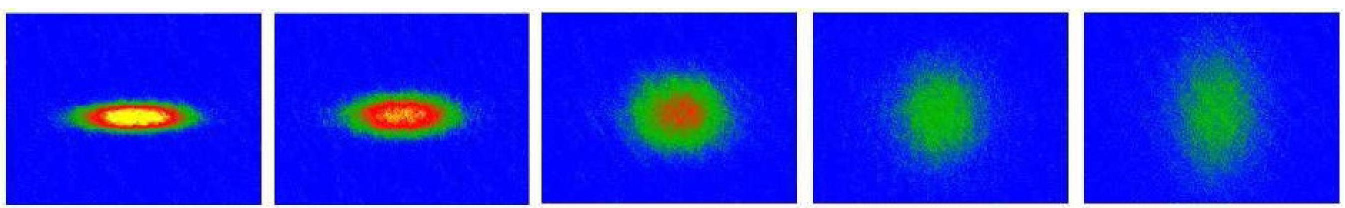


$$F = A\,\eta\,\frac{\partial v_x}{\partial y}$$

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

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

Kinetic theory (Boltzmann equation) prediction: $\eta = n\bar{p}l_{\text{mfp}}$



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

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

KSS conjecture

[Kovtun, Son, Starinets, PRL (2005)]

shear viscosity

entropy density

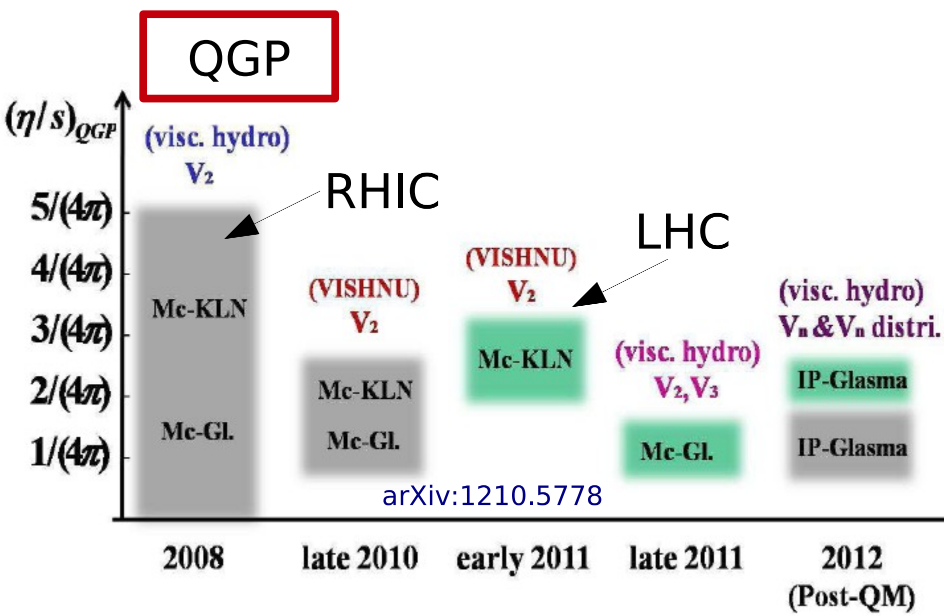
$$\frac{\eta}{s} \geq \frac{1}{4\pi}\frac{\hbar}{k_B}$$

Minimum defines a “perfect” fluid

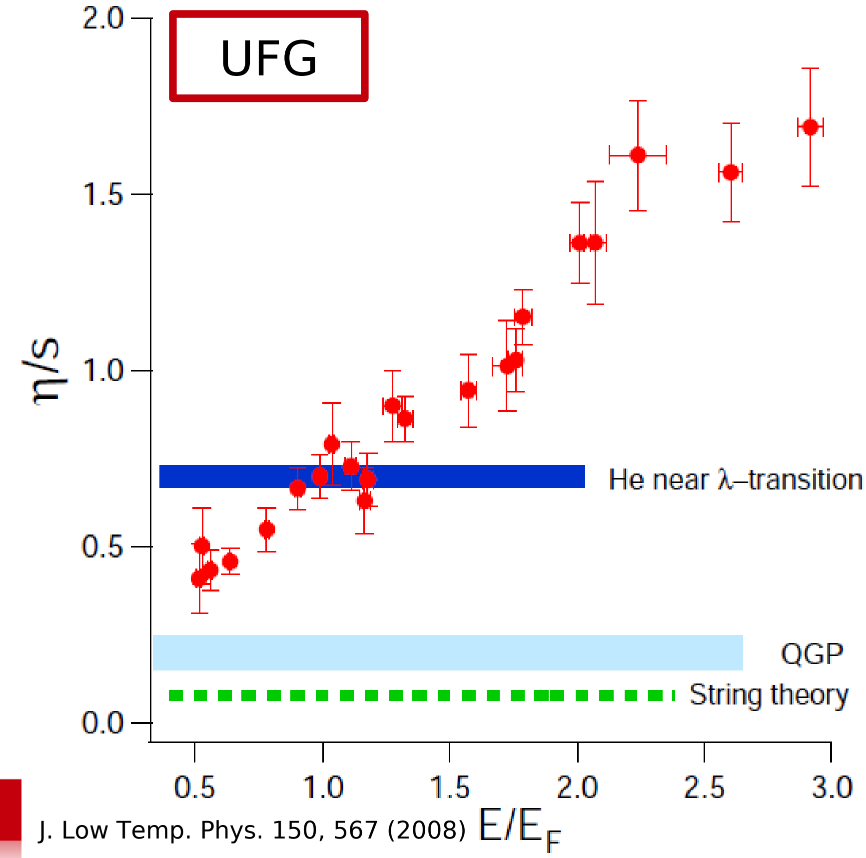
Bound has been proposed on the basis of string theory.

Valid for large class of (string) theories.

Saturated for the case of strongly coupled theory.



arXiv:1210.5778

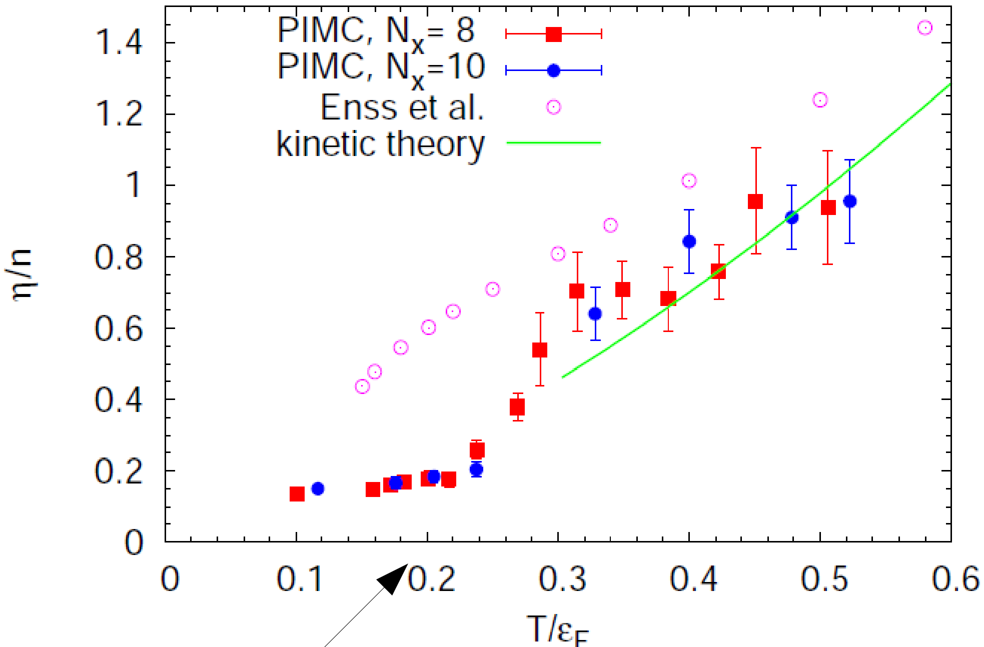


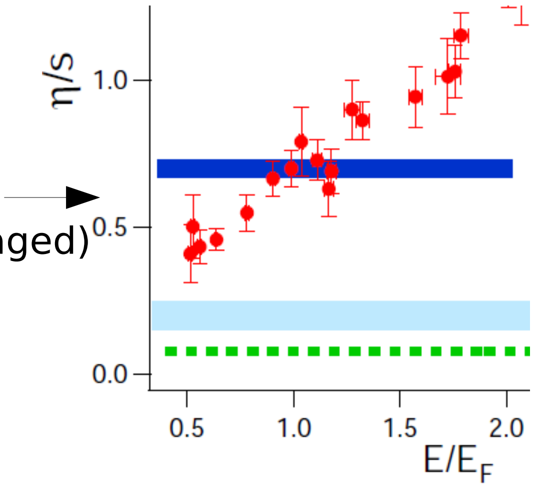
J. Low Temp. Phys. 150, 567 (2008)

Shear viscosity from QMC

(Technically very similar to computation of the spin conductivity)

(We compute stress tensor-stress tensor correlator + tail asymptotic
+ sum rule)

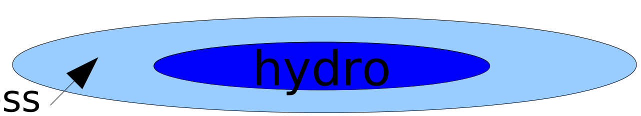




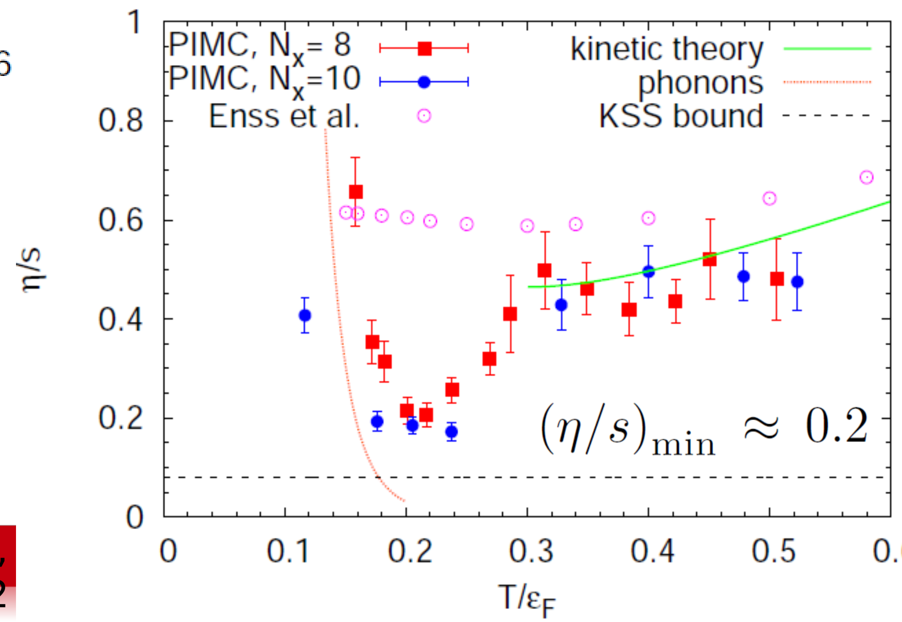
Exp
(trap-averaged)

Problem with averaging procedure of the uniform results

Hydrodynamic description breaks down at the edges.

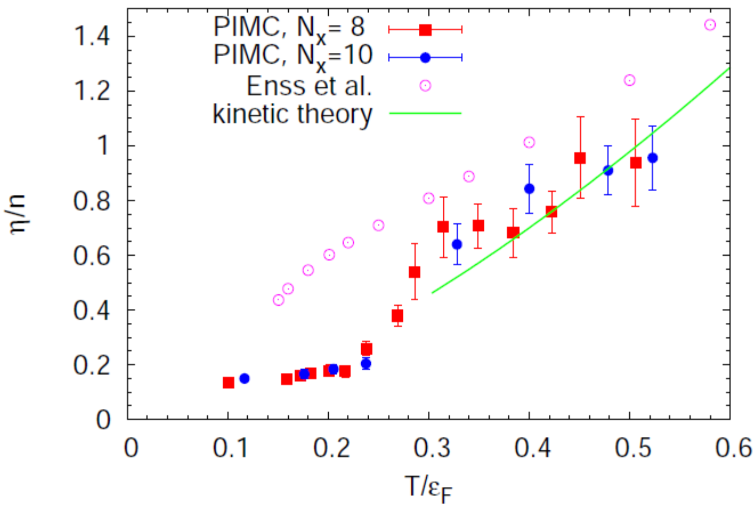


collisionless

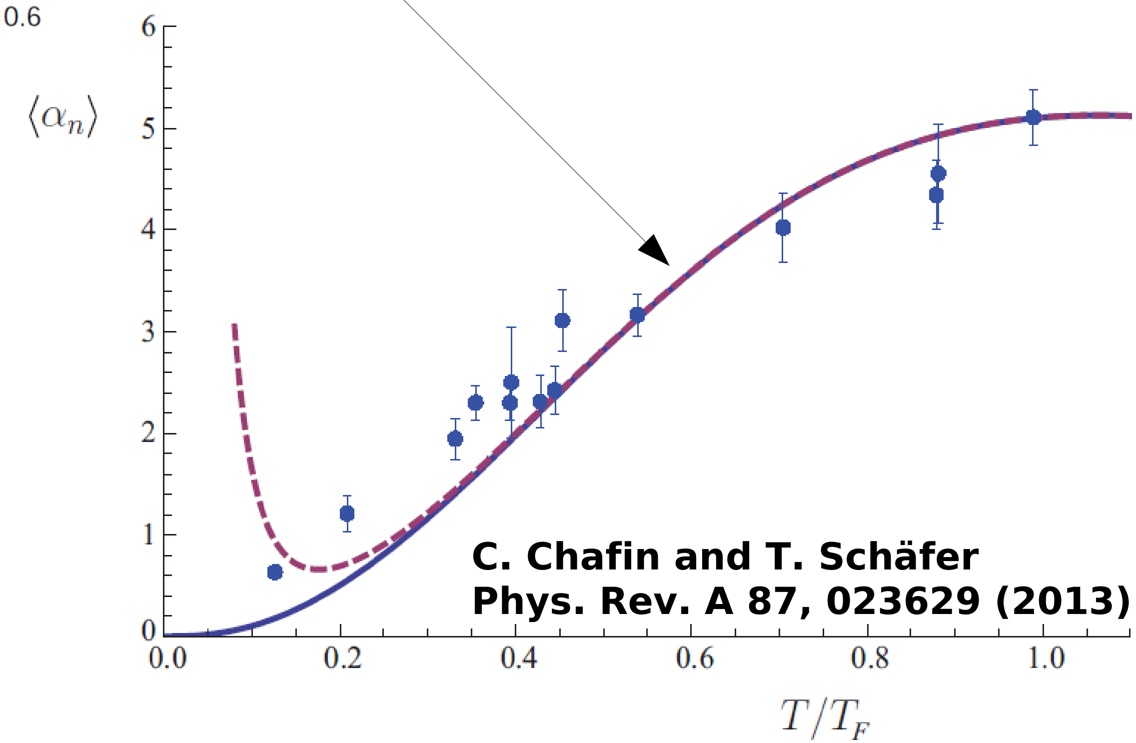


G. Wlazłowski, P. Magierski, J.E. Drut,
Phys. Rev. Lett. 109:020406, 2012

Shear viscosity from QMC

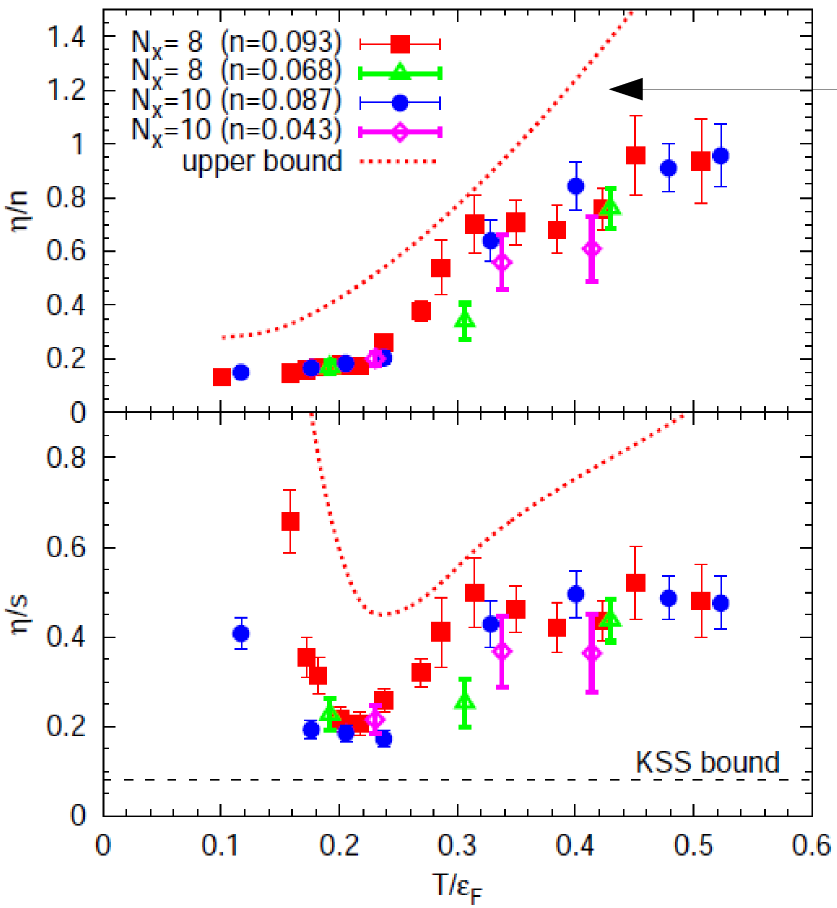


Trap averaged of
the kinetic theory results



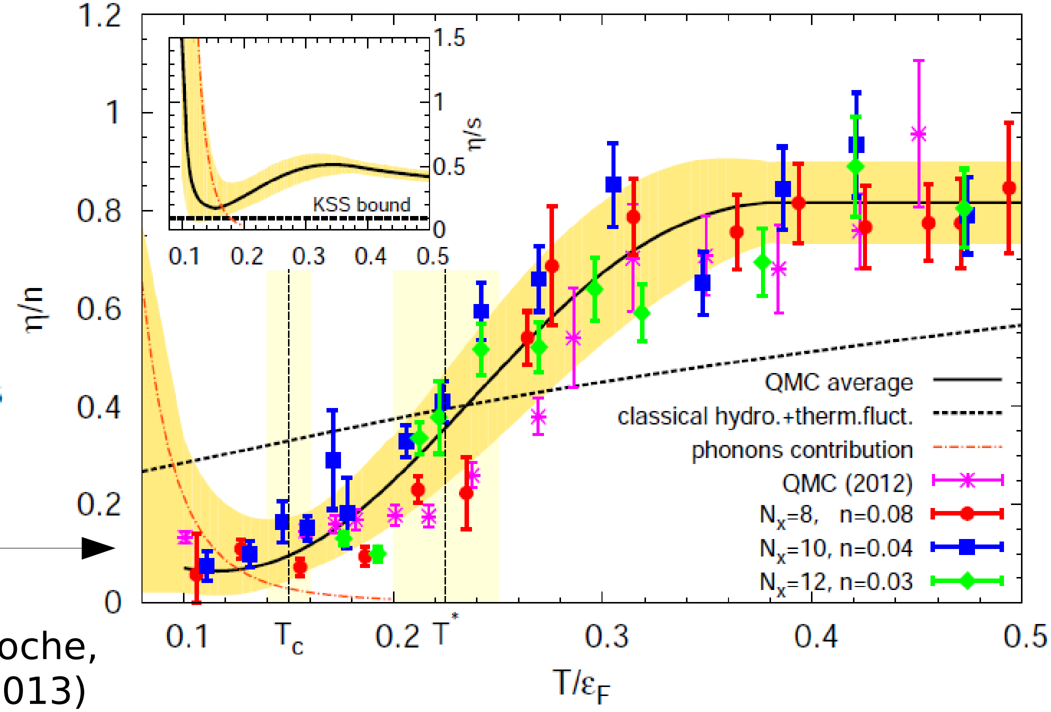
C. Chafin and T. Schäfer
Phys. Rev. A 87, 023629 (2013)

Shear viscosity from QMC



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

Recent simulations



G. Wlazłowski, P. Magierski, A. Bulgac, K.J. Roche, Phys. Rev. A 88, 013639 (2013)

Spectral function (see talk: P. Magierski)

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

$$\mathcal{G}(\boldsymbol{p},\tau) = \langle \psi^\dagger(\boldsymbol{p},\tau)\psi(\boldsymbol{p},0)\rangle_0$$

One-body temperature Green's (Matsubara) function

Inverse problem

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

Constraints:

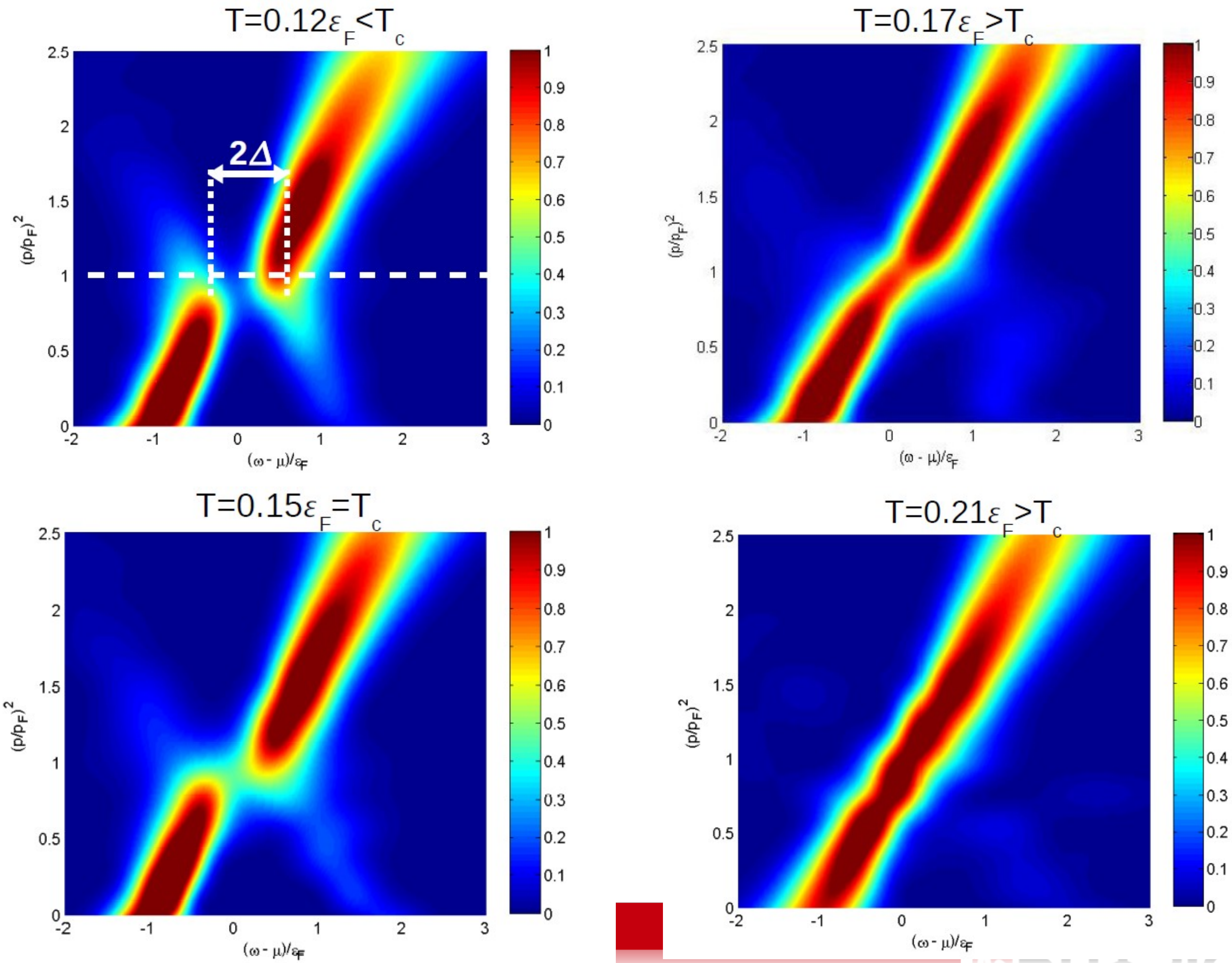
$$A(\boldsymbol{p},\omega) \geq 0, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\boldsymbol{p},\omega) = 1,$$

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

Model:

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

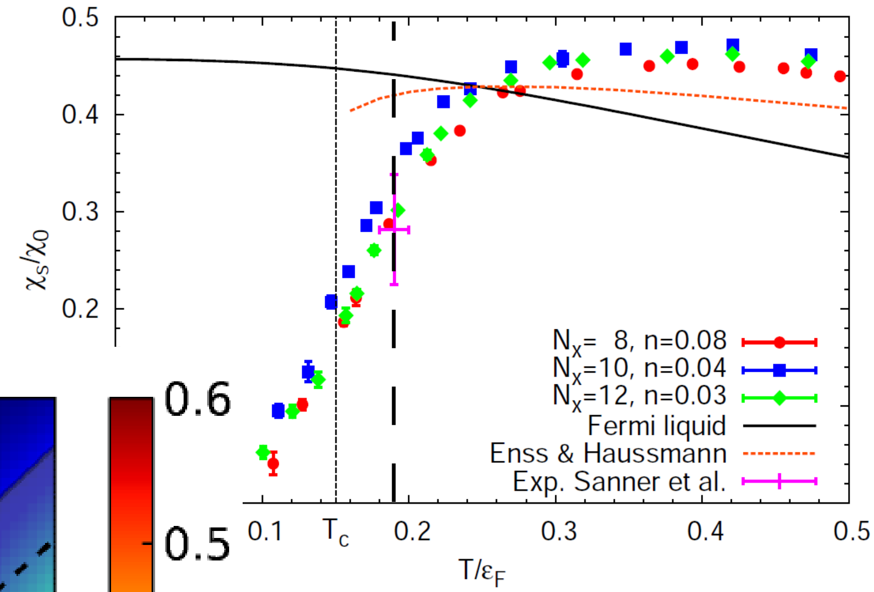
Spectral function

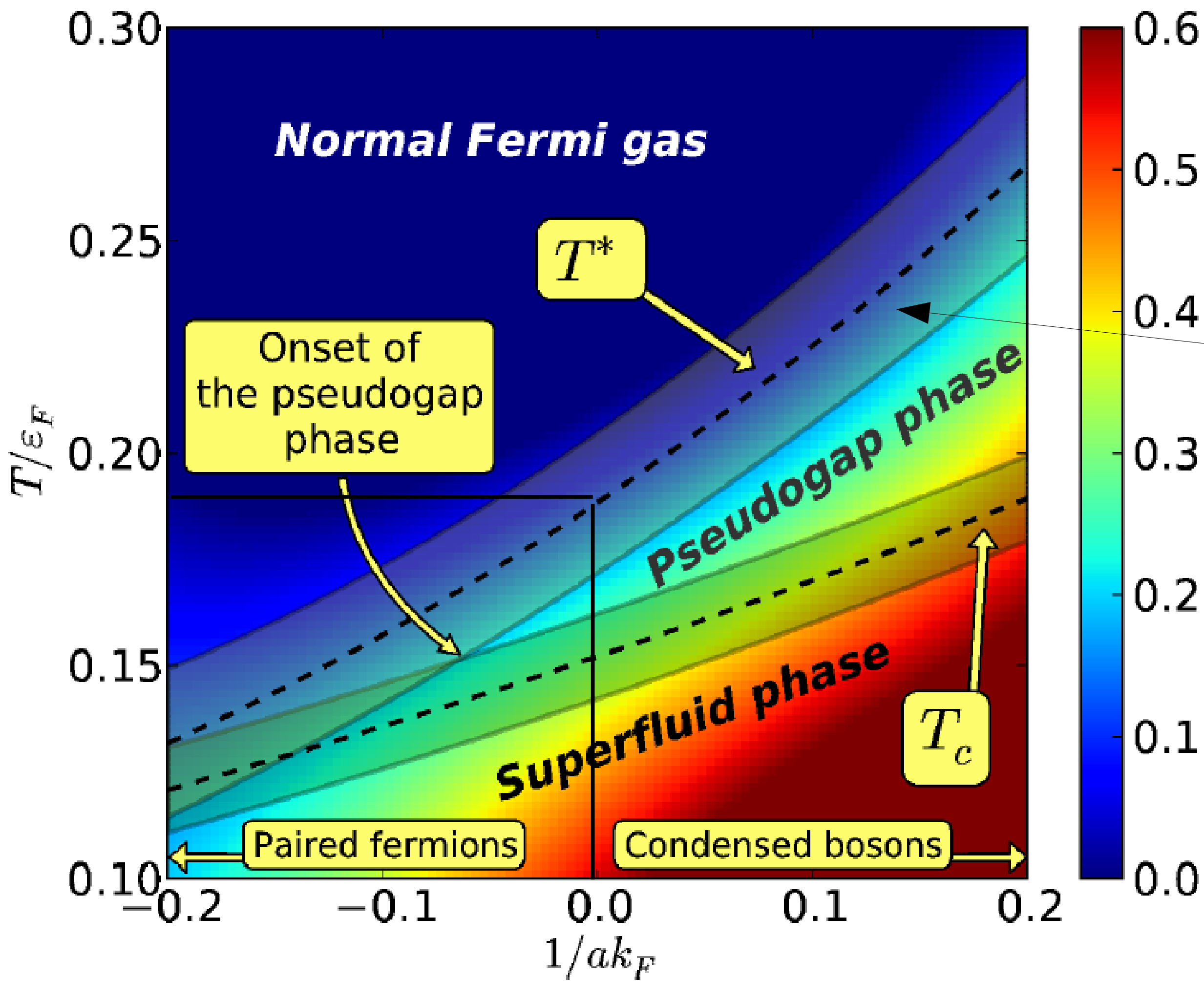


Huge pairing gap helps!

T_c & T^*

P. Magierski, G. Wlazłowski, A. Bulgac
Phys. Rev. Lett. 107, 145304 (2011)





Lower limit for T^*:
due to finite resolution of the analytic continuation procedure

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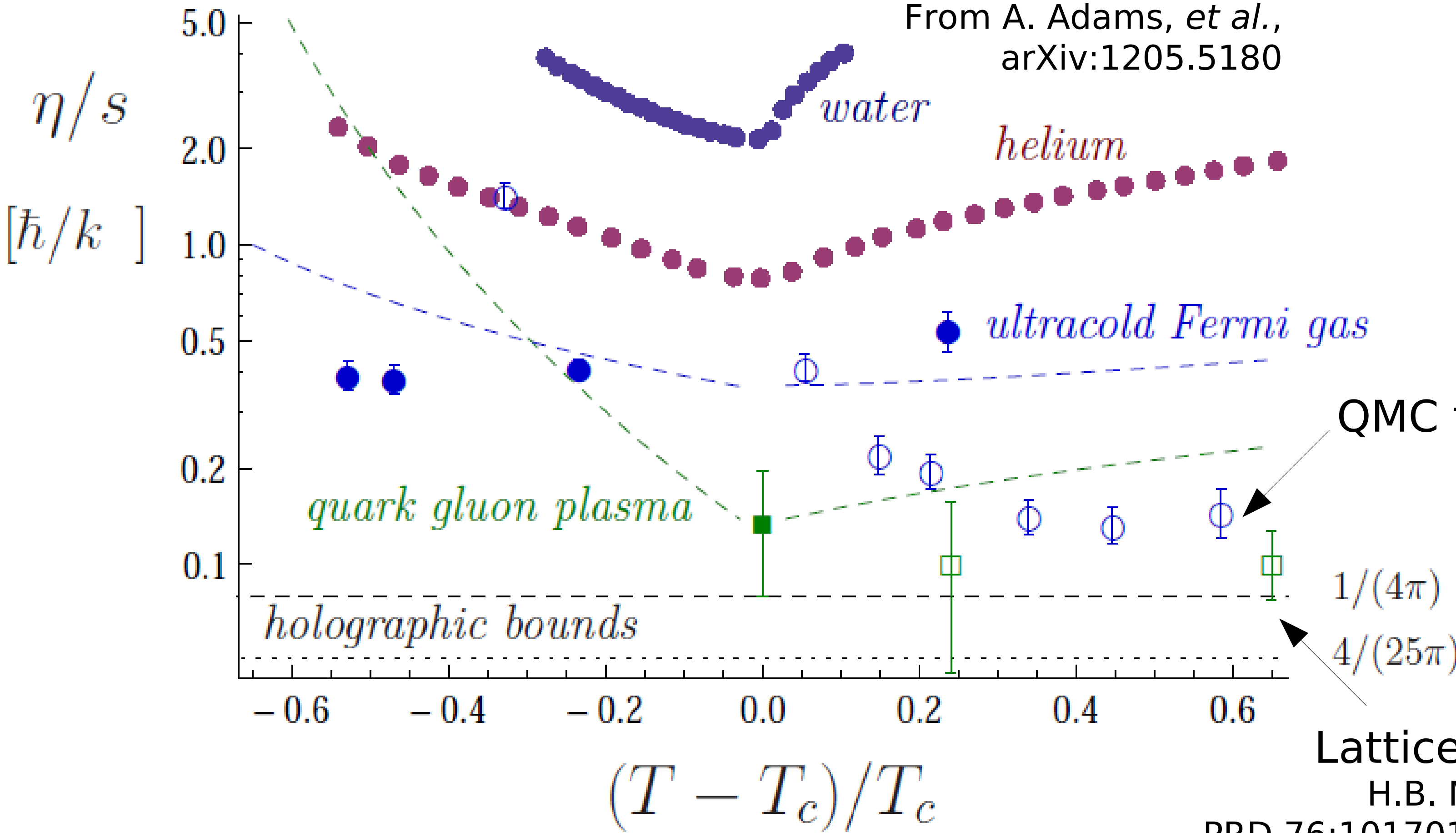
Searching for perfect fluid...

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



QMC for UFG

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

THANK YOU ...