Title: The unitary Fermi gas across the superfluid transition

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Abstract: Quantum Monte Carlo is a versatile tool for studying strongly interacting theories in condensed matter physics from first principles. A prominent example is the unitary Fermi gas: a two-component system of fermions interacting with divergent scattering length. I will present numerical results for different properties of the homogeneous, spin-balanced unitary Fermi gas across the superfluid transition, such as the critical temperature, the equation of state and the temperature dependence of the contact density. Our values show good agreement with recent experimental data.

Ultracold quantum gases

Motivation: quantum mechanics on a macroscopic scale
many-body physics

Dilute systems:

- particles move almost freely
- rare (2-body) collisions
- particles almost uncorrelated

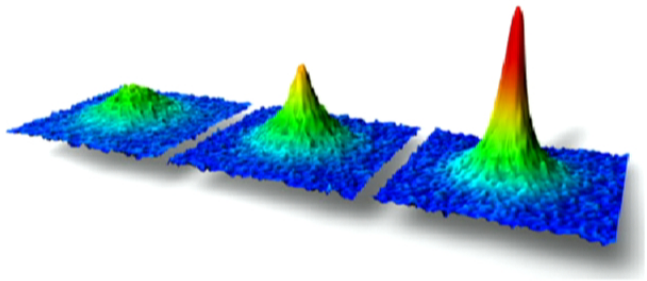
Ultracold gases are:

- simple: direct realisation of basic quantum mechanical models
- tunable: easy to manipulate in an experiment
  - interaction strength
  - temperature
  - external potential
  - dimension,...
- versatile: many real-world analogues

Fermi gases

Examples:

- electrons inside a metal
- quark-gluon plasma in the inner core of a neutron star
- atomic gas e.g. of ^{40}K or ^{6}Li atoms ($\Rightarrow$ experiment!)

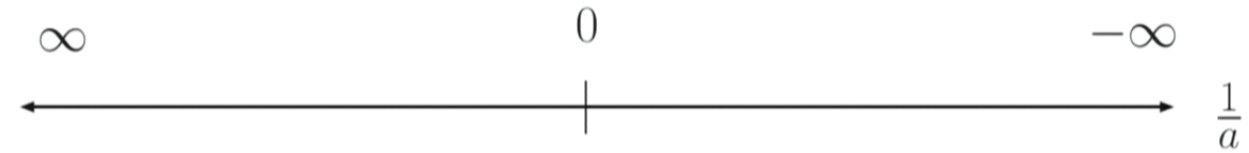


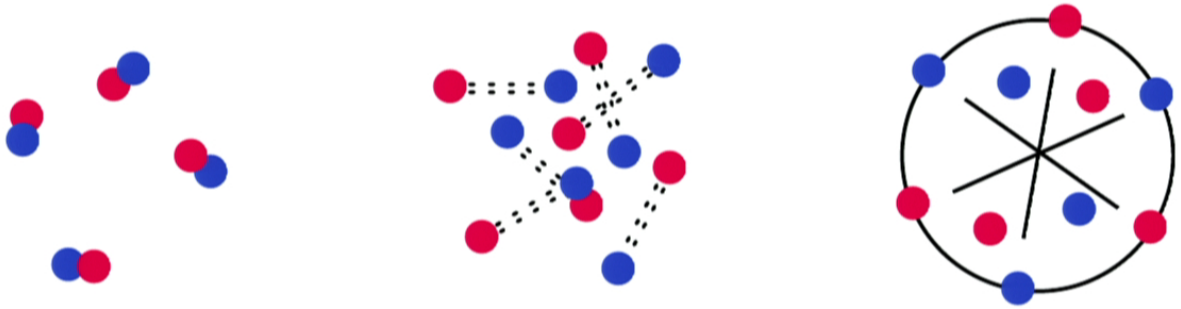
experiment by the JILA group (University of Colorado)

low temperature: quantum phenomena become important
identical fermions $\Rightarrow$ no s-wave scattering $\Rightarrow$ ideal gas model

The unitary Fermi gas

Fermions of two species $\Rightarrow$ interactions become important
Low-energy interactions are characterised by the scattering length a





BEC regime
strongly bound (bosonic) molecules of two fermions

UNITARITY
strongly interacting fermions

BCS regime
pairs of fermions weakly bound in momentum space

What is interesting about unitarity?

- System is dilute and strongly interacting at the same time
- No length scales associated with interactions
  $\Rightarrow$ universal behaviour
- Only relevant parameters: temperature and density
- High-temperature superfluidity

neutron star	$T_c = 10^6$K	$T_c = 10^{-5}\,T_F$
high-T_c superconductor	$T_c = 10^2$K	$T_c = 10^{-3}\,T_F$
atomic Fermi gas	$T_c = 10^{-7}$K	$T_c = 10^{-1}\,T_F$

- Experimental data available

What is interesting about unitarity?

strong interactions $\Rightarrow$ no small parameter for perturbation theory

No exact theory for the Fermi gas at unitarity!

What to do?

- Approximate schemes (e.g. mean-field theory) involve uncontrolled approximations
- Numerical methods
  $\Longrightarrow$ good results for critical temperature and other quantities

Project: Thermodynamic properties of the unitary Fermi gas at and near the critical point
Method: Determinant Diagrammatic Monte Carlo (DDMC) algorithm [Burovski, Prokof'ev, Svistunov, Troyer (2006)]

The Fermi-Hubbard model

Simplest lattice model for two-particle scattering

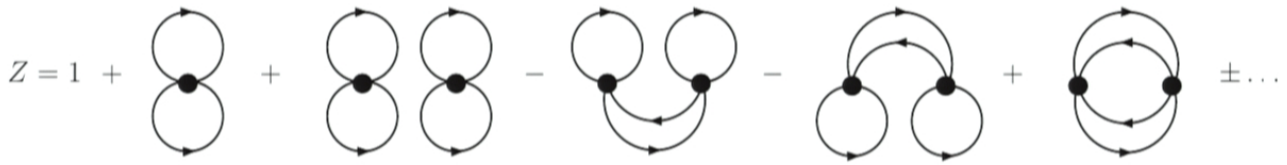
- Non-relativistic fermions
- Contact interaction between spin up and spin down
- On-site attraction $U < 0$ tuned to describe unitarity
- Grand canonical ensemble
- Finite 3D simple cubic lattice, periodic boundary conditions
- Continuum limit can be taken by extrapolation to zero density

$$H = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{x}} c^{\dagger}_{\mathbf{x}\uparrow} c_{\mathbf{x}\uparrow} c^{\dagger}_{\mathbf{x}\downarrow} c_{\mathbf{x}\downarrow},$$

where $\epsilon_{\mathbf{k}} = \frac{1}{m} \sum_{j=1}^{3} (1 - \cos k_j)$ is the discrete FT of $\frac{-\nabla^2}{2m}$.

Finite temperature formalism

Grand canonical partition function in imaginary time interaction picture: $Z = \mathrm{Tr} e^{-\beta H}$:



Sign problem!

The diagrams of each order can be written as the product of two matrix determinants [Rubtsov, Savkin, Lichtenstein (2005)]

$$Z = \sum_{p, S_p} (-U)^p \det \mathbf{A}^{\uparrow}(S_p) \det \mathbf{A}^{\downarrow}(S_p),$$

where S_p is the vertex configuration and the matrix entries are free (finite temperature) propagators

Order parameter of the phase transition

Anomalous correlations in the superfluid phase:

$\Rightarrow$ Introduce pair annihilation/creation operators P and $P^\dagger$:

$$P(\mathbf{x},\tau) = c_{\mathbf{x}\uparrow}(\tau)c_{\mathbf{x}\downarrow}(\tau) \quad \text{and} \quad P^\dagger(\mathbf{x}',\tau') = c^\dagger_{\mathbf{x}'\uparrow}(\tau')c^\dagger_{\mathbf{x}'\downarrow}(\tau')$$

Order parameter is obtained from the pair correlation function

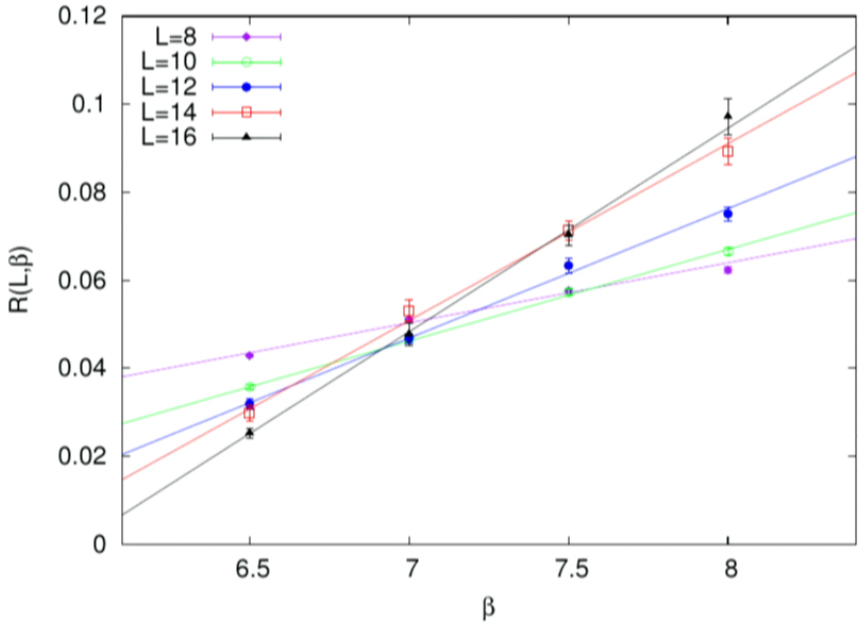
$$G_2(\mathbf{x}\tau;\mathbf{x}'\tau') = \left\langle \mathbf{T}_\tau P(\mathbf{x},\tau)P^\dagger(\mathbf{x}',\tau') \right\rangle$$

Order parameter of the phase transition

$\Rightarrow$ the rescaled integrated correlation function

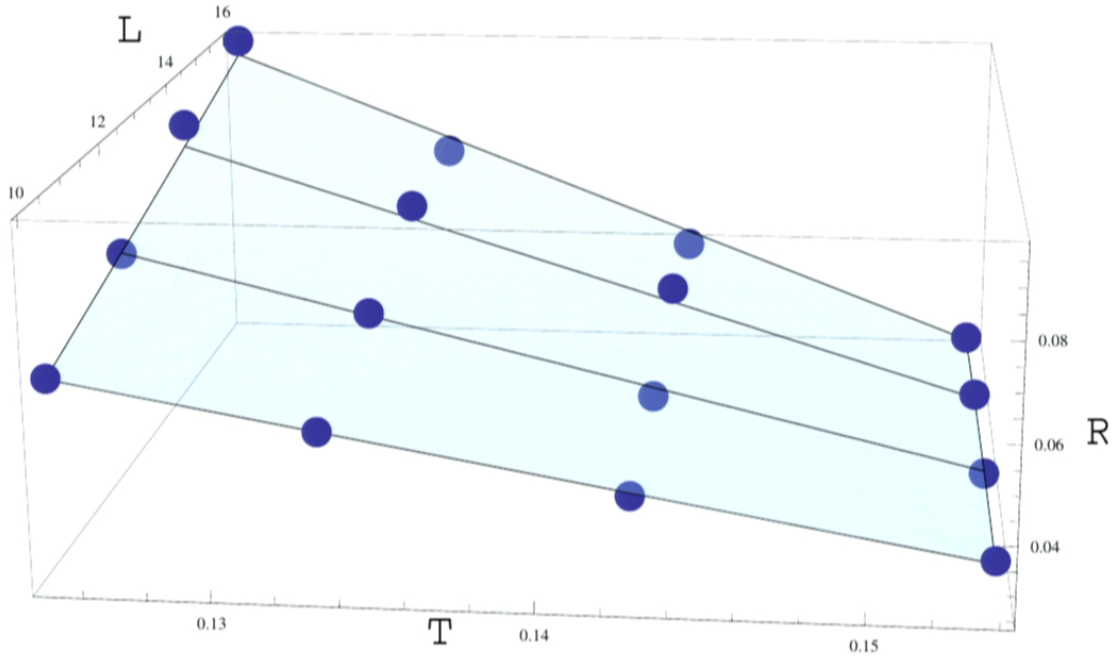
$$R(L,T) = L^{1.038}\overline{G_2(\mathbf{x}\tau;\mathbf{x}'\tau')}$$

becomes independent of lattice size L at the critical point



Order parameter of the phase transition

Example: nonlinear fit of the rescaled integrated correlator $R(L, T)$

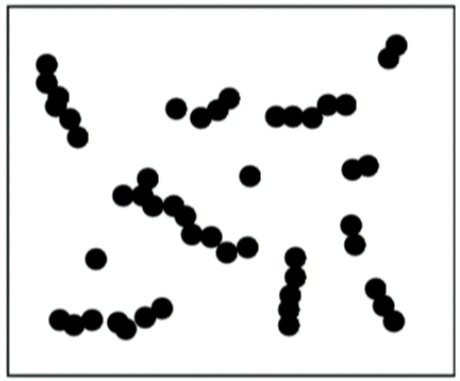


(data taken at 4 different temperatures and 4 different lattice sizes)

Diagrammatic Monte Carlo

Burovski, Prokof'ev, Svistunov and Troyer (2006):

- sampling via a Monte Carlo Markov chain process
- configuration space: spacetime positions of interaction vertices
- extension of the configuration space $\rightarrow$ worm vertices

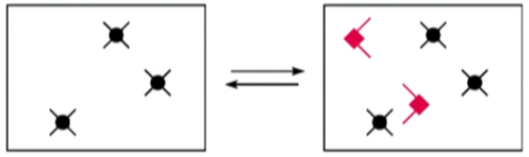


- physical picture: at low densities multi-ladder diagrams dominate
- updates designed to favour prolonging existing vertex chains

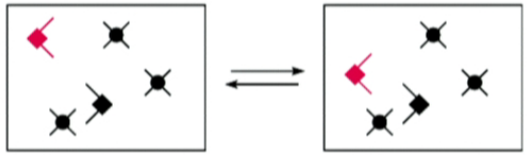
Diagrammatic Monte Carlo

Original set of updates (Burovski et al. 2006):

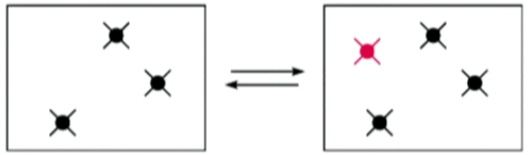
- inserting/removing worm vertices



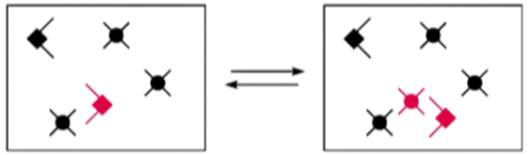
- shifting the worm vertex



- changing the diagram order
  - diagonal version

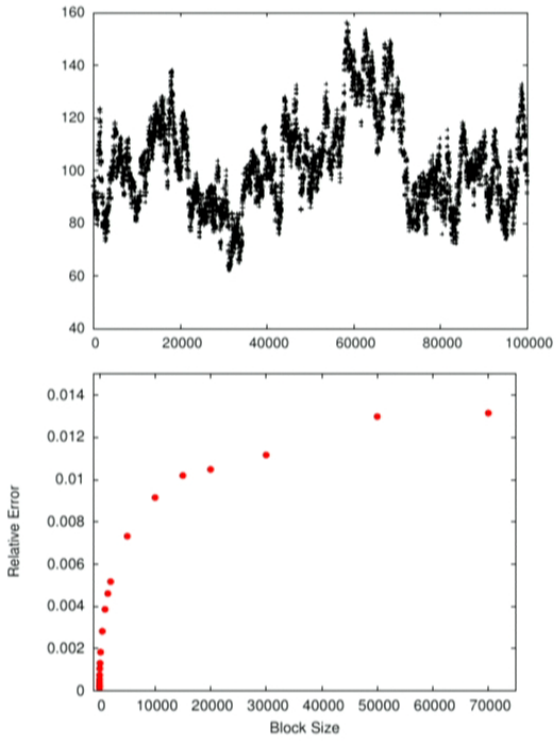


  - worm version

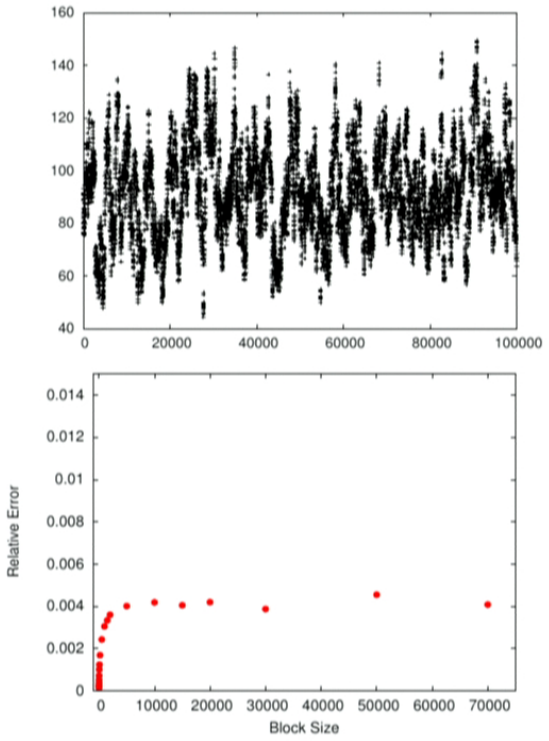


Diagrammatic Monte Carlo

Autocorrelations in the interaction energy ($\propto$ diagram order)



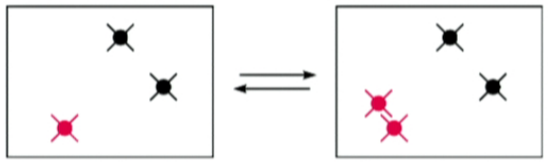
Worm updates

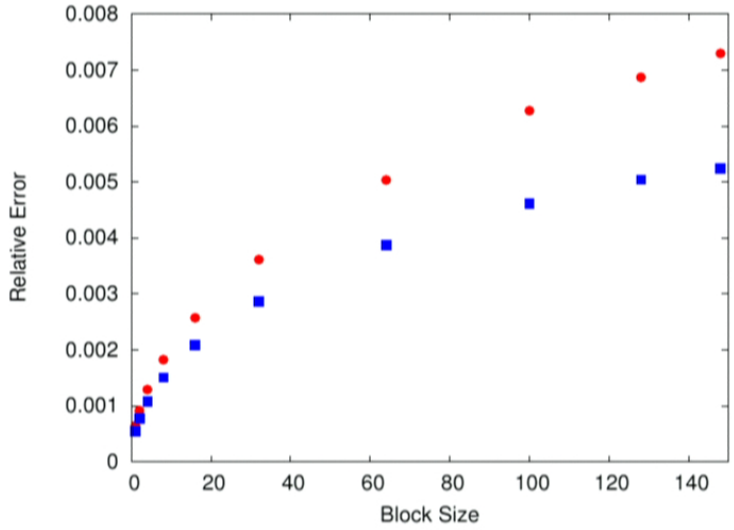


Diagonal updates

Diagrammatic Monte Carlo

Alternative worm-type updates



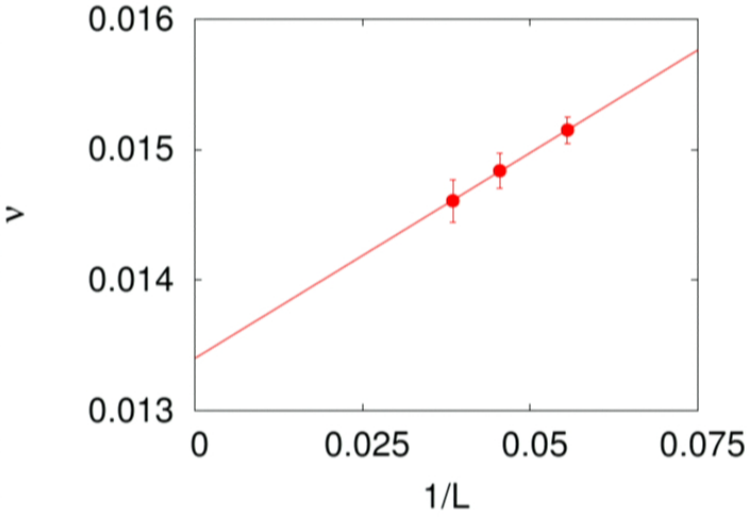


- diagonal setup
- alternative worm setup

at low filling factor

Thermodynamic limit

Extrapolation from finite to infinite system size:

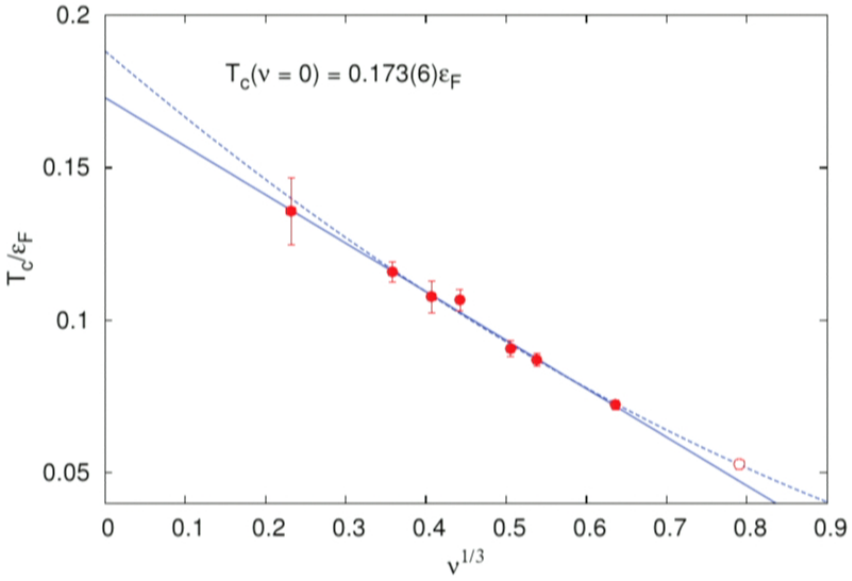


Filling factor $\nu = \langle \sum_\sigma c^\dagger_{\mathbf{x}\sigma} c_{\mathbf{x}\sigma} \rangle$

- small lattices $\Rightarrow$ higher ν
- linear fit of ν versus $1/L$
- extrapolate $\nu(1/L \to 0)$ to get ν in the thermodynamic limit

ν determines the energy scale via $\varepsilon_F = (3\pi^2\nu)^{2/3}/2m$

Continuum limit



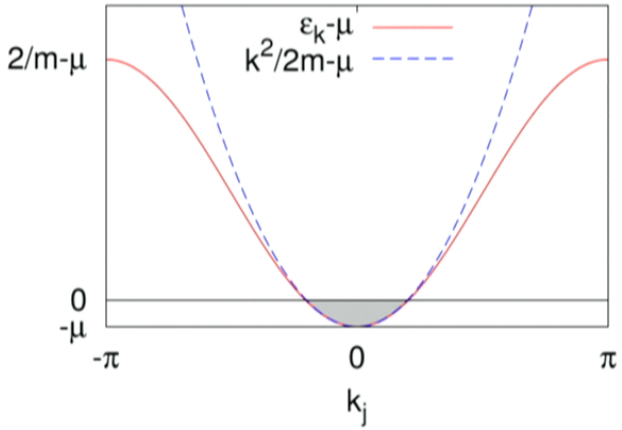
physical scale $\nu = nb^3$

- $\nu = \langle \sum_\sigma c^\dagger_{\mathbf{x}\sigma} c_{\mathbf{x}\sigma} \rangle$ dimensionless filling factor
- n particle density
- b lattice spacing

- continuum limit $b \to 0$ corresponds to $\nu \to 0$
- leading order lattice corrections $\propto b \propto \nu^{1/3}$

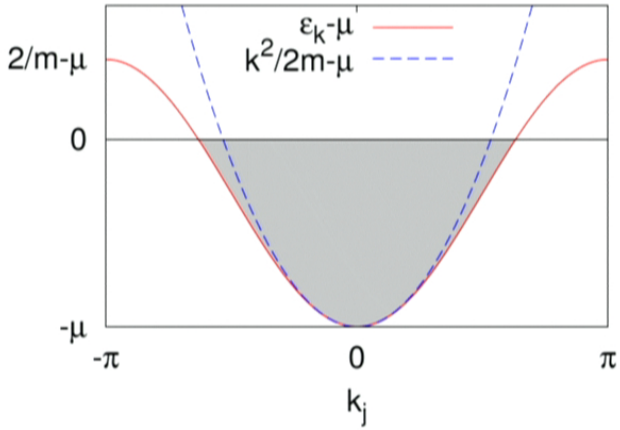
Continuum limit

small μ, dilute



$\Rightarrow$ linear regime

large μ, dense



$\Rightarrow$ nonlinear regime

Results at T_c

Results at the critical point:

$$\begin{aligned} T_c/\varepsilon_F &= 0.171(5) \\ \mu/\varepsilon_F &= 0.429(7) \\ E/E_{\mathrm{FG}} &= 0.440(15) \\ \mathcal{C}/k_F^4 &= 0.1101(9) \end{aligned}$$

and generalisation to the imbalanced case ($\mu_\uparrow \neq \mu_\downarrow$) for small imbalances

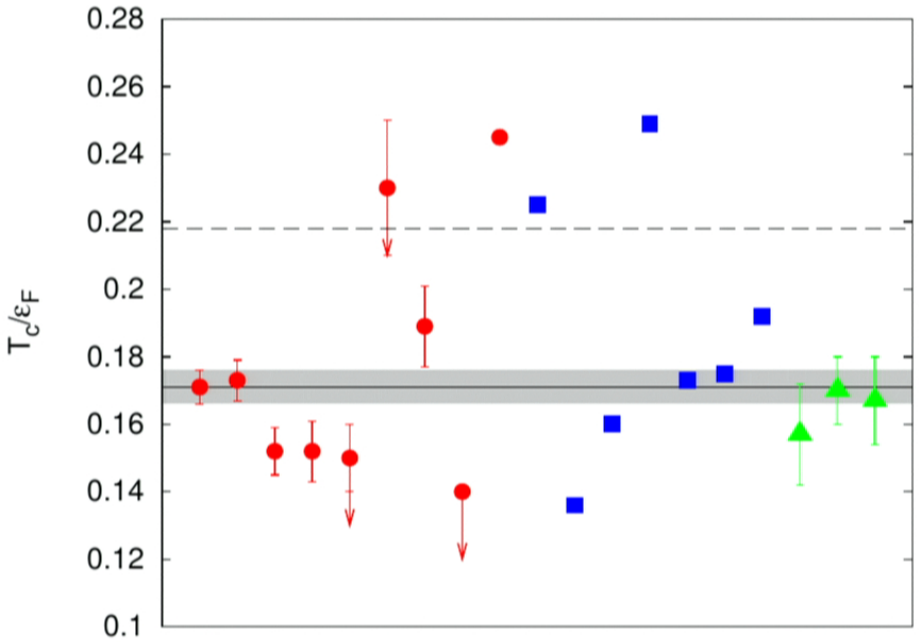
[Phys. Rev. A **82**, 053621 (2010), PoS(Lattice 2010)187]

Results: Critical temperature

Comparison with other numerical studies and experiment:

- Crossings
  - Burovski, Prokof'ev, Svistunov, Troyer (DDMC) 0.152(7)
  - Burovski, Kozik, Prokof'ev, Svistunov, Troyer 0.152(9)
  - Bulgac, Drut, Magierski 0.15(1)
- Full fit
  - Abe, Seki 0.189(12)
  - Goulko, Wingate (DDMC) 0.171(5)
- Experiment
  - Nascimbene, Navon, Jiang, Chevy, Salomon 0.157(15)
  - Horikoshi, Nakajima, Ueda, Mukaiyama 0.17(1)
  - Ku, Sommer, Cheuk, Zwierlein 0.167(13)

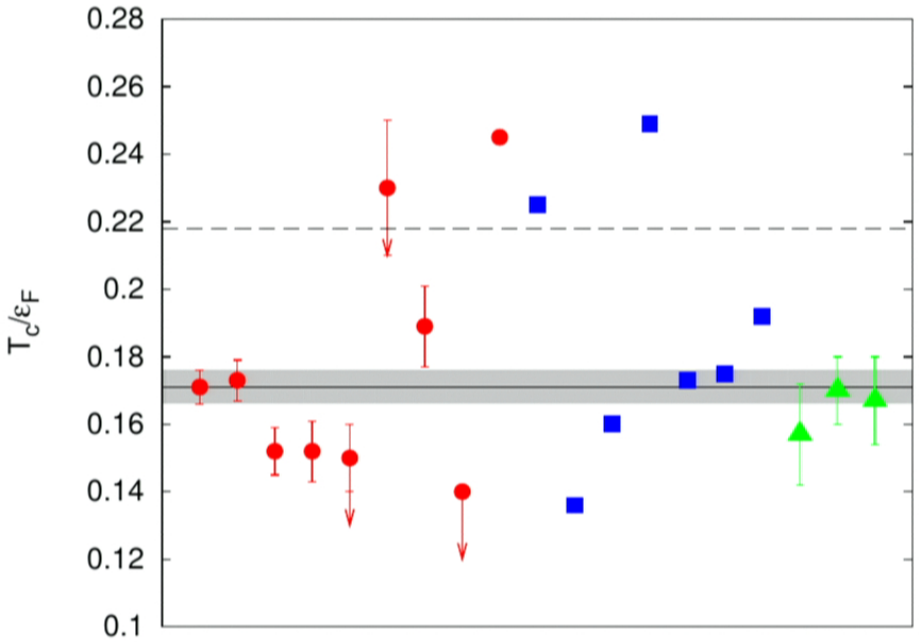
Results: Critical temperature



from left to right:

- numerical: this work (with and without imbalance); Burovski et al. (discrete and continuous space DDMC); Bulgac et al. (auxiliary field MC, 2008 and 2006); Abe and Seki (neutron matter); Lee and Schaefer (hybrid MC); Akkineni et al. (restricted path integral MC)
- analytical: Hu et al. (beyond MF); Nikolic and Sachdev ($1/N$ expansion); Haussmann et al. (self-consistent); 4 results from the ε-expansion by Nishida and Son
- experiment: Nascimbene et al. (ENS); Horikoshi et al. (Tokyo); Ku et al. (MIT)
- – – – BEC limit

Results: Critical temperature



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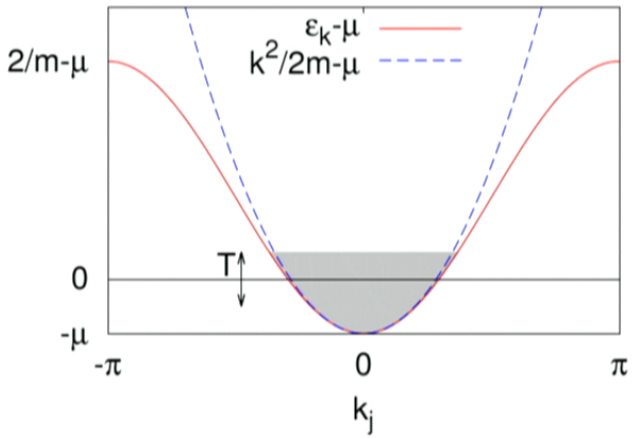
Temperatures beyond T_c

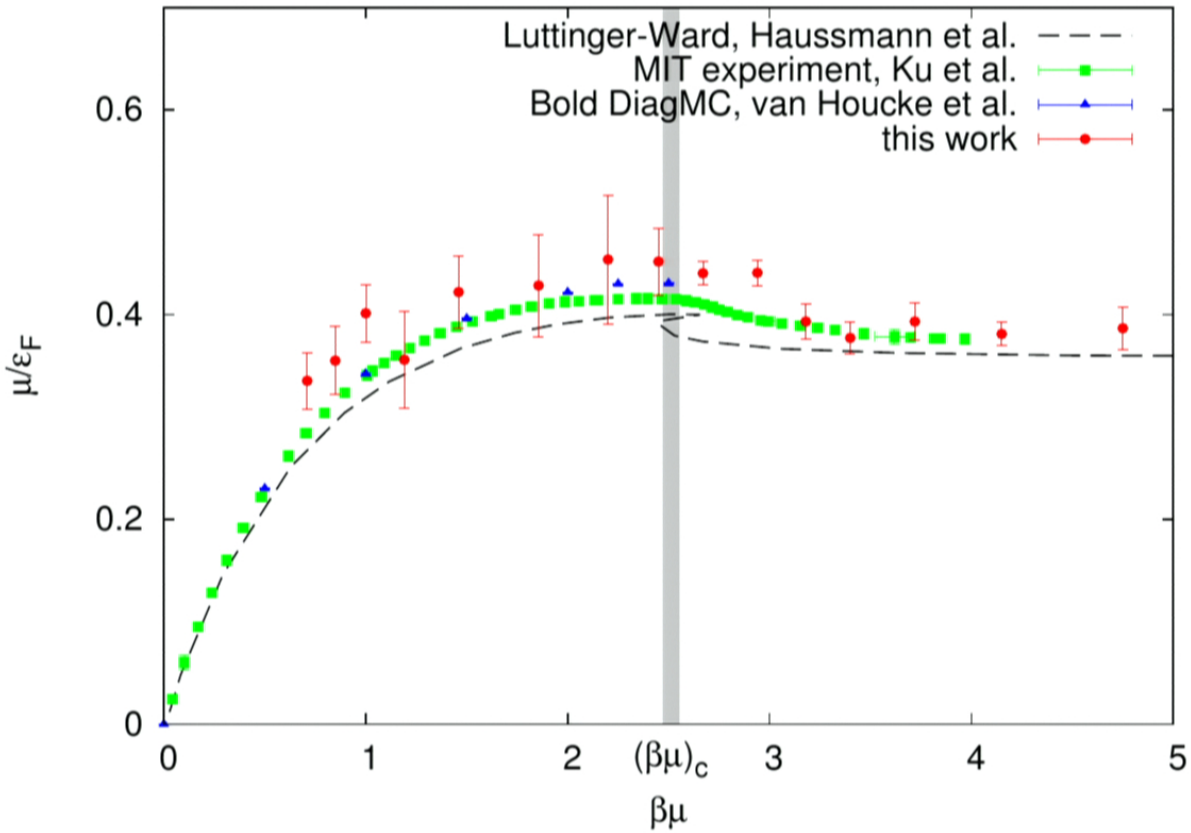
Challenges:

- Fixing the temperature scale (at $T \neq T_c$ there is no order parameter to fix the curves of constant physics)
- Discretisation errors increase with increasing temperature

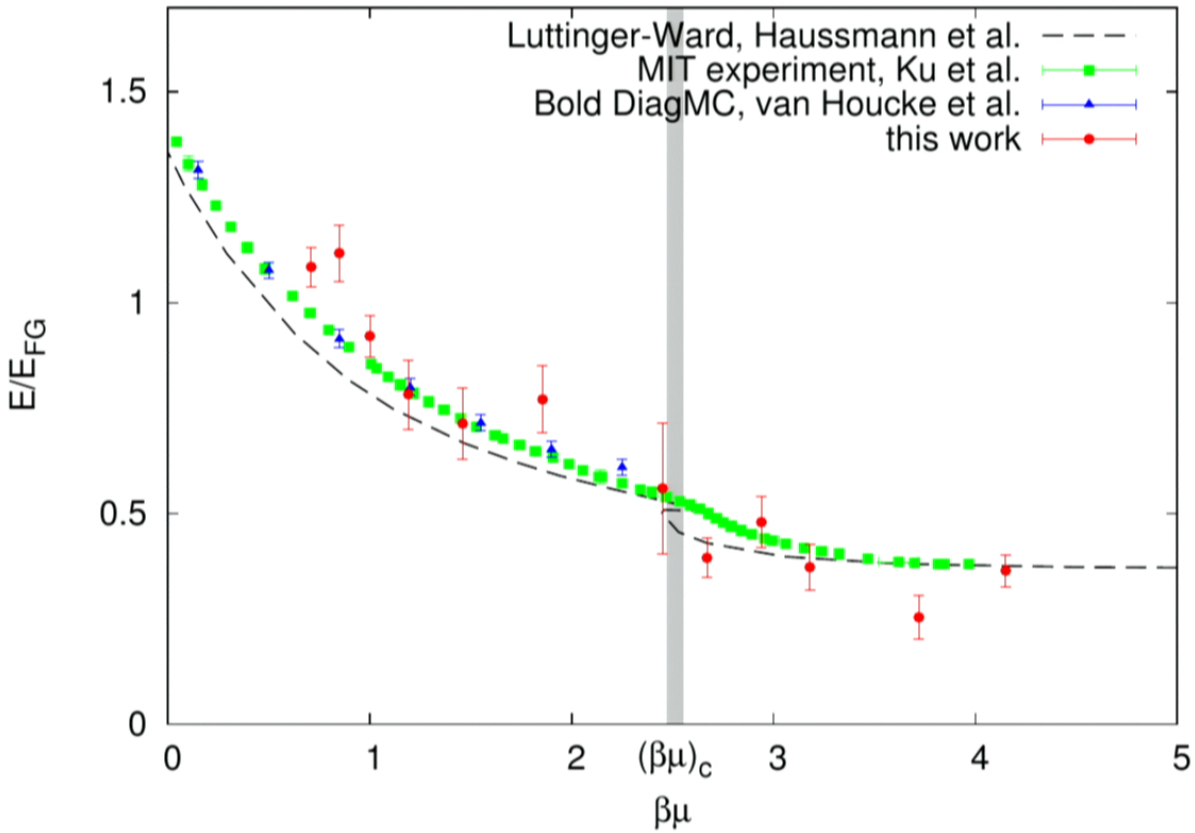


- use the dimensionless $\beta\mu$ to fix the temperature scale by linearly extrapolating along curves of constant $\beta\mu$

Results: Chemical potential



Results: Energy per particle



Contact density

The contact can be interpreted as a measure for the local pair density [Tan (2008), Braaten (2010)].

Definition contact [Werner and Castin (2010)]:

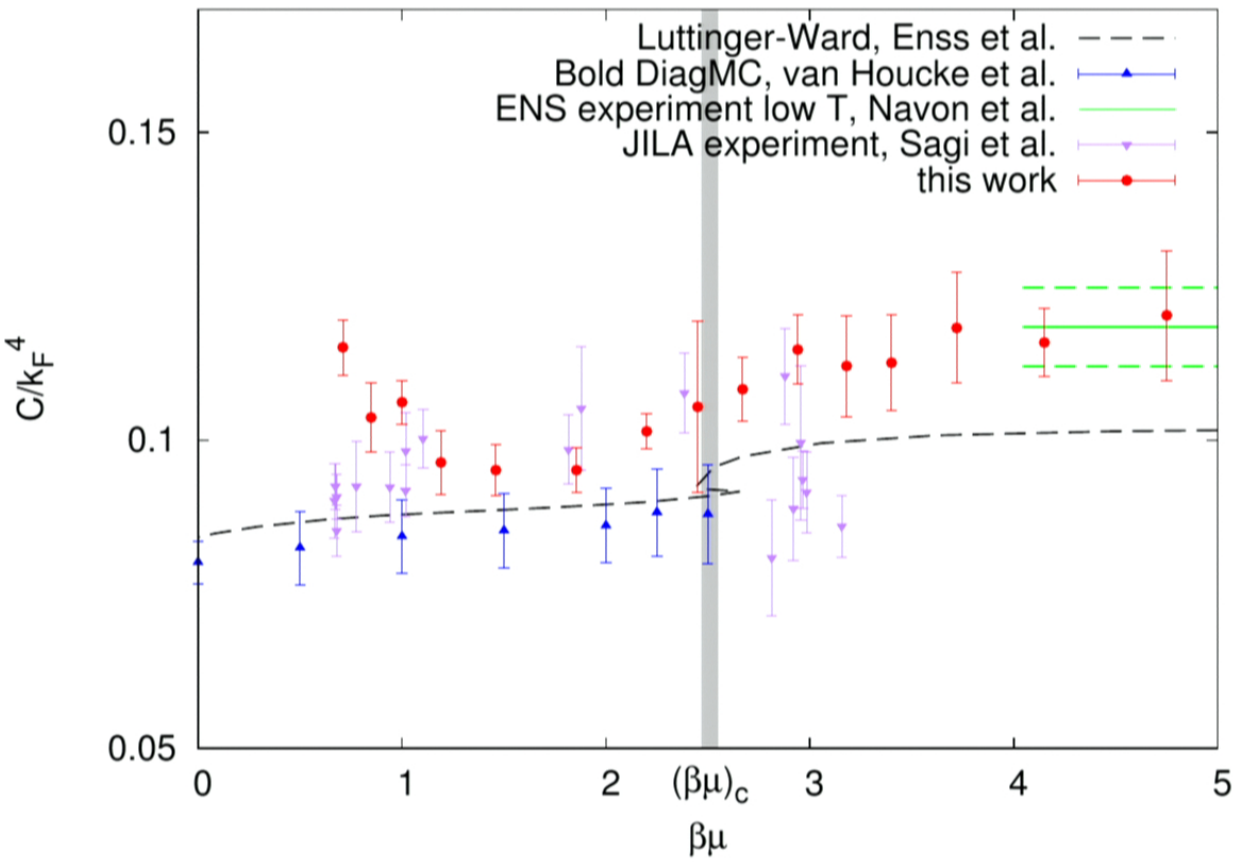
$$C = m^2 g_0 E_{\text{int}},$$

where g_0 is the physical coupling constant.

The contact density is $\mathcal{C} = C/V$ and has units k_F^4.

Expressed through lattice quantities: $\mathcal{C}/k_F^4 = \frac{UE_{\text{int}}}{4L^3 k_F^4}$

Results: Contact density



Summary

- First principles study of the unitary Fermi gas with a Diagrammatic Monte Carlo algorithm
- Precise calculation of the critical temperature
- Generalisation to temperatures above and below T_c
- Temperature dependence of the chemical potential, the contact density and the energy density