LA-UR-13-27192
Approved for public release; distribution is unlimited.

Title: Quantum Monte Carlo study of strongly interacting Fermi gases

Author(s): Gandolfi, Stefano

Intended for: XVII. International Conference on Recent Progress in Many-Body Theories, 2013-09-08/2013-09-13 (Rostock, Germany)

Issued: 2013-10-04 (rev.1)

Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer,is operated by the Los Alamos National Security, LLC for the National NuclearSecurity Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Departmentof Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

QMC study of strongly interacting Fermi gases

Stefano Gandolfi

Los Alamos National Laboratory (LANL)

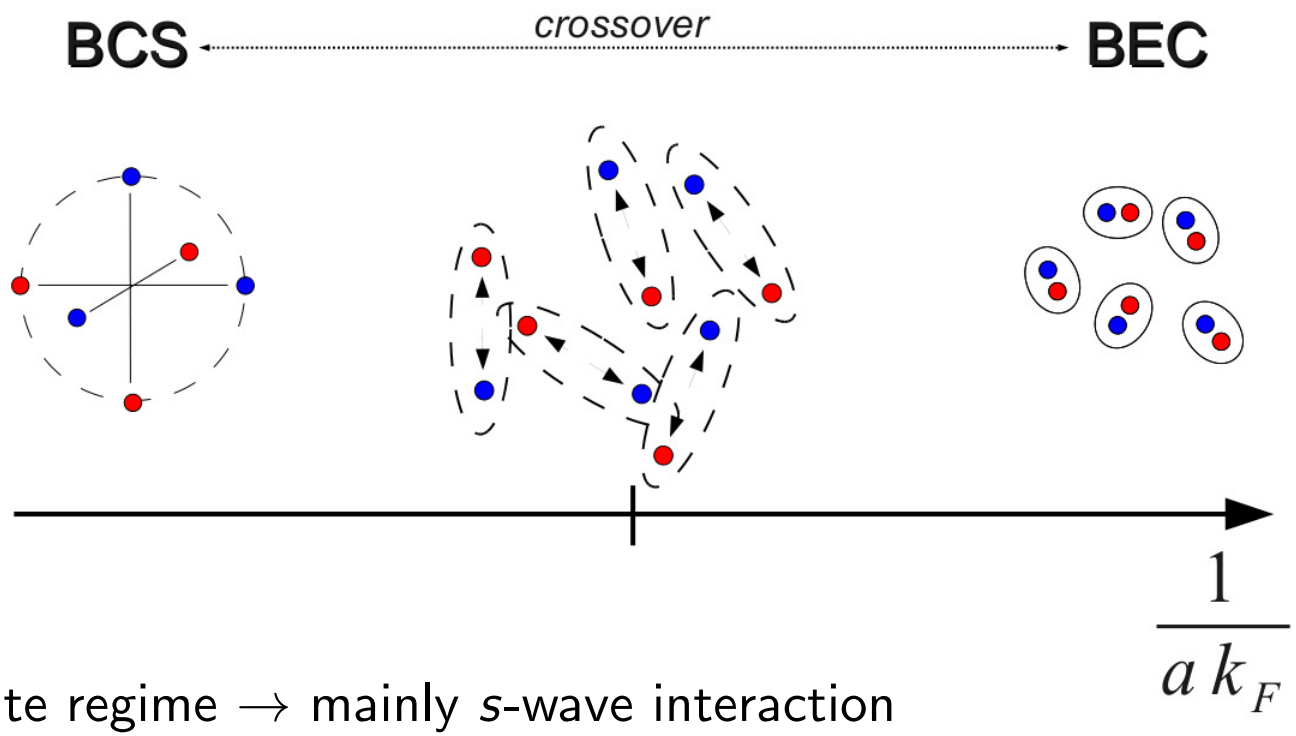
XVII. International Conference on Recent Progress in Many-Body Theories,
September 8-13, 2013, Rostock, Germany.

Los Alamos NATIONAL LABORATORY EST. 1943

NUCLEI
Nuclear Computational Low-Energy Initiative

www.computingnuclei.org

Introduction



- Dilute regime $\rightarrow$ mainly s-wave interaction
- T fraction of T_F $\rightarrow$ T $\sim$0
- Experimentally tunable interaction
- Crossover from weakly interacting Fermions (paired) to weakly repulsive Bosons (molecules)

Cold atoms

Example of Fermionic superfluids:

- Superconductors, $\Delta/E_F \sim 10^{-4}$
- Liquid ^3He, $\Delta/E_F \sim 10^{-3}$
- High-T_C superconductors, $\Delta/E_F \sim 10^{-2}$
- Cold Fermi gases, $\Delta/E_F \sim 0.5$
- Neutron matter, $\Delta/E_F \sim 0.35$

Systems very interesting to study:

- Tunable interaction (Feshbach resonances)
- Universality connecting free Fermions (BCS) to free Bosons (BEC)
- Experiments (EOS, the contact parameter, various responses, ...)
- Very similar to low-density neutron matter

Overview

- The model and Quantum Monte Carlo methods
- The unitary limit and the BCS-BEC crossover
- Contact parameter
- Static response to external potentials
- Density and spin response functions
- Conclusions

Background

Unitary limit:

$$r_{eff} \ll r_0 \ll |a| \,, \quad r_{eff} = 0 \,, \; |a| = \infty$$

Only one scale: $\rightarrow E = \xi E_{FG}$

The model:

$$H = -\frac{\hbar^2}{2m_l} \sum_{i=1}^{N_l} \nabla_i^2 + \frac{\hbar^2}{2m_h} \sum_{i=1}^{N_h} \nabla_i^2 + \sum_{i,j} v(r_{ij})$$

Ideally: $v(r) \sim \delta(r)$

System strongly interacting and non-perturbative
$\rightarrow$ Quantum Monte Carlo methods

Quantum Monte Carlo

Evolution of Schrodinger equation in imaginary time **t**:

$$\psi(t) = e^{-(H-E_T)t}\psi(0)$$

At $t \to \infty$ we get $\psi(t) \to \phi_0$ if not orthogonal to $\psi(0)$.

Propagation performed by

$$\psi(R,t) = \langle R|\psi(t)\rangle = \int dR' G(R,R',t)\psi(R',0)$$

where $G(R,R',t)$ is an approximate propagator known in the small-time limit:

$$G(R,R',\Delta t) = \langle R|e^{-H\Delta t}|R'\rangle \approx \langle R|e^{-p^2\Delta t}|R'\rangle\langle R|e^{-V\Delta t}|R'\rangle$$

Then we need to iterate the above integral equation many times in the small time-step limit.

Monte Carlo methods

- Diffusion Monte Carlo: coordinate space (continuum). Fixed-node approximation (upperbound).

  A careful optimization of ψ_T is very important.

$$\psi_T(R) = \prod_{i,j} f(r_{ij})\, \Phi_{BCS}\,, \qquad \phi_{pair}(r_{ij}) = \sum_n c_n \exp(i\mathbf{k_n}\mathbf{r_{ij}}) + \beta(r_{ij})$$

  $f(r_{ij})$ contains both short- and long-range correlations.

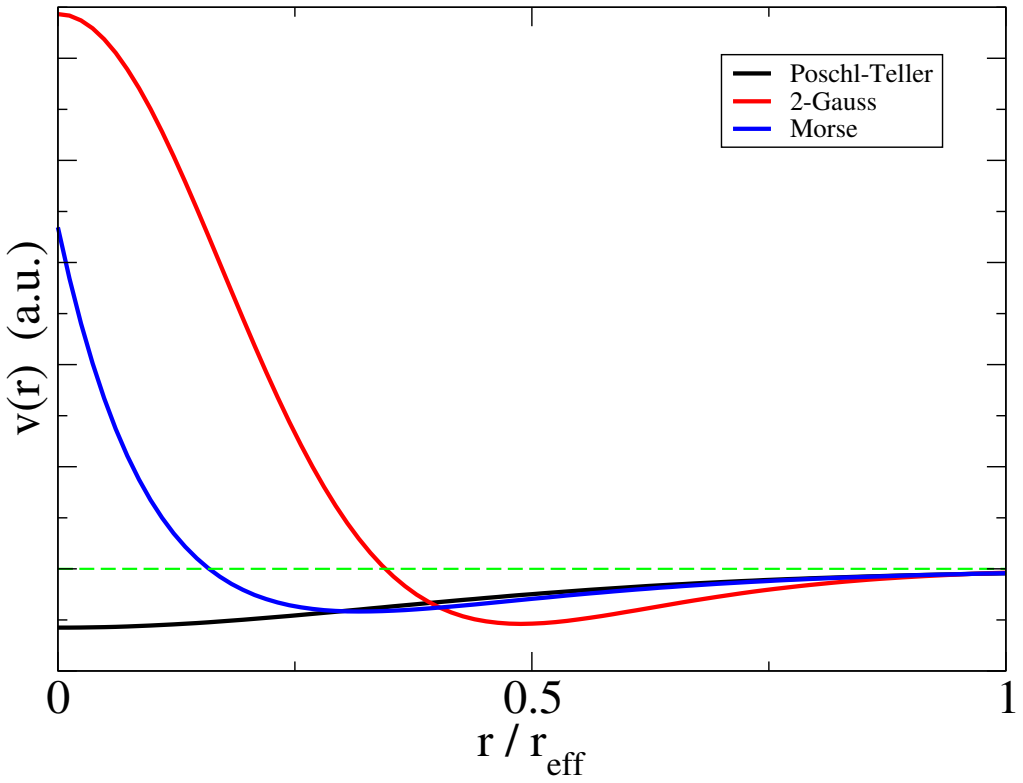
  $\sim$15-20 parameters to variationally optimize.

- Auxiliary Field Monte Carlo: orbitals (lattice). Exact for unpolarized systems with attractive interaction. Results independent to the trial wave function (but for the variance it matters).

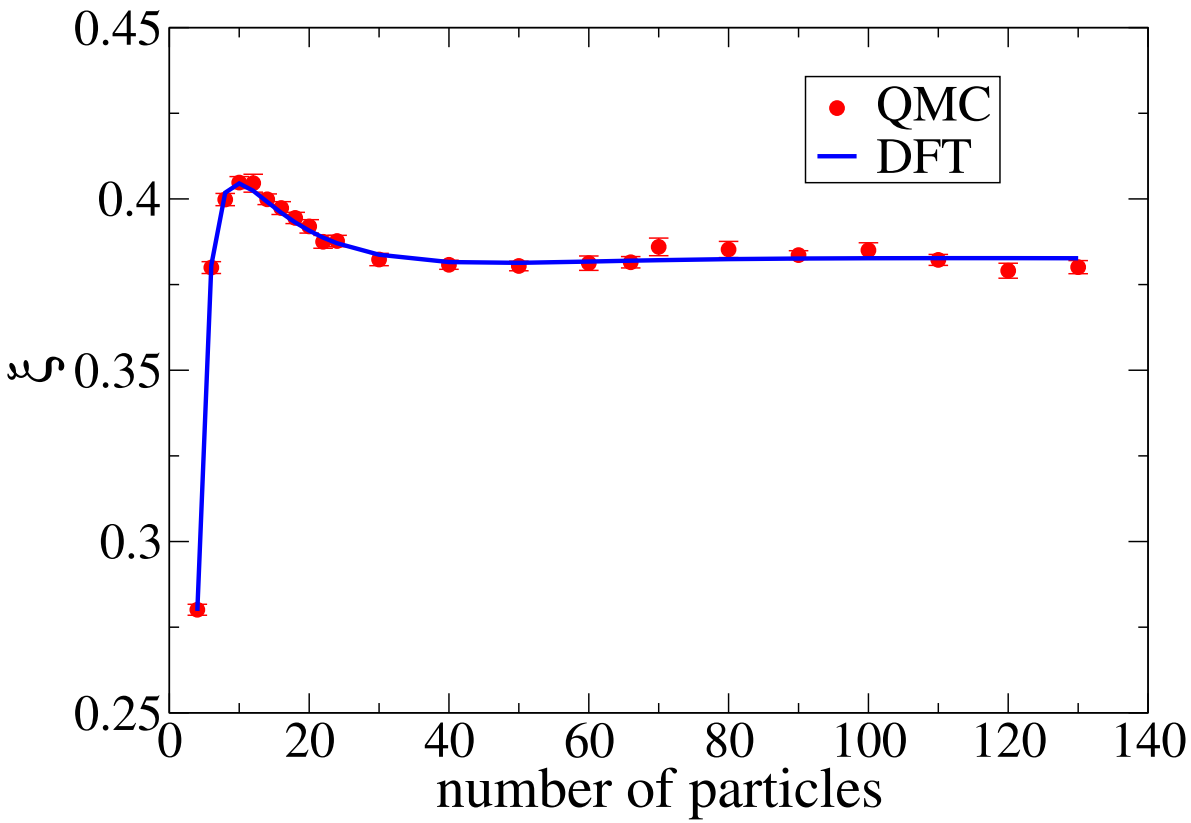
Short range potential

Models of $v(r)$:

- $\sim -V_0 \cosh^{-2}(\mu r)$
- $\sim -V_0[\exp(-(\mu r)^2/4) - 4\exp(-(\mu r)^2)]$
- $\sim -V_0[\exp(-\mu r) - 2\exp(-2(\mu r))]$



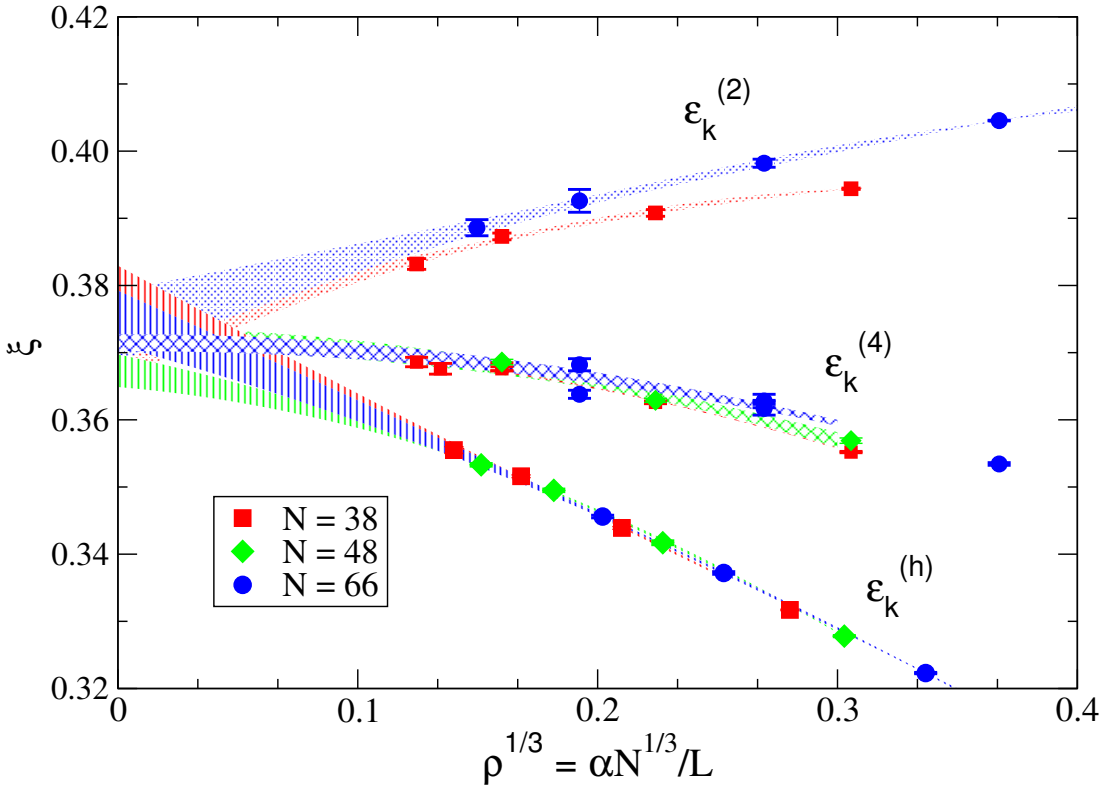
Unitary Fermi gas - finite size effects



Forbes, Gandolfi, Gezerlis PRL 106, 235303 (2011).

Finite size effects well under control in QMC using pairing orbitals.

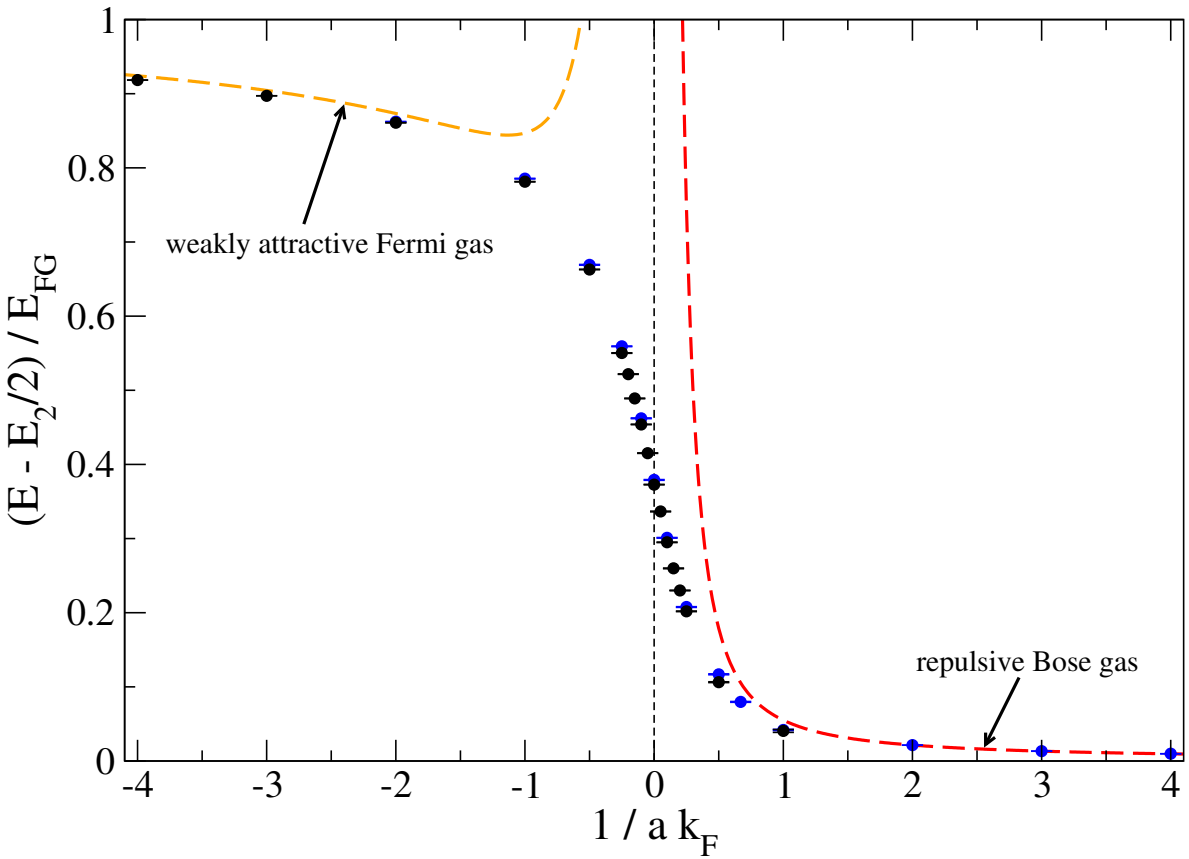
Unitary Fermi gas - Exact calculation of ξ



$\xi = 0.372(5)$ Carlson, Gandolfi, Schmidt, Zhang PRA 84, 061602 (2011)
$\xi = 0.376(5)$ subsequent experiment at MIT (Ku, Sommer, Cheuk, Zwierlein, Science (2012))

Predictive power of QMC confirmed by experiments!

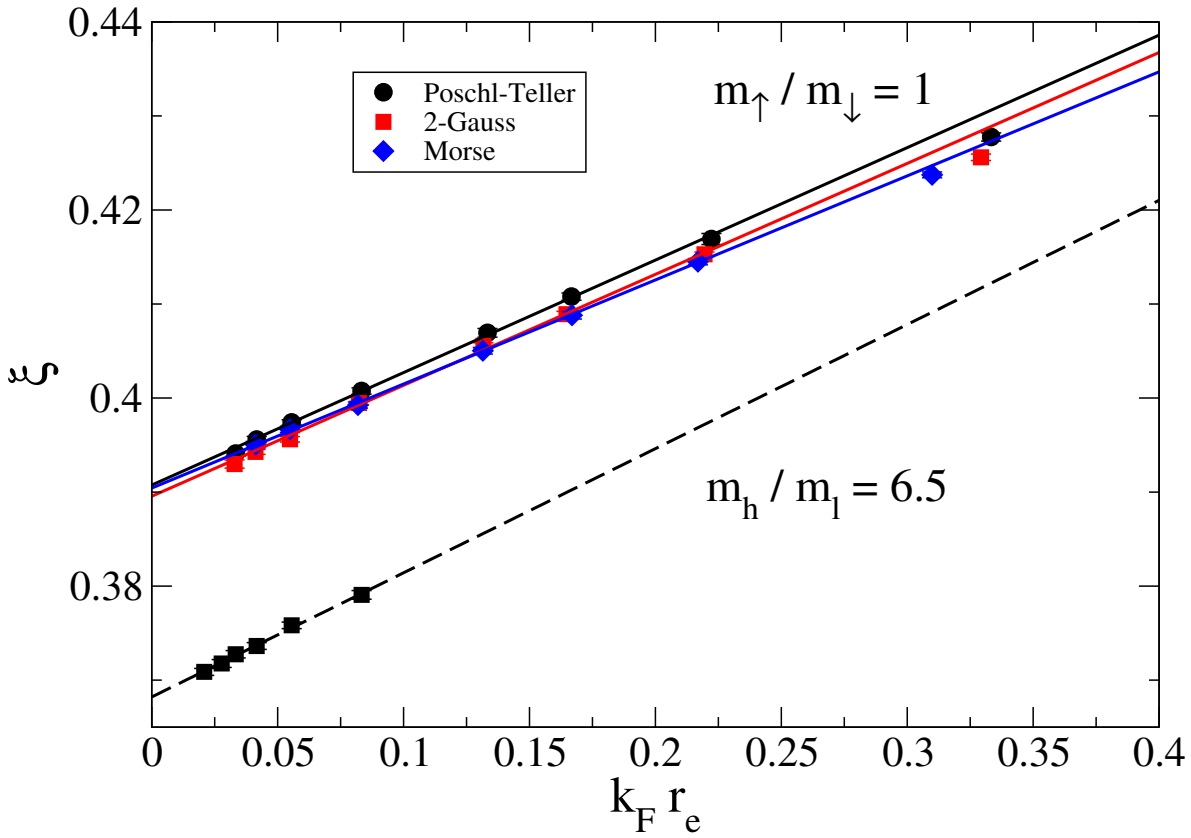
BCS-BEC crossover



Fixed-node DMC results:

$m_\uparrow/m_\downarrow = 1$: $\xi = 0.389(1)$ $\qquad$ $m_h/m_l = 6.5$: $\xi = 0.368(1)$

Unitary Fermi gas - Effective range extrapolation

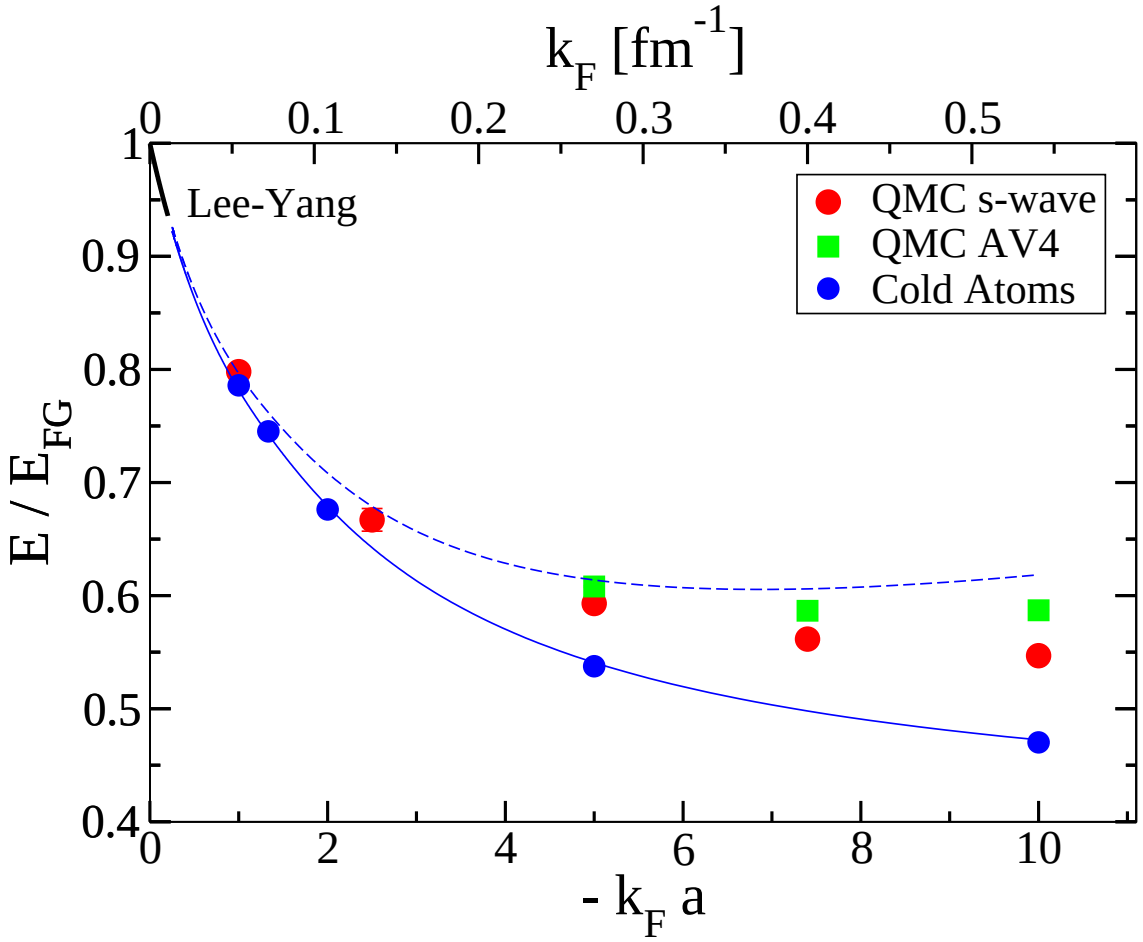


$$\xi = \xi_0 + S\, k_F r_{eff} + \cdots$$

In this range $S = 0.12(2)$, independent to $v(r)$ and to m_h/m_l.

AFMC: $S = 0.11(3)$, Carlson, Gandolfi, Schmidt, Zhang, PRA 84, 061602 (2011).

Fermi gas and neutron matter



Carlson, Gandolfi, Gezerlis, PTEP 01A209 (2012).

Contact parameter

Tan universal relations:

$$\frac{E}{E_{FG}} = \xi - \frac{\zeta}{k_F a} - \frac{5\nu}{3(k_F a)^2} + \dots, \qquad \frac{C}{N k_F} = \frac{6}{5}\pi\zeta$$

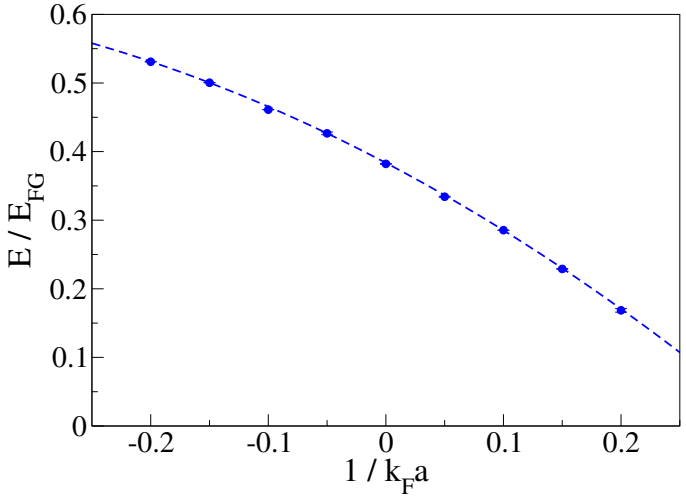
$$N(k) \to \frac{8}{10\pi}\zeta\frac{k_F^4}{k^4} = \frac{2}{3\pi^2}\frac{C}{N k_F}\frac{k_F^4}{k^4}$$

$$g_{\uparrow\downarrow}(r) \to \frac{9\pi}{20}\zeta(k_F r)^{-2} = \frac{3}{8}\frac{C}{N k_F}(k_F r)^{-2}$$

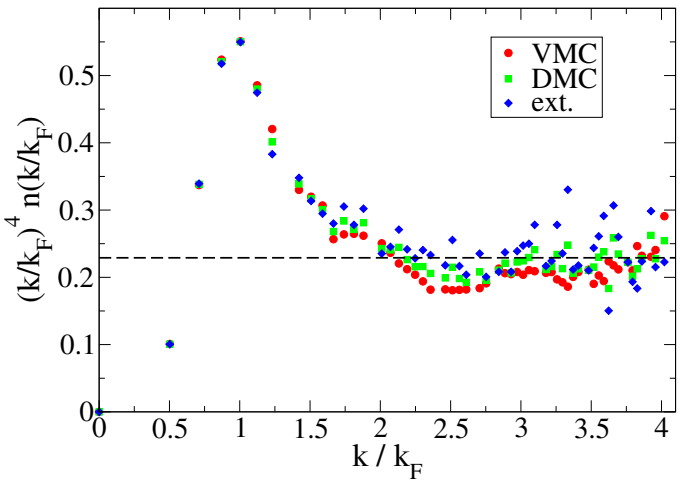
$$S_{\uparrow\downarrow}(k) \to \frac{3\pi}{10}\zeta\frac{k_F}{k} = \frac{1}{4}\frac{C}{N k_F}\frac{k_F}{k}$$

Shina Tan, Ann. Phys. (2008).

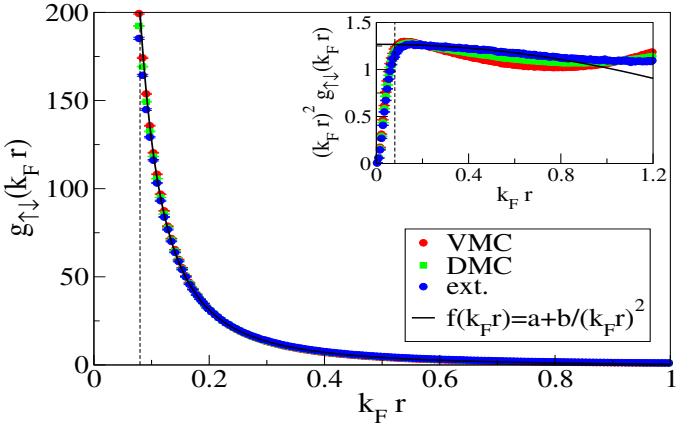
Contact parameter



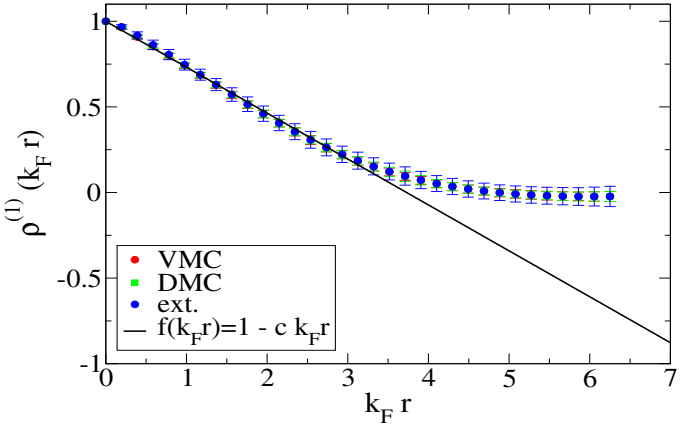
Equation of state



Momentum distribution



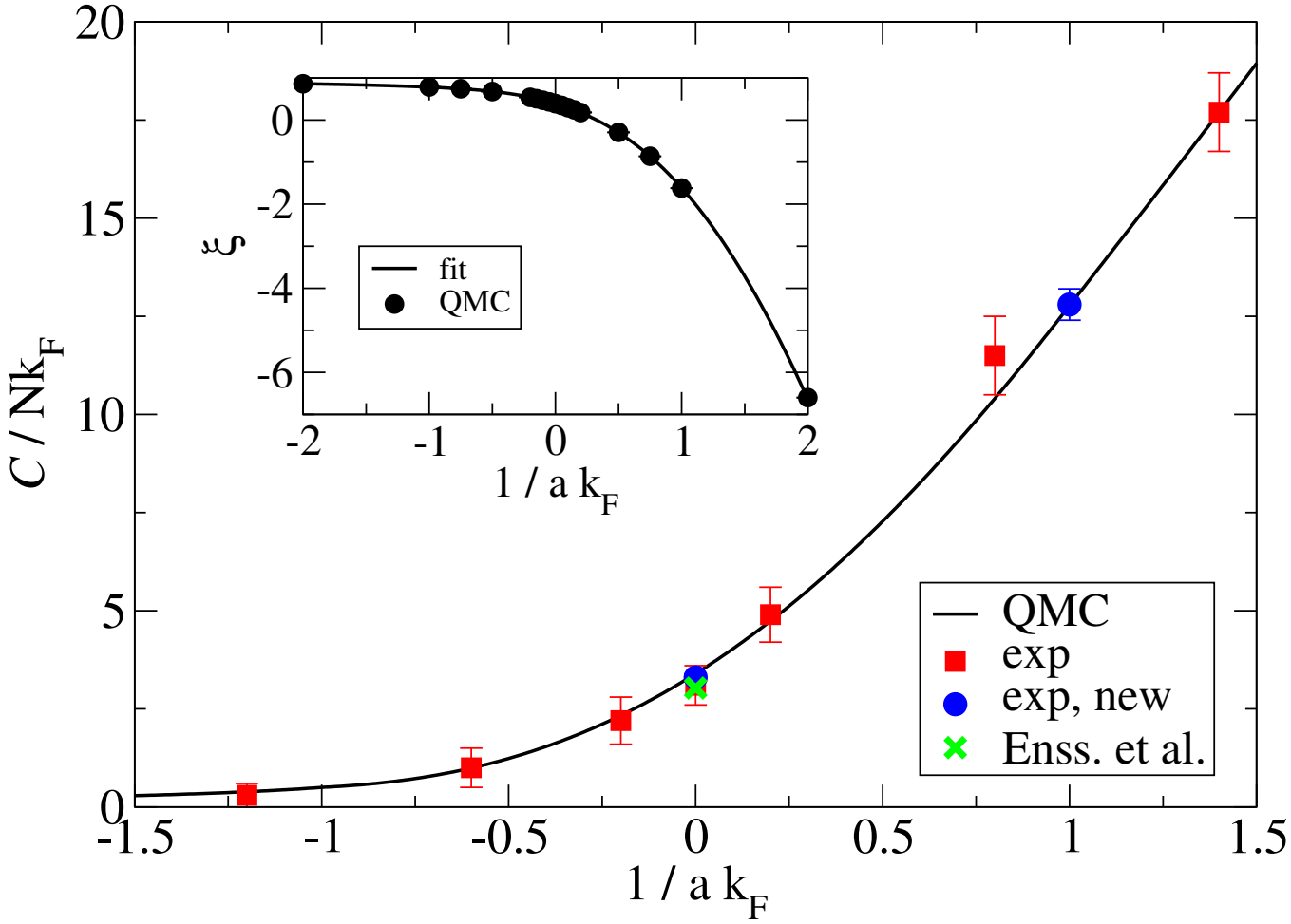
Pair distribution function



One-body density matrix

$C/Nk_F = 3.39(1)$, Gandolfi, Schmidt, Carlson, PRA 83, 041601 (2011).

Contact parameter



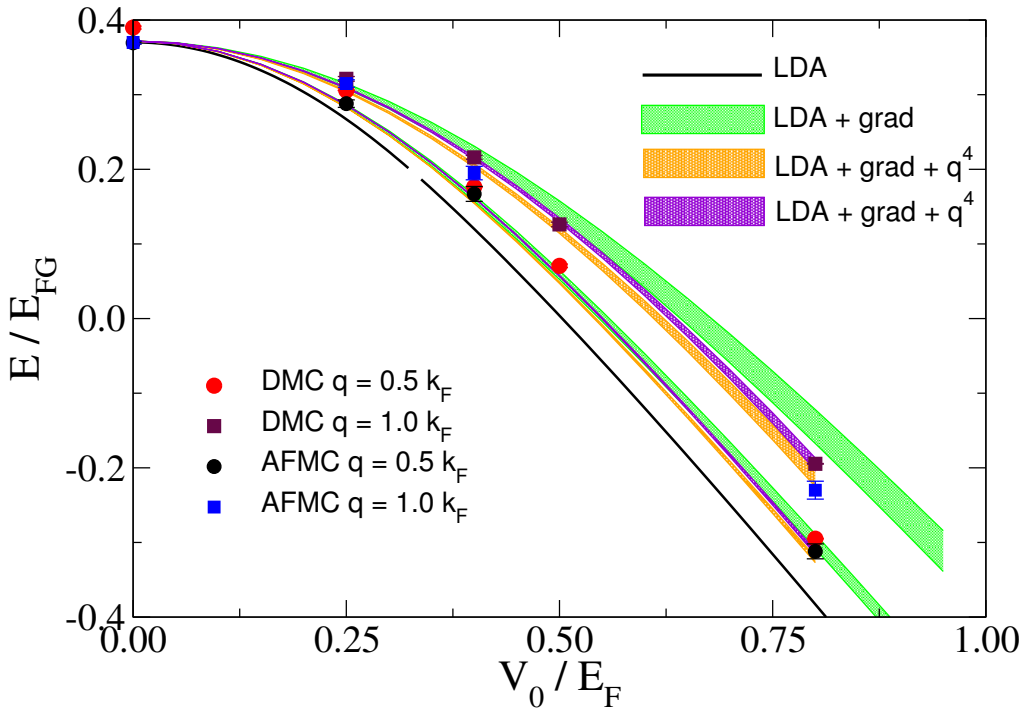
Hoinka, Lingham, Fenech, Hu, Vale, Drut, Gandolfi, PRL 110, 055305 (2013).

Green point: Enss, Haussmann, Zwerger, Ann. Phys. 326, 770 (2011).

Static response

H scale invariant, functional should work for any external potential.

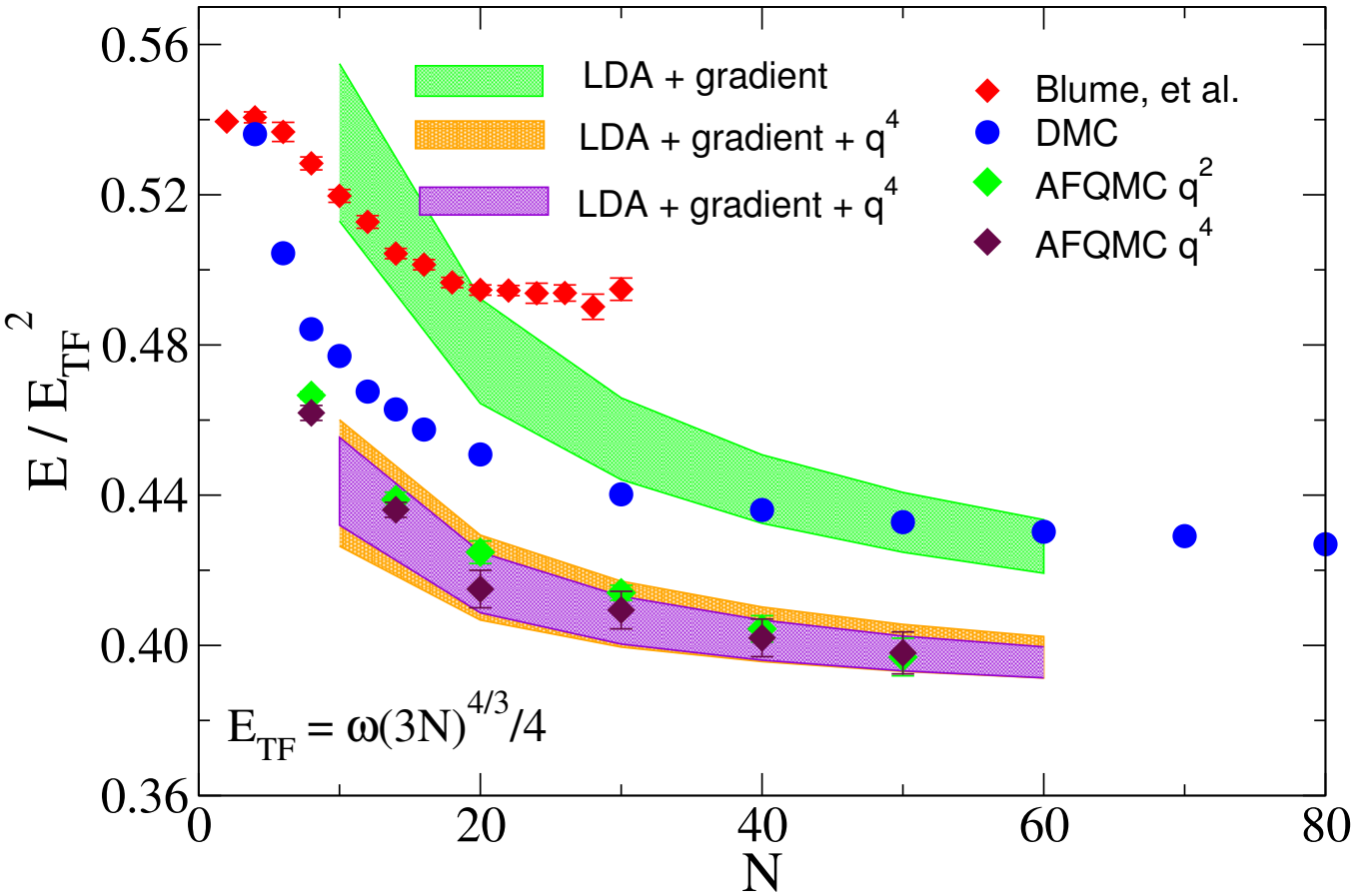
Static response to an external potential $V = -V_0 \sum \cos(\mathbf{q} \cdot \mathbf{r})$



Carlson, Gandolfi, in preparation.

$$\mathcal{E}_g = \int V_{ext}(r)\rho(r) + \xi \frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3} + c_g \nabla\rho^{1/2} \cdot \nabla\rho^{1/2} - c_4 \frac{\nabla^2\rho^{1/2}\nabla^2\rho^{1/2}}{\rho^{2/3}}$$

Unitary gas in a trap



Carlson, Gandolfi, in preparation.

Dynamic response functions

Response to an operator $\hat{S}$:

$$S(q,\omega) = \sum_n \left| \langle \psi_n | \hat{S}(q) | \psi_0 \rangle \right|^2 \delta(E_n - E_0 - \omega)$$

Euclidean (or imaginary-time) response:

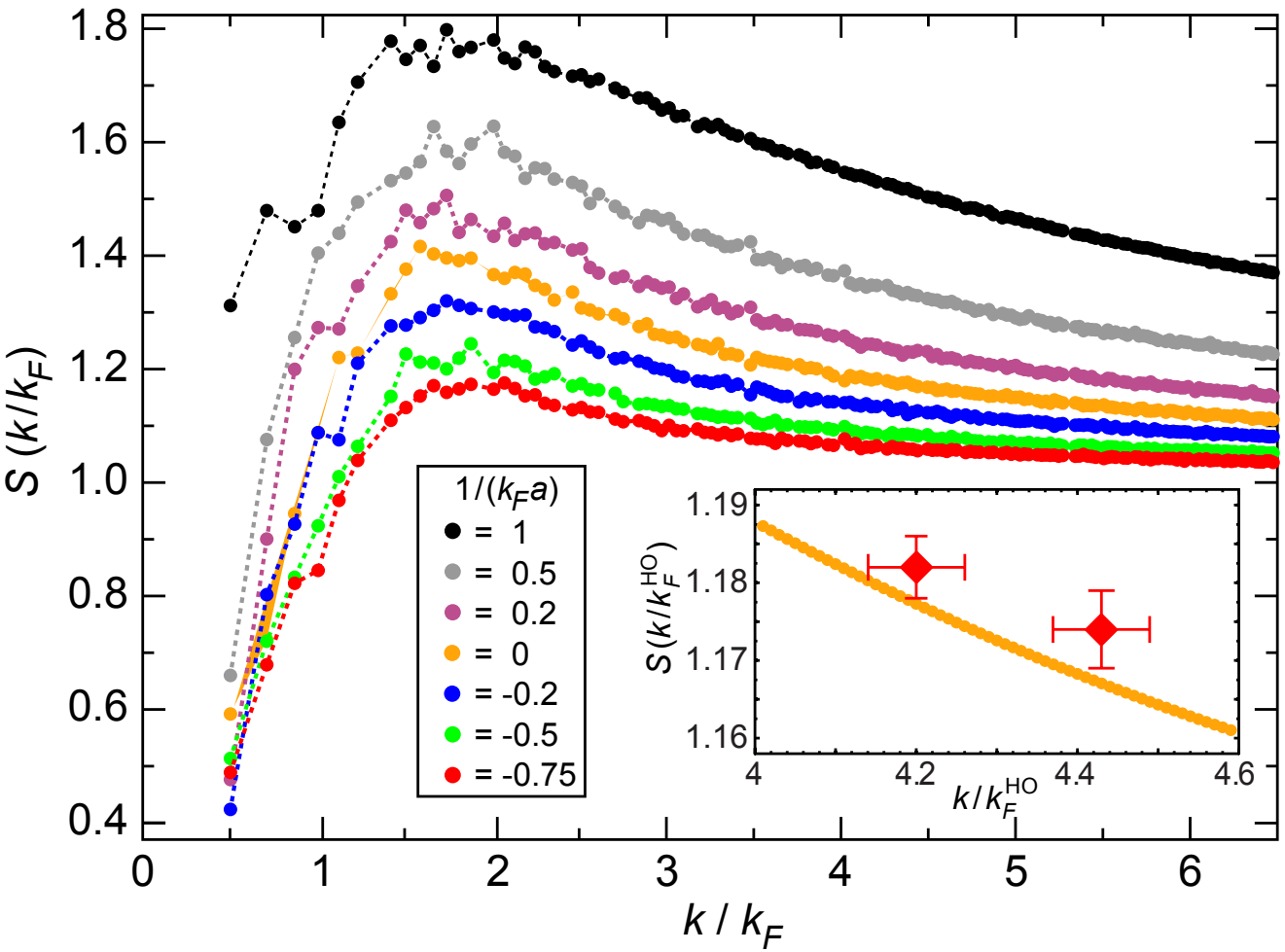
$$S(q,\tau) = \int d\omega \, K(\omega,\tau) S(q,\omega) = \langle \psi_0 | \hat{S}^\dagger(q) K(H,\tau) \hat{S}(q) | \psi_0 \rangle$$

where the density- and spin-density response operators are:

$$\hat{S}_\rho(q) = \sum_i e^{i\vec{q}\vec{r}_i} \qquad \hat{S}_\sigma(q) = \sum_i \sigma_i^z e^{i\vec{q}\vec{r}_i}$$

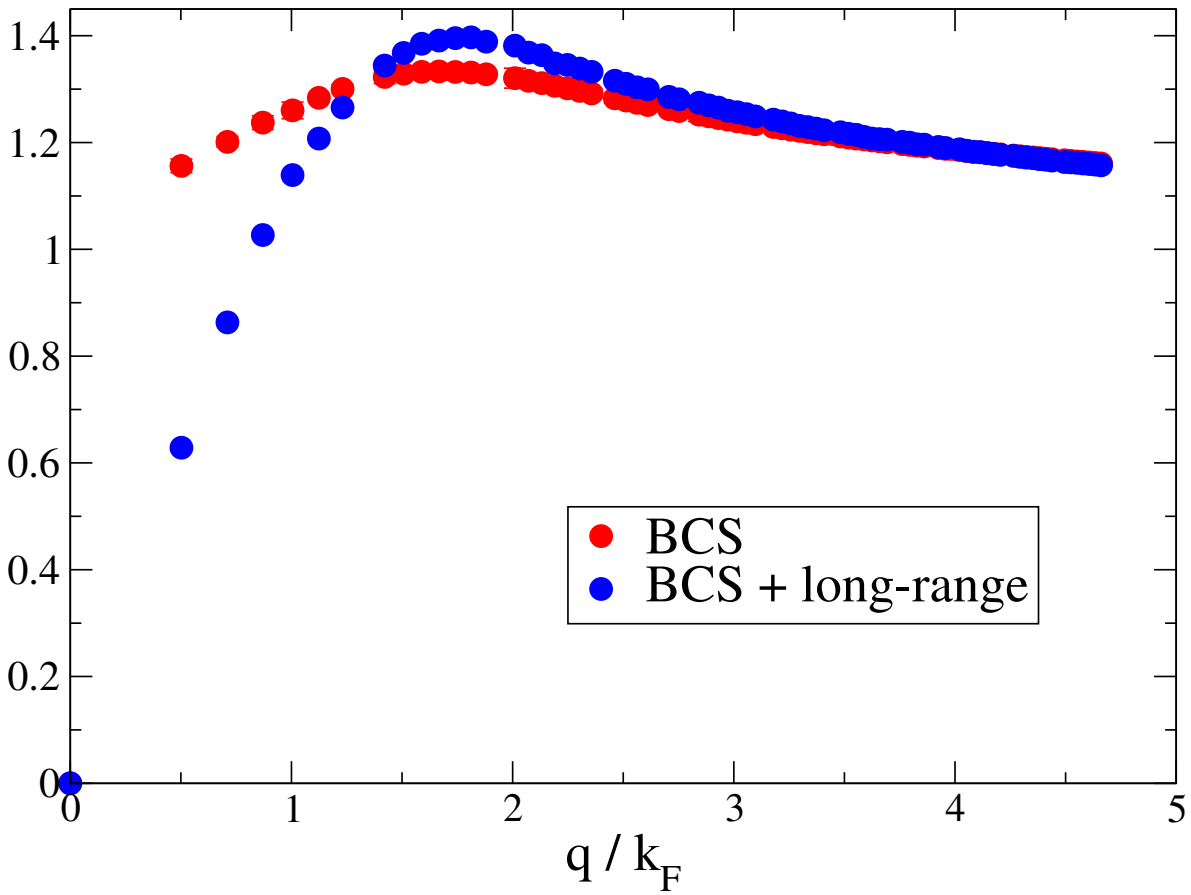
Note: $S(q,\tau=0)$ gives the sum rule of $\hat{S}$.

Static Structure Function - density-response sum rule



Hoinka, Lingham, Fenech, Hu, Vale, Drut, Gandolfi, PRL 110, 055305 (2013).

Static Structure Function



$$\Psi(\mathbf{R}) = \prod_{i<j} \exp\left[\gamma \sum_n \frac{\exp(-\beta|\mathbf{q_n}|)}{|\mathbf{q_n}|} \exp(-i\mathbf{q}\cdot\mathbf{r_{ij}})\right] \Psi_{box}(\mathbf{R})$$

Dynamic response functions

Calculation of $S(q,\tau)$ possible with QMC, but the inversion of imaginary-time response is a very difficult task.

- Sumudu kernel (Roggero, Pederiva, Orlandini, arXiv:1209.5638), resolution controllable with respect Laplace

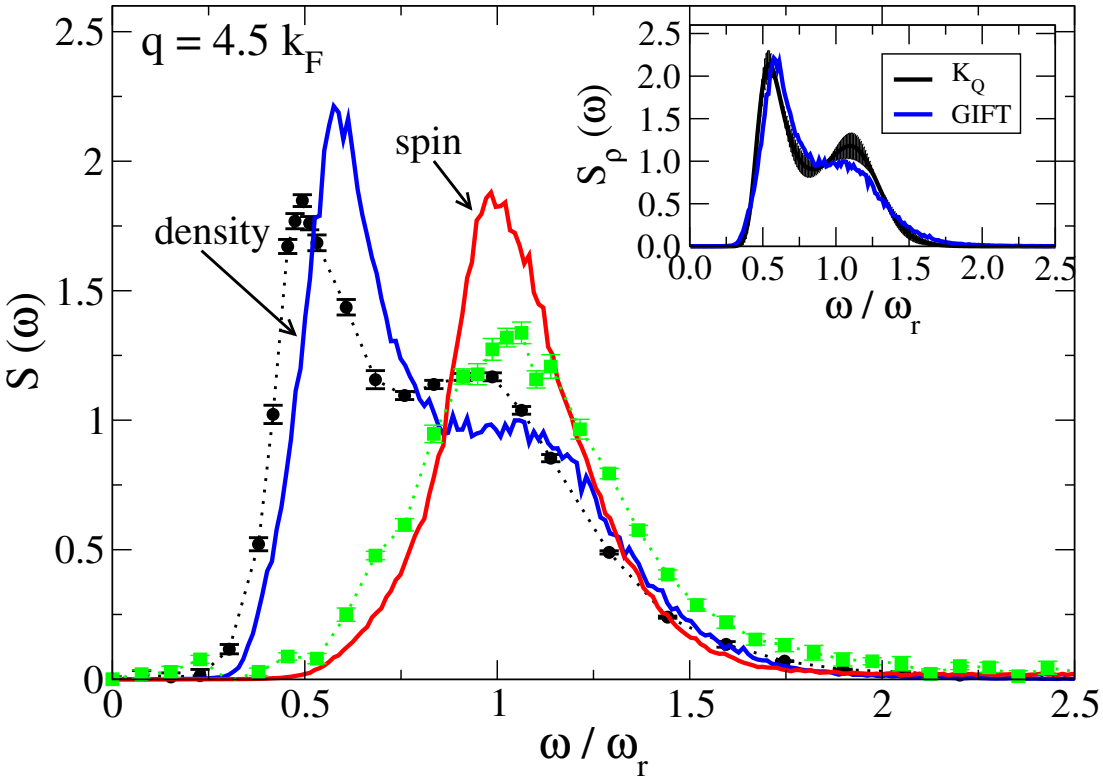
$$K_Q(\omega,\tilde{\tau}) = N\left(e^{-\mu\frac{\omega}{\tilde{\tau}}} - e^{-\nu\frac{\omega}{\tilde{\tau}}}\right)^P$$

  combined with a maximum-entropy like method

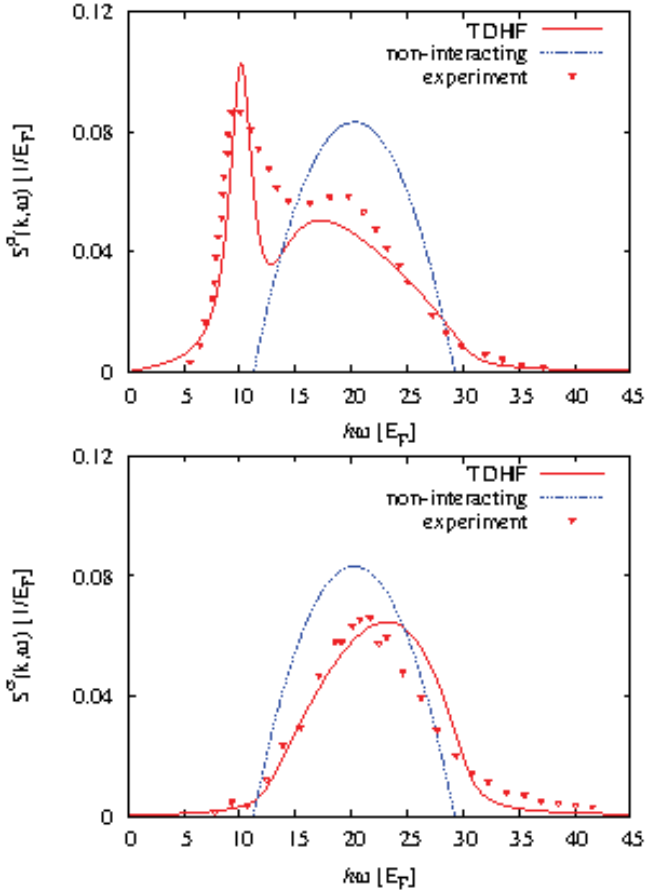
- Genetic Inversion via Falsification of Theories (GIFT) method (Vitali, Rossi, Reatto, Galli, PRB 82, 174510, 2010), where $S(\omega)$ is a sampled histogram to have

$$\chi_i^2(S) \propto \sum_j \left[S_i(\tau_j) - \int d\omega\, e^{-\omega\tau_j} S(\omega)\right]^2 \approx 1$$

Density and spin response



Carlson, Gandolfi, Orlandini, Pederiva, Roggero, Vitali, in preparation.

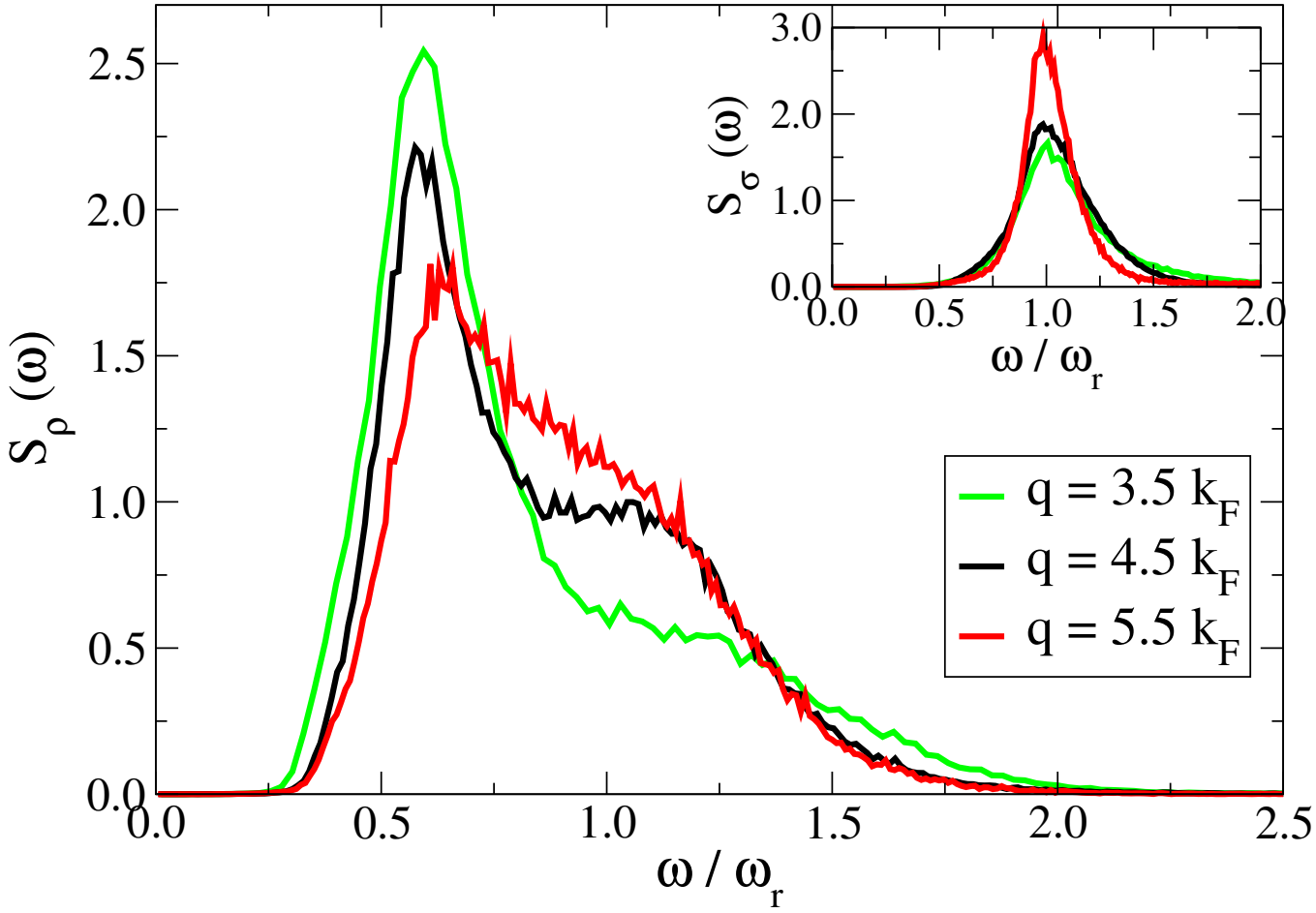


TDHF (DMC+CBF)

Exp: q=4.2k_F Hoinka, et *al*., PRL 110, 055305 (2013).

See also Astrakharchik, Boronat, Krotscheck, Lichtenegger, arXiv (2013).

Density and spin response



Carlson, Gandolfi, Orlandini, Pederiva, Roggero, Vitali, in preparation.

Conclusions

- QMC methods very successful to calculate the BCS-BEC crossover of strongly interacting Fermi gases.
- Contact parameter and structure factor in good agreement with experimental measurements.
- Long-range correlations very important to describe $S(q)$ at low q.
- Static response useful to constrain density functionals and describe systems in a trap.
- Calculation of dynamic density- and spin-response functions in progress.

Thank you!

Los Alamos NATIONAL LABORATORY EST. 1943

NUCLEI Nuclear Computational Low-Energy Initiative

www.computingnuclei.org