The nature of superfluidity in the cold atomic unitary Fermi gas

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

- The *trapped* unitary Fermi gas

  Configuration-interaction (CI) shell model formulation
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- The *homogenous* unitary Fermi gas

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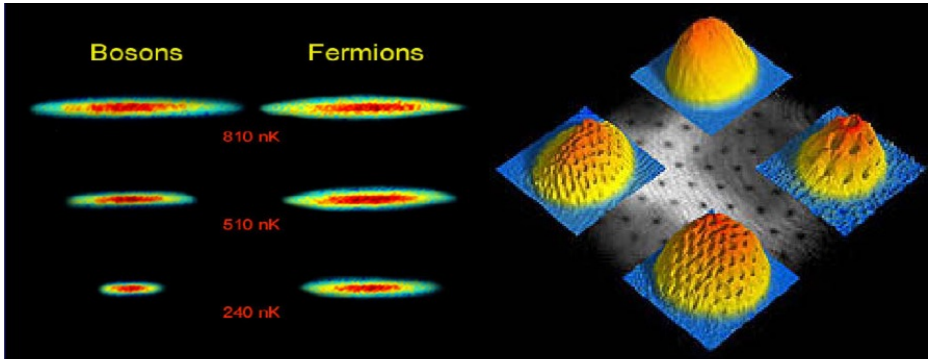
Introduction

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



Of particular interest is the unitary limit of strongest interaction $a \to \infty$

Many interesting properties: universality, scale invariance,…

- A challenging non-perturbative many-body problem

A variety of quantum Monte Carlo methods have been used: auxiliary field, diagrammatic, diffusion, Green's functions, variational, …

We have used auxiliary-field Monte Carlo methods to study two systems at unitarity:

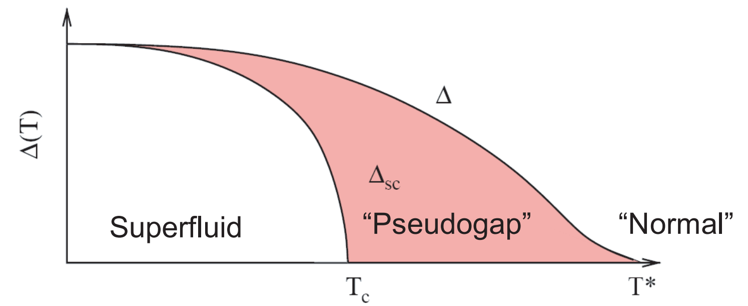
(i) Trapped gas in a spherical harmonic trap
(ii) Homogenous gas in a box

Thermodynamics at unitarity

- Superfluid phase transition below a critical temperature T_c.

  However, its nature remains incompletely understood.

- A pseudogap phase above T_c was proposed in the unitary gas, but is still debated both theoretically and experimentally.



Pseudogap phase or non-Fermi liquid above T_c

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

Gaebler et al, Nature Phys 2010
RF spectroscopy experiments

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

Fermi liquid behavior above T_c

Nascimbene et al, PRL 2011
Spin response compatible with Fermi Liquid behavior

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

Review: E.J. Mueller, arXiv:1701.04838 (2017)

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

The AFMC method enables calculations in spaces that are many orders of magnitude larger than those that can be treated by conventional methods.

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 $\sigma(\tau)$

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

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

- Exact up to statistical errors

Recent review of AFMC: Y. Alhassid, arXiv:1607.01870, chapter in a book (2017)

Thermal expectation values of observables

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

where $\langle \hat{O} \rangle_\sigma \equiv \mathrm{Tr}\,(\hat{O}\hat{U}_\sigma)/\mathrm{Tr}\,\hat{U}_\sigma$

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

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

Canonical quantities are calculated by an exact particle-number projection

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

- The high-dimensional integration over σ is evaluated by Monte Carlo methods.

The trapped Fermi gas: a configuration-interaction (CI) approach

C.N. Gilbreth and Y. Alhassid, Phys. Rev. A **88**, 063643 (2013)

We use as a single-particle basis the eigenstates $n\,l\,m$ of the harmonic trap and construct Slater determinants for the many-particle basis.

Single-particle basis is truncated to $N_{\max}$ harmonic oscillator shells.

The contact interaction $V_0\delta(\mathbf{r}-\mathbf{r}')$ is non-vanishing only in the s-wave channel

- Renormalization: V_0 is determined by for each $N_{\max}$ to reproduce the exact ground-state energy of the two-particle system ($2\hbar\omega$ in the unitary limit).

- The attractive contact interaction has a good Monte Carlo sign for $N_\uparrow = N_\downarrow$

  $\Rightarrow$ accurate calculations

Thermodynamic observables of the trapped gas

(i) Model-independent pairing gap

We define the energy-staggering pairing gap by

$$\Delta_{gap} = [2E(N,N-1) - E(N,N) - E(N-1,N-1)]/2$$

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

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

(ii) 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)]

(iii) Condensate fraction

Pair correlation matrix for good angular momentum L

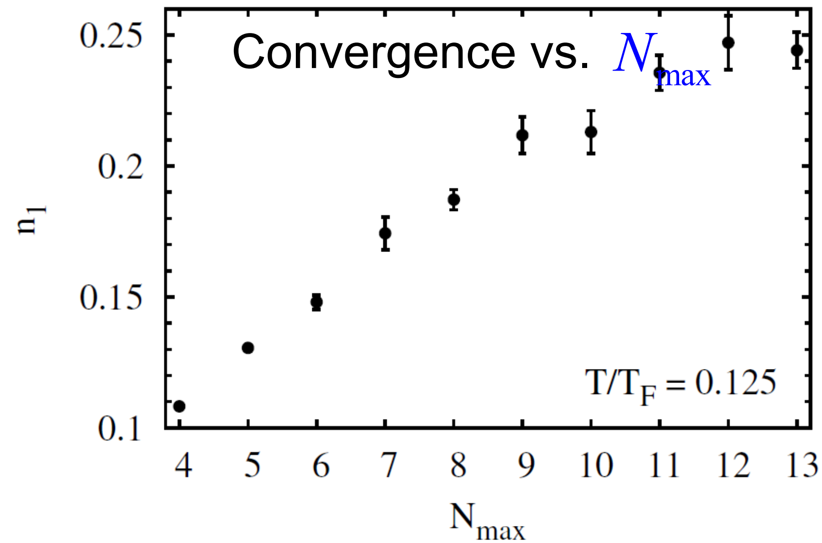
$$C_L(ab,cd) = < A^{\dagger}_{LM\uparrow\downarrow}(ab) A_{LM\uparrow\downarrow}(cd) >$$

$A^{\dagger}_{LM\uparrow\downarrow}(ab)$ is a pair creation operator of particles in orbitals a and b

Maximal eigenvalue occurs for $L=0$ and defines the condensate $B^{\dagger}$

For interacting fermions: $0 \le \langle B^{\dagger} B \rangle \le N/2$

$\Rightarrow$ Condensate fraction: $n = \langle B^{\dagger} B \rangle / (N/2)$



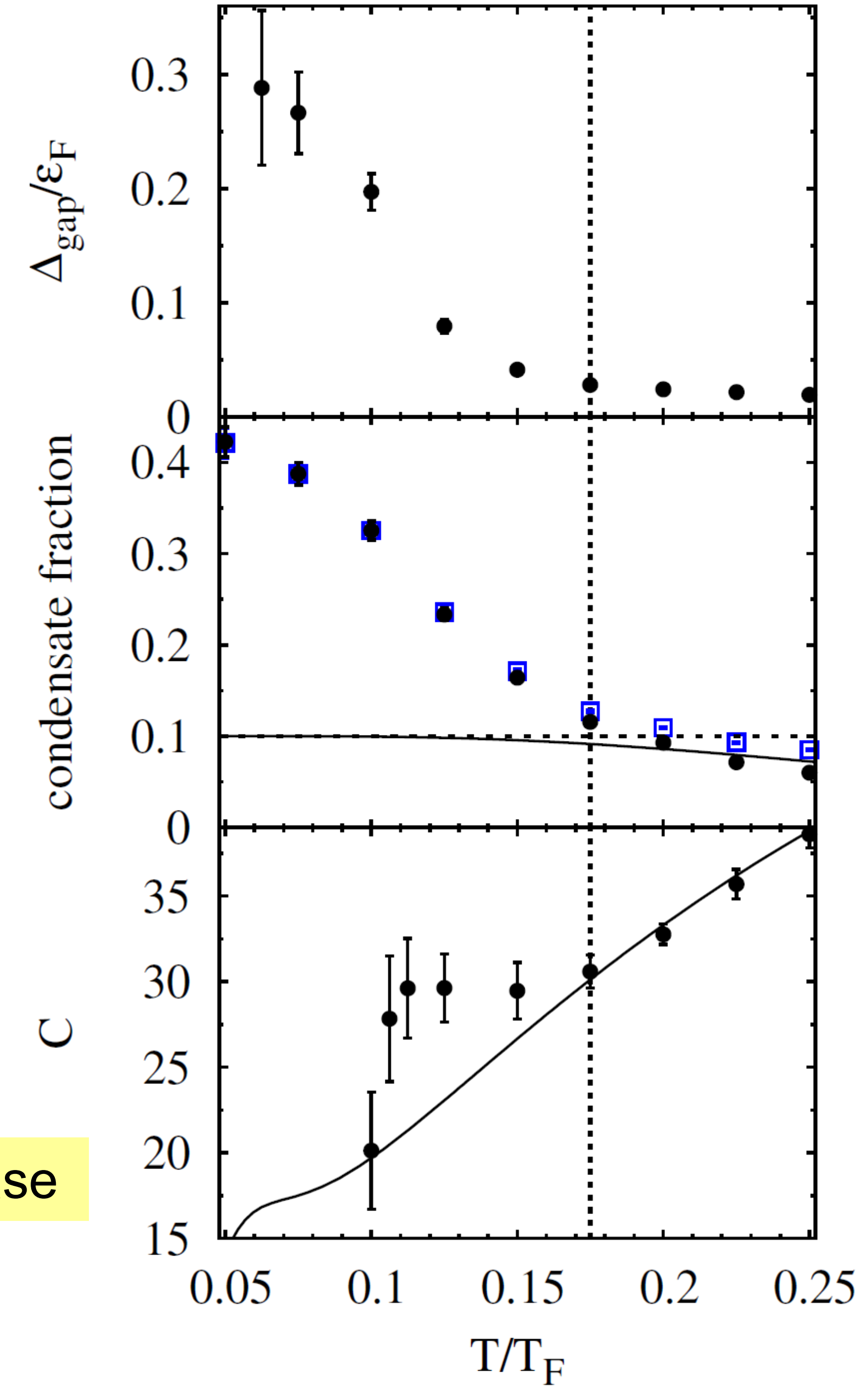
Equivalent to theory of off-diagonal long-range order (C.N. Yang, RMP 1962)

N = 20 atoms in the spin-balanced unitary gas

- Clear signatures of the superfluid phase transition

• However, the gap does not appear to lead the condensate fraction as the temperature decreases.

⇒ No clear signature of a pseudogap phase



Homogenous Fermi gas: a lattice approach

S. Jensen, C.N. Gilbreth, and Y. Alhassid

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:

$$\frac{1}{V_0} = \frac{m}{4\pi\hbar^2 a} - \frac{mK_3}{4\pi\hbar^2 \delta x}$$ where (for a cube in $\mathbf{k}$) $K_3 = 2.4427$... (Werner, Castin, 2012)

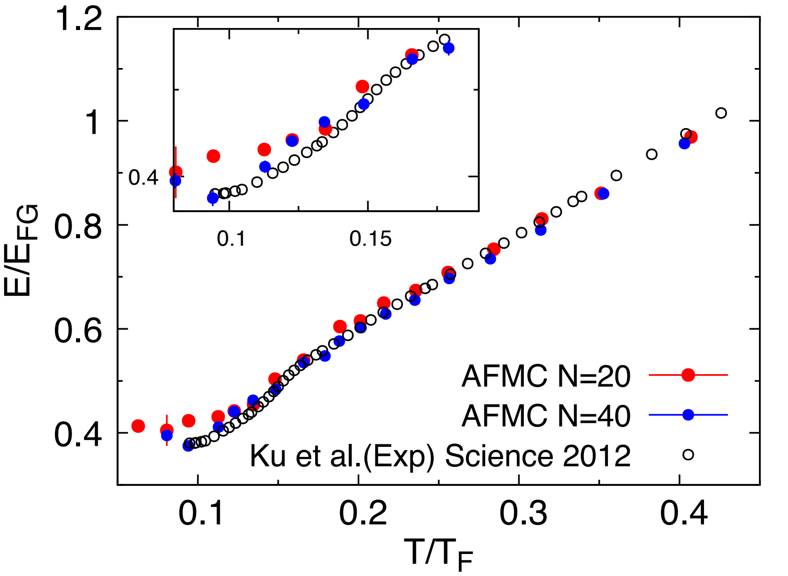
For a *spherical cutoff* with $k_c = \pi / \delta x$, we have $K_3 = 2$

Thermodynamic observables of the homogenous gas

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

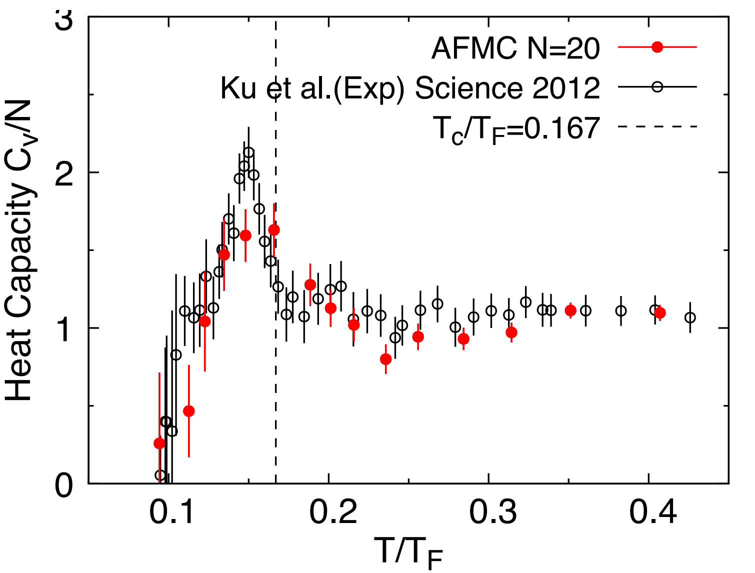
(i) Energy

The thermal energy for $N=40\,(N_x=9)$ is in good agreement with the MIT experiment



(ii) Heat capacity

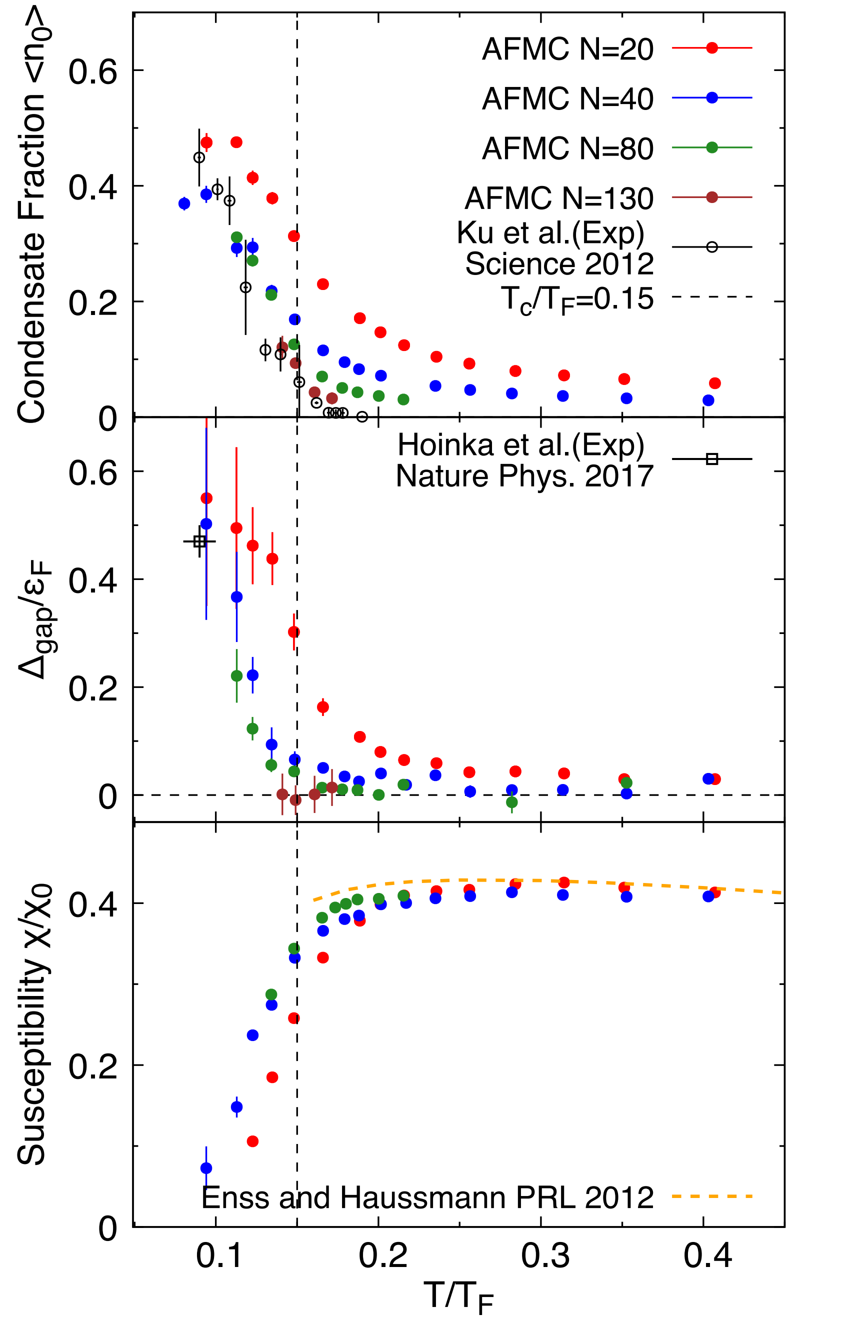
First *ab initio* calculation of the heat capacity in good agreement with the MIT experiment (lambda point).



(iii) Condensate fraction

Calculated from the largest eigenvalue of the pair correlation matrix

$$\langle a^{\dagger}_{\mathbf{k}_1\sigma_1} a^{\dagger}_{\mathbf{k}_2\sigma_2} a_{\mathbf{k}_4\sigma_4} a_{\mathbf{k}_3\sigma_3} \rangle$$



(iv) Energy-staggering pairing gap

Approaches zero at T_c as the number of particles and lattice size increase

(v) Static spin susceptibility

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

Spin-flip excitations require the breaking of pairs and leads to suppression of the spin susceptibility.

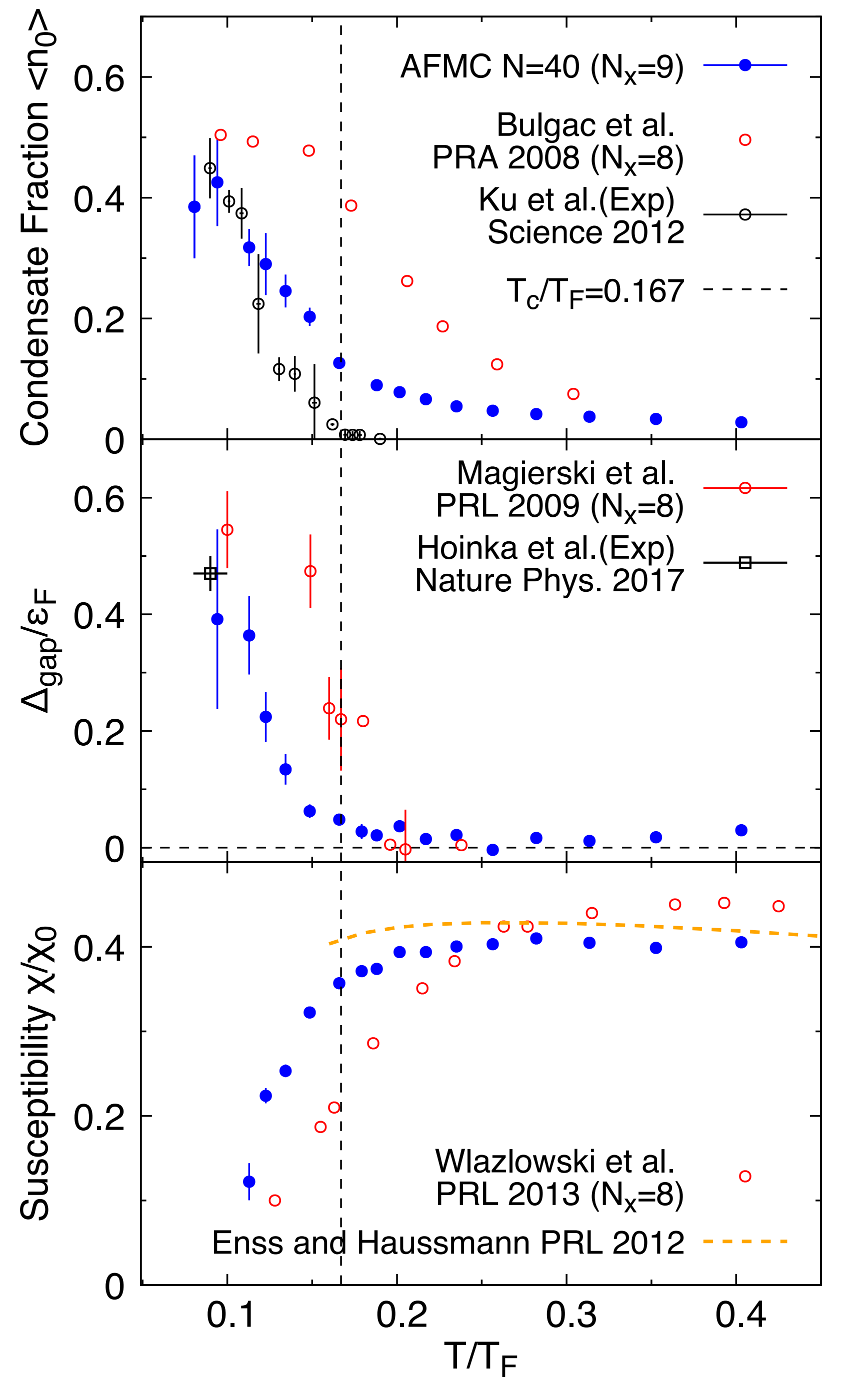
Is there a pseudogap phase at unitarity?

We have compared our AFMC results (blue solid circles, no cutoff) with Bulgac, Drut et al.(red open circles, spherical cutoff)

We observe no signature of a non-zero pairing gap above T_c.

We observe no significant suppression of the spin susceptibility above T_c.

- In contrast to the Seattle group, we do not observe clear signatures of a pseudogap phase.



Conclusion

- Auxiliary-field Monte Carlo (AFMC) methods enable accurate *ab initio* thermodynamic studies of the unitary Fermi gas.
- Clear signatures of the superfluid phase transition (heat capacity, condensate fraction, gap, and spin susceptibility).
- No clear signatures of a pseudogap phase in the unitary gas.
- Lattice AFMC studies must be carried out in the complete conjugate momentum space (no spherical truncation).
- Good agreement with experimental data for the condensate fraction, heat capacity, and low-temperature pairing gap.

Outlook

- Carry out AFMC calculations for larger lattices and particle number.
- Redo finite-size scaling (Burovski et al, PRL 2008) with no spherical cutoff.
- More experiments are needed: spin susceptibility and gap vs. temperature.