Precision thermodynamics of the strongly interacting Fermi gas

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Precision Thermodynamics of the strongly interacting Fermi gas

- Introduction: the strongly interacting Fermi gas in 3D (unitary Fermi gas) and in 2D
- Canonical-ensemble auxiliary-field Monte Carlo (AFMC) method
- Lattice formulation and continuum limit
- The contact
- Pseudogap regime
- Conclusion and outlook

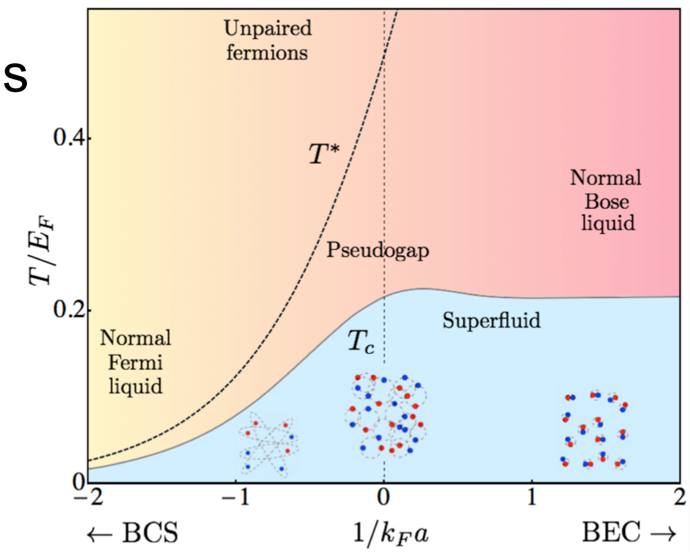
Introduction

Consider a 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 .

Three spatial dimensions (3D)

- A two-particle bound state for $a>0$
- The scattering amplitude at low momentum k is

$$f(k)=\frac{1}{-1/a-ik}$$



Randeria and Taylor, 2014

- A crossover from BCS for $(k_F a)^{-1} \sim -\infty$ to BEC for $(k_F a)^{-1} \sim +\infty$
- Phase transition to a superfluid below a critical temperature T_c

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

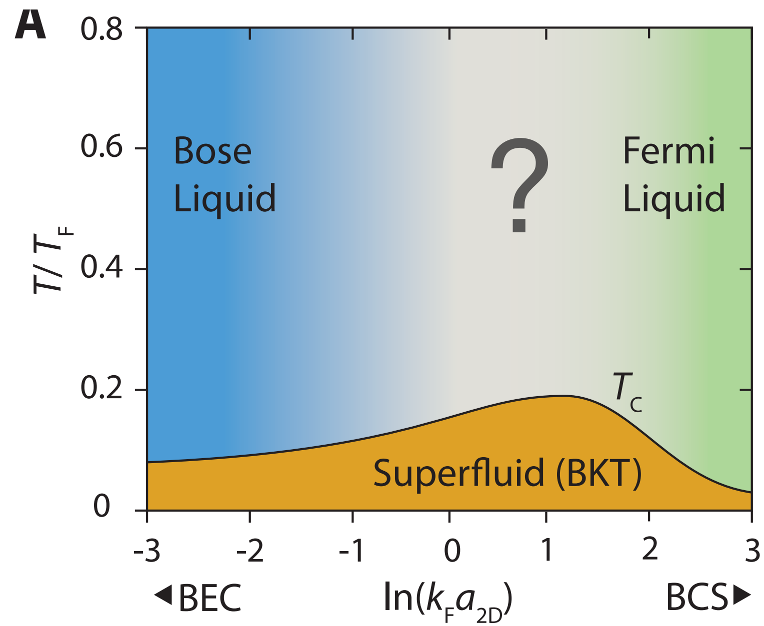
Of interest for high-T_c superconductivity, nuclear matter, and other strongly interacting Fermi systems

Two spatial dimensions (2D)

- There is a bound two-particle state for arbitrarily weak interaction strength
- The scattering amplitude at low momentum k is given by

$$f(k) = \frac{2\pi}{[\ln(2/kae^{\gamma}) + i\pi/2]}$$

- A crossover from BEC to BCS as a function of $\ln(k_F a)$
- The phase transition to superfluidity is of the Berezinskii-Kosterlitz-Thouless type
- Strong coupling regime: $\ln(k_F a) \sim 1$



Murthy et al, Science 2018

Many theoretical methods have been used to study the thermodynamics of the strongly coupled Fermi gas:

Strong-coupling theories:

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

T-matrix approaches

Self-consistent Luttinger-Ward theory

…

Quantum Monte Carlo methods:

Lattice diagrammatic Monte Carlo (LDMC)

Bold diagrammatic Monte Carlo (BDMC)

Auxiliary-field quantum Monte Carlo (AFMC)

...

The contact C

A fundamental thermodynamic property of quantum many-body systems with short-range interactions

- The contact C describes the short-range pair correlation at distance $r \to 0$

3D: $\langle n_\uparrow(r) n_\downarrow(0) \rangle \sim \dfrac{C}{4\pi r^2}$ 2D: $\langle n_\uparrow(r) n_\downarrow(0) \rangle \sim \dfrac{C}{(2\pi)^2} \ln^2 r$

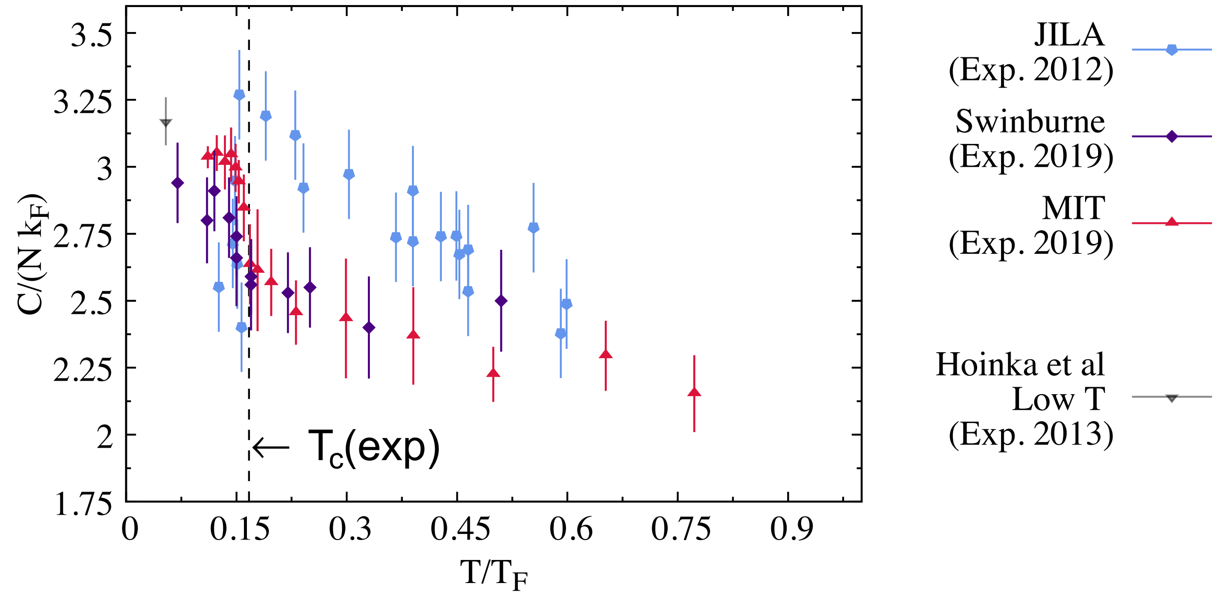
- Characterizes the tail of the momentum distribution $n_\sigma(k) \sim \dfrac{C}{k^4}$
- Characterizes the high-frequency tail of the shear viscosity spectral function
- Can be expressed as the adiabatic derivative of the energy with respect to the inverse scattering length (3D) or $\ln a$ (2D)

3D: $C = \dfrac{4\pi m}{\hbar^2} \dfrac{\partial E}{\partial(-1/a)}$ 2D: $C = \dfrac{4\pi m}{\hbar^2} \dfrac{\partial E}{\partial \ln a}$

The measurement and theoretical calculation of the temperature dependence of the contact has been a major challenge in the last decade

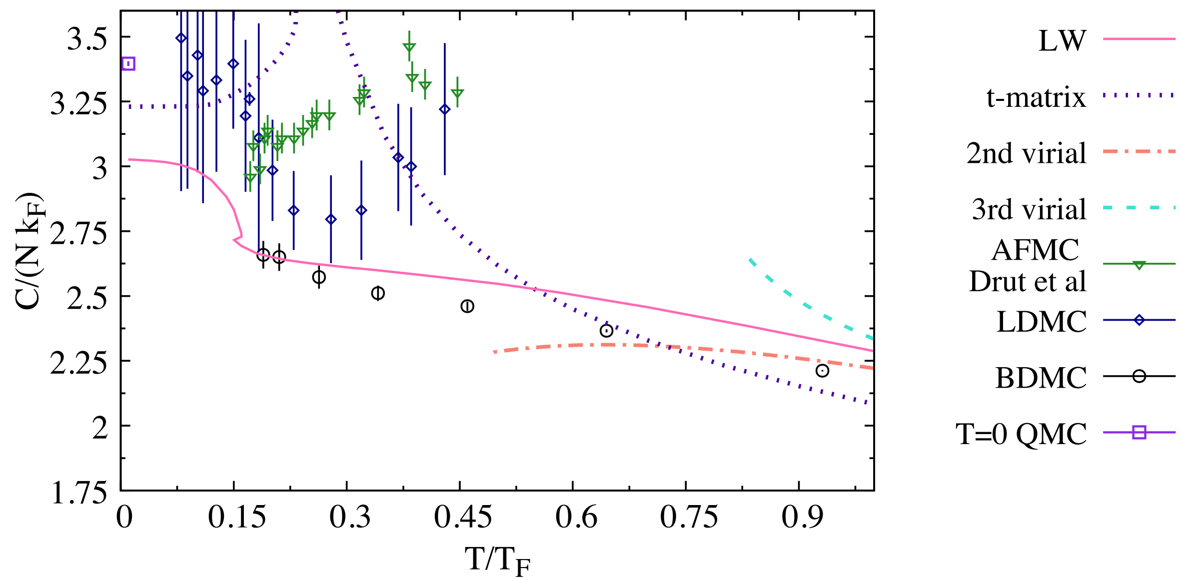
Experiment (UFG)

The results of the two recent precision experiments (Swinburne and MIT, 2019) differ substantially from the those of the original JILA experiment (2012).



Theory (UFG)

Theoretical calculations differ widely, even on a qualitative level.



Many of the strong coupling theories are based on uncontrolled approximations

Canonical ensemble 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 $\sigma(\tau)$

- The integrand reduces to matrix algebra in the single-particle space.

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

We implemented the canonical ensemble by exact particle-number projection.

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

Lattice formulation

S. Jensen, C.N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **124** (2020)

We use a discrete spatial lattice with spacing δx

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

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

- The interaction constant V_0 is normalized to reproduce the two-particle scattering length a on the lattice.

- Two important limits must be taken:

(i) Continuum limit $\delta x \to 0$ or filling factor $\nu \to 0$ at a fixed particle number N

(ii) Thermodynamic limit of large particle number $N \to \infty$

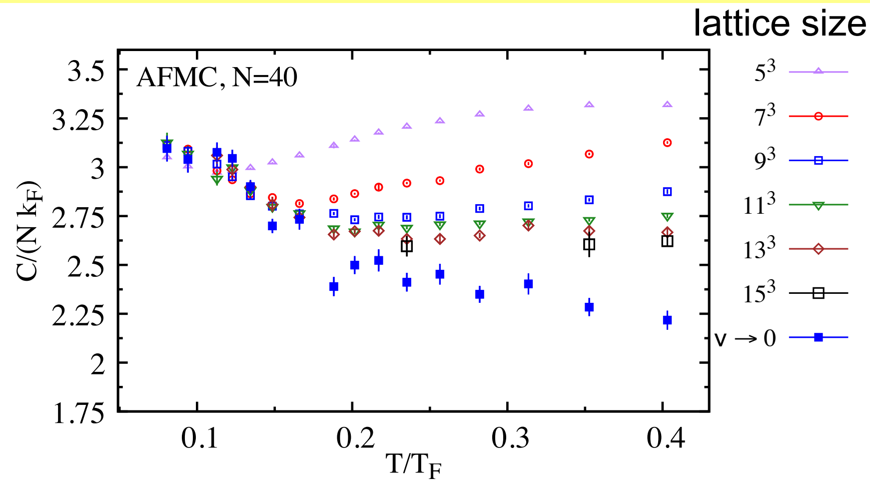
Continuum limit

S. Jensen, C.N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **125** (2020)

The continuum limit (filling factor $\nu \to 0$) is major challenge requiring AFMC calculation on large lattices.

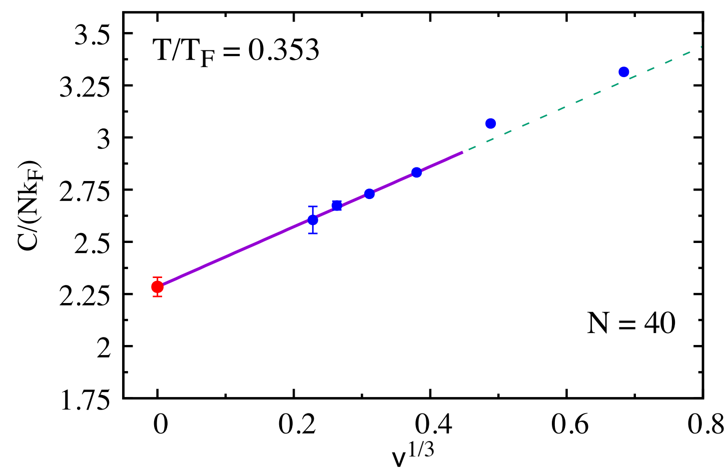
We introduced a novel method that ignores the (almost) unoccupied single-particle states, enabling large lattice calculations (Comp. Phys. Comm. 2021)

The contact is sensitive to the filling factor, and the extrapolation is crucial



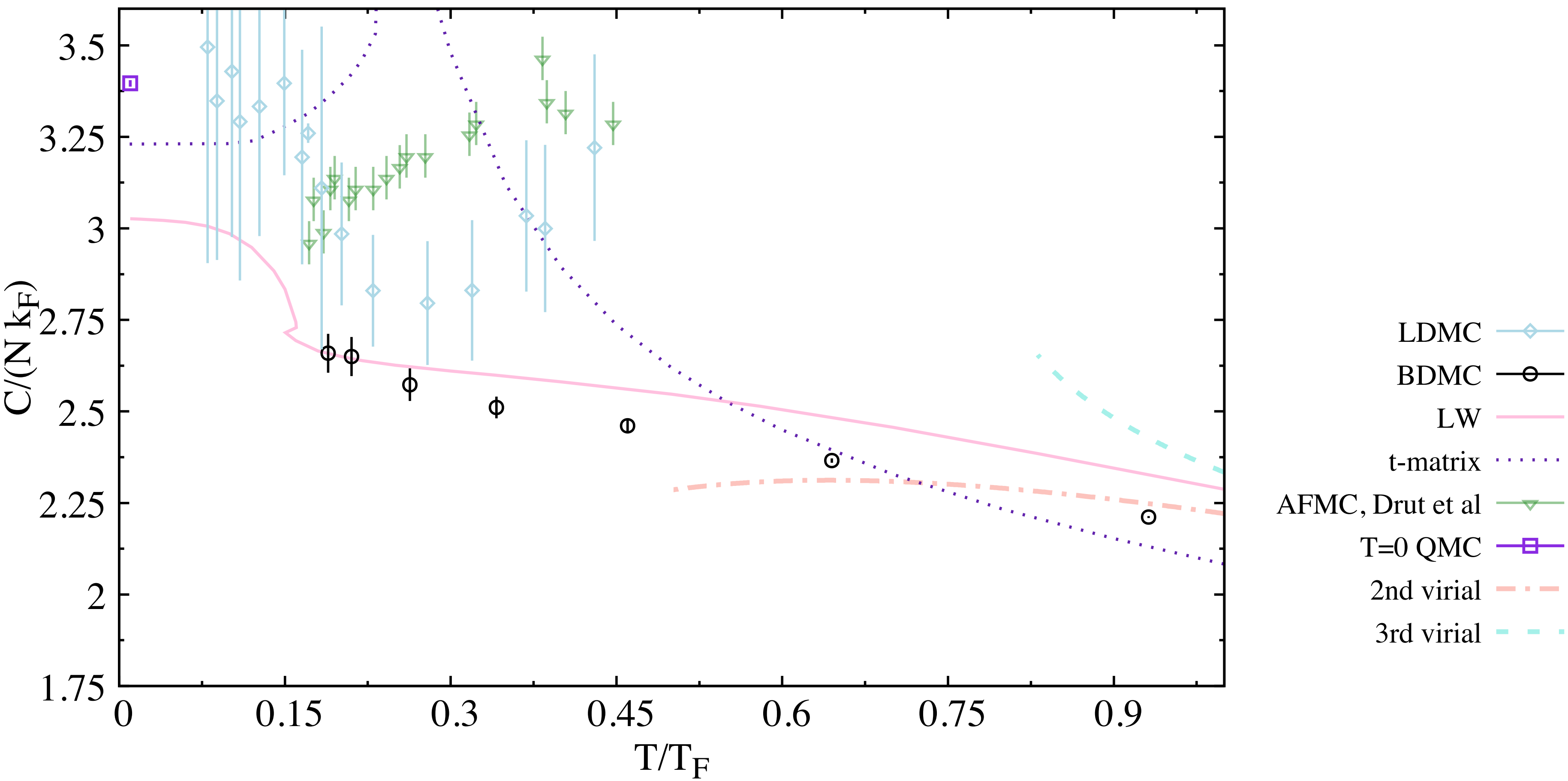
In 3D, the extrapolation is linear in $\nu^{1/3}$

In 2D, the extrapolation is linear in ν



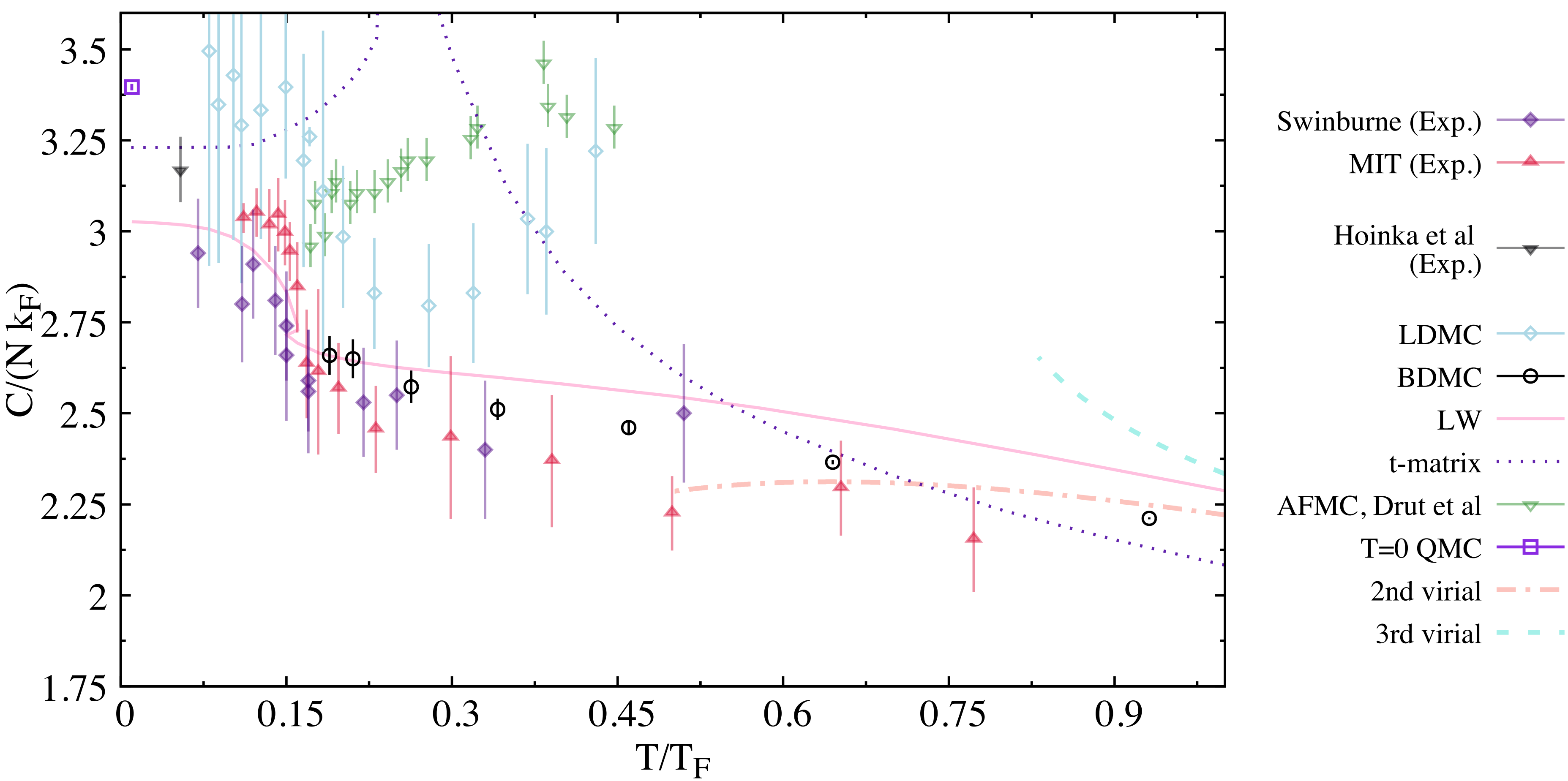
The contact: UFG

Previous theory results



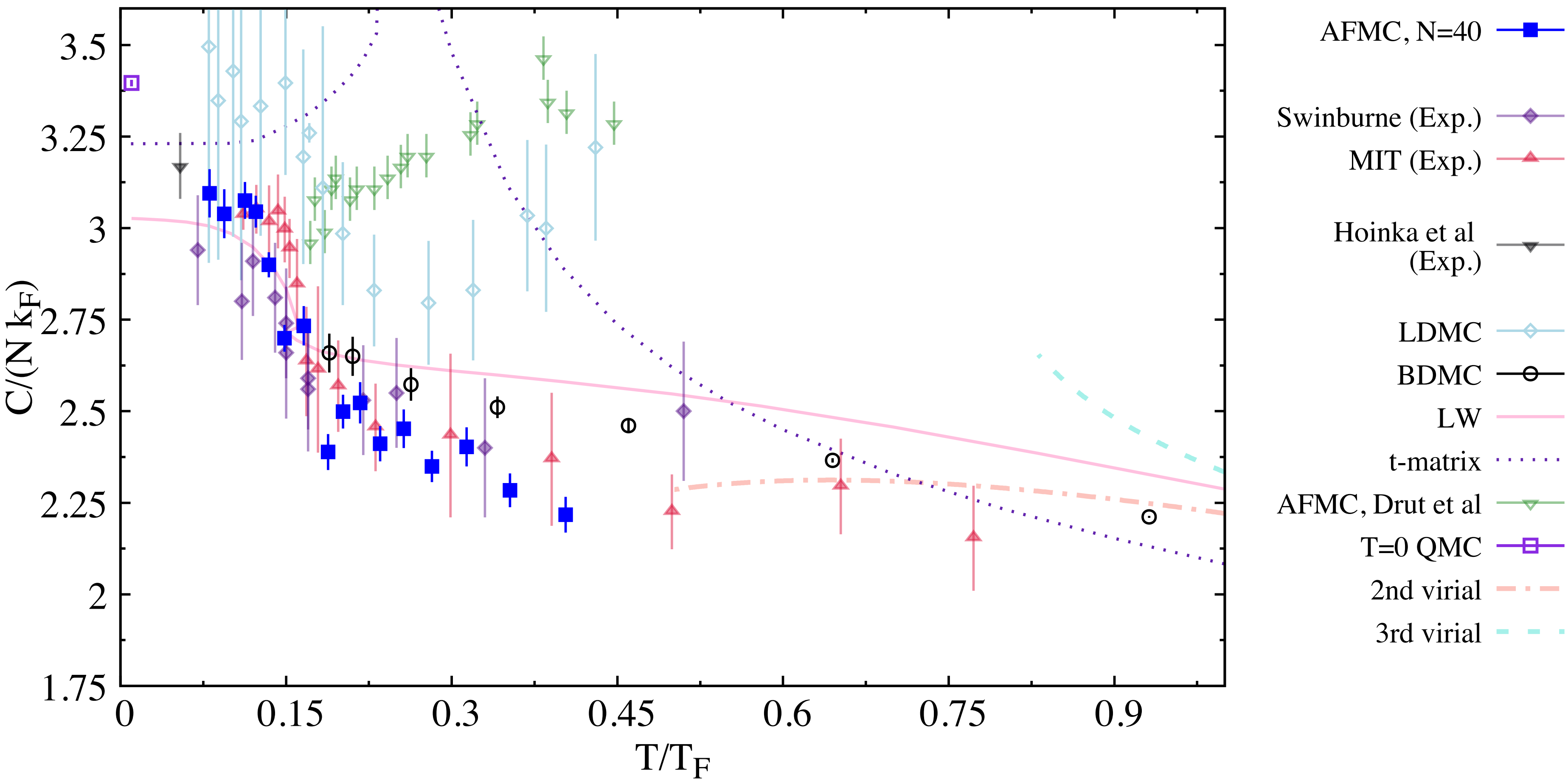
The contact: UFG

Previous theory results + recent experiments



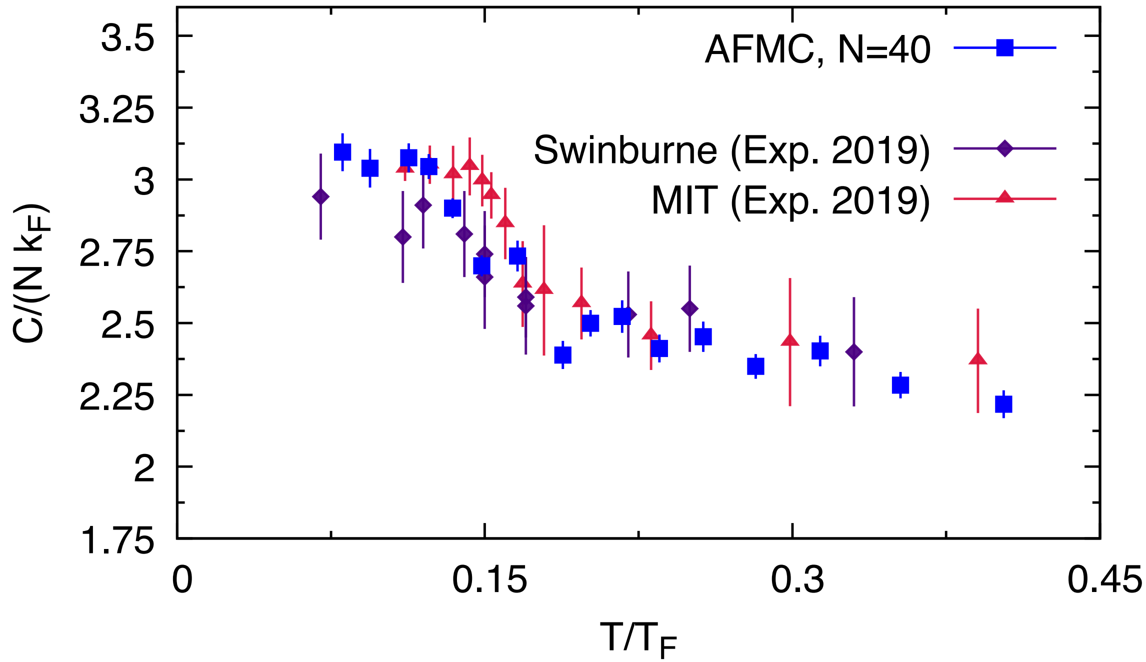
The contact: UFG

Previous theory results + recent experiments + our AFMC results

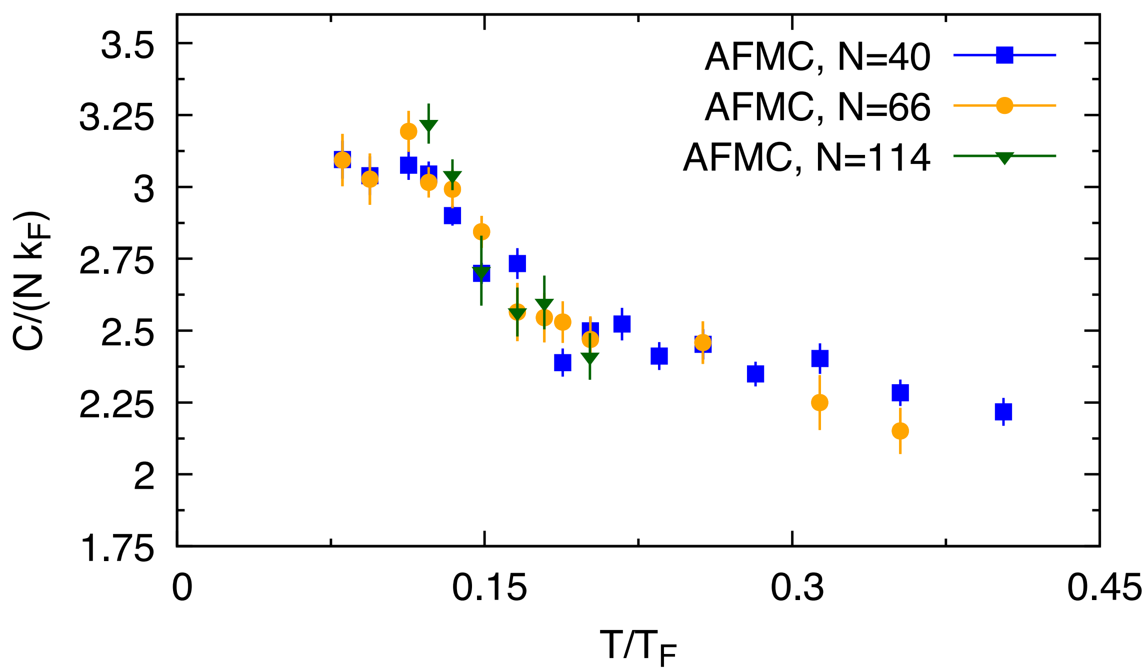


When compared to previous calculations, our continuum limit results provide the best quantitative agreement with the recent precision experiments.

AFMC results in comparison with the Swinburne and MIT experiments



AFMC results for N=40, 66 and 114 particles

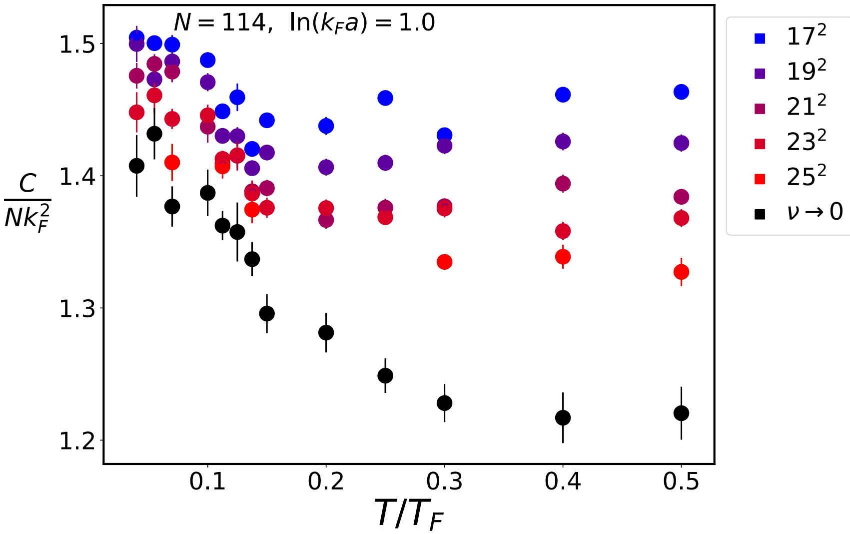


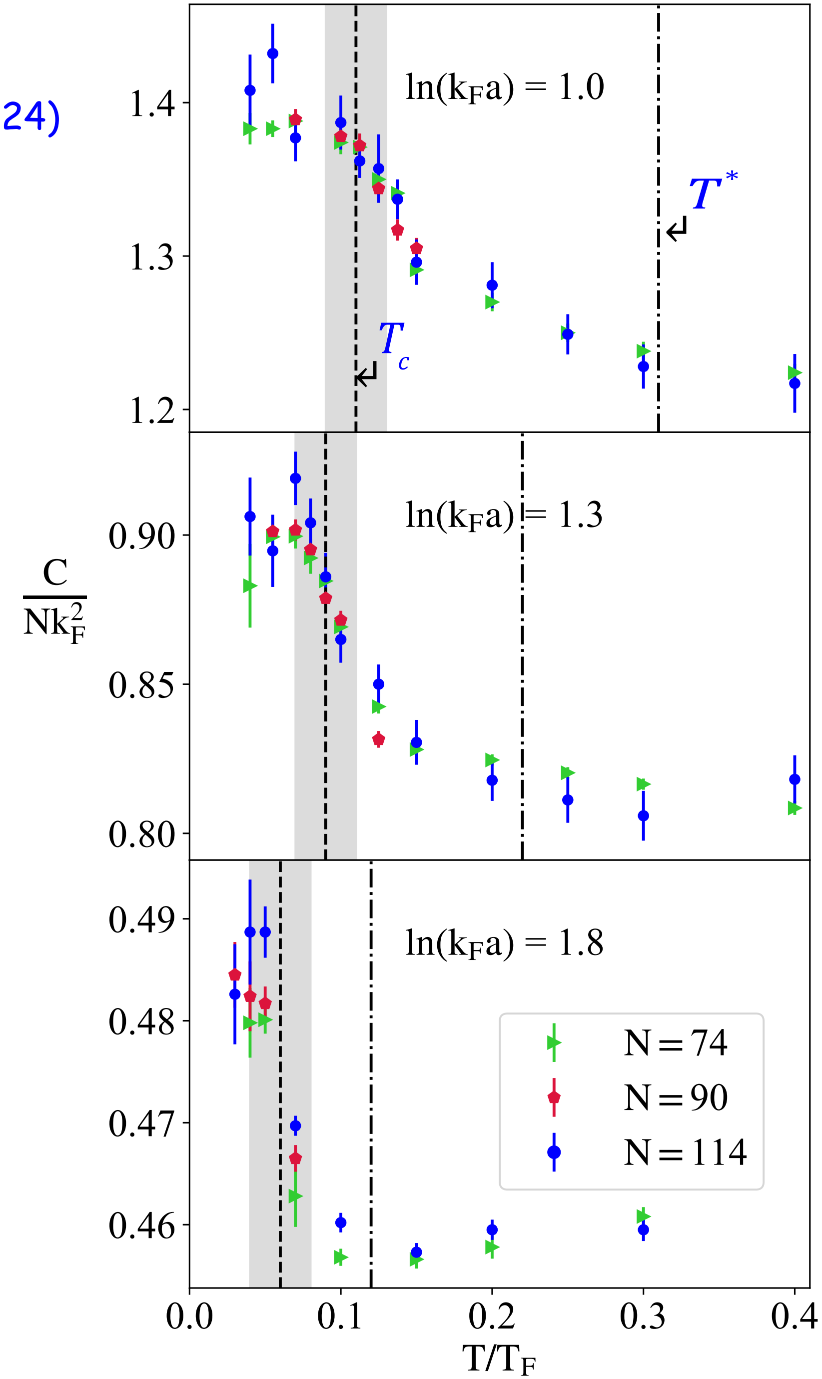
Weak dependence on number of particles N
⇒ results are close to the thermodynamic limit

Contact in 2D Fermi gas

S. Ramachandran, S. Jensen, Y. Alhassid, PRL 133, 143405 (2024)

Continuum extrapolations:

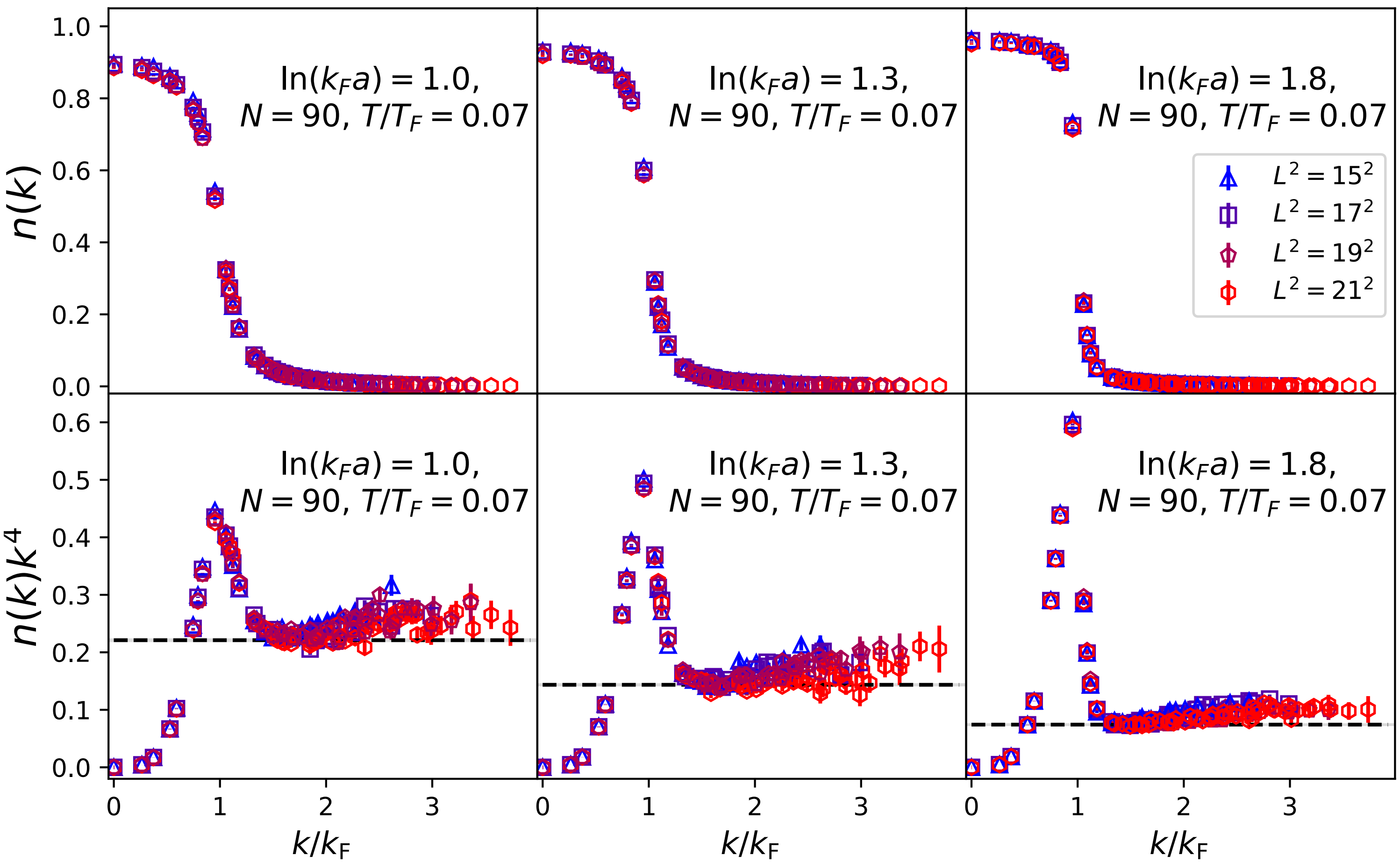




- A rapid increase below T_c for all couplings
- Magnitude becomes smaller towards the BCS side

Single-particle momentum distribution

For large k: $n(k) = \frac{C}{k^4}$



Pseudogap regime

Are there signatures of a pseudogap regime above the critical temperature in which pairing correlations survive?

Spin susceptibility

$$\chi \propto \beta \langle (N_\uparrow - N_\downarrow)^2 \rangle$$

Pairing correlations suppress the spin susceptibility

Model-independent pairing gap

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

-- requires the canonical ensemble

Free energy gap

$$\Delta_F = [2F(N_\uparrow, N_\downarrow - 1) - F(N_\uparrow, N_\downarrow) - F(N_\uparrow - 1, N_\downarrow - 1)]/2$$

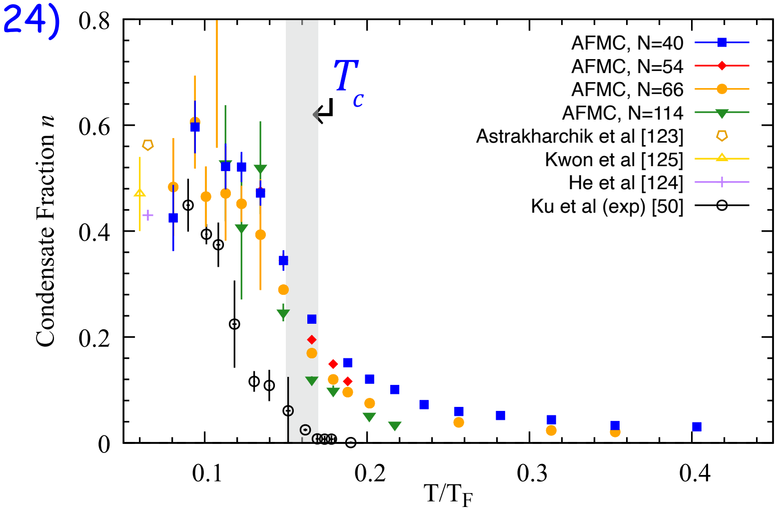
-- Calculated from ratios of canonical partition functions – most accurate

Pseudogap regime in the continuum limit: (i) unitary Fermi gas

S. Jensen, C.N. Gilbreth, Y. Alhassid, arXiv:2408.16676 (2024)

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 $n = \lambda_{\max}/(N/2)$



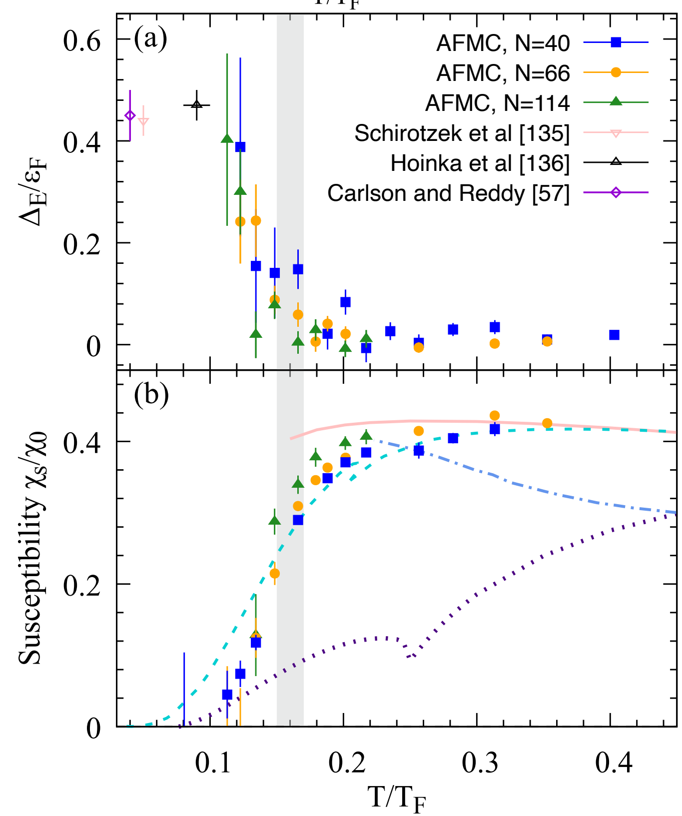
Model-independent pairing gap Δ_E

- The pairing gap vanishes above $0.2\,T_F$

Spin susceptibility

Pair correlations suppress the spin susceptibility

- Spin susceptibility is suppressed below $0.2\,T_F$

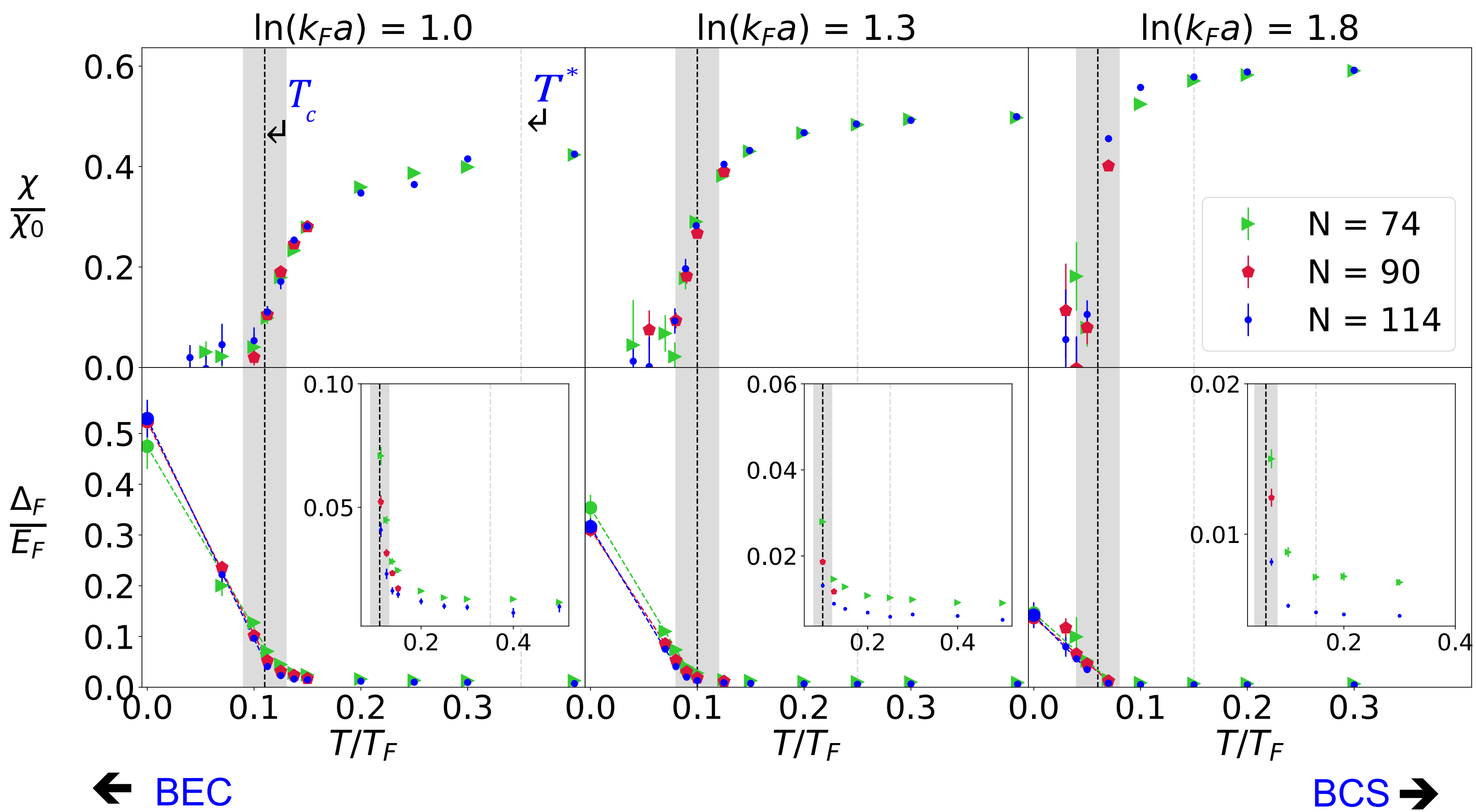


Pseudogap regime below $T^* \sim 0.2\,T_F$
-- much narrower than previously estimated

(ii) Strongly coupled 2D Fermi gas

S. Ramachandran, S. Jensen, Y. Alhassid, PRL 133, 143405 (2024)

Spin susceptibility (top) and free energy gap (bottom) vs. temperature



The regime $T_c < T < T^*$ in which the spin susceptibility is suppressed (spin gap) is substantial for $\ln(k_F a) = 1$ and becomes narrower on the BCS side

The free energy gap increases as T decreases towards T_c in the spin gap regime

Conclusion

Precision thermodynamics of the interacting Fermi gas has been a major challenge to both experimentalists and theorists.

- Most theoretical methods use uncontrolled approximations and lead to widely different results
- We performed accurate auxiliary-field Monte Carlo (AFMC) calculations on the lattice, eliminating systematic errors associate with finite lattice spacing
- Our calculations for the contact of the unitary Fermi gas (UFG) provide the best quantitative agreement with recent precision experiments
- We determined the UFG pseudogap regime in the continuum limit (long debated)
- We find a significant pseudogap regime for the 2D Fermi gas at $\ln(k_F a) \sim 1$ that becomes narrower towards the BCS side

Outlook

- Calculate dynamical observables in AFMC: spectral weight, shear viscosity,...
- Carry out precision experiments in a uniform trap (3D and 2D)