The pseudogap regime in the unitary Fermi gas using canonical-ensemble quantum Monte Carlo

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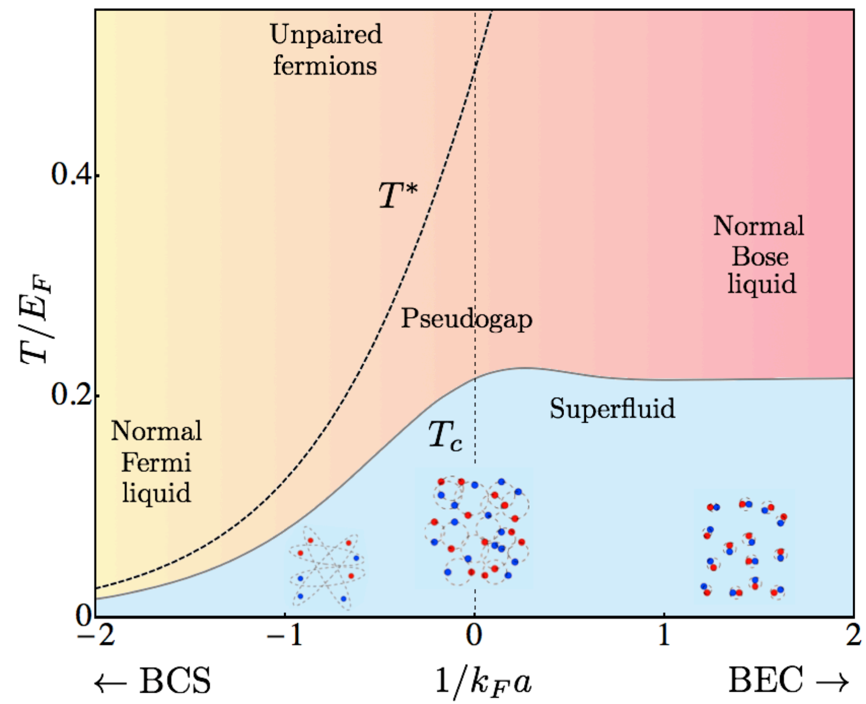
- Introduction
- Thermodynamics of the unitary Fermi gas: experiment and theory
- Canonical-ensemble auxiliary-field Monte Carlo (AFMC) method
- The homogenous unitary Fermi gas: lattice formulation
- Signatures of superfluidity
- Is there *a pseudogap* regime in the unitary gas?
- Conclusion and outlook

Introduction

Two-component (spin up/down) fermionic atoms interacting with a short-range interaction $V_0\delta(\mathbf{r}-\mathbf{r}')$ characterized by a scattering length a.

A crossover from BCS for $(k_F a)^{-1} \sim -\infty$ to BEC for $(k_F a)^{-1} \sim +\infty$

Of particular interest is the unitary Fermi gas (UFG) describing the limit of strongest interaction $a \to \infty$ or $(k_F a)^{-1} = 0$



Randeria and Taylor (2014)

Many interesting properties: universality, scale invariance,…

- A challenging non-perturbative many-body problem

A variety of theoretical methods have been used to study the thermodynamics of the UFG:

Strong-coupling theories:

Early theories: Leggett (1980), Nozieres and Schmidt-Rink (1985)

T-matrix approaches

Self-consistent Luttinger-Ward theory

Quantum Monte Carlo methods:

Diagrammatic Monte Carlo

Auxiliary-field Monte Carlo (AFMC)

Diffusion Monte Carlo (at T=0)

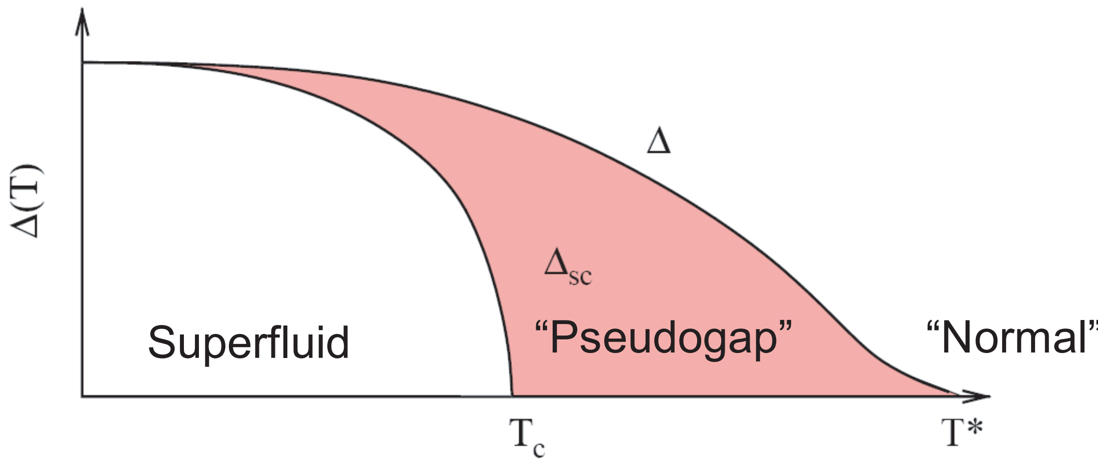
We use finite-temperature AFMC methods in the canonical ensemble of fixed particle numbers.

Thermodynamics of the UFG

- Superfluid phase transition below a critical temperature T_c.

  However, its nature remains incompletely understood.

- A pseudogap regime above T_c and below T^* was proposed in the UFG, in which pairing correlations exist even though the condensate vanishes.



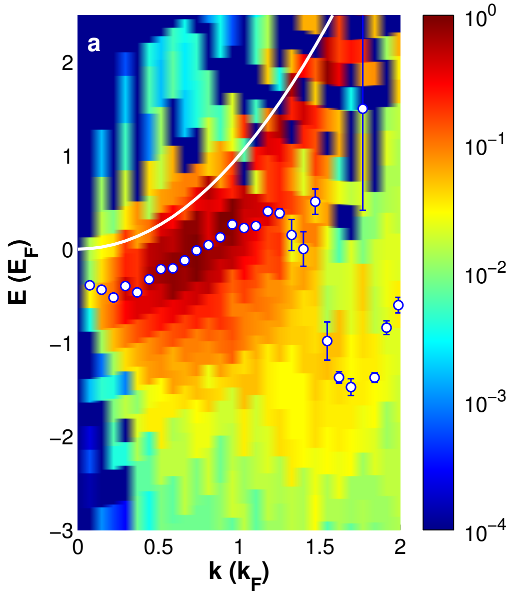
A pseudogap regime is known from high-T_c superconductors

The psedogap regime and its extent in the UFG is debated both theoretically and experimentally.

Recent review: S. Jensen, C.N. Gilbreth and Y. Alhassid, arXiv:1807.03913

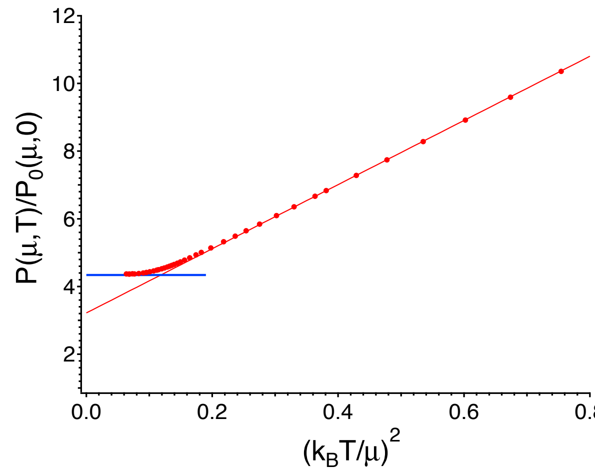
Experiment

Pseudogap regime above T_c



Sagi et al, Boulder (PRL 2015):
Backbending above T_c in photoemission spectroscopy

Fermi liquid behavior above T_c

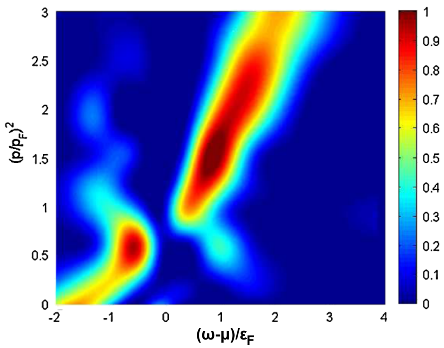


Ku et al, MIT (Science 2012):
Equation of state is well described by Fermi liquid theory

Nascimbene et al, Paris (PRL 2011):
Spin response compatible with Fermi liquid behavior

Theory

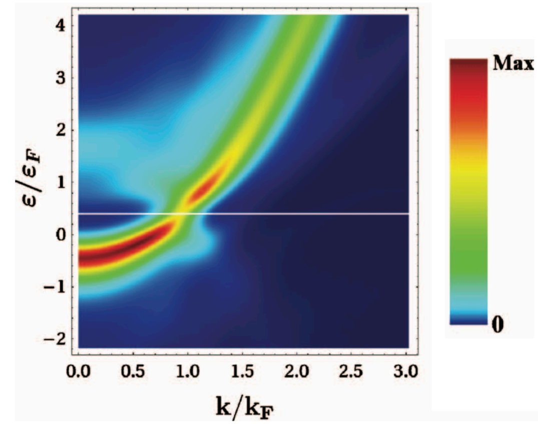
Pseudogap regime above T_c



Magieriski et al (PRL 2009):
Non-zero gap above T_c
(quantum Monte Carlo)

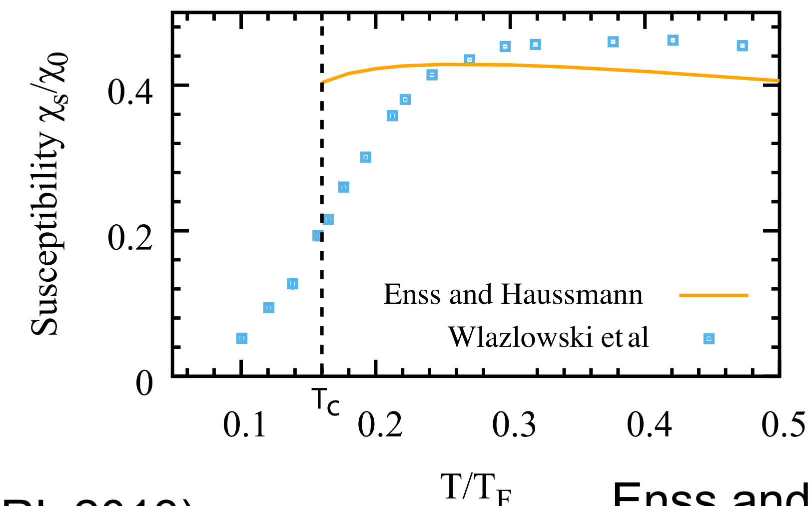
Spectral weight

Fermi liquid behavior above T_c



Haussmann et al (PRA 2009):
No pronounced pseudogap

Spin susceptibility



Wlazłowski et al (PRL 2013):
suppression of spin susceptibility above T_c
(quantum Monte Carlo)

Enss and Haussmann (PRL 2012):
No suppression of spin susceptibility
(Luttinger-Ward theory)

Finite-temperature auxiliary-field Monte Carlo (AFMC) method

AFMC is based on the Hubbard-Stratonovich transformation, which describes the Gibbs ensemble $e^{-\beta H}$ at inverse temperature $\beta = 1/T$ as a path integral over time-dependent auxiliary fields $\sigma(\tau)$

$$e^{-\beta H} = \int D[\sigma]\, G_\sigma U_\sigma$$

G_σ is a Gaussian weight and U_σ is a propagator of *non-interacting* particles moving in external auxiliary fields $\sigma(\tau)$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\,(\hat{O} e^{-\beta \hat{H}})}{\mathrm{Tr}\,(e^{-\beta \hat{H}})} = \frac{\int \mathcal{D}[\sigma] G_\sigma \langle \hat{O} \rangle_\sigma \mathrm{Tr}\,\hat{U}_\sigma}{\int \mathcal{D}[\sigma] G_\sigma \mathrm{Tr}\,\hat{U}_\sigma} \quad \text{where} \quad \langle \hat{O} \rangle_\sigma \equiv \mathrm{Tr}\,(\hat{O}\hat{U}_\sigma)/\mathrm{Tr}\,\hat{U}_\sigma$$

Grand-canonical quantities in the integrands can be expressed in terms of the *single-particle* representation matrix $\mathbf{U}_\sigma$ of the propagator :

$$Tr\, U_\sigma = \det(1 + \mathbf{U}_\sigma)$$

The high-dimensional integration over σ is evaluated by importance sampling.

Canonical-ensemble AFMC

We use exact particle-number projection in the HS transformation

Grand-canonical traces are replaced by canonical traces $Tr \to Tr_N$

For a finite number M of single-particle states, this can be done by an exact discrete Fourier transform

$$Tr_N U_\sigma = \frac{e^{-\beta\mu N}}{M} \sum_{m=1}^{M} e^{-i\varphi_m N} \det(1 + e^{i\varphi_m} e^{\beta\mu} \mathbf{U}_\sigma) \quad \text{where} \quad \varphi_m = 2\pi m / M$$

- The integrand in the HS transformation reduces to matrix algebra in the single-particle space (of typical dimension ~ 100 - 1000).

- $O(M^4)$ scaling reduced to $O(M^3)$

[C.N. Gilbreth and Y. Alhassid, Comp. Phys. Comm. (2015)]

Recent review of AFMC: Y. Alhassid, in *Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling,* ed. K.D. Launey (World Scientific 2017)

Homogenous Fermi gas: a lattice approach

S. Jensen, C.N. Gilbreth, and Y. Alhassid, arXiv:1801.06163

We use a discrete spatial lattice with spacing δx and linear size $L = N_x \delta x$

The lattice Hamiltonian for a contact interaction has the form

$$H = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{V_0}{2(\delta x)^3} \sum_{\mathbf{x}_i \sigma} \psi^\dagger_{\mathbf{x}_i \sigma} \psi^\dagger_{\mathbf{x}_i \sigma'} \psi_{\mathbf{x}_i \sigma'} \psi_{\mathbf{x}_i \sigma}$$

where $\mathbf{k},\sigma$ is a single-particle state with momentum $\mathbf{k}$ and spin σ and $\psi^\dagger_{\mathbf{x}_i \sigma}$ is a creation operator at site $\mathbf{x}_i$ and spin σ.

- Our single-particle model space is the complete first Brillouin zone B in $\mathbf{k}$

- a cube with side $k_c = \pi / \delta x$

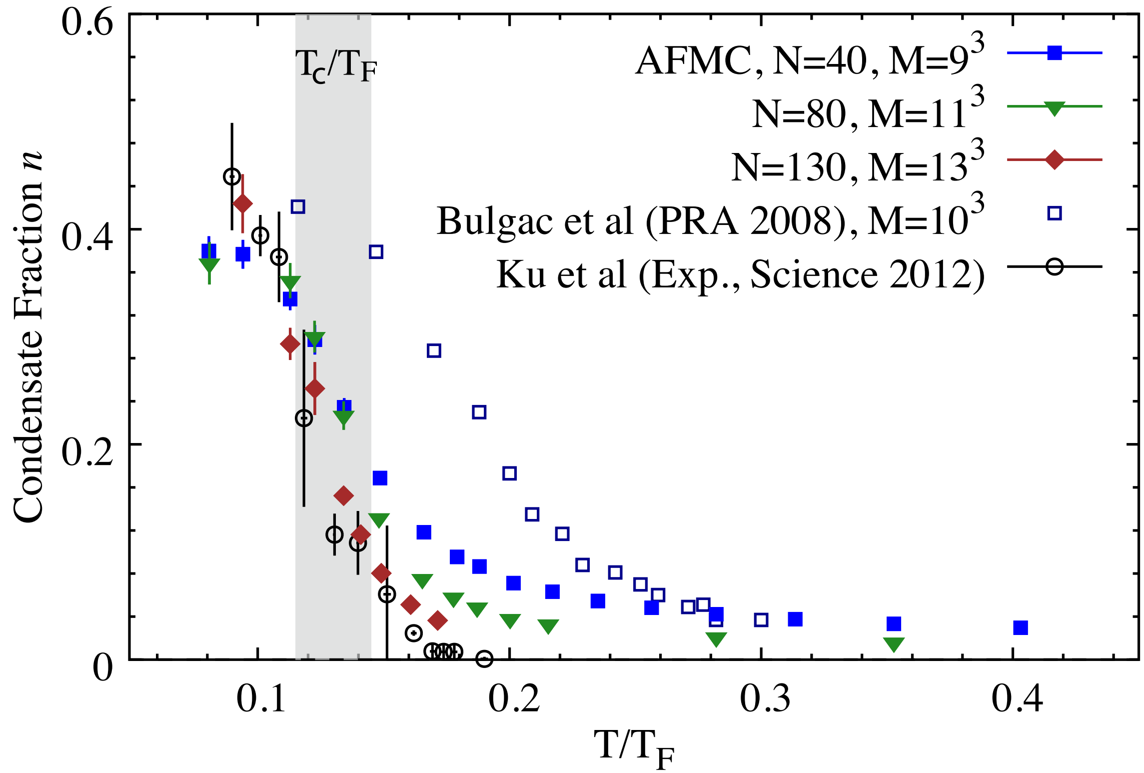
The interaction is normalized to reproduce the two-particle scattering length a on the lattice:

$$\frac{1}{V_0} = \frac{m}{4\pi\hbar^2 a} - \frac{m K_3}{4\pi\hbar^2 \delta x}$$ where (for a cube in $\mathbf{k}$) $K_3 = 2.4427\ldots$ (Werner, Castin, 2012)

Thermodynamic observables

We carried out AFMC calculation for N=20, 40, 80 and 130 atoms on lattices of size $M = 7^3, 9^3, 11^3$ and 13^3, respectively, so the filling factor $\nu = N/M$ remains constant at ~ 0.06.

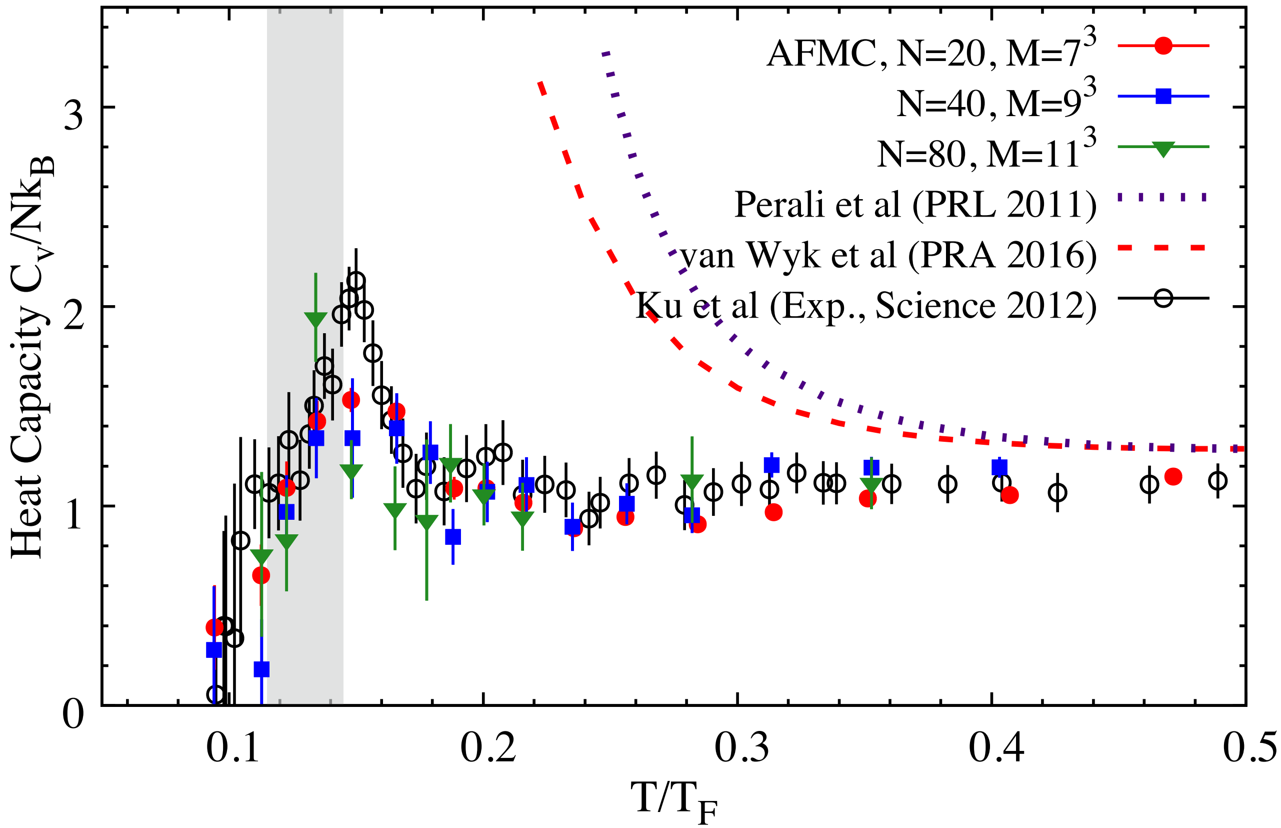
(i) Condensate fraction n



Calculated from the largest eigenvalue $\lambda_{\max}$ of the pair correlation matrix $\langle a^\dagger_{\mathbf{k}_1\sigma_1} a^\dagger_{\mathbf{k}_2\sigma_2} a_{\mathbf{k}_4\sigma_4} a_{\mathbf{k}_3\sigma_3} \rangle$ using $n = \lambda_{\max}/(N/2)$

We used finite-size scaling to estimate a critical temperature of $T_c = 0.130(15)\, T_F$ at a filling factor of $\nu \approx 0.06$

(i) Heat capacity



Numerical differentiation *inside* the path integral using the same fields at T and $T+dT$, and taking into account *correlated* errors: reduces the statistical errors by an order of magnitude [Liu and Alhassid, PRL **87**, 022501 (2001)]

First *ab initio* calculation of the heat capacity in AFMC in good agreement with the MIT experiment (lambda point).

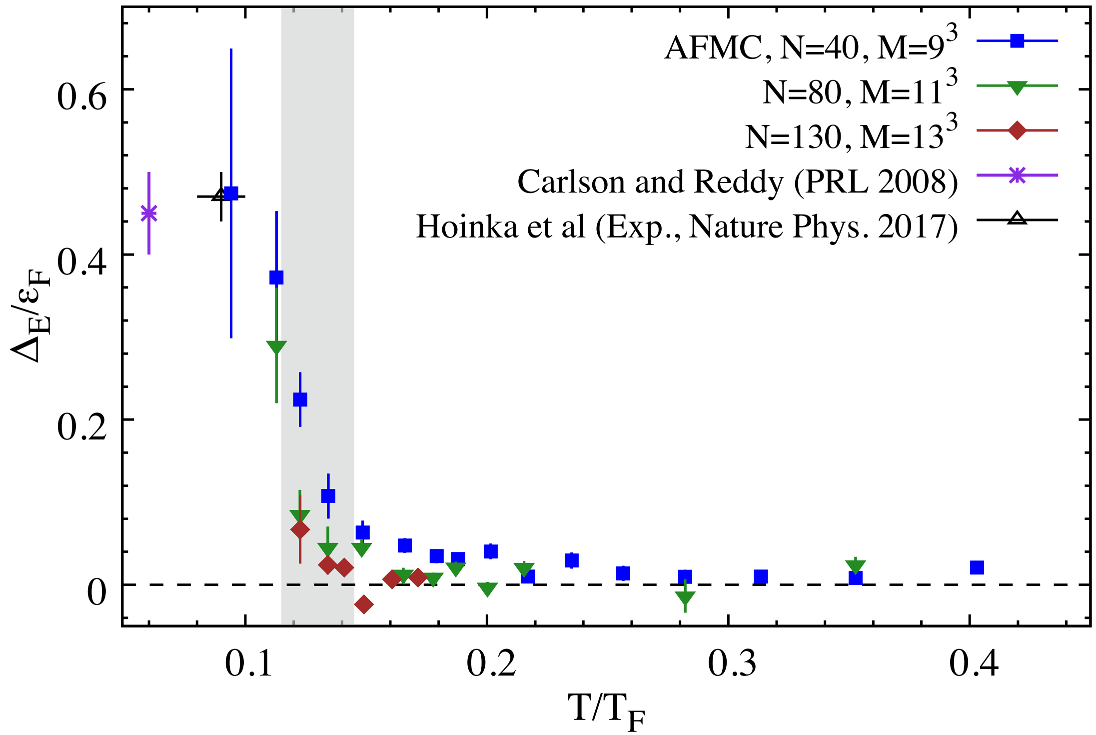
(iii) Model-independent pairing gap

We define the energy-staggering pairing gap by

$$\Delta_E = [2E(N_\uparrow, N_\downarrow - 1) - E(N_\uparrow, N_\downarrow) - E(N_\uparrow - 1, N_\downarrow - 1)]/2$$

where $E(N_\uparrow, N_\downarrow)$ is the energy for $N_\uparrow$ spin-up and $N_\downarrow$ spin-down atoms.

First calculation of the energy-staggering pairing gap for the UFG at finite temperature

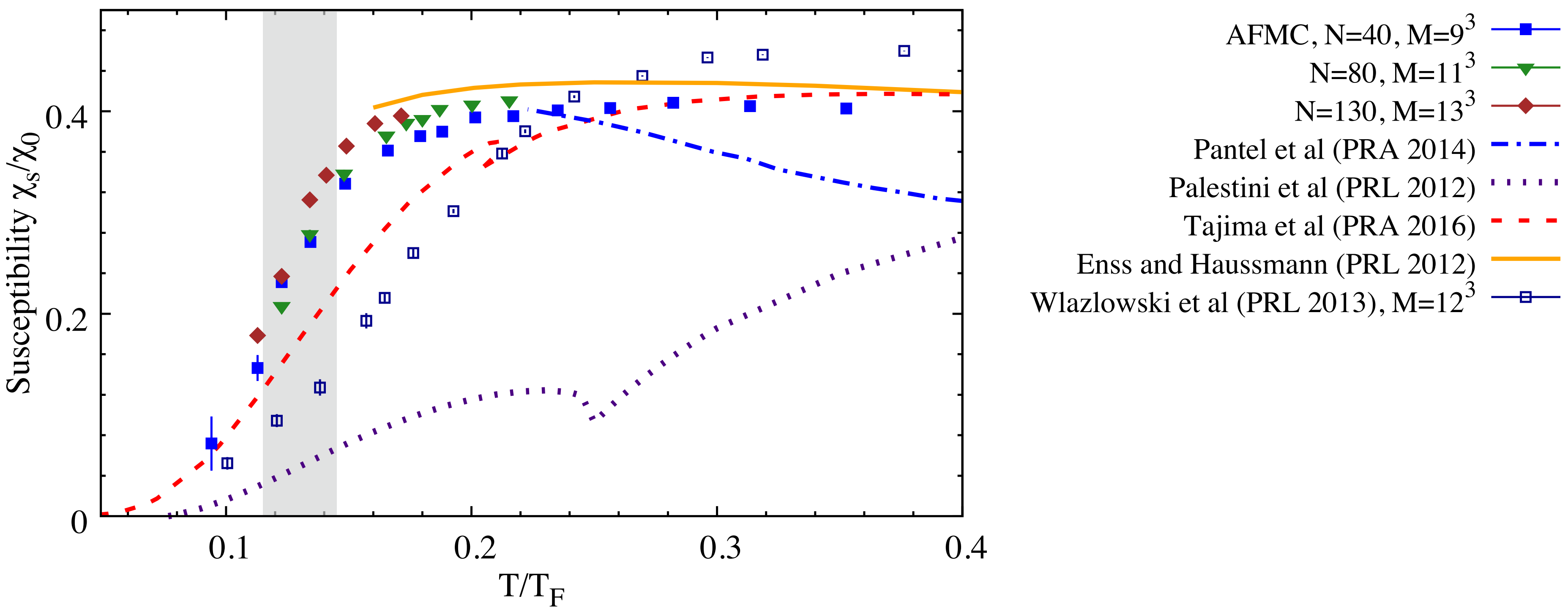


- Requires the canonical ensemble of fixed particle numbers and uses a reprojection method [Alhassid, Liu and Nakada, PRL **83**, 4265 (1999)]

(iv) Static spin susceptibility

$$\chi_s = \frac{2\beta}{V}\langle (N_\uparrow - N_\downarrow)^2 \rangle$$

Spin-flip excitations require the breaking of pairs
⇒ pairing correlations suppress the spin susceptibility

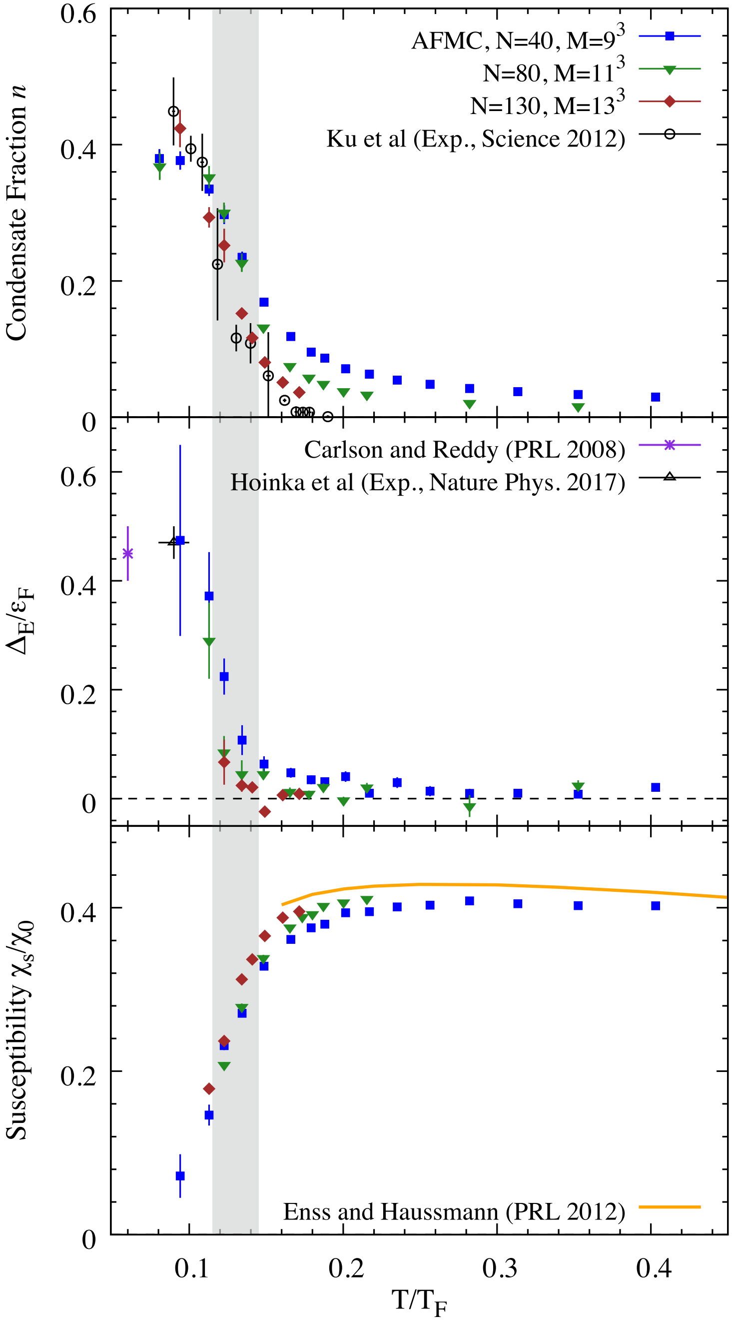


Is there a pseudogap regime in the UFG?

- Pairing gap vanishes above T_c
- Moderate suppression of the spin susceptibility above T_c

$\Longrightarrow \quad T^* \leq 0.16\, T_F$ for $\nu \approx 0.06$

No clear evidence of pseudogap effects



Two-particle scattering on the lattice

[Werner and Castin (PRA 2012)]

Inverse scattering amplitude (s wave) at relative momentum k

$$f_k^{-1} = -ik + k\cot\delta = -ik - \frac{1}{a} + \frac{1}{2} r_e k^2 + \ldots$$ where r_e is the effective range

On a lattice with spacing δx: $r_e \approx 0.337\,\delta x$

The above expression for f_k^{-1} holds when the complete first Brillouin zone in momentum space is used.

However, when a spherical cutoff of $\pi/\delta x$ is used for the single-particle momentum

$$f_k^{-1} = -ik + \frac{K}{2\pi} - \frac{1}{a} + \frac{1}{2} r_e k^2 + \ldots$$ where K is the center of mass momentum

A K-dependent shift that does not vanish in the continuum limit $\delta x \to 0$

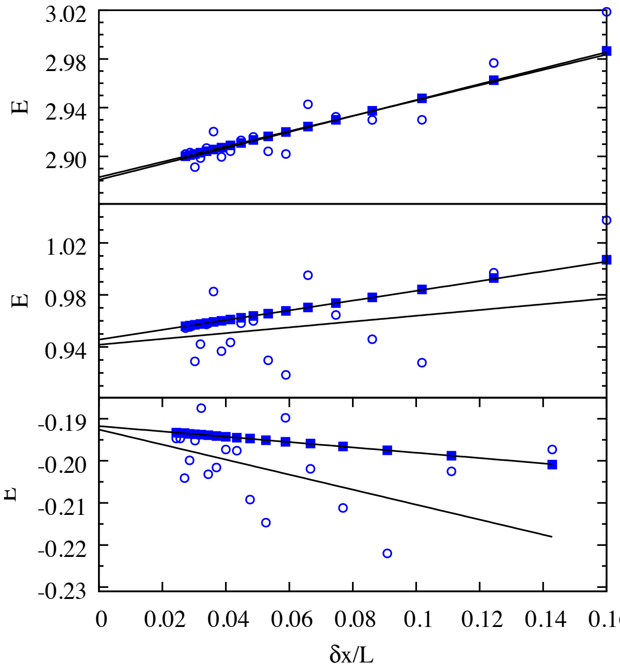
- The spherical cutoff does not reproduce the unitary limit

Numerical scattering on the lattice

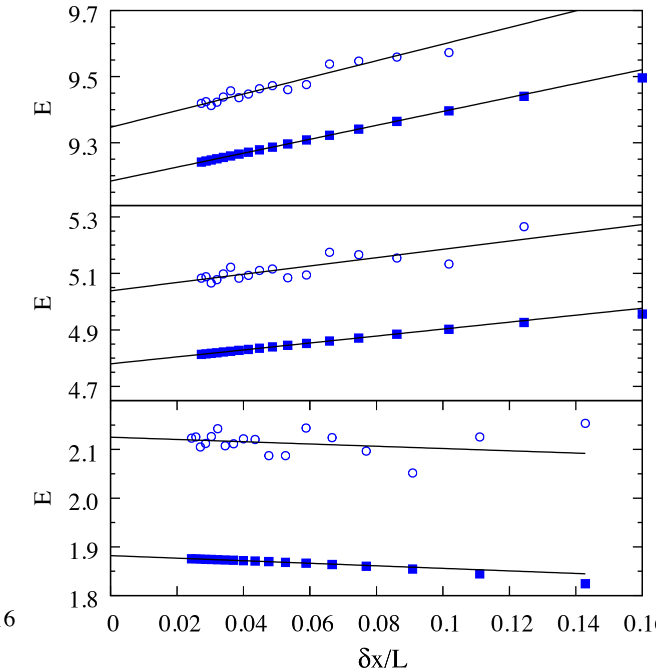
Low-lying energies of the two-particle system

no cutoff ■
spherical cutoff ○

$K = 0$

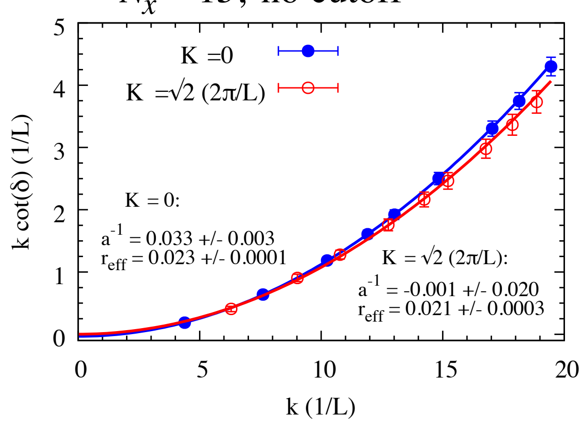


$K = \frac{2\pi}{L}(1,1,1)$



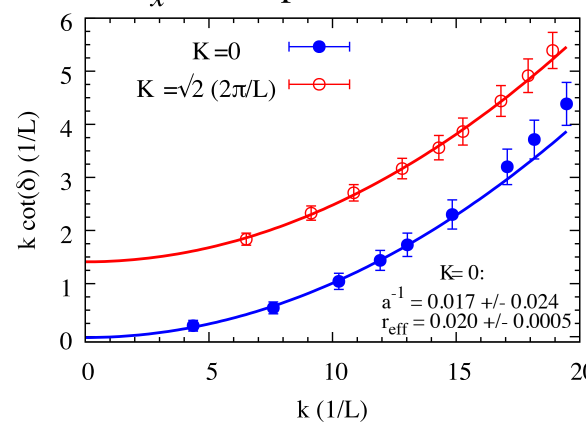
$k \cot \delta$ vs. k

$N_x = 15$, no cutoff



K independent

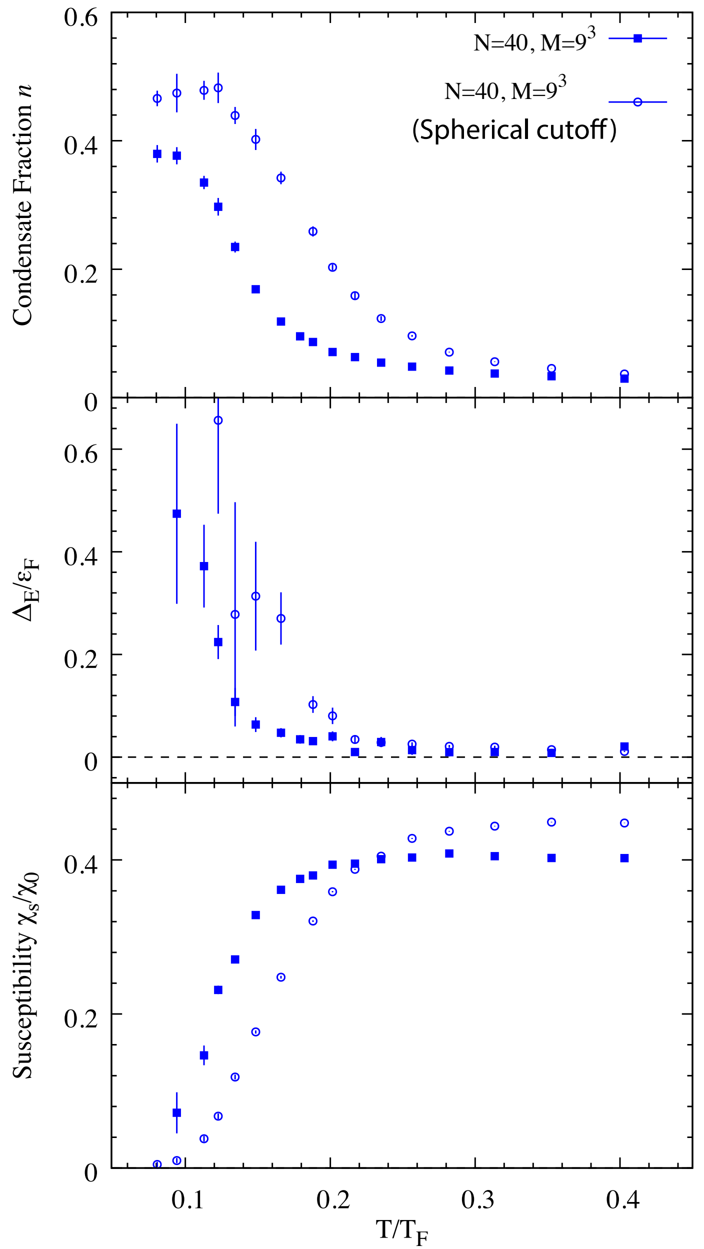
$N_x = 15$, spherical cutoff



K-dependent shift

Thermodynamic observables: no cutoff versus spherical cutoff results

Canonical-ensemble calculations for N=40 particles on $M=9^3$ lattice



Conclusion

- We carried out accurate finite-temperature AFMC calculations of the unitary Fermi gas.
- Clear signatures of the superfluid phase transition: heat capacity, condensate fraction, pairing gap, and spin susceptibility
- No clear evidence of a pseudogap regime: pairing gap vanishes and moderate suppression of the spin susceptibility above T_c
- Good agreement with experimental data for the condensate fraction, heat capacity, and low-temperature pairing gap

Outlook

- Extrapolate AFMC calculations to zero density (continuum limit) and thermodynamic limit: a major challenge
- More experiments are needed:
  (i) uniform trap
  (ii) spin susceptibility and pairing gap vs. temperature