Nature of pairing correlations in the homogeneous Fermi gas at unitarity

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arXiv:1801.06163

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ECT* 2018

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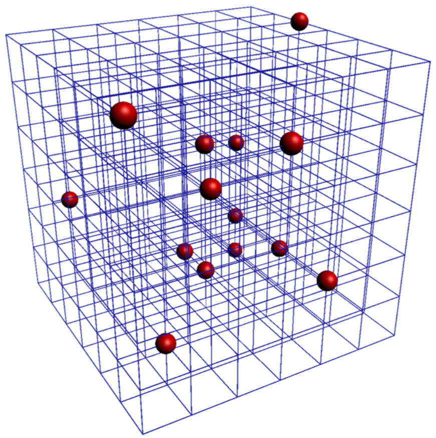
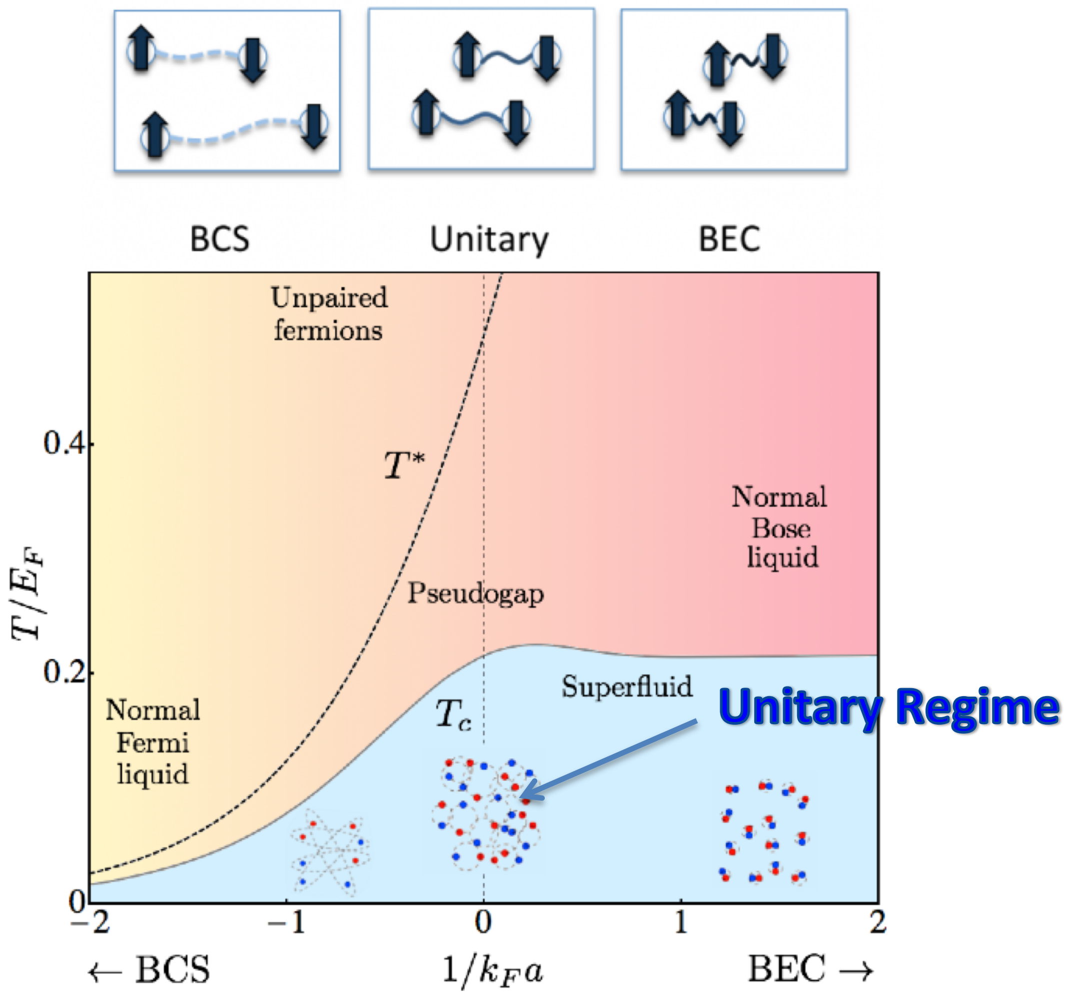
Outline

- BCS-BEC crossover and the unitary Fermi gas
- What is a pseudogap?
- Lattice Model
- Canonical ensemble AFMC method
- Pseudogap regime in the unitary Fermi gas?



Two-component homogeneous Fermi gas with contact interaction

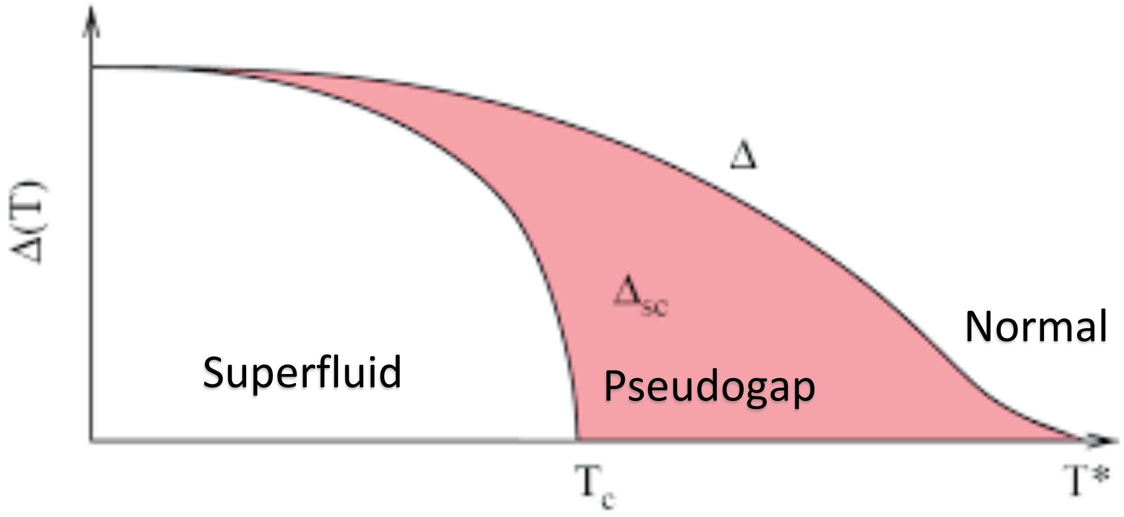
- Two-species up/down fermions (neutral cold atomic hyperfine states of ^{6}Li and ^{40}K) with contact interactions $V = V_0\delta(\mathbf{r} - \mathbf{r}')$.
- Interaction can be tuned to describe the crossover from Cooper pairing in the BCS regime to weakly interacting dimers in the BEC regime.
- Strong correlations in the unitary limit of infinite scattering length $a \to \infty$.



Randeria and Taylor (2014)

Pseudogap

- High transition temperature $T_c = 0.167(13)T_F$
(Ku et al Science 2012)

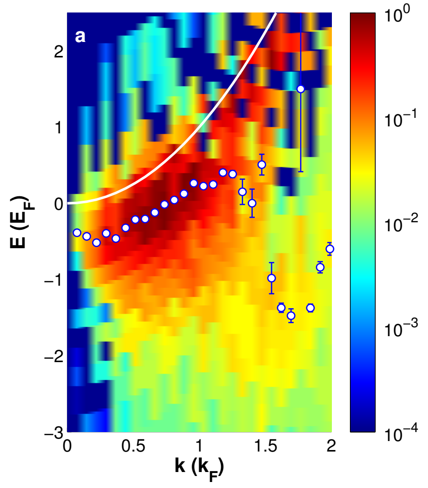


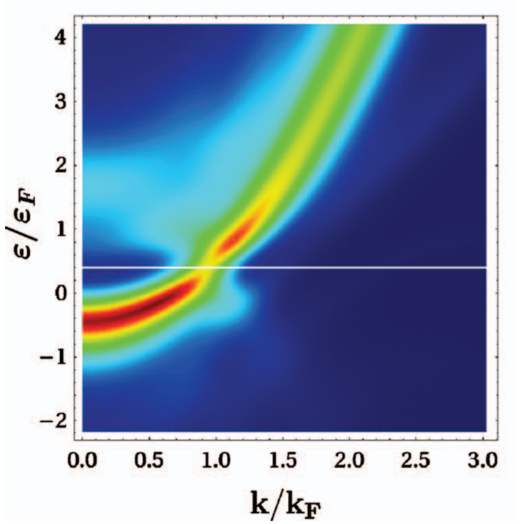
A pseudogap regime has been proposed to exist for the unitary Fermi gas, but is still debated both experimentally and theoretically.

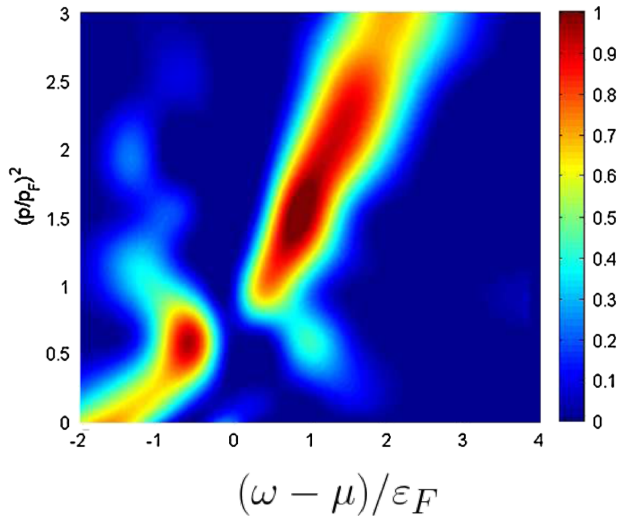
Observables for pseudogap

- Spectral function
- Density of states
- Spin susceptibility
- Heat capacity
- Pairing gap

Pseudogap spectral function







Experiment
(Sagi et al, PRL 2015):

Backbending in Photoemission spectroscopy

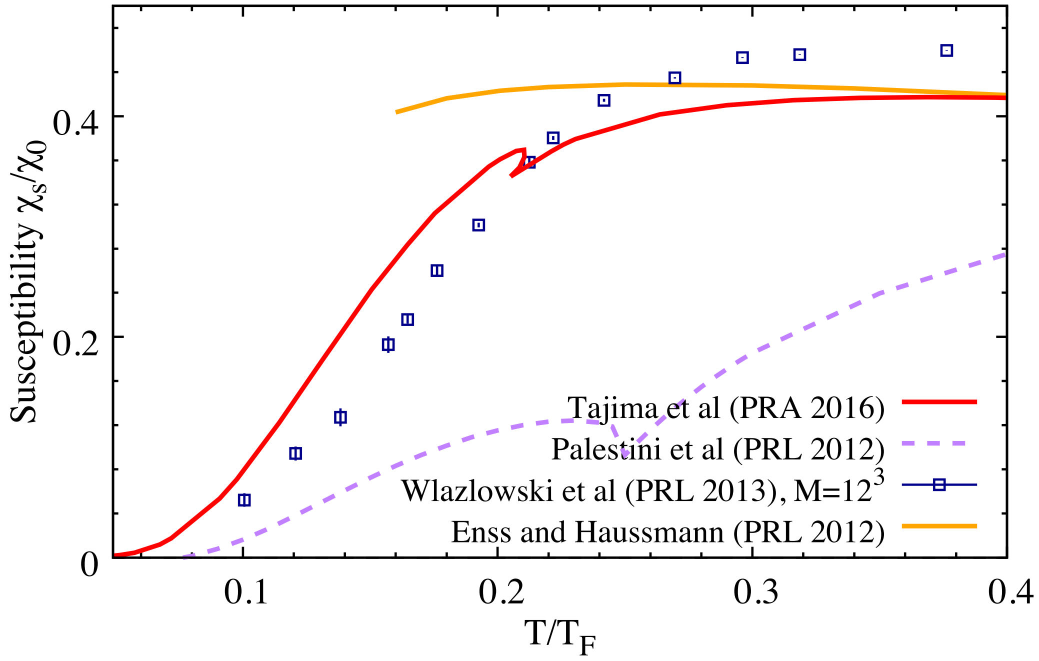
Self-consistent field theory (Haussmann et al, PRA 2009):

Only weak suppression at T_c and no pronounced pseudogap.

Quantum Monte Carlo (Magierski et al, PRL 2009):

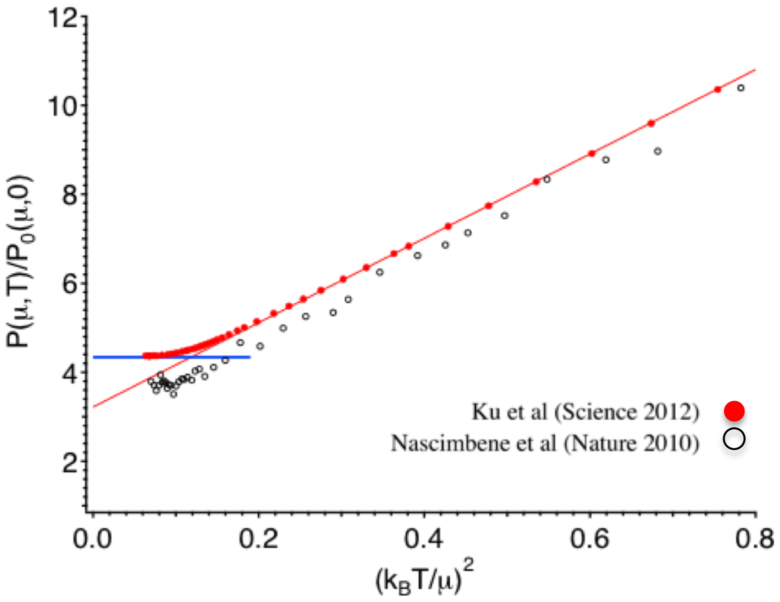
Non-zero gap above T_c

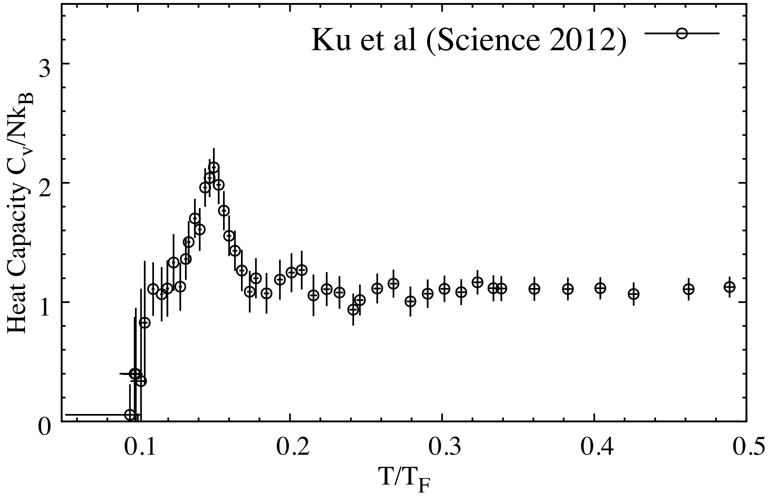
Pseudogap Thermodynamics



Suppression of spin susceptibility above Tc

Equation of state is well described by normal Fermi liquid behavior





Heat capacity displays no pronounced dip above T_c

Lattice Description

Contact interaction: $V = V_0 \delta(\mathbf{r} - \mathbf{r}')$

Lattice spacing: $\delta x = L/N_L$

Box length

Hamiltonian: $\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k},\sigma} \hat{a}_{\mathbf{k},\sigma} + \frac{V_0}{(\delta x)^3} \sum_{\mathbf{x}} \hat{n}_{\mathbf{x},\uparrow} \hat{n}_{\mathbf{x},\downarrow}$

Lattice spacing

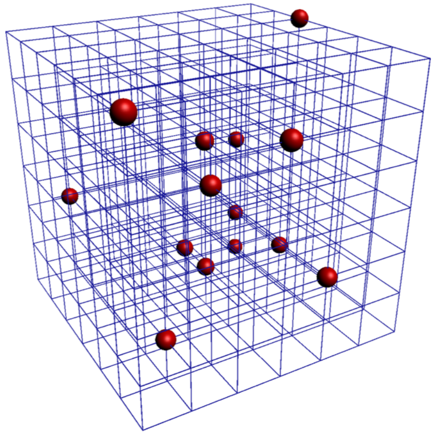
Renormalization condition: $\frac{1}{V_0} = \frac{m}{4\pi\hbar^2 a} - \int_B \frac{d^3k}{(2\pi)^3 2\epsilon_{\mathbf{k}}}$

F. Werner and Y. Castin (PRA 2012)

Scattering length

Brillouin Zone

Single-particle dispersion: $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$



Calculations performed for finite number of particles N and lattice size $M=N_L^3$ using the complete first Brillouin zone of single-particle states in momentum space (no spherical cutoff).

Auxiliary-field Monte Carlo method

- Trotter decomposition
- Hubbard-Stratonovich transformation
- Gaussian quadratures
- Metropolis algorithm

$\beta = 1/k_B T$ is the inverse temperature

One-body propagator of non-interacting particles coupled to external auxiliary fields σ

$$e^{-\beta \hat{H}} = \int \mathcal{D}[\sigma] \underbrace{G_\sigma}_{\text{Gaussian weight}} \overbrace{\hat{U}_\sigma}^{}$$

Gaussian weight

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

where $\langle \hat{O} \rangle_\sigma = \dfrac{\mathrm{Tr}(\hat{O}\hat{U}_\sigma)}{\mathrm{Tr}(\hat{U}_\sigma)}$

- Integrands can be calculated by matrix algebra in the single-particle space

$$\mathrm{Tr}(\hat{U}_\sigma) = \det[\mathrm{I} + \mathbf{U}_\sigma]$$

→ Matrix in single-particle space

Particle-Number Projection

- Two particle-number projection (on $N_\uparrow$ and $N_\downarrow$) for heat capacity, ODLRO, and pairing gap
- One particle-number projection (on total N) for spin susceptibility
- Chemical potential is a free parameter adjusted for numerical stability
- Algorithm O(M^3) allows large lattice size simulations with the canonical ensemble

$$\mathrm{Tr}_N \hat{X} = \mathrm{Tr}(\hat{P}_N \hat{X})$$

Projection Operator: $$\hat{P}_N = \frac{e^{-\beta\mu N}}{2M} \sum_{m=1}^{2M} e^{-i\varphi_m N} e^{(\beta\mu + i\varphi_m)\hat{N}}$$

$$M = N_L^3 \qquad \varphi_m = \frac{2\pi m}{2M}$$

$$\frac{1}{2M} \sum_{m=1}^{2M} e^{i\varphi_m(N-A)} = \delta_{N,A}$$

(C. Gilbreth, Y. Alhassid, Computer Physics Communications, 2015)

Projection on fixed numbers of protons and neutrons is crucial in nuclei
-- methods to optimize particle-number projection in cold atoms have been implemented in nuclear AFMC

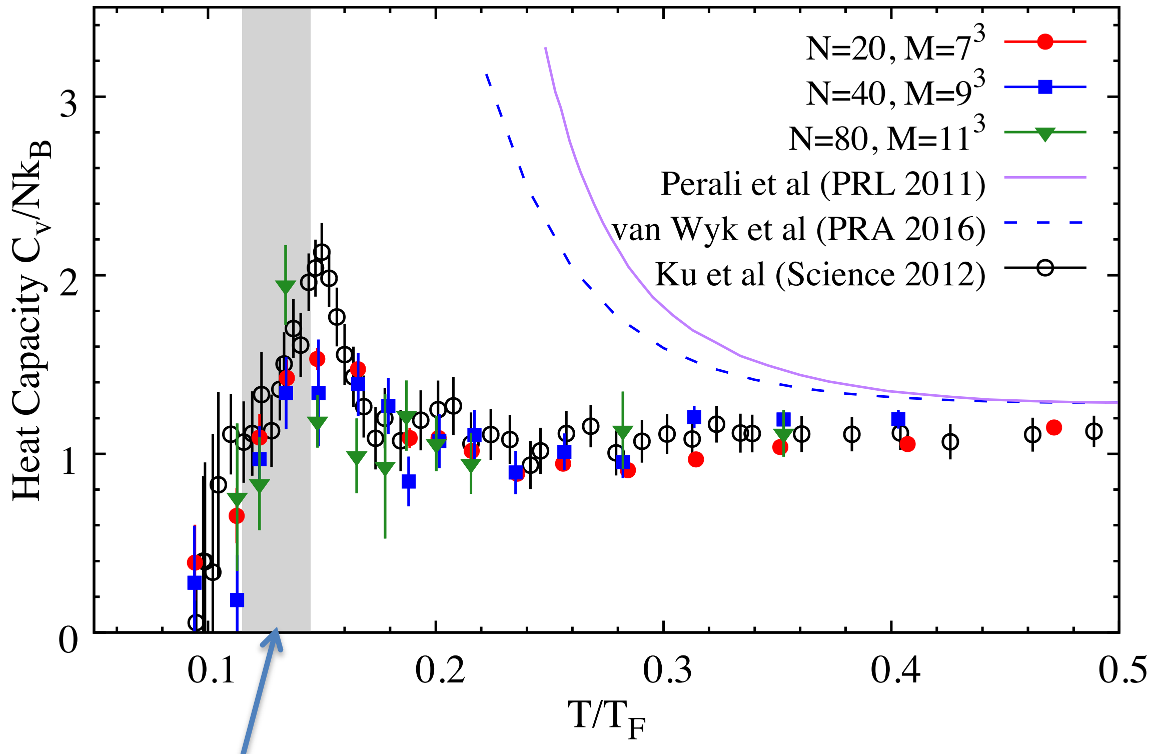
Observables: (i) Heat Capacity

- Canonical ensemble
- N=20,40,80,130 particles on lattices of size $M=7^3, 9^3, 11^3, 13^3$, respectively,

$$N/M \simeq 0.06 \ (k_F r_e \simeq 0.41)$$

Heat capacity: $$C = \frac{E(T+\triangle T) - E(T-\triangle T)}{2 \triangle T}$$

- First quantum Monte Carlo result for the heat capacity of the homogeneous unitary Fermi gas.
- Large reduction of statistical errors by taking derivative inside the HS integral using the same auxiliary fields, Liu and Alhassid (PRL 2001).



T_c from finite-size scaling of condensate fraction

(ii) Condensate Fraction

Off-Diagonal Long-Range Order

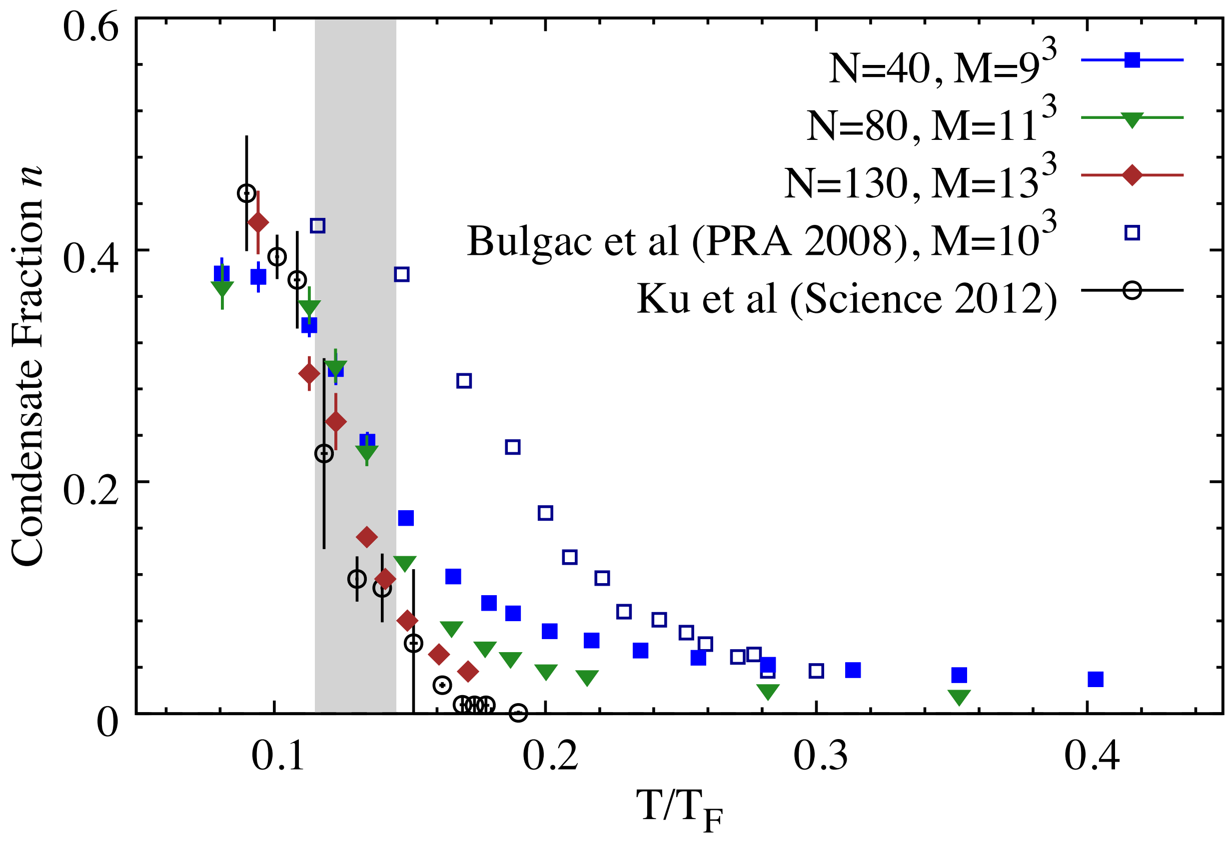
Two-body density matrix: $\langle \hat{\psi}^\dagger_{\mathbf{k_1},\uparrow} \hat{\psi}^\dagger_{\mathbf{k_2},\downarrow} \hat{\psi}_{\mathbf{k_3},\downarrow} \hat{\psi}_{\mathbf{k_4},\uparrow} \rangle$

Condensate Fraction: $n = \lambda/(N/2) \leq 1$

Max eigenvalue

Particle number

C.N. Yang, Rev. Mod. Phys. 34, 694 (1962)



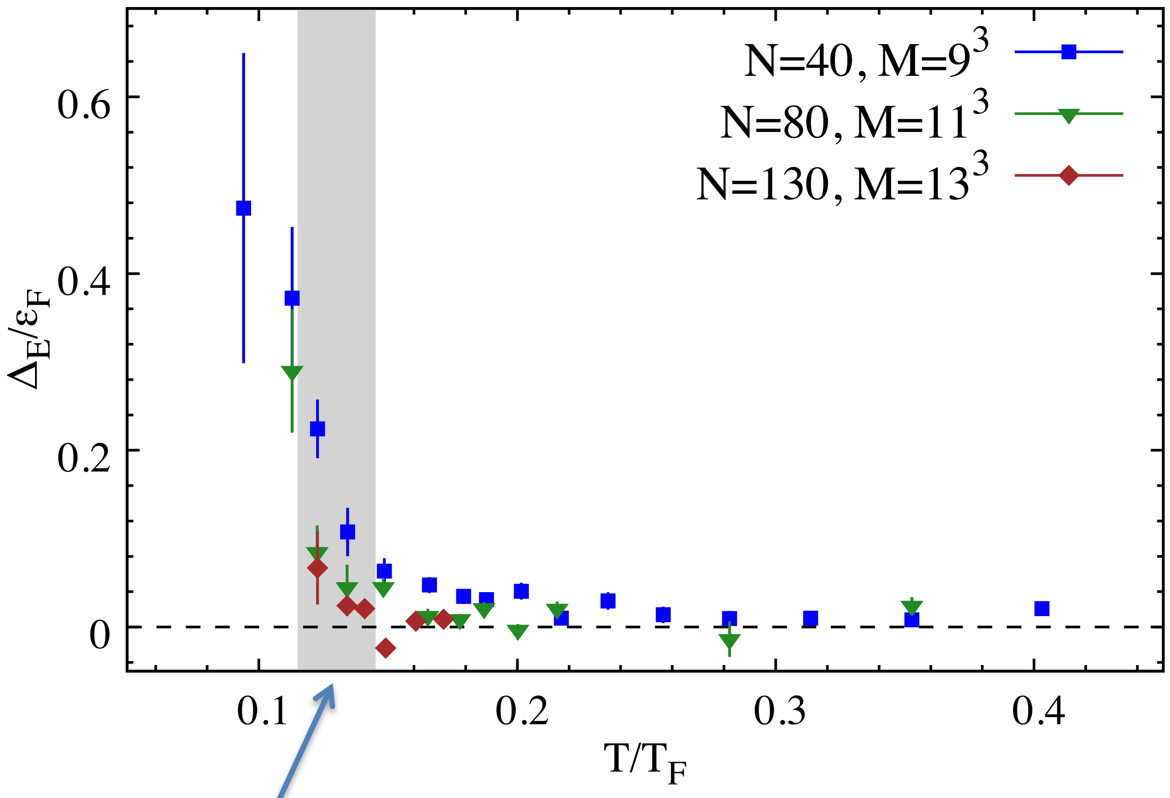
(iii) Pairing Gap

Model-independent pairing gap:
(no analytic continuation necessary!)

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

Thermal energy

Number of spin up Fermions



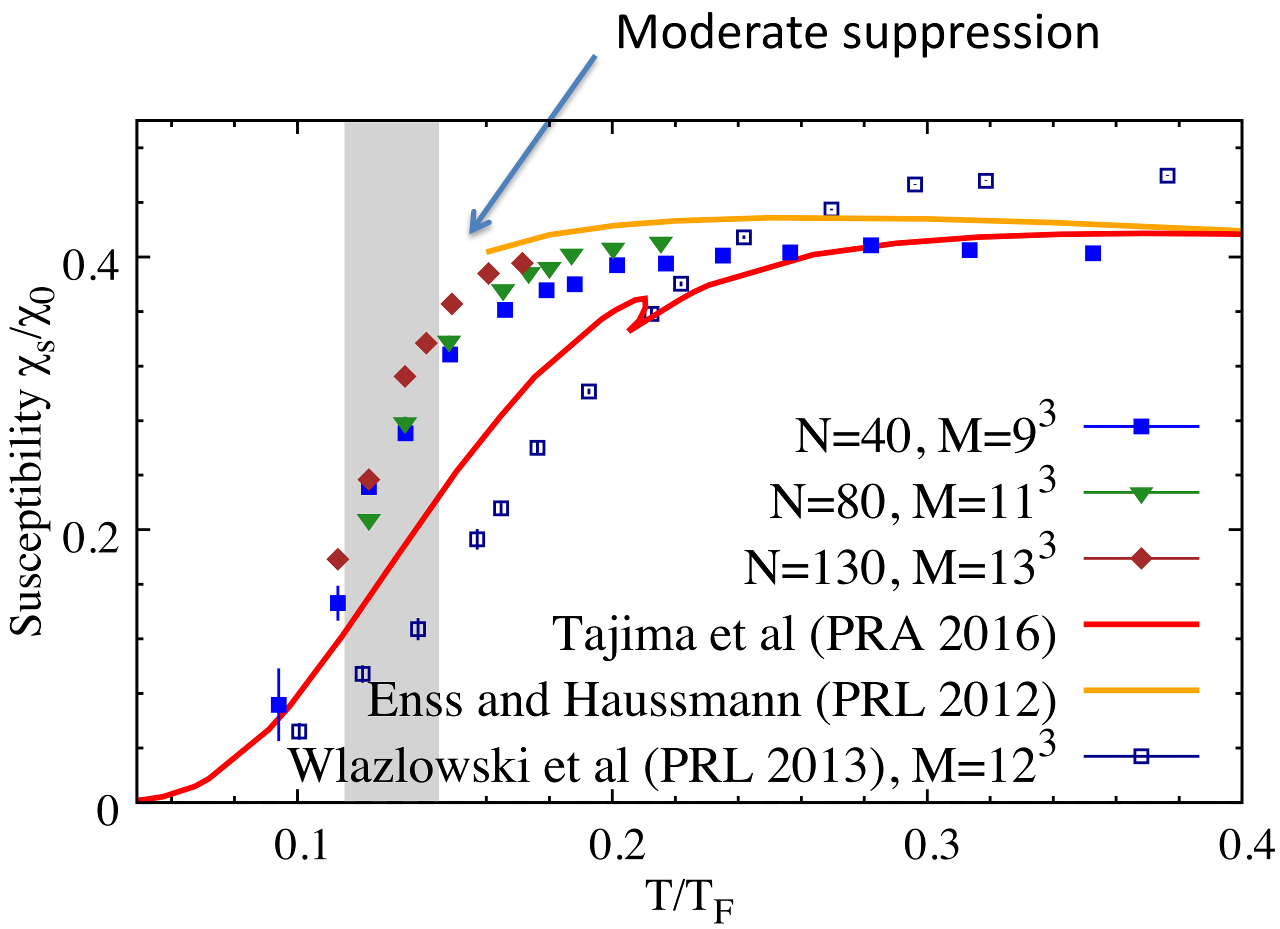
Gap vanishing above T_c

- First calculation of the energy-staggering pairing gap for the unitary Fermi gas.
- Requires the canonical ensemble.

(iv) Spin Susceptibility

Spin susceptibility: $\chi_s = \frac{\beta}{V}\langle(\hat{N}_\uparrow - \hat{N}_\downarrow)^2\rangle$

Volume



- Spin-flip excitations require s-wave pair breaking leading to suppression of the spin susceptibility.
- Spin susceptibility agrees well with Luttinger-Ward approach, Enss and Haussmann (PRL 2012).

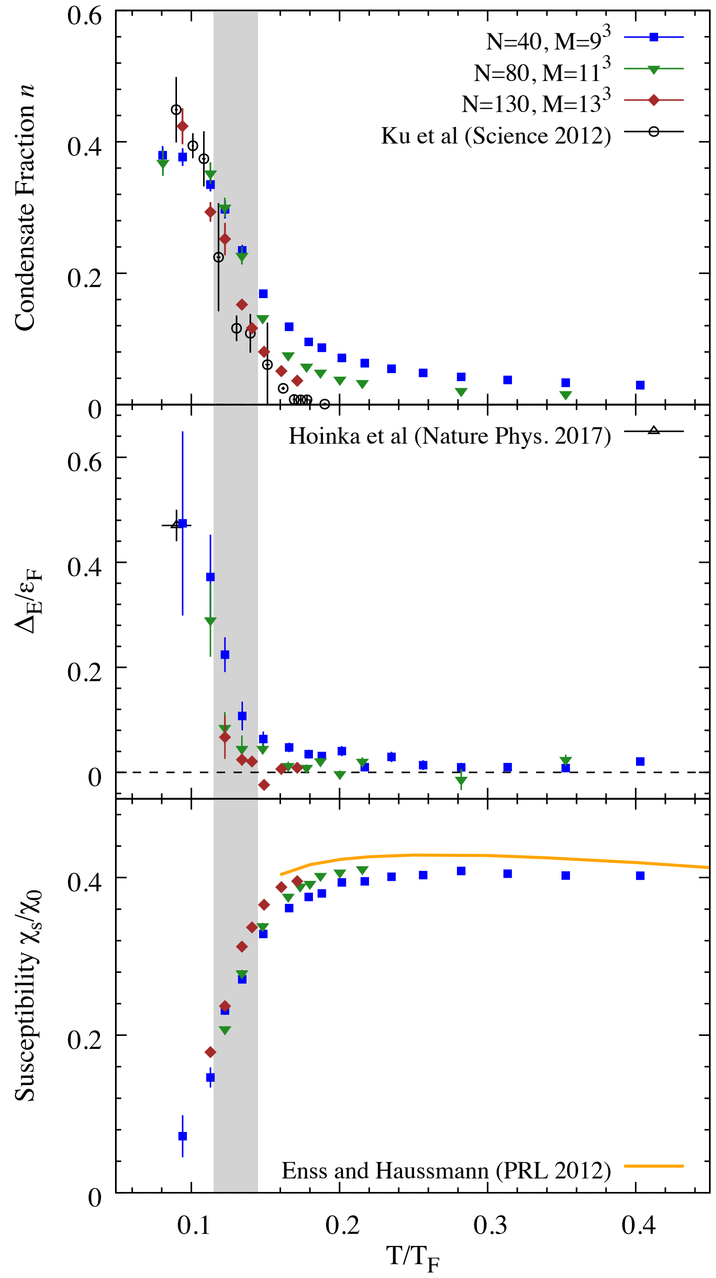
Summary

- First auxiliary-field Monte Carlo (AFMC) calculation of the heat capacity and energy-staggering pairing gap for the unitary gas at finite temperature.

- Thermodynamic observables in the canonical ensemble show clear signatures of the superfluid phase transition.

- No clear evidence of the pseudogap in AFMC simulations of the pairing gap at $N/M \simeq 0.06$.

- Moderate suppression of the spin susceptibility above T_c and below $\sim 0.17 T_F$.



Future Work

- Study larger number of particles and lattice sizes with lower filling factor for extrapolation to the dilute gas limit $k_F r_e \to 0$.
- Finite-size scaling with larger lattice sizes
- Pairing gap from spectral weight
- Momentum distribution and contact
- Pseudogap physics in lower spatial dimension