The Imbalanced Fermi Gas at Unitarity

Olga Goulko
in collaboration with Matthew Wingate

DAMTP, University of Cambridge

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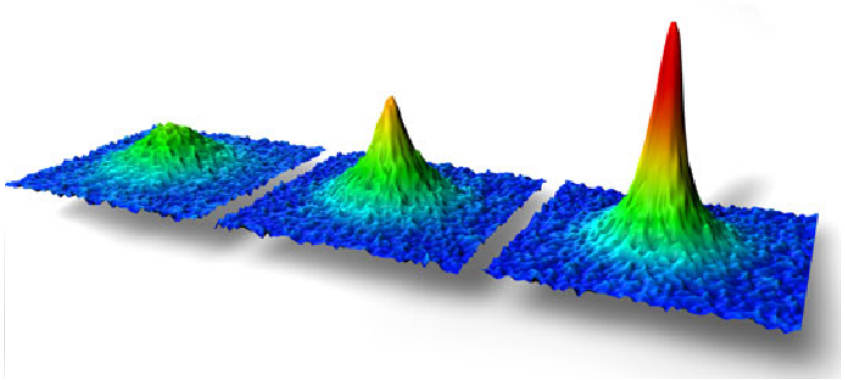
What is a Fermi gas?

A Fermi gas is a dilute system of fermions

Examples:

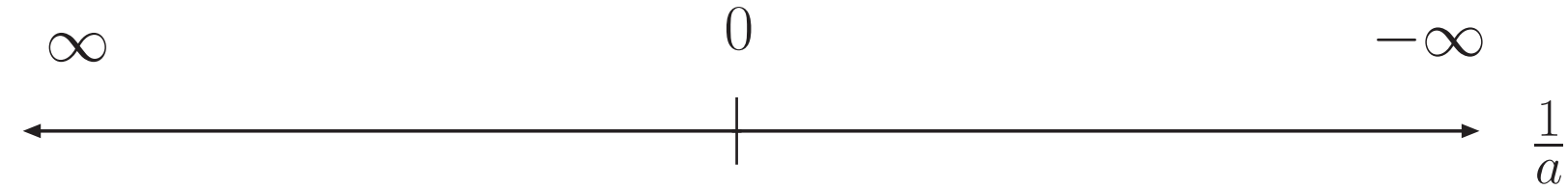
- electrons inside a metal
- quark-gluon plasma in the inner core of a neutron star
- atomic gas e.g. of ^{40}K or ^{6}Li atoms ($\Rightarrow$ experiment!)

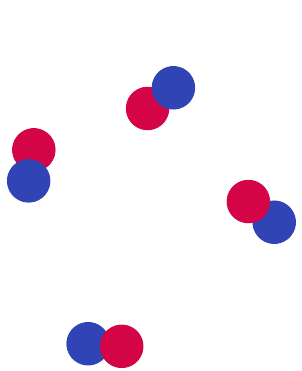


low temperature: quantum phenomena become important
identical fermions $\Rightarrow$ no s-wave scattering $\Rightarrow$ ideal gas model

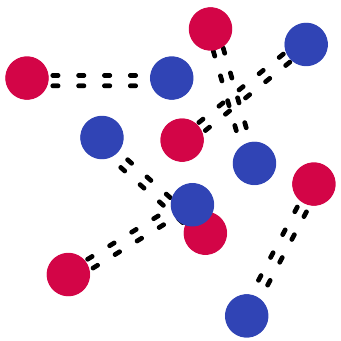
What is a unitary Fermi gas?

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

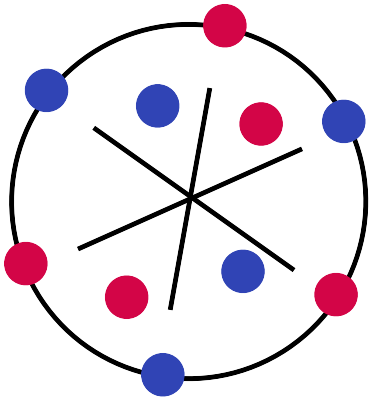




BEC regime
strongly bound
(bosonic) molecules
of two fermions



UNITARITY
strongly
interacting
fermions



BCS regime
pairs of fermions
weakly bound in
momentum space

What is interesting about unitarity?

- System is dilute (range of potential $\ll$ interparticle distance) and strongly interacting (interparticle distance $\ll$ scattering length) at the same time
- No length scales associated with interactions $\Rightarrow$ universal behaviour
- Only relevant parameters: temperature and density
- High-temperature superfluidity

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

- Experimental data available

What is interesting about unitarity?

Strong interactions $\Rightarrow$ No small parameter for perturbation theory

No exact theory for 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

Our project: Calculating the critical temperature of the imbalanced unitary Fermi gas with the Determinant Diagrammatic Monte Carlo (DDMC) algorithm [Burovski et al. cond-mat/0605350v2]

The Fermi-Hubbard model

Simplest lattice model for two-particle scattering

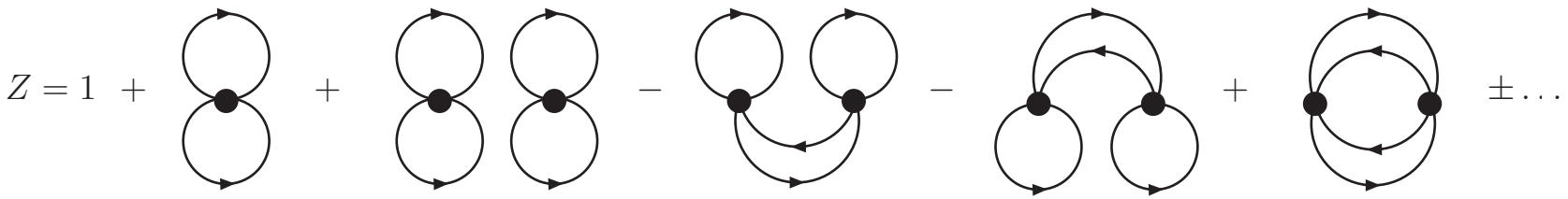
- Non-relativistic fermions
- Contact interaction between spin up and spin down
- On-site attraction $U < 0$ tuned to describe unitarity
- Grand canonical ensemble
- Finite 3D simple cubic lattice, periodic boundary conditions
- Continuum limit can be taken by extrapolation to zero density

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

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 et al. cond-mat/0411344]

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

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 $P^\dagger$:

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

At the critical point the correlation function

$$G_2(\mathbf{x}\tau;\mathbf{x}'\tau') = \left\langle \mathbf{T}_\tau P(\mathbf{x},\tau)P^\dagger(\mathbf{x}',\tau') \right\rangle = \frac{1}{Z}\mathrm{Tr}\mathbf{T}_\tau P(\mathbf{x},\tau)P^\dagger(\mathbf{x}',\tau')e^{-\beta H}$$

is proportional to $|\mathbf{x}-\mathbf{x}'|^{-(1+\eta)}$ as $|\mathbf{x}-\mathbf{x}'| \to \infty$
(in 3 spatial dimensions, where $\eta \approx 0.038$ for U(1) universality class)

Order parameter of the phase transition

$\Rightarrow$ the rescaled integrated correlation function

$$R(L,T) = L^{1+\eta}\overline{G_2(\mathbf{x}\tau;\mathbf{x}'\tau')}$$

becomes independent of lattice size at the critical point

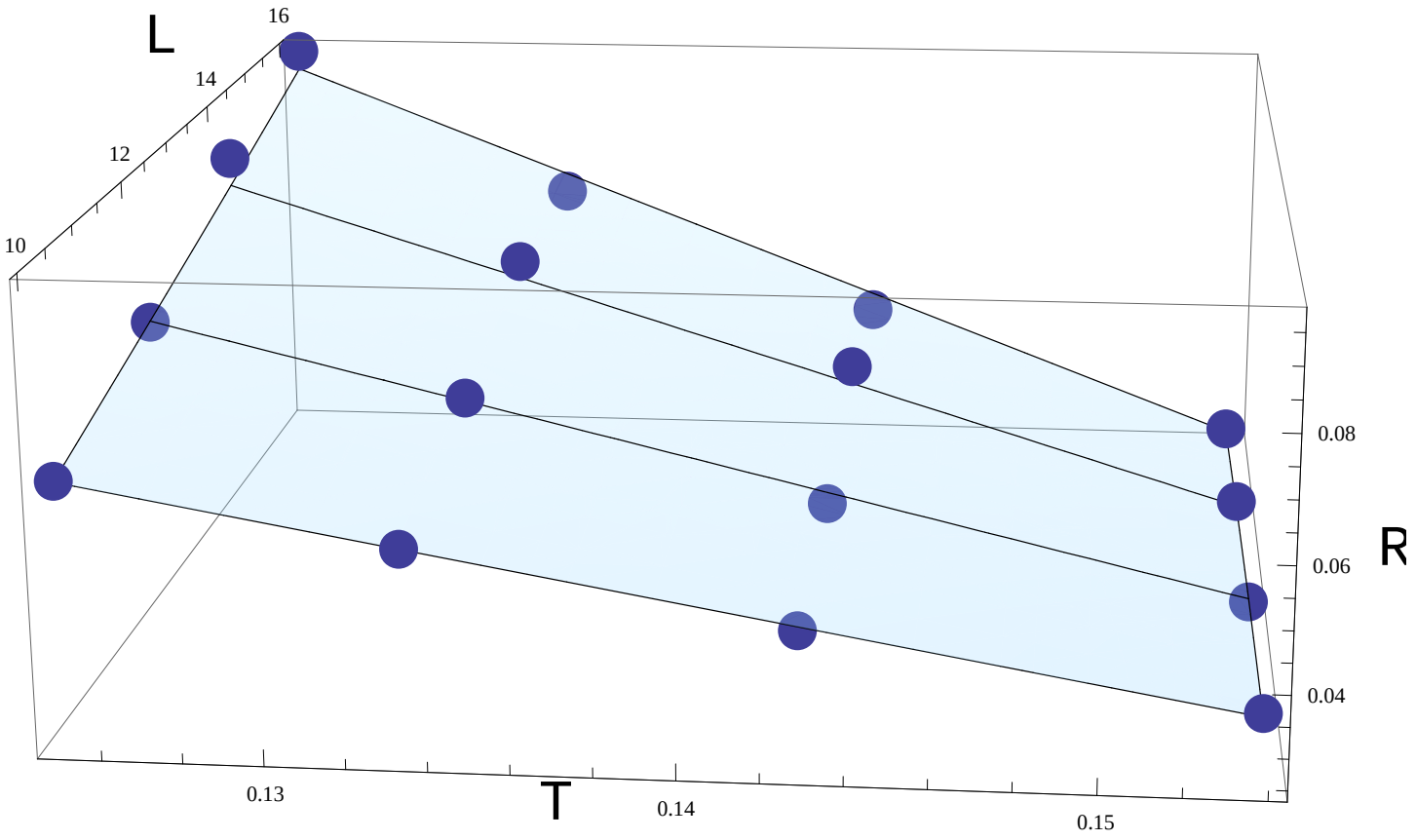
Finite-size corrections:

$$R(L,T) = \underbrace{(f_0 + f_1(T-T_c)L^{1/\nu_\xi} + \ldots)}_{\text{universal scaling function}}\underbrace{(1 + cL^{-\omega} + \ldots)}_{\text{finite-size scaling}}$$

- Critical exponents for the U(1) universality class: $\nu_\xi \approx 0.67$ and $\omega \approx 0.8$
- Non-universal constants to be determined: T_c, f_0, f_1, c (to first order)

Order parameter of the phase transition

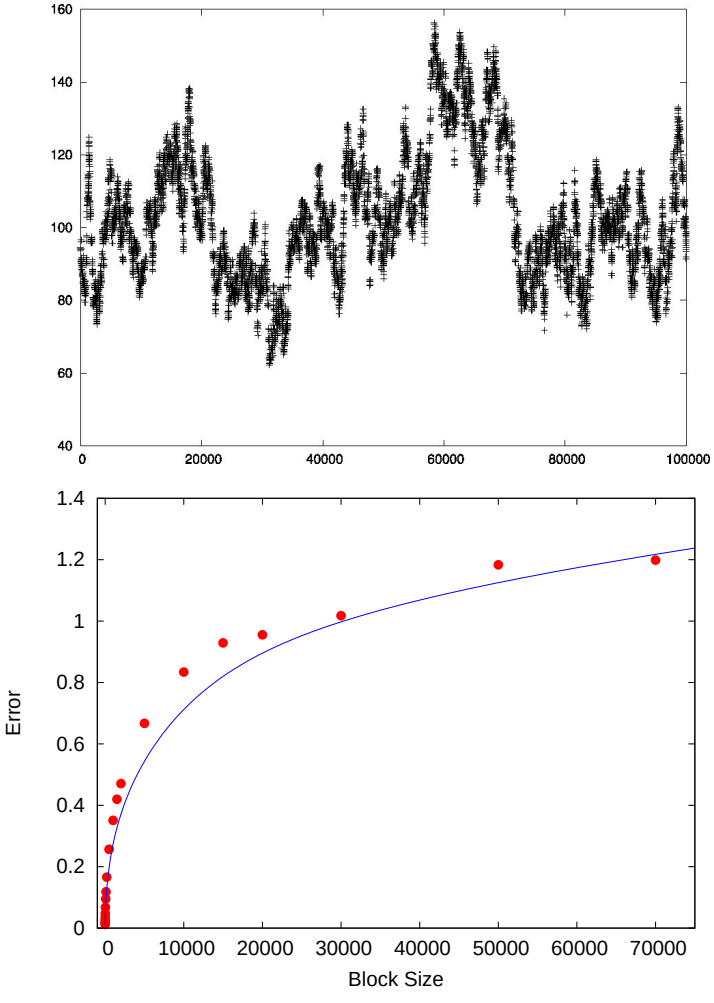
Example: fit of the rescaled integrated correlator $R(L, T)$



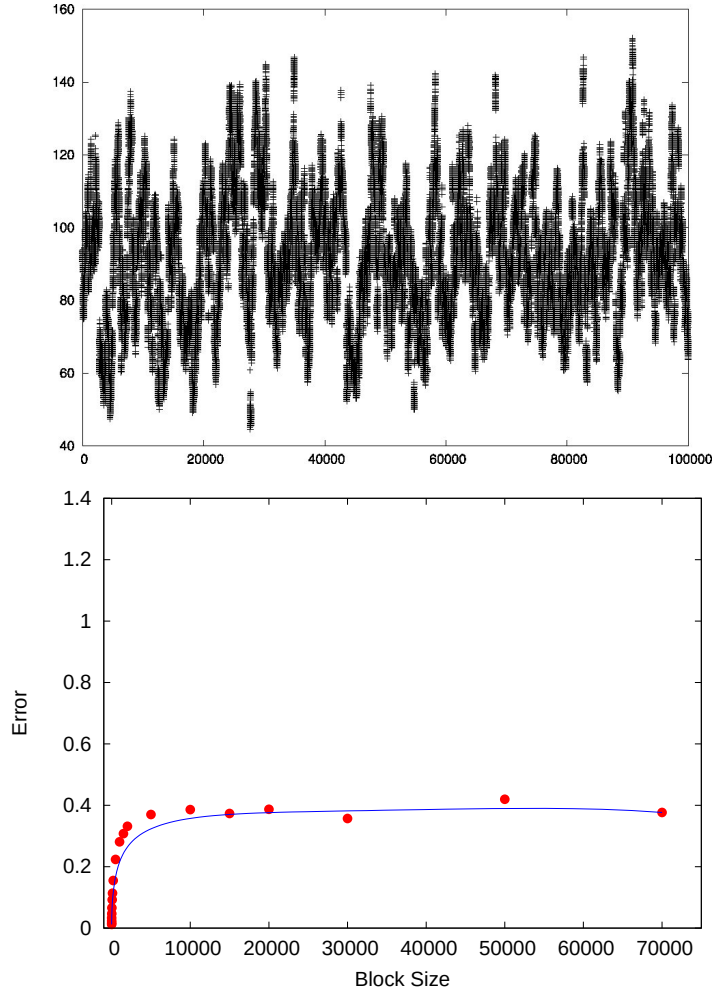
(data taken at 4 different temperatures and 4 different lattice sizes)

Autocorrelations

The original worm algorithm achieved high acceptance ratios, but at the cost of strongly autocorrelated results:



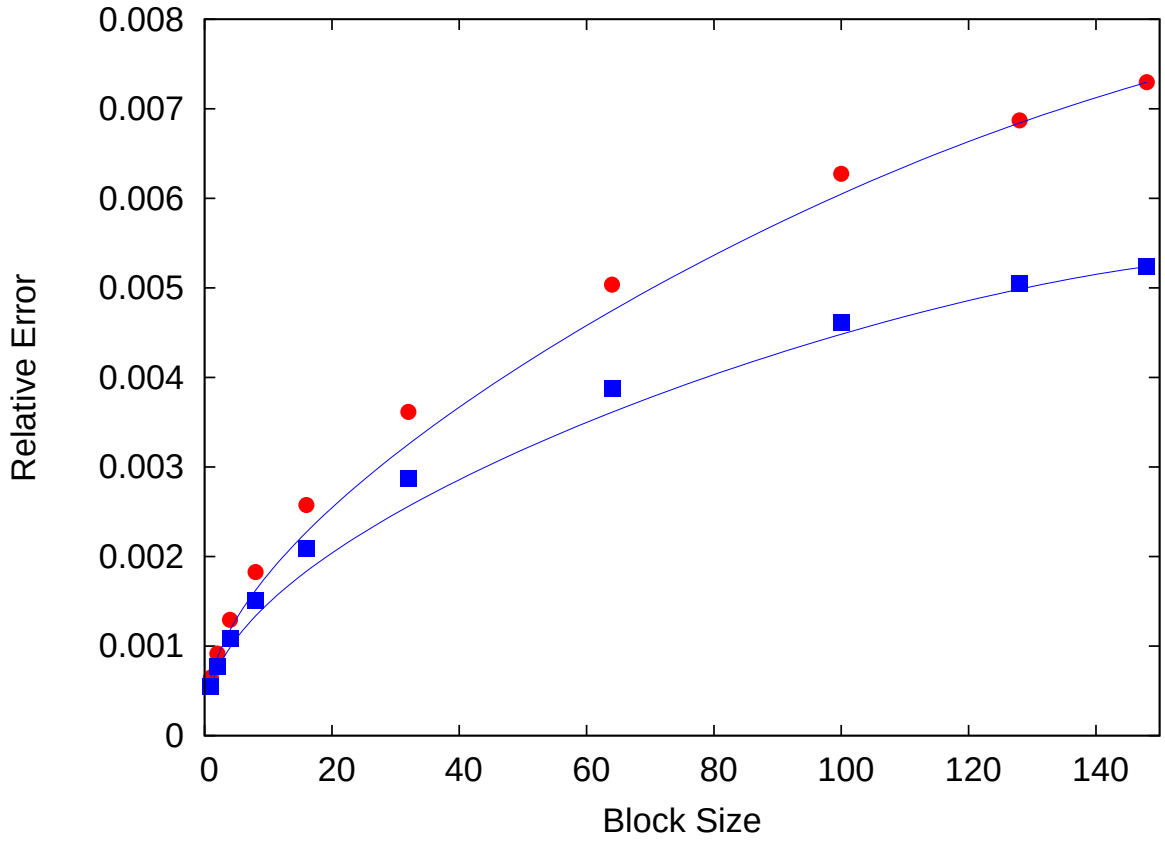
Worm updates



Diagonal updates

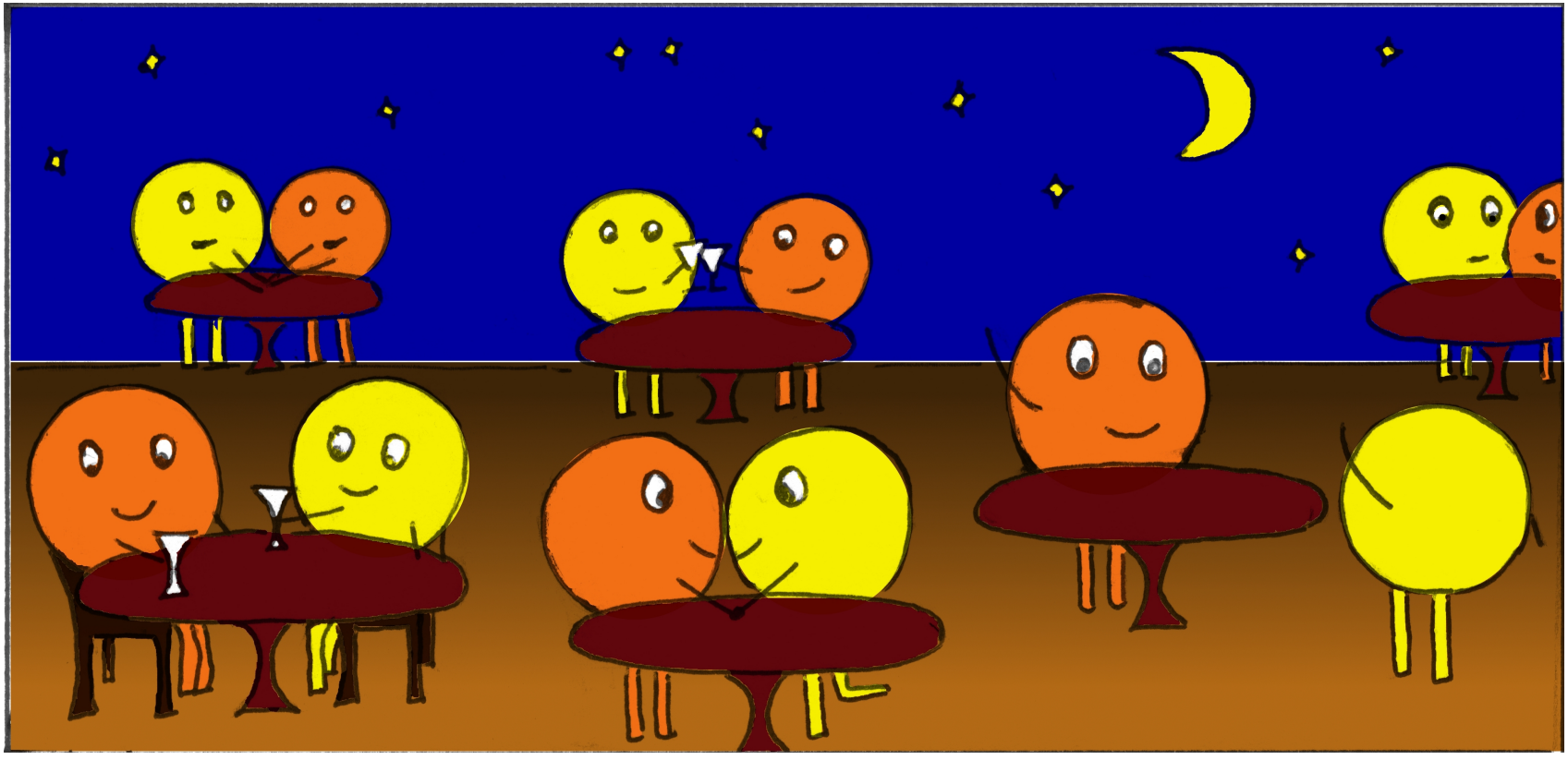
Alternative updates

Alternative set of updates: both weak autocorrelations and high acceptance rates [Goulko and Wingate, arXiv:0910.3909].



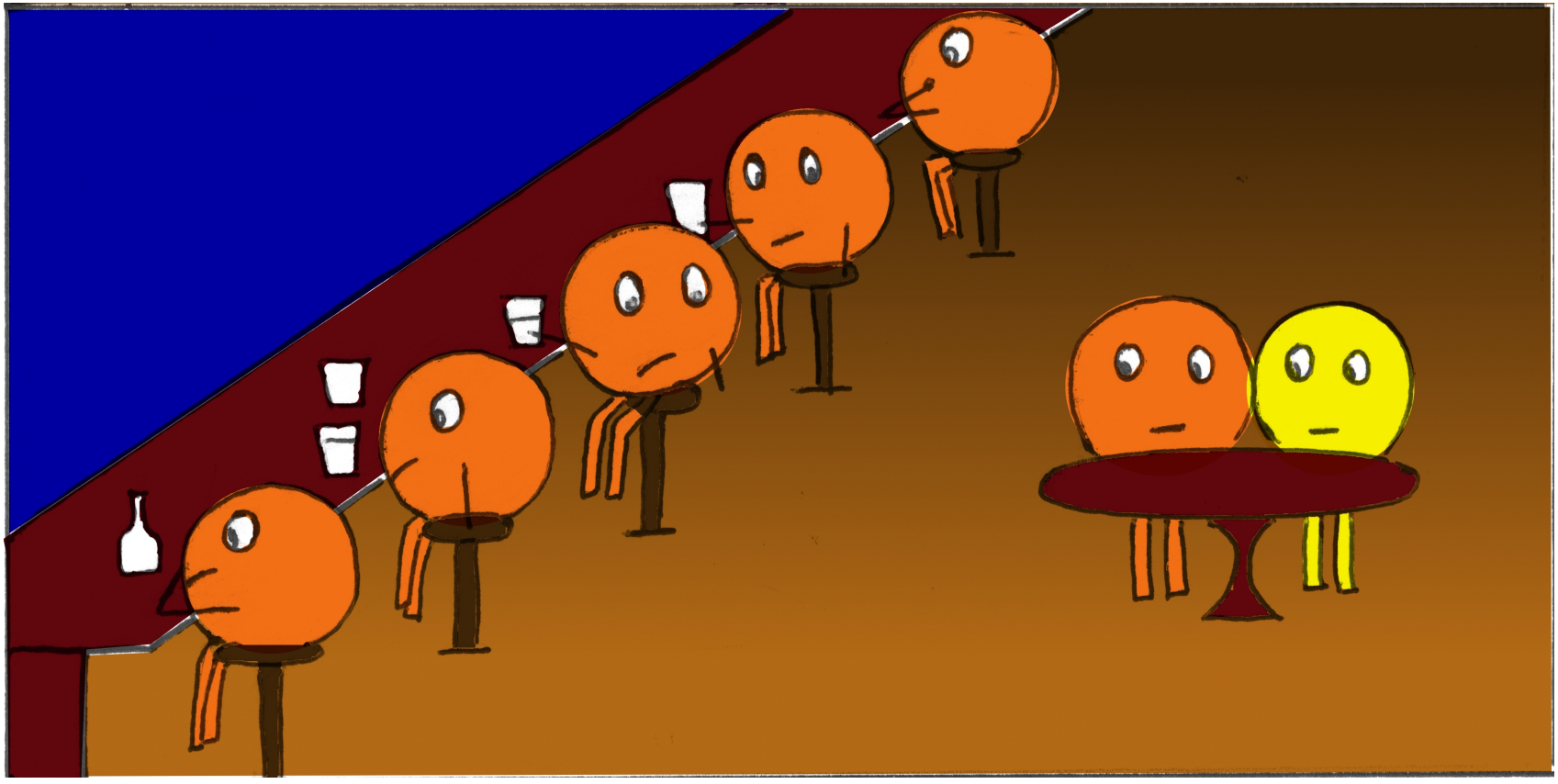
Comparison between diagonal setup (red circles) and alternative worm setup (blue squares) at low filling factor

The balanced Fermi gas



An interacting system with equal number of spin up and spin down fermions ($\mu_\uparrow = \mu_\downarrow$)

The imbalanced Fermi gas



Interactions are suppressed in presence of an imbalance ($\mu_\uparrow \neq \mu_\downarrow$)

The imbalanced Fermi gas

Thermal probability distribution:

$$\rho(S_p) = \frac{1}{Z}(-U)^p \det \mathbf{A}^{\uparrow}(S_p) \det \mathbf{A}^{\downarrow}(S_p)$$

Sign problem: $\mu_{\uparrow} \neq \mu_{\downarrow} \Rightarrow \det \mathbf{A}^{\uparrow} \det \mathbf{A}^{\downarrow} \neq |\det \mathbf{A}|^2$

Sign quenched method: write $\rho(S_p) = |\rho(S_p)|\text{sign}(S_p)$ and use $|\rho(S_p)|$ as the new probability distribution

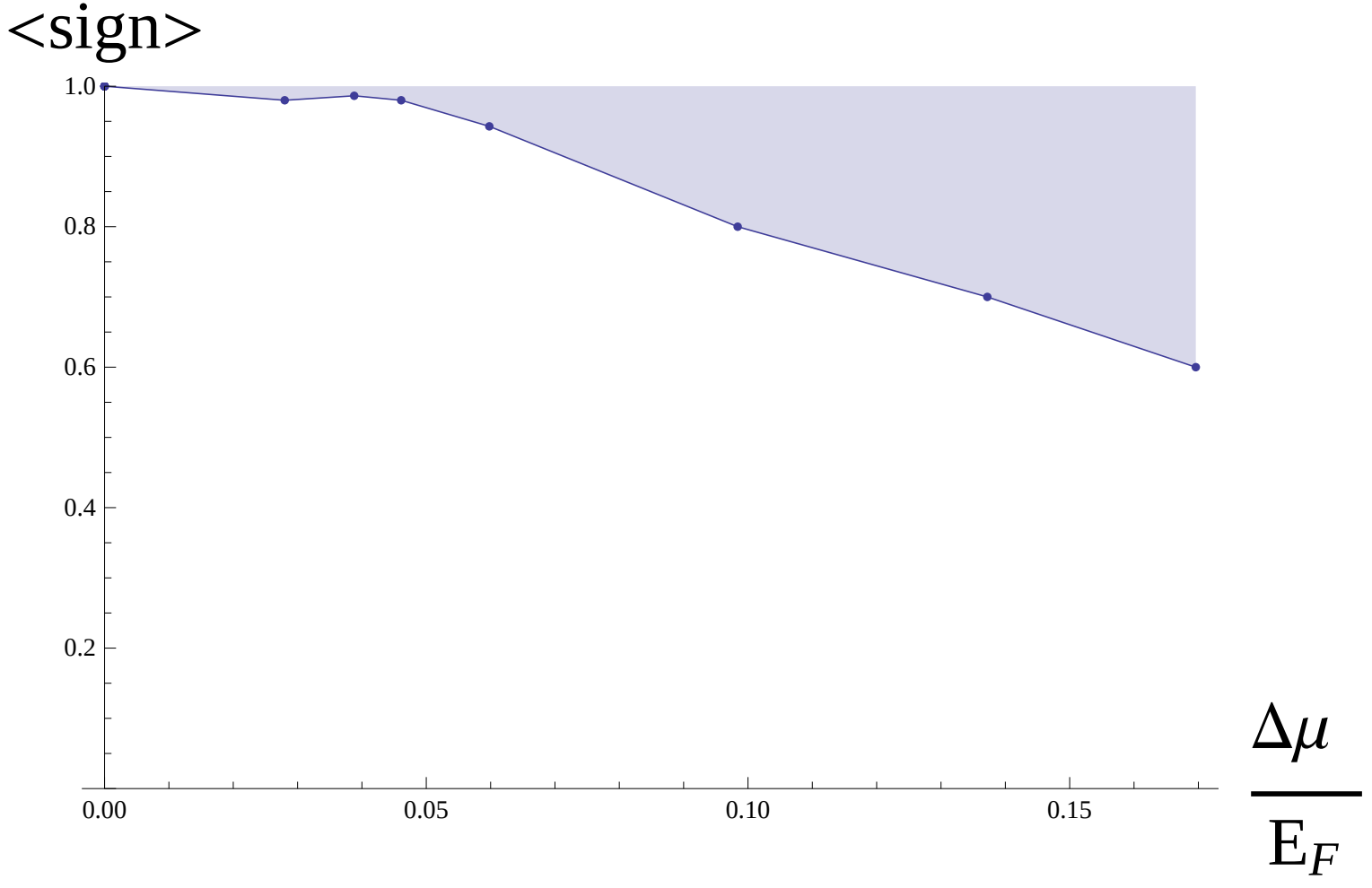
$$\langle X \rangle_{\rho} = \frac{\sum X(S_p)\rho(S_p)}{\sum \rho(S_p)} = \frac{\sum X(S_p)|\rho(S_p)|\text{sign}(S_p)}{\sum |\rho(S_p)|\text{sign}(S_p)} = \frac{\langle X\text{sign} \rangle_{|\rho|}}{\langle \text{sign} \rangle_{|\rho|}}$$

Problems can arise if $\langle \text{sign} \rangle \approx 0$

But for the unitary Fermi gas $\langle \text{sign} \rangle_{|\rho|} \approx 1$ for a wide range of $\Delta\mu$

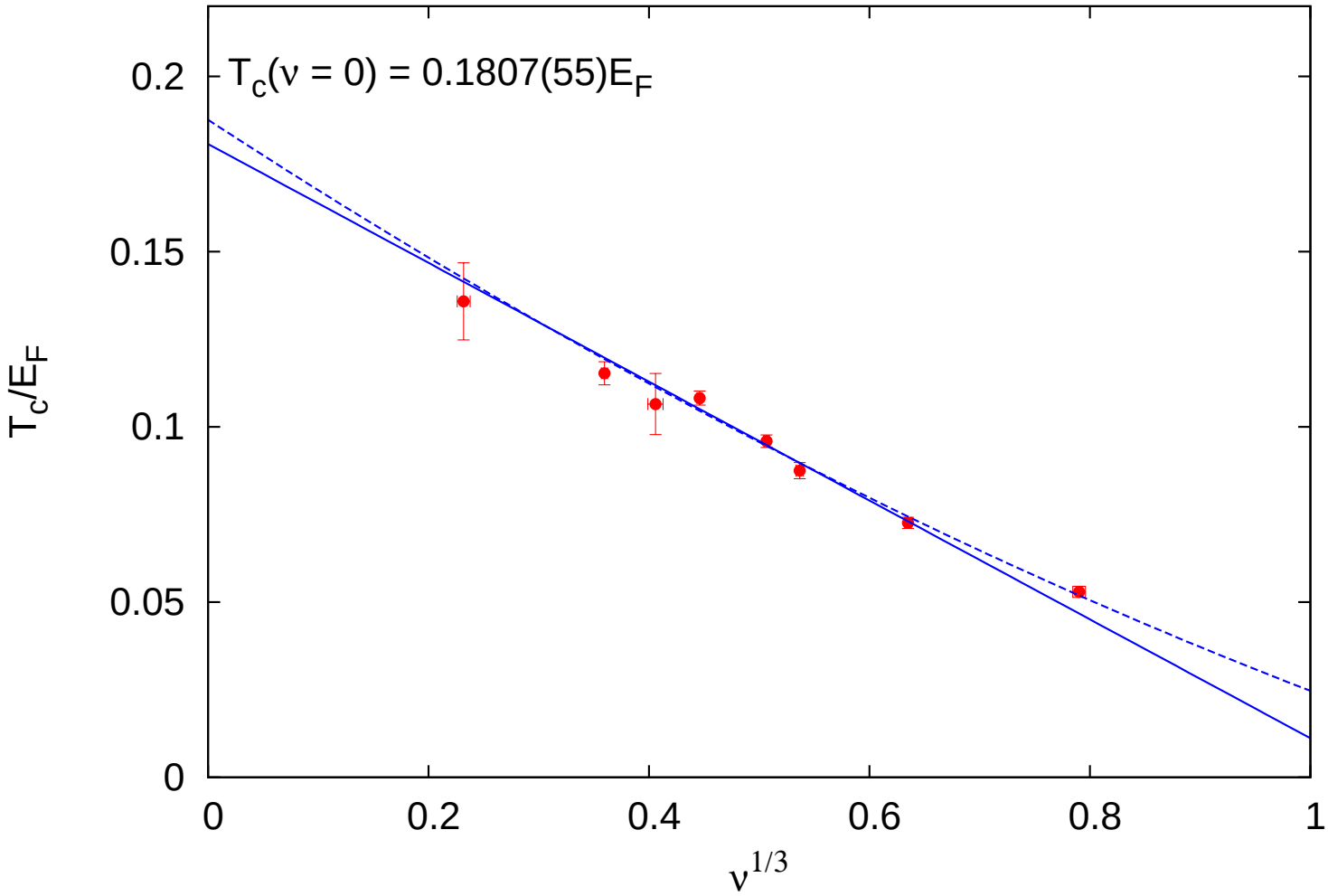
The imbalanced Fermi gas

Schematic plot of the average sign at the critical point and at the largest lattice size used



Results

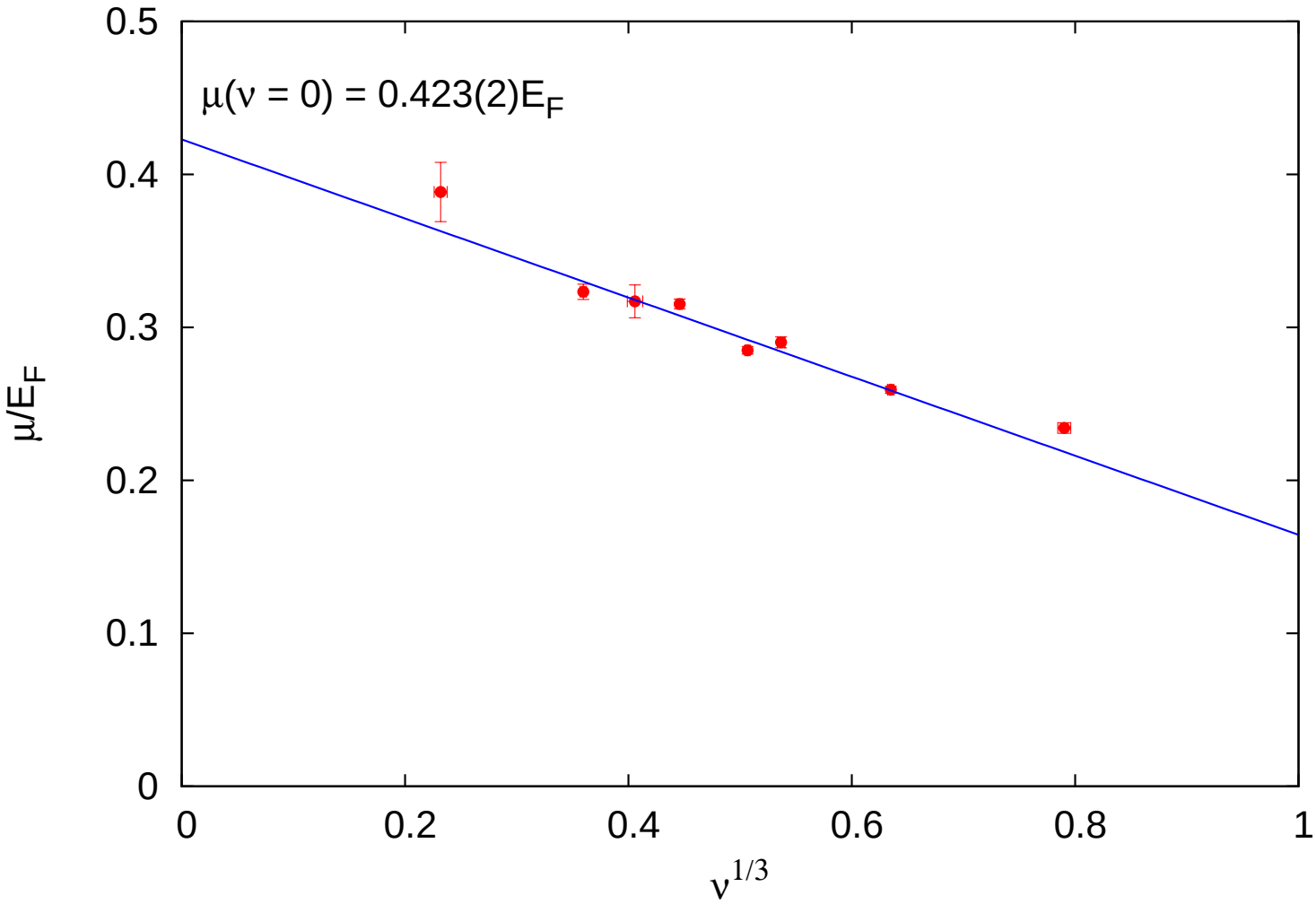
Reproducing the critical temperature in the balanced case



$\nu \longrightarrow 0$ corresponds to the continuum limit

Results

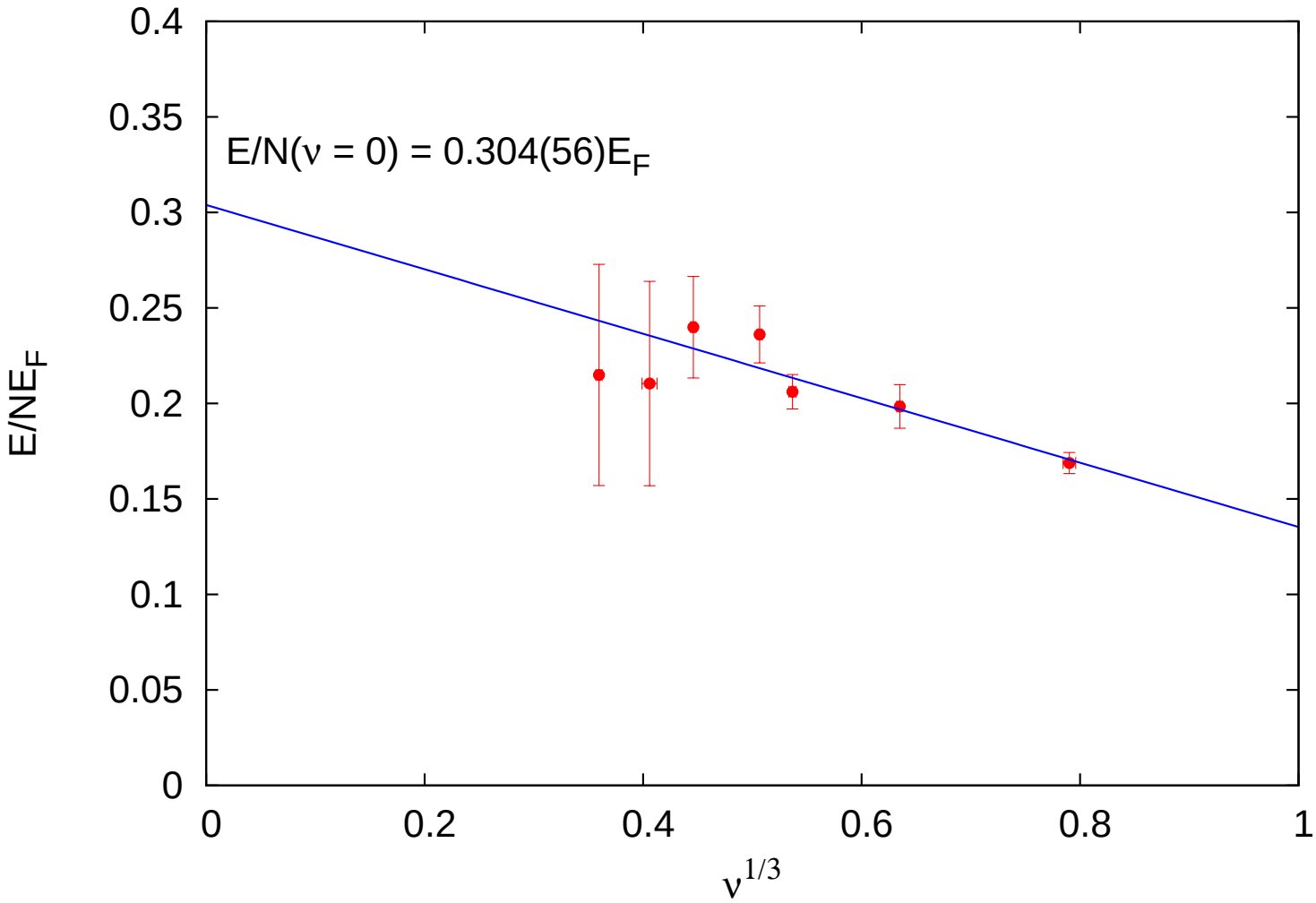
The chemical potential in the balanced case



$\nu \longrightarrow 0$ corresponds to the continuum limit

Results

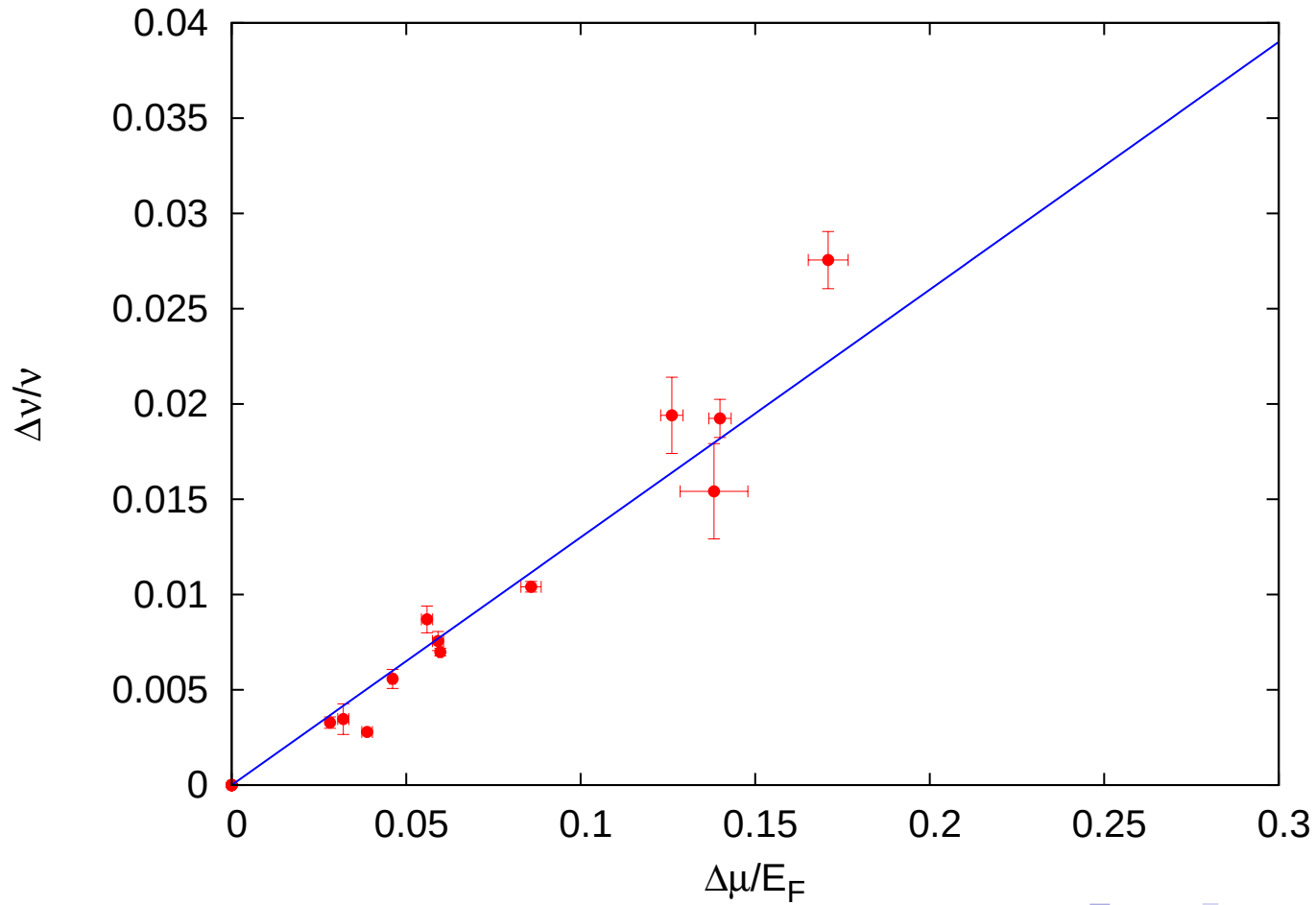
The energy per particle in the balanced case



$\nu \longrightarrow 0$ corresponds to the continuum limit

Results

Relationship between $\Delta\mu/E_F = |\mu_\uparrow - \mu_\downarrow|/E_F$ and $\delta\nu/\nu = |\nu_\uparrow - \nu_\downarrow|/(\nu_\uparrow + \nu_\downarrow)$



Results

Surface fit of the critical temperature as a function of filling factor $\nu^{1/3}$ and imbalance $h = \Delta\mu/E_F$.

- At fixed imbalance the critical temperature is a linear function of $\nu^{1/3}$, with slope $\alpha(h)$.
- $T_c(h)$ and $\alpha(h)$ viewed as functions of the imbalance h are analytic and can thus be Taylor expanded.
- Due to symmetry in h all odd powers in the Taylor expansion of $T_c(h)$ have to vanish.

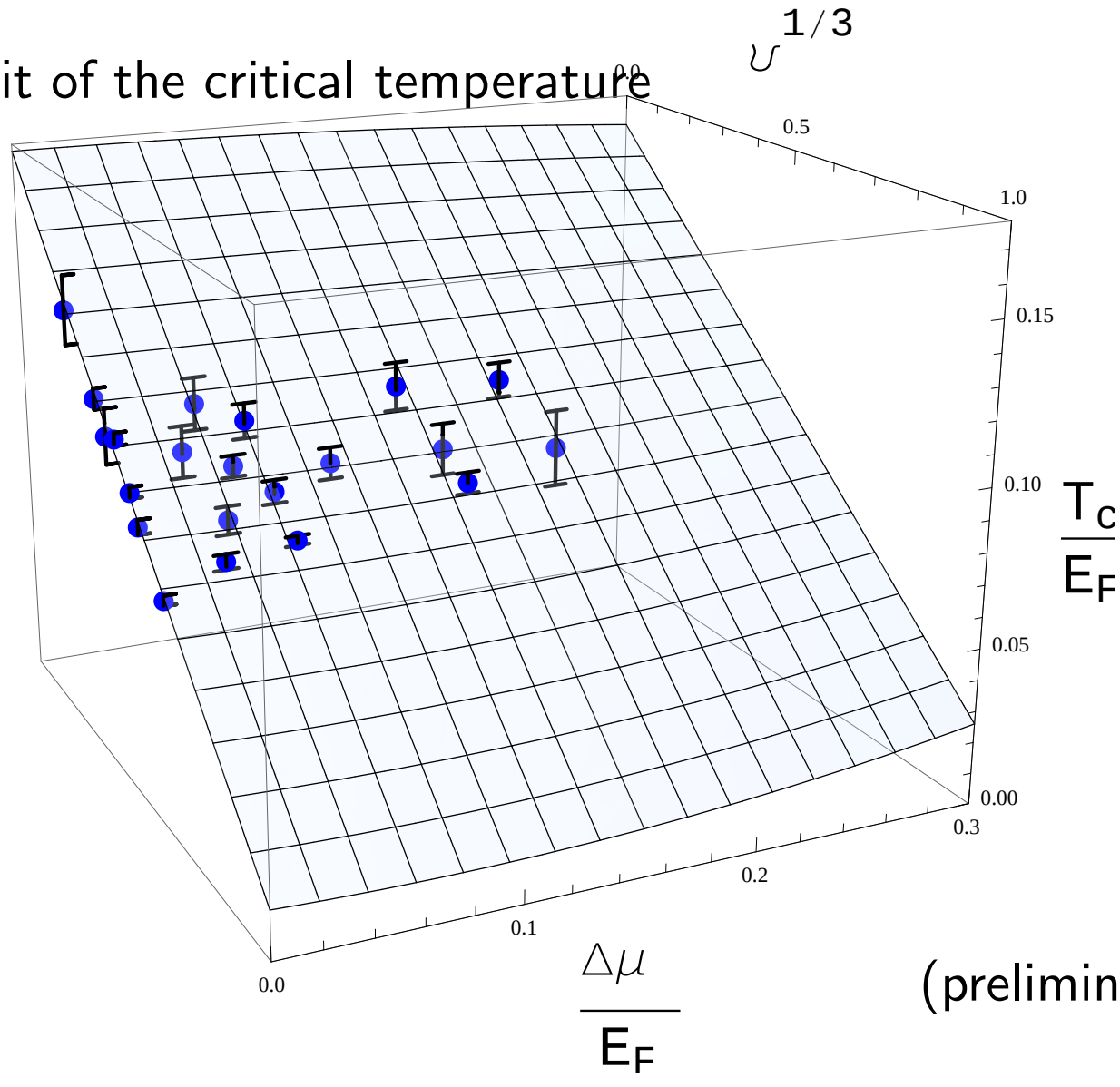
Hence the fitted function takes the form

$$T_c(\nu, h) = T_c(h) + \alpha(h)\nu^{1/3}$$

We will expand the functions $T_c(h)$ and $\alpha(h)$ to second order in h.

Results

Surface fit of the critical temperature



(preliminary data)

Conclusions

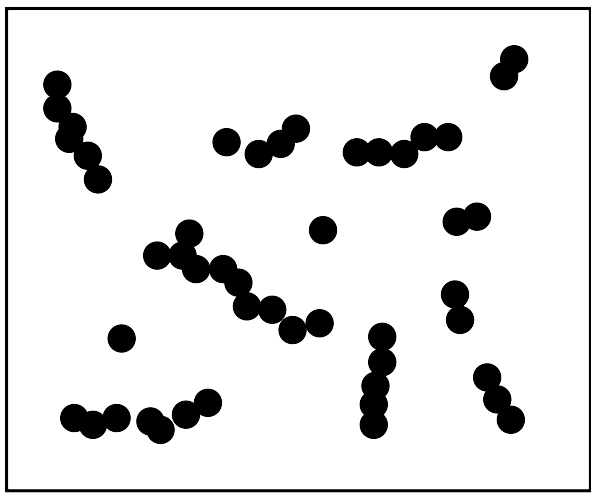
- Lattice Field Theory is a useful tool for studying strongly interacting systems in condensed matter physics
- The DDMC algorithm can be applied to calculate the critical temperature of the Fermi gas at unitarity
- Result for the balanced case: $T_c/E_F = 0.1807(55)E_F$
- Imbalanced case with the sign quenched method

Thank you!

Bonus slides

Bonus slides: Diagrammatic Monte Carlo

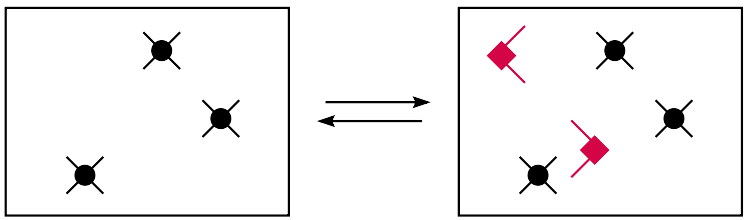
- sampling via a Monte Carlo Markov chain process
- the configuration space is extended $\longrightarrow$ worm vertices



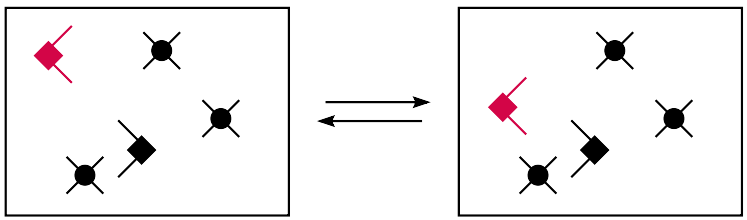
- physical picture: at low densities multi-ladder diagrams dominate
- updates designed to favour prolonging existing vertex chains

Bonus slides: The worm updates

Updates only concerning the worm vertices:



Worm creation/annihilation: insert/remove the pair $P(\mathbf{x}, \tau)$, $P^\dagger(\mathbf{x}', \tau')$ into/from the configuration

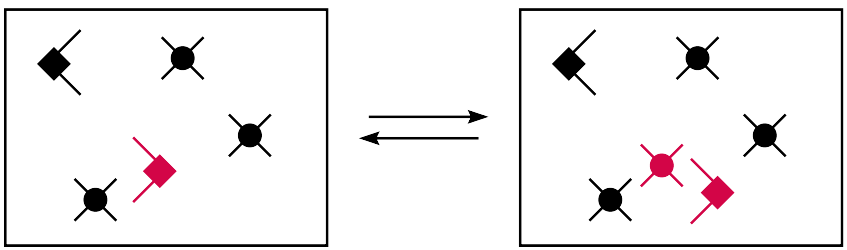


Worm shift: Shift the $P^\dagger(\mathbf{x}', \tau')$ vertex to other coordinates

Bonus slides: The worm updates

Updates of the regular 4-point vertices: **adding/removing a 4-point vertex** (changes the diagram order)

- Diagonal version: add or remove a random vertex
- Alternative using worm: move the $P(\mathbf{x}, \tau)$ vertex to another position and insert a 4-point vertex at its old position.
  $\Rightarrow$ choose new coordinates of P very close to its initial coordinates
  $\Rightarrow$ the removal update always attempts to remove the nearest neighbour of P



Bonus slides: Alternative updates

Combine the advantages of the diagonal setup (weak autocorrelations) with the ones of the worm setup (high acceptance ratios)

- Choose a random 4-point vertex from the configuration (will act as a worm for this step).
- Addition: add another 4-point vertex on the same lattice site and in some time interval around the worm.
- Removal: remove the nearest neighbour of the worm vertex

This setup still prolongs existing vertex chains, but autocorrelations are reduced since the worm changes with every update.