The Imbalanced Fermi Gas at Unitarity

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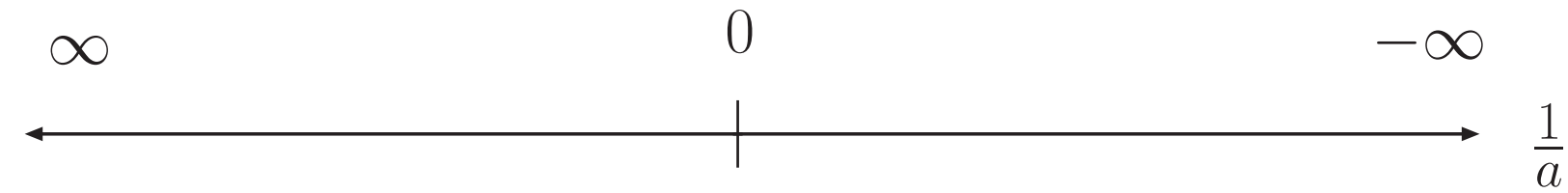
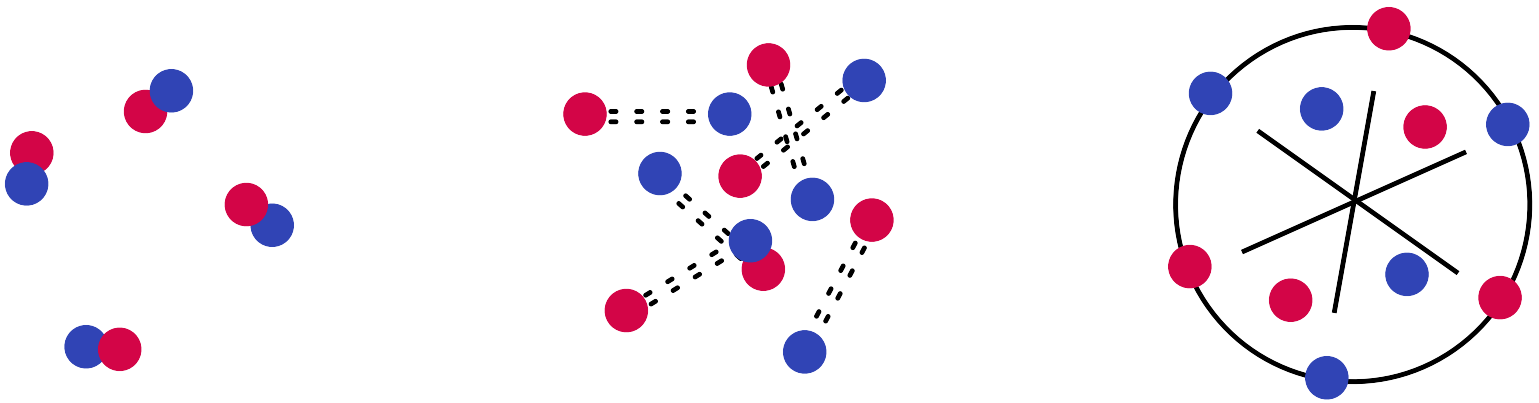
The unitary Fermi gas

Interacting system of two-component fermions:
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

Methods to study 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, Prokof'ev, Svistunov, Troyer (2006)]

The Fermi-Hubbard model

Simplest lattice model for two-particle scattering

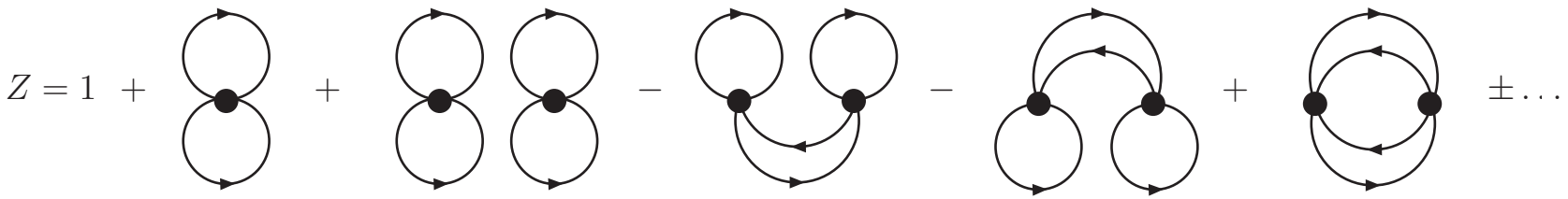
- Non-relativistic fermions
- Contact interaction between spin up and spin down
- On-site attraction $U < 0$ tuned to describe unitarity
- Grand canonical ensemble
- Finite 3D simple cubic lattice, periodic boundary conditions
- Continuum limit can be taken by extrapolation to zero density

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

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 $P^\dagger$:

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

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

Crossing of $R(L,T)$ curves for 2 lattice sizes L_i, L_j:

$$R(L_i, T_{ij}) = R(L_j, T_{ij}) \Rightarrow T_{ij} - T_c = \text{const.} \cdot g(L_i, L_j)$$

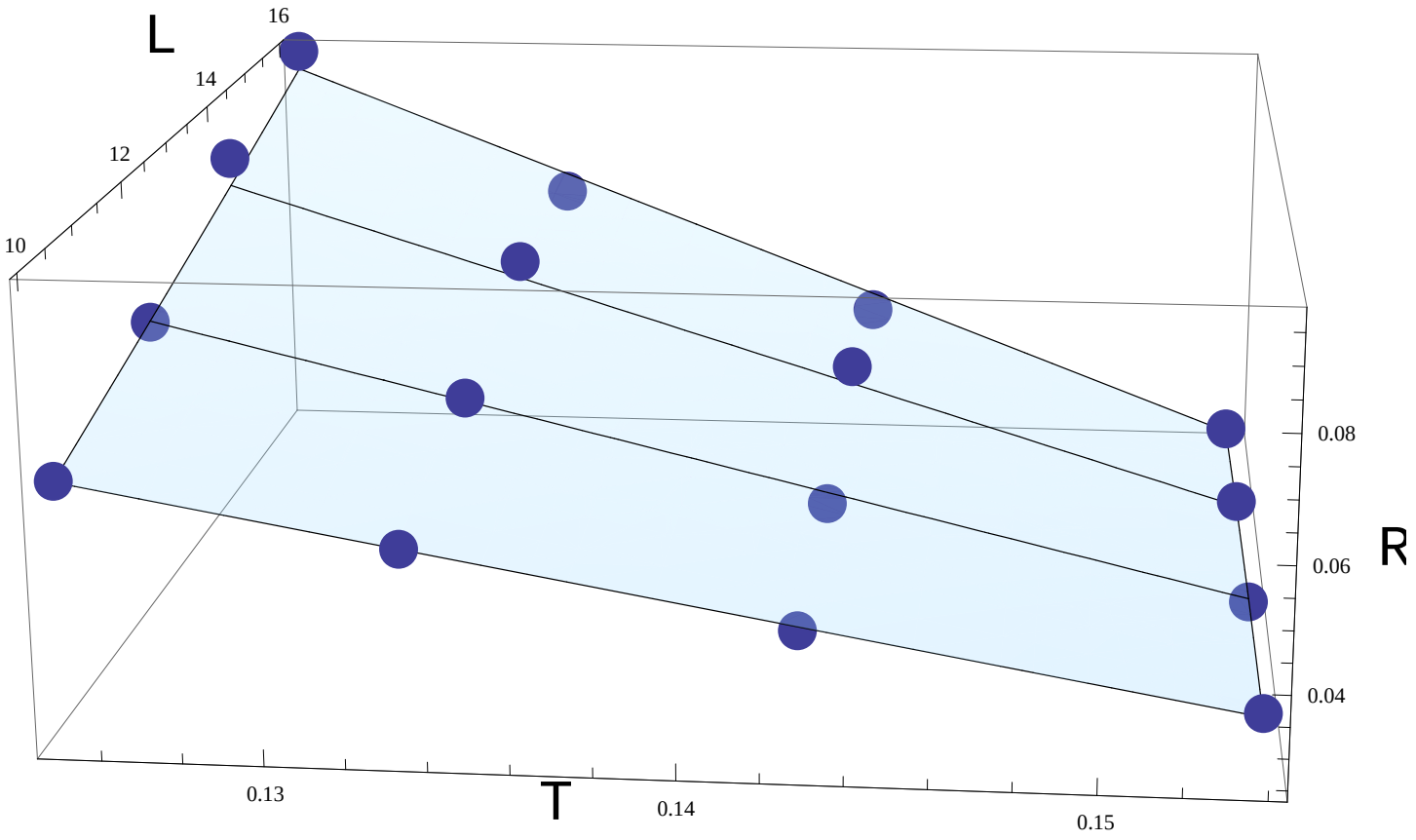
with

$$g(L_i, L_j) = \frac{(L_j/L_i)^{\omega} - 1}{L_j^{\frac{1}{\nu_\xi}+\omega}\left(1 - (L_i/L_j)^{\frac{1}{\nu_\xi}}\right) + \underbrace{cL_j^{\frac{1}{\nu_\xi}}\left(1 - (L_i/L_j)^{\frac{1}{\nu_\xi}-\omega}\right)}_{\text{neglect?}}}$$

c can take values of $O(1) \Rightarrow$ perform non-linear fit to 4 parameters instead

Order parameter of the phase transition

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

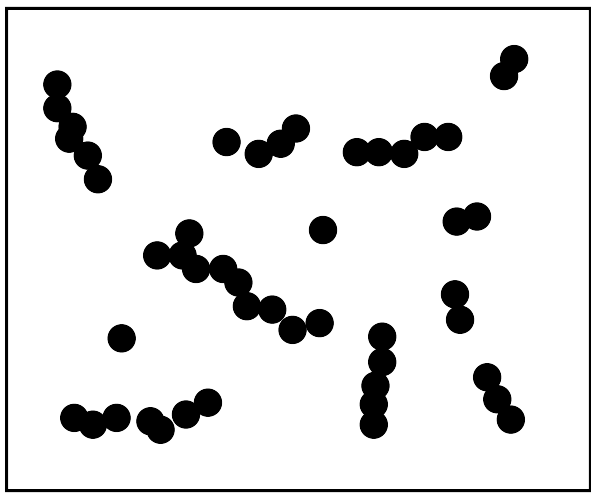


(data taken at 4 different temperatures and 4 different lattice sizes)

Diagrammatic Monte Carlo

Burovski et al. (2006):

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

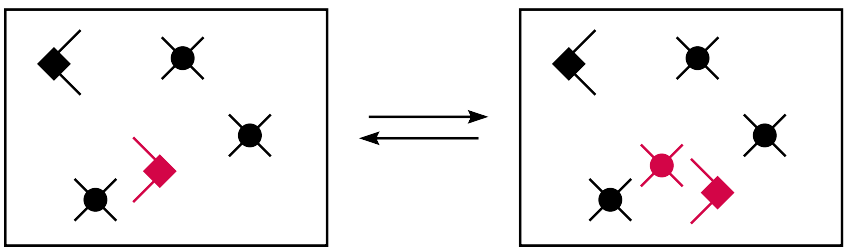


- physical picture: at low densities multi-ladder diagrams dominate
- updates designed to favour prolonging existing vertex chains

The worm updates

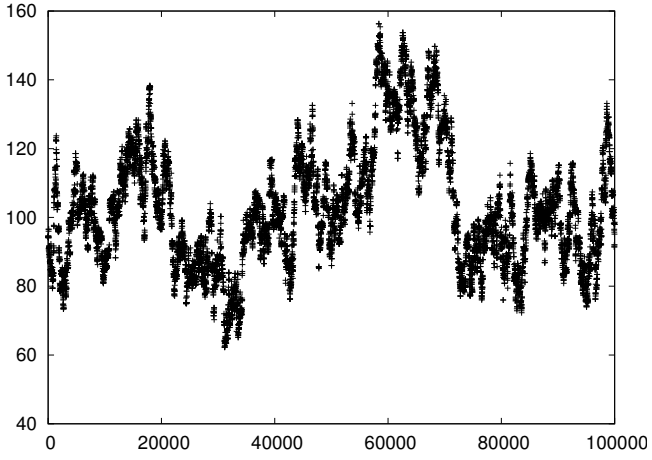
Updates of the regular 4-point vertices: **adding/removing a 4-point vertex** (changes the diagram order)

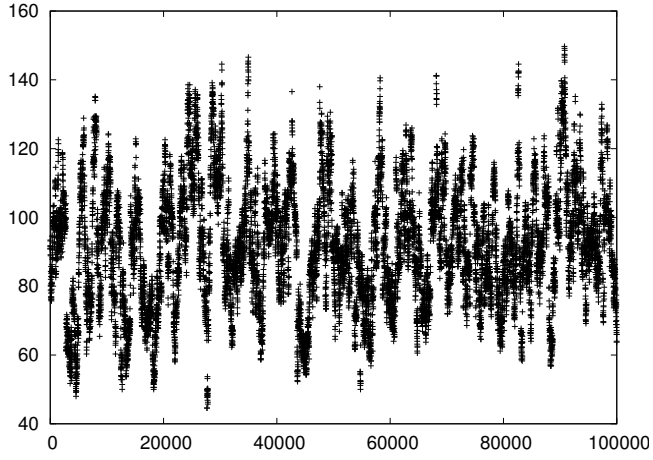
- Diagonal version: add or remove a random vertex
- Alternative using worm: move the $P(\mathbf{x}, \tau)$ vertex to another position and insert a 4-point vertex at its old position.
  $\Rightarrow$ choose new coordinates of P very close to its initial coordinates
  $\Rightarrow$ the removal update always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

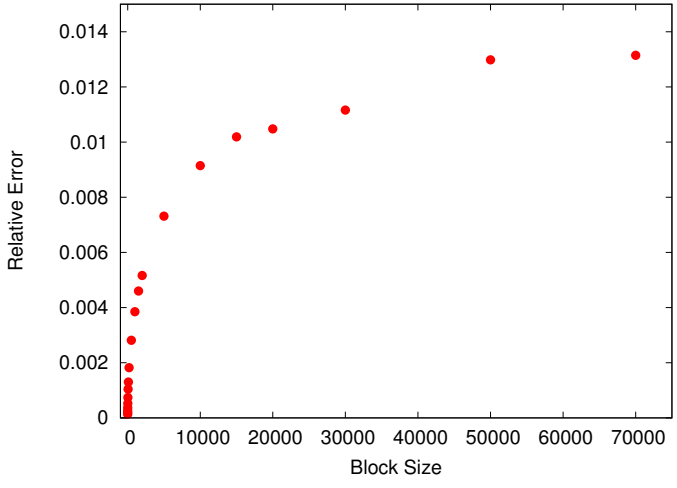


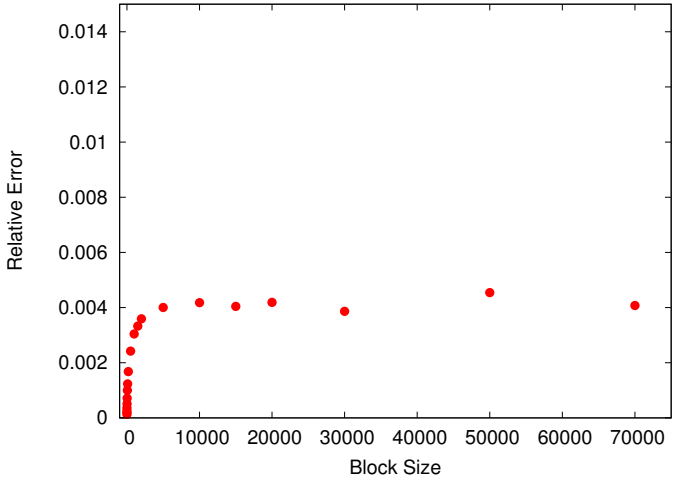
Autocorrelations

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









Worm updates

Diagonal updates

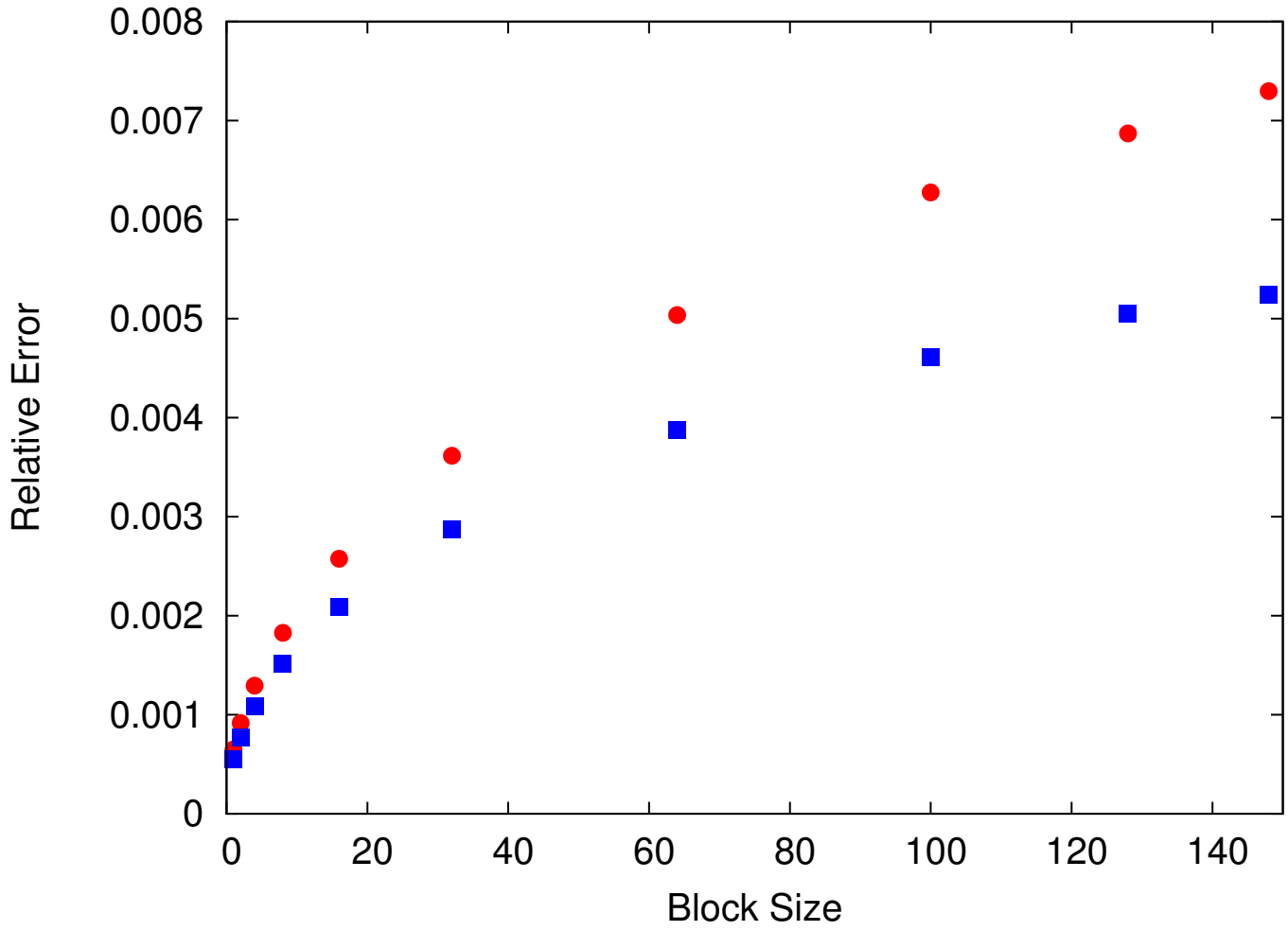
Alternative updates

Alternative set of updates: both weak autocorrelations and high acceptance rates [Goulko and Wingate (2009)].

- 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

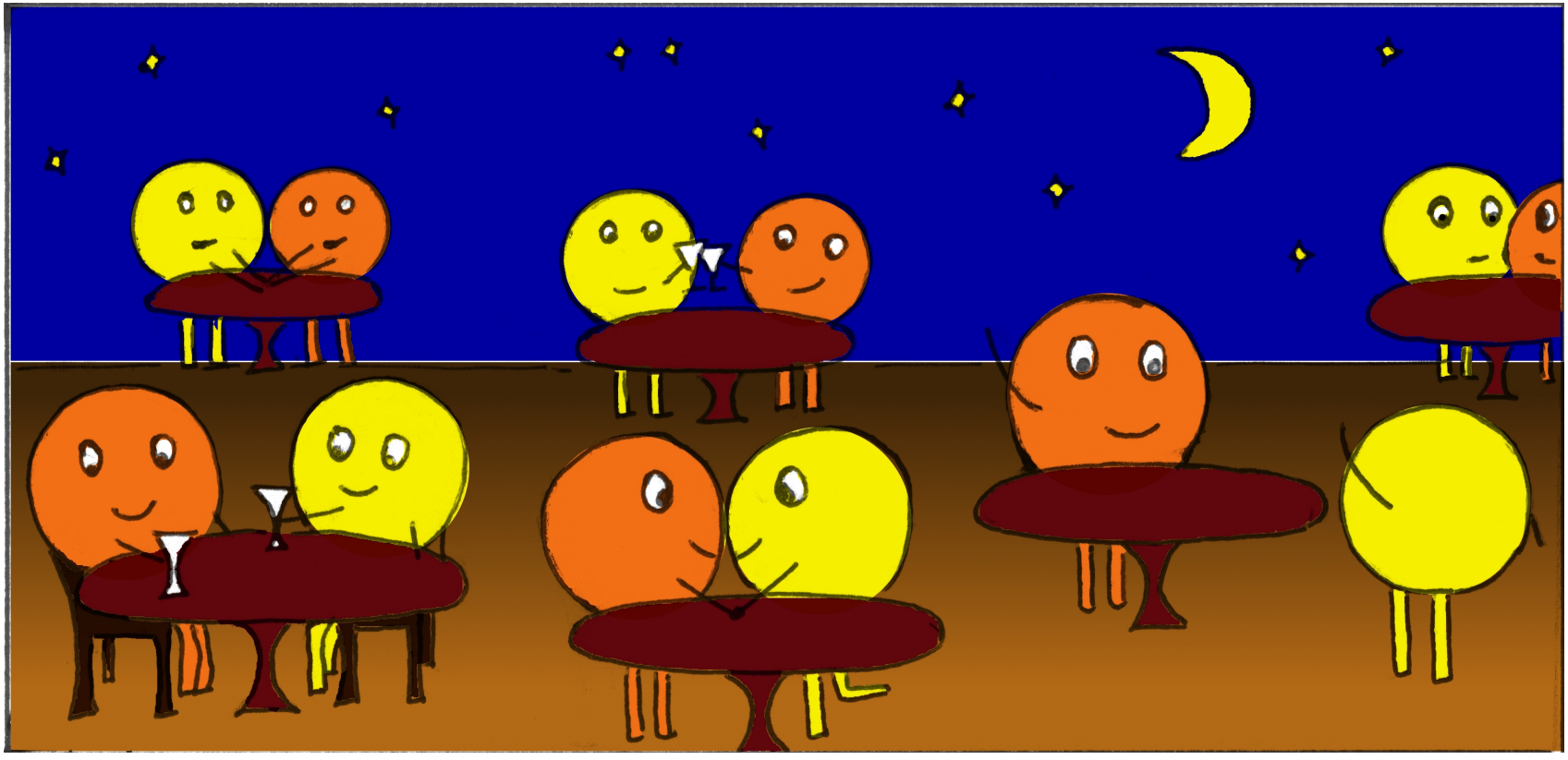
This setup still prolongs existing vertex chains, but autocorrelations are reduced since the worm changes with every update.

Alternative updates



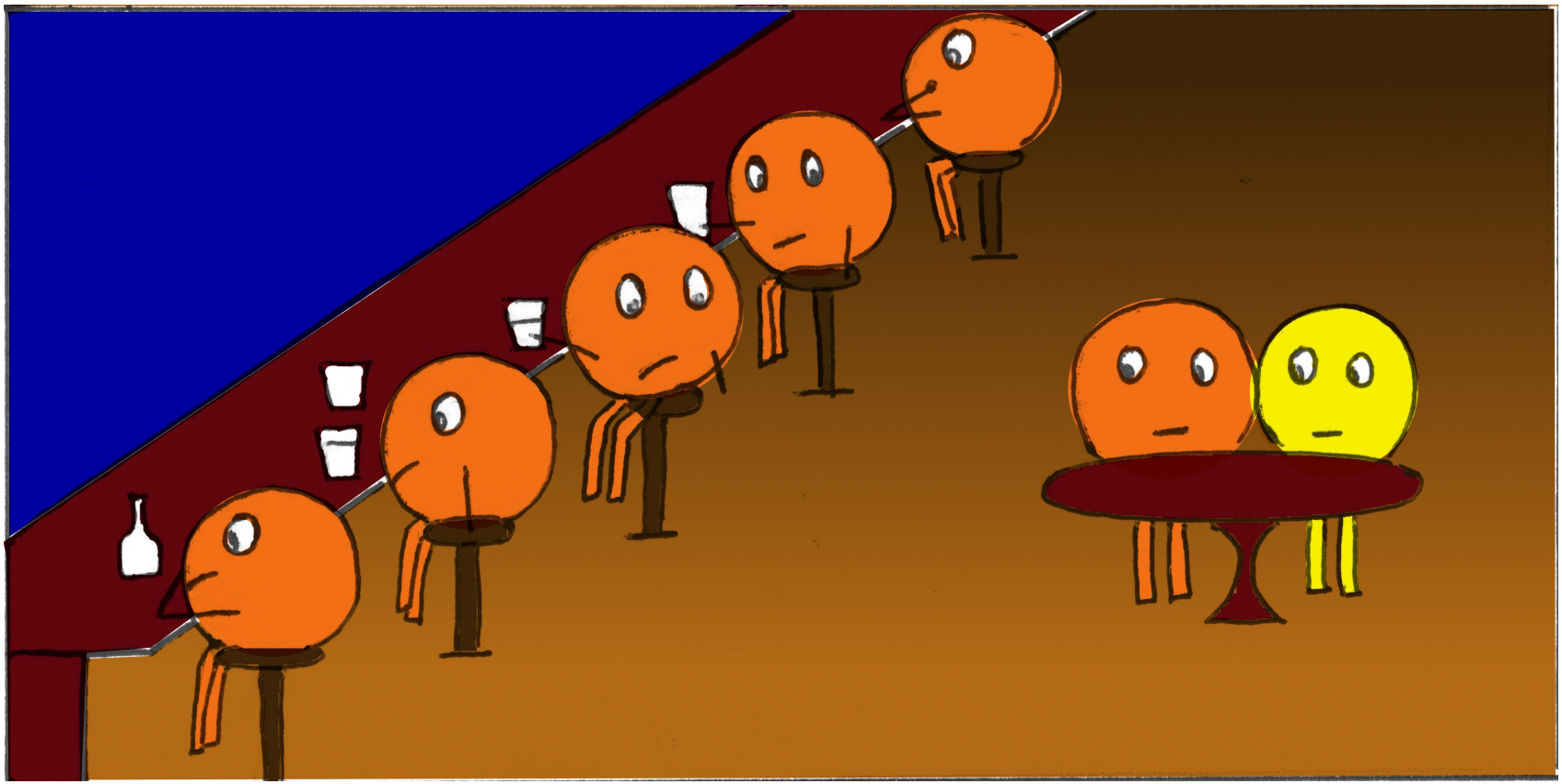
Comparison between diagonal setup (red circles) and alternative worm setup (blue squares) at low filling factor

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

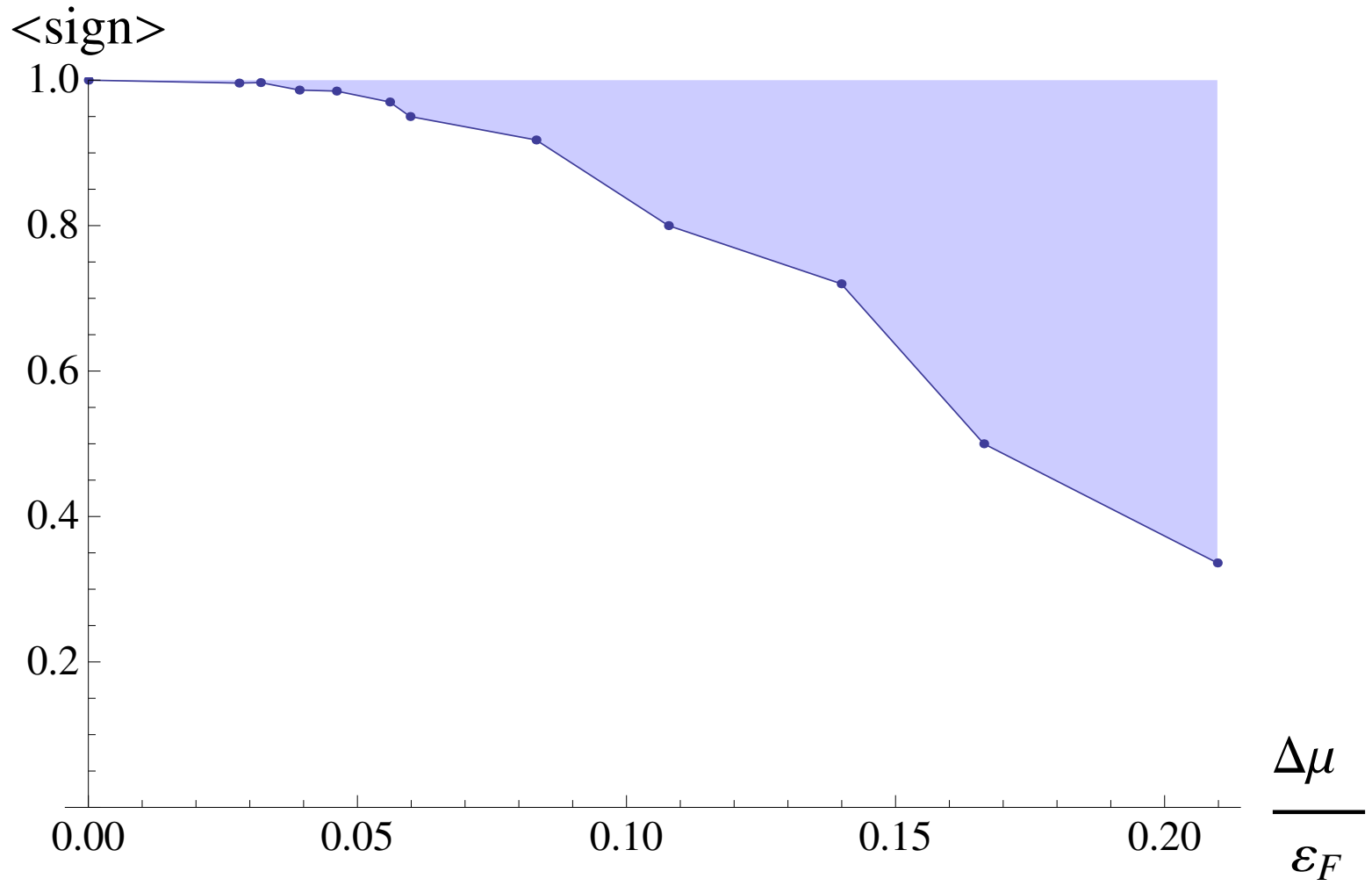
$$\langle X \rangle_{\rho} = \frac{\sum X(S_p)\rho(S_p)}{\sum \rho(S_p)} = \frac{\sum X(S_p)|\rho(S_p)|\text{sign}(S_p)}{\sum |\rho(S_p)|\text{sign}(S_p)} = \frac{\langle X\text{sign} \rangle_{|\rho|}}{\langle \text{sign} \rangle_{|\rho|}}$$

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

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

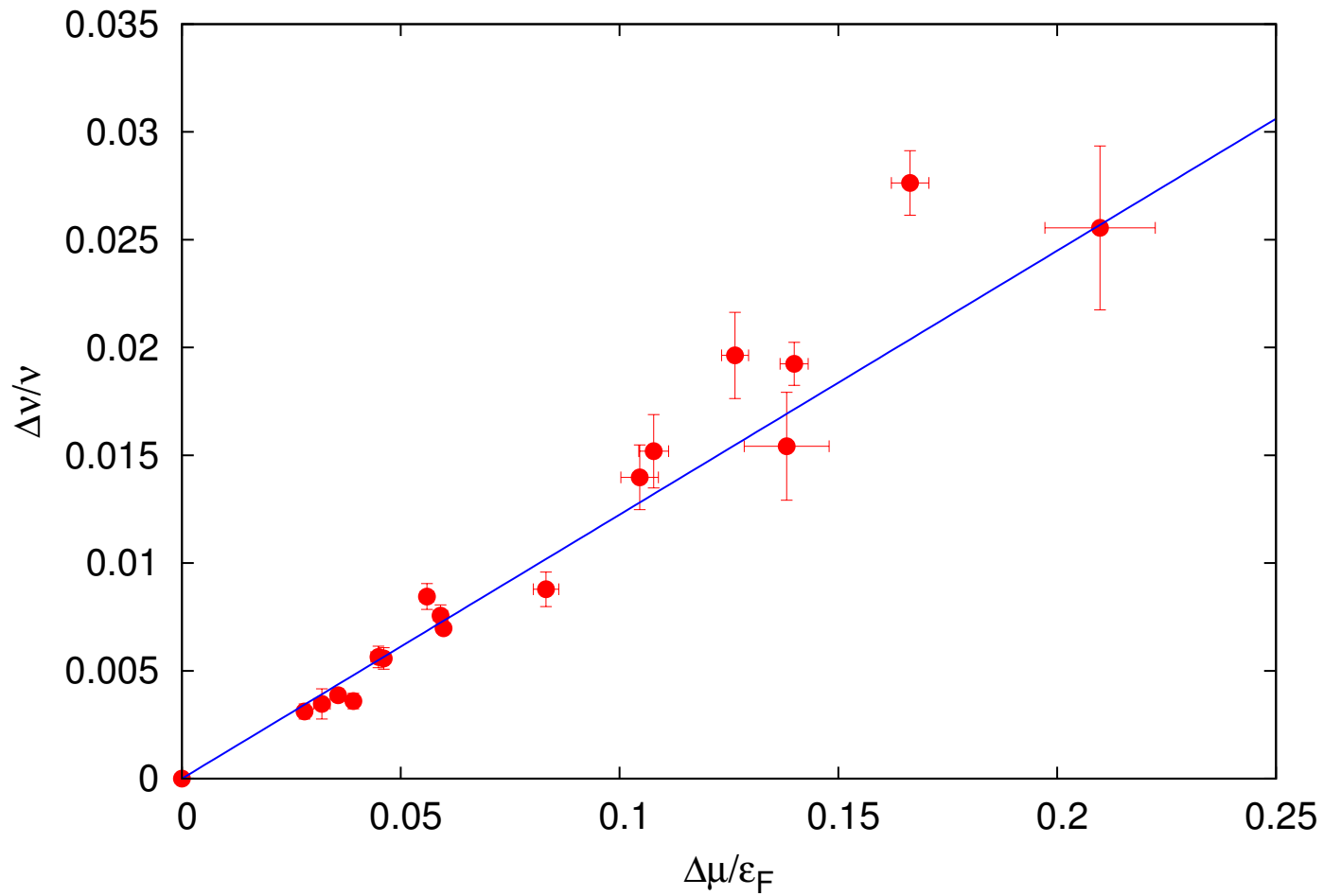
The imbalanced Fermi gas

Schematic plot of the sign near the critical point:



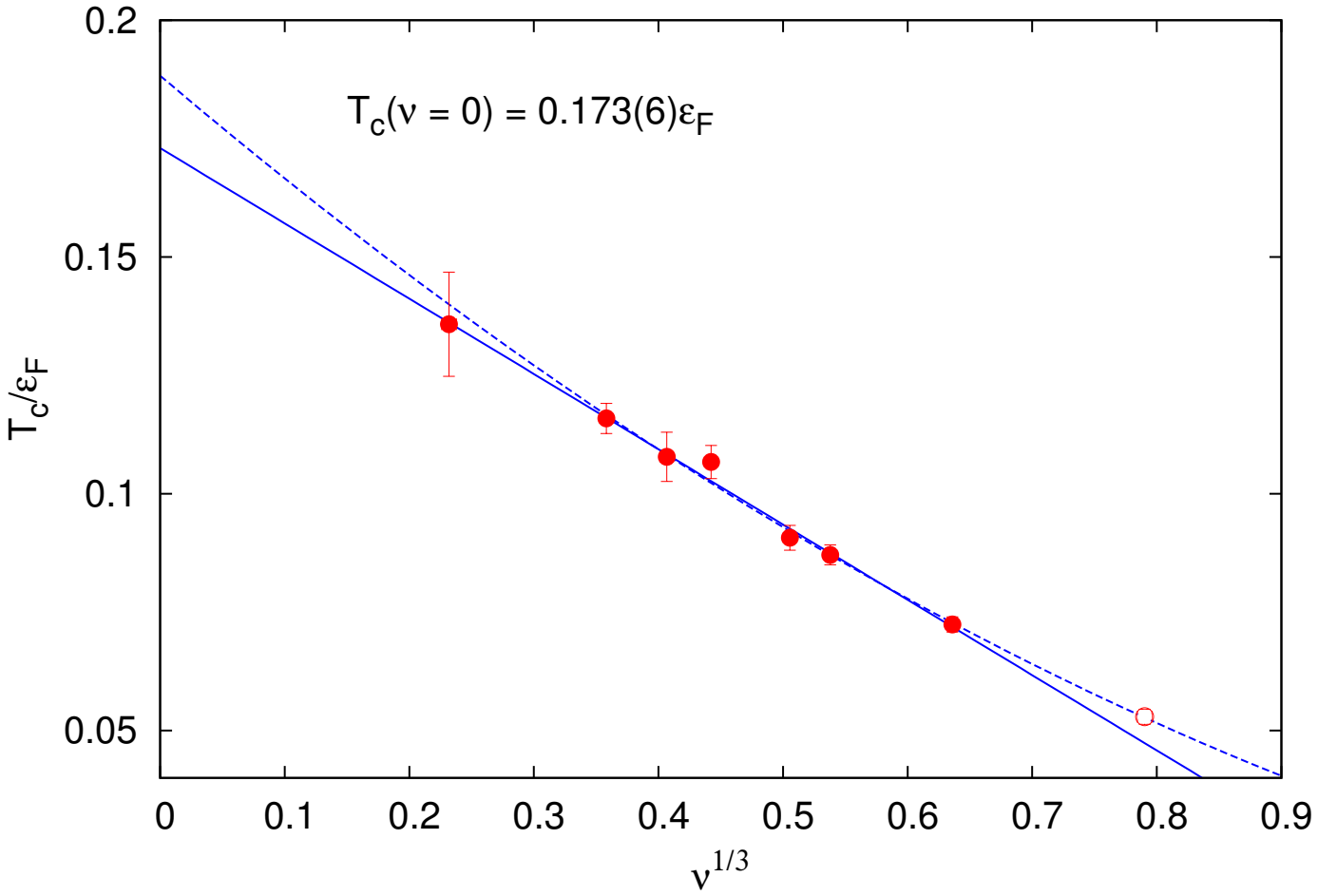
Results

Relationship between $\Delta\mu/\varepsilon_F = |\mu_\uparrow - \mu_\downarrow|/\varepsilon_F$ and $\delta\nu/\nu = \frac{|\nu_\uparrow - \nu_\downarrow|}{\nu_\uparrow + \nu_\downarrow}$



Results: the critical temperature

The critical temperature using only balanced data:



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

Surface fits for the imbalanced gas

Surface fit of a physical observable X as a function of filling factor $\nu^{1/3}$ and imbalance $h = \Delta\mu/\varepsilon_F$:

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

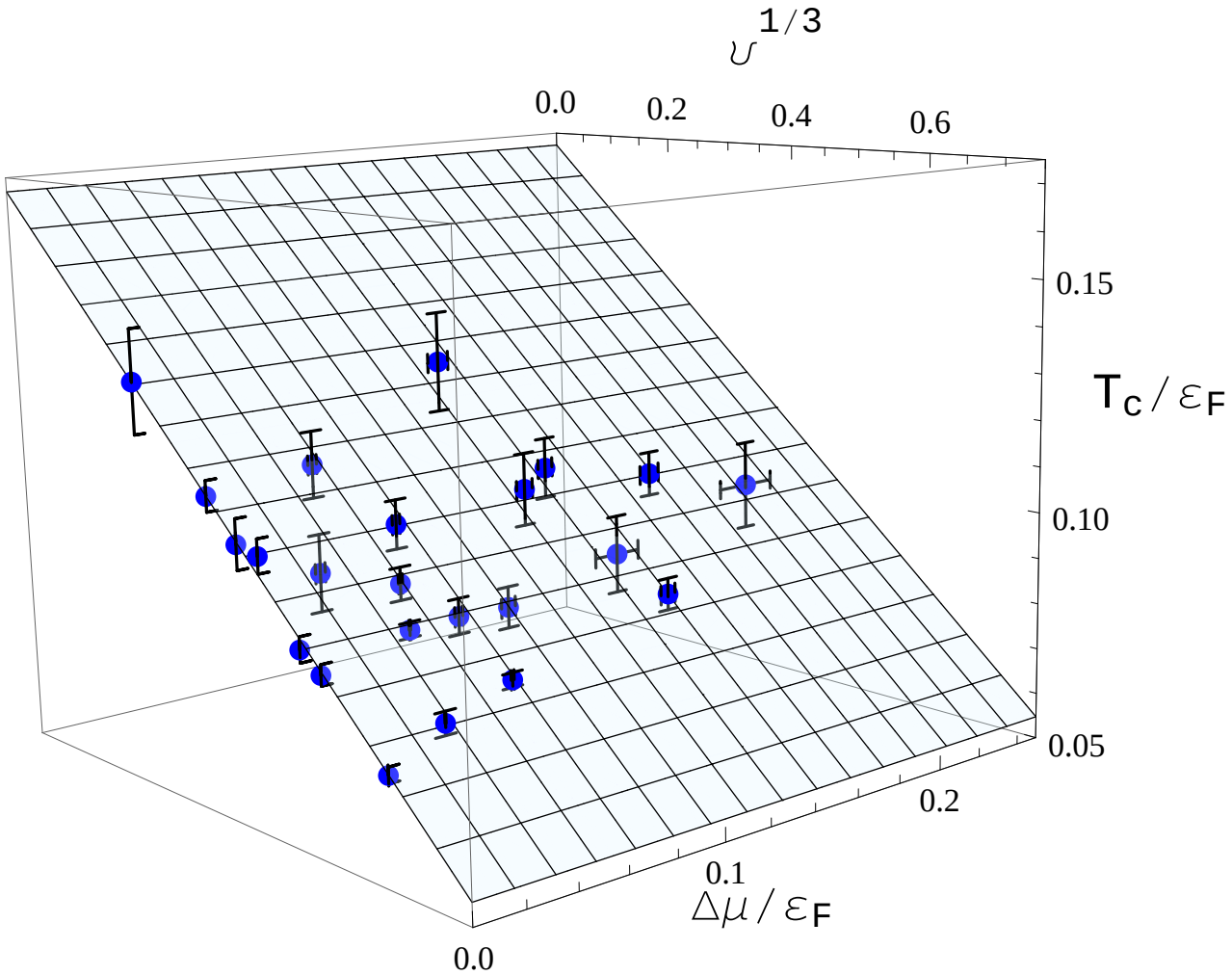
Hence the fitted function takes the form

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

We will expand the functions $X(h)$ and $\alpha^{(X)}(h)$ to 2nd order in h.

Results: the critical temperature

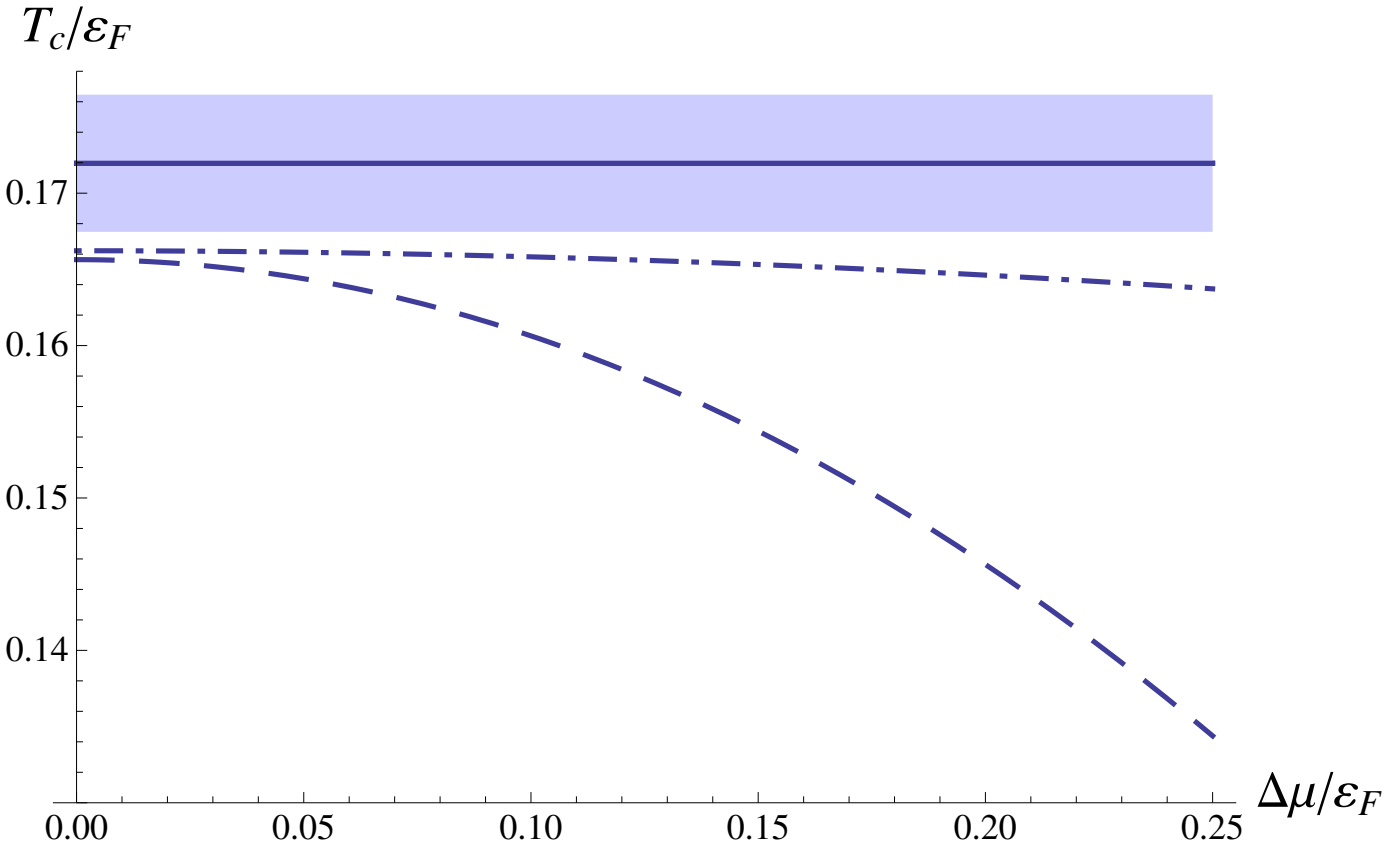
Surface fit of the critical temperature versus $\nu^{1/3}$ and h:



Data is consistent with $T_c(\nu = 0) = 0.171(5)\varepsilon_F$, independent of h.

Results: the critical temperature

Lower bounds for the deviation of T_c from the balanced limit:



lower bound: $T_c(h) - T_c(0) > -0.5\varepsilon_F h^2$,
with additional assumption: $T_c(h) - T_c(0) > -0.04\varepsilon_F h^2$

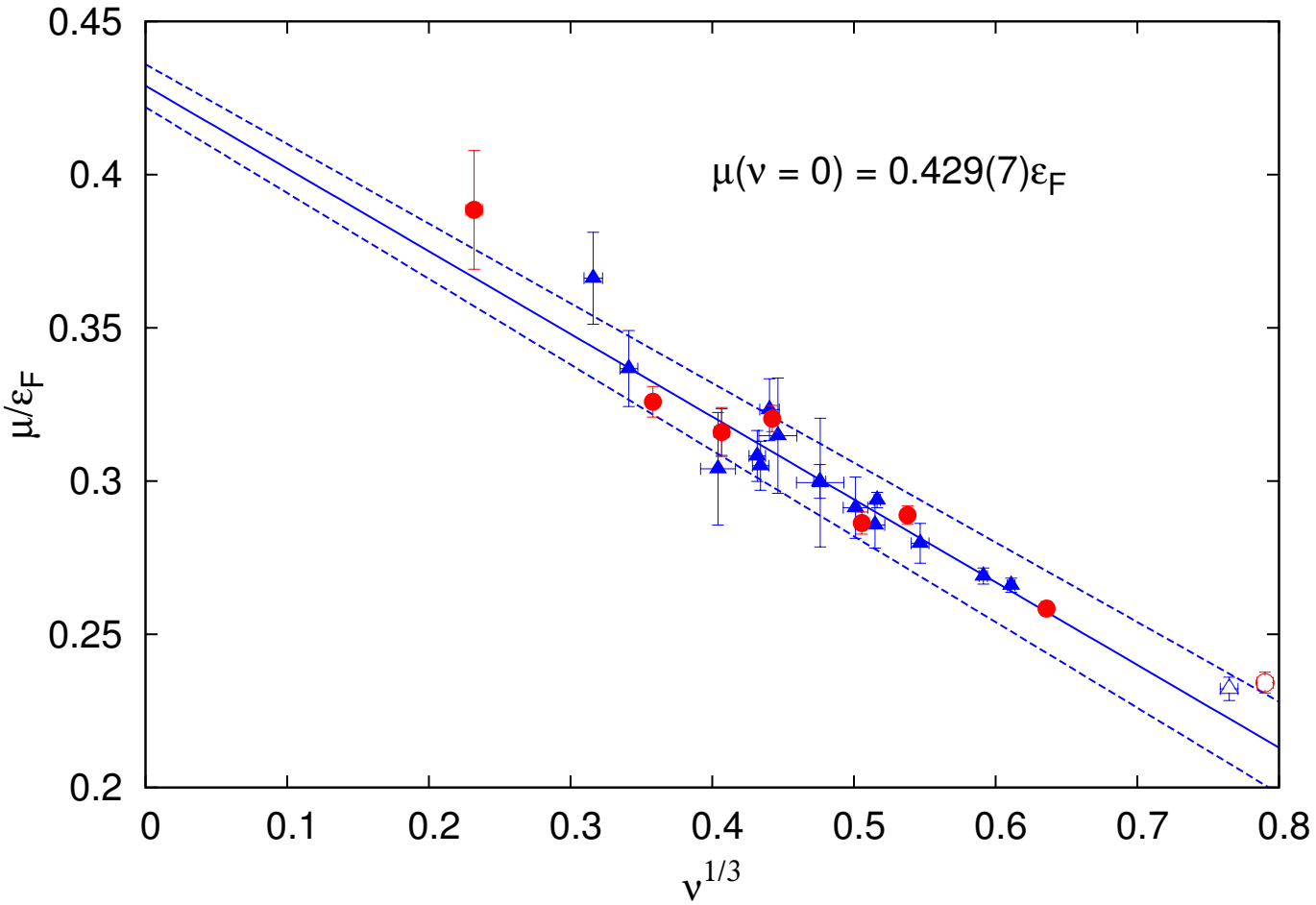
Results: the critical temperature

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)

Results: the chemical potential

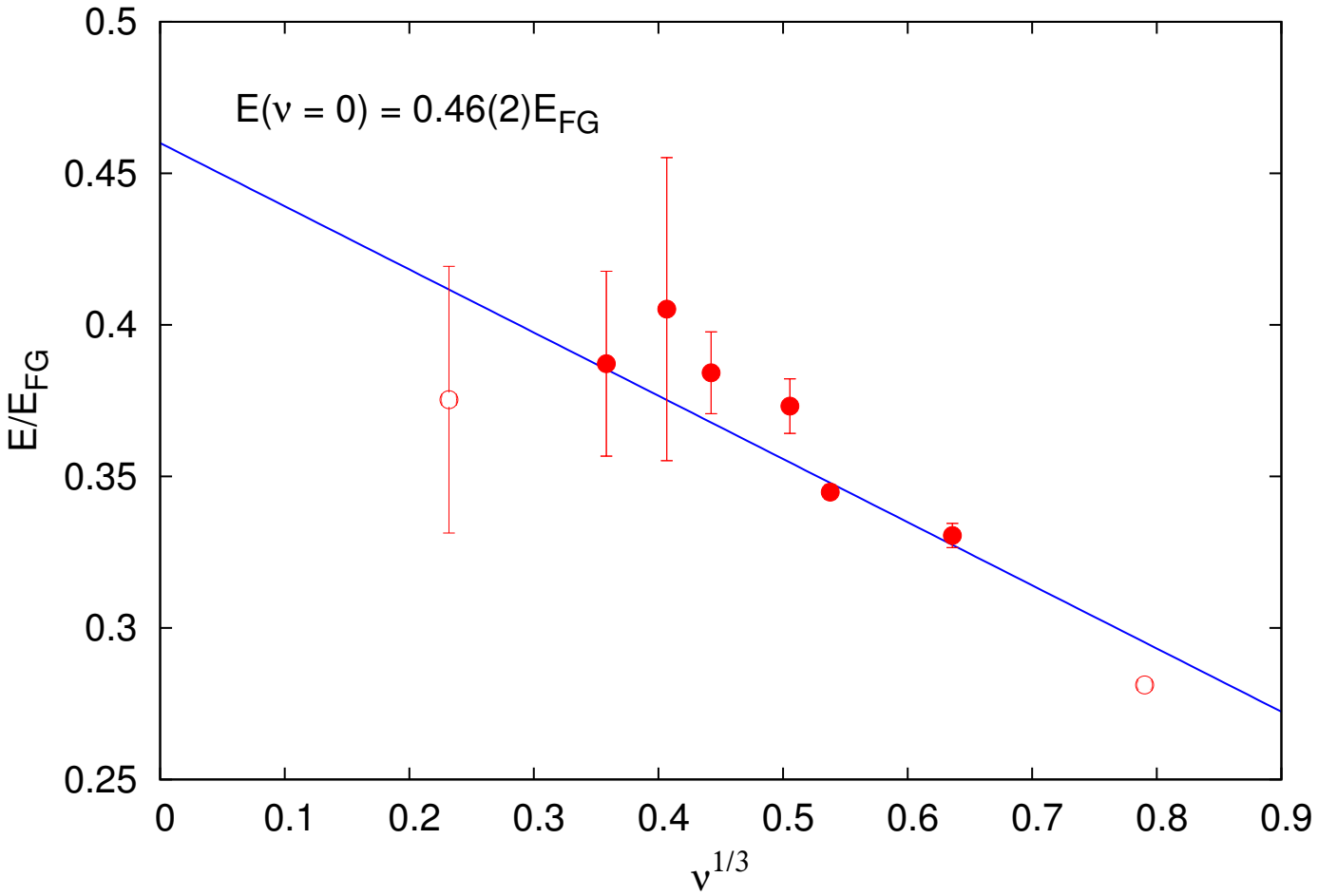
The average chem. pot. projected onto the $(\nu^{1/3} - \mu)$ plane:



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

Results: the energy per particle

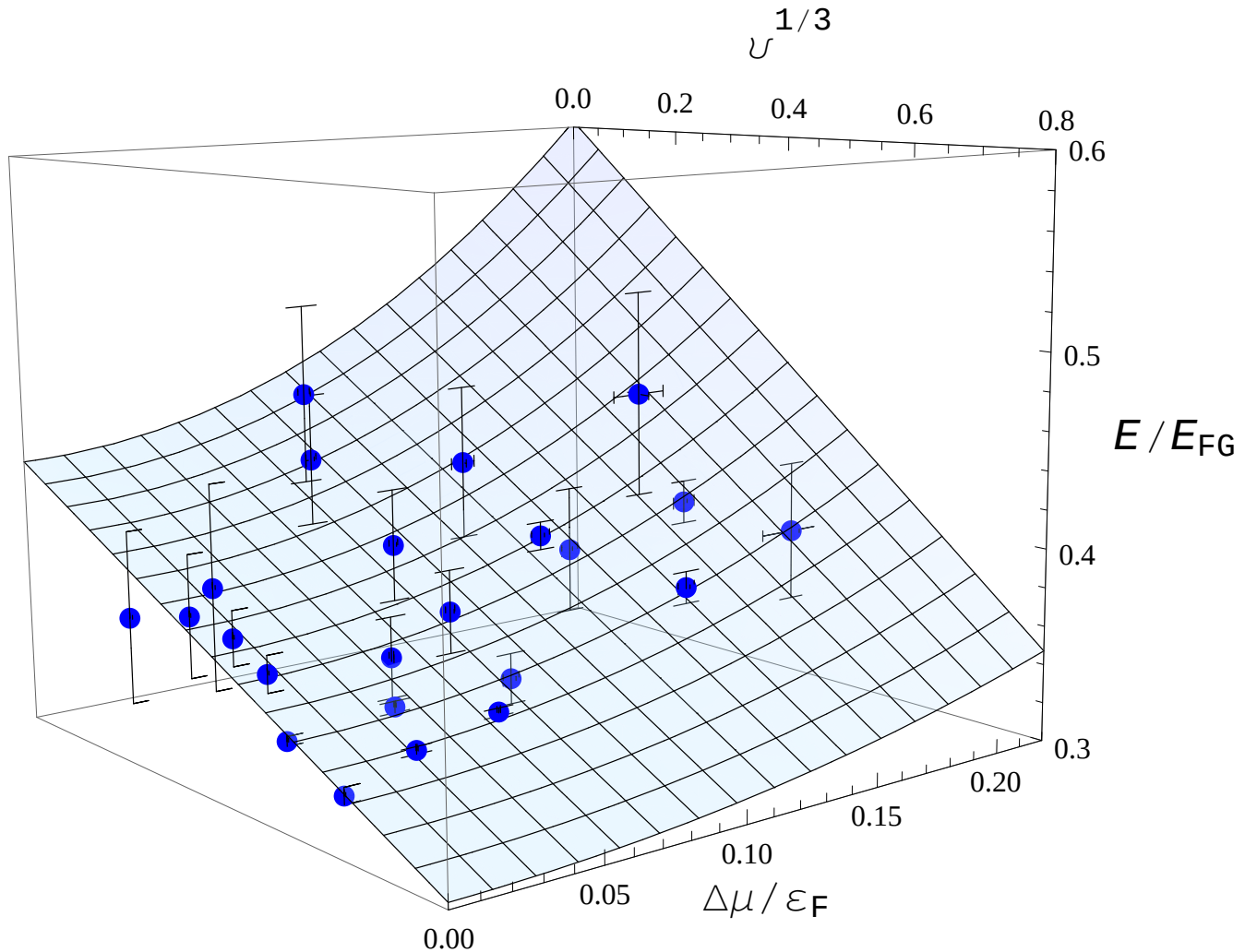
The energy per particle using only balanced data:



$\nu \to 0$ corresponds to the continuum limit; $E_{FG} = (3/5)N\varepsilon_F$

Results: the energy per particle

Surface fit of the energy per particle versus $\nu^{1/3}$ and h:



Results: the 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)]:

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

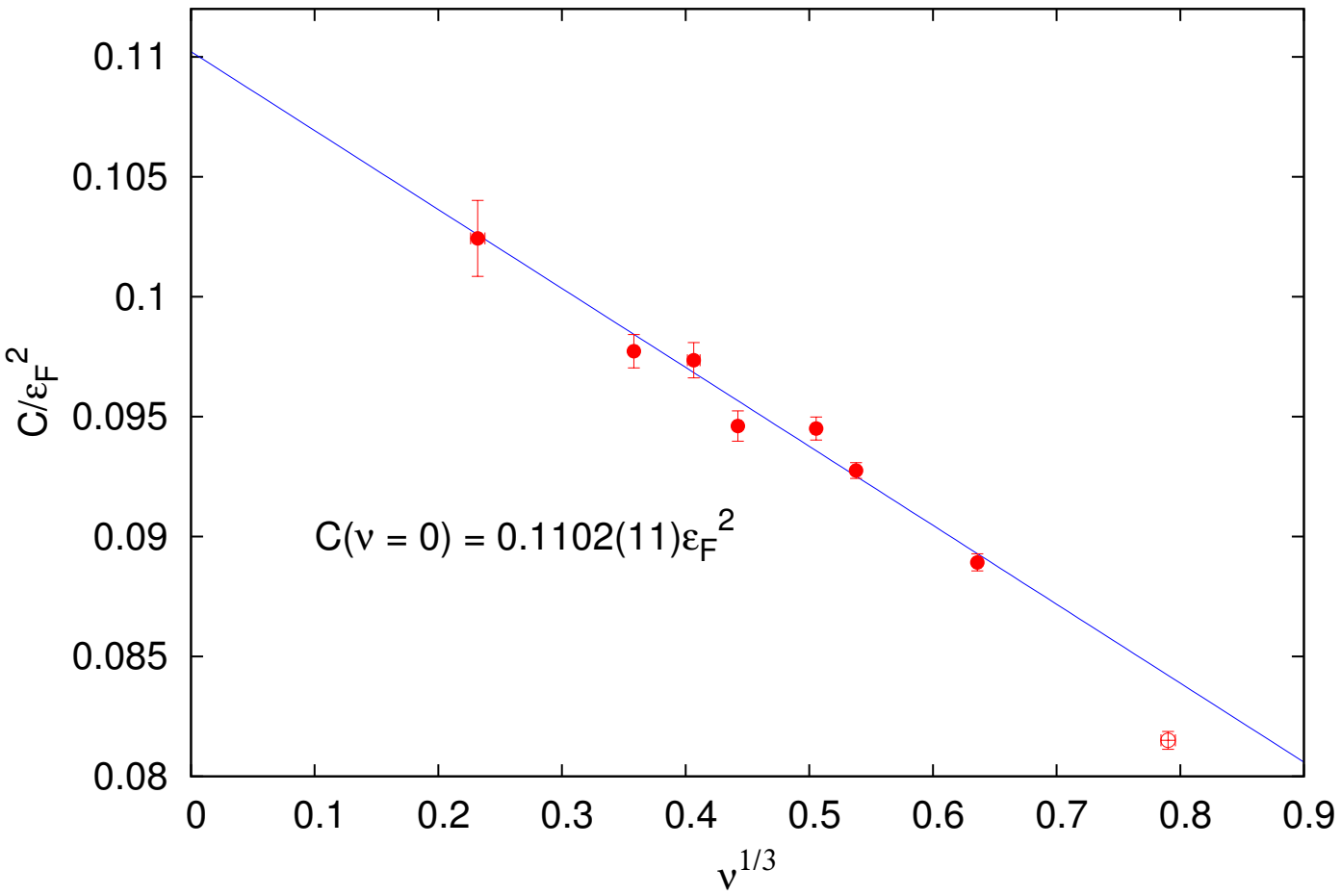
where g_0 is the physical coupling constant.

The contact density is $\mathcal{C} = C/V$ and has units ε_F^2.

This was the first numerical calculation of the contact density at finite temperature [Goulko and Wingate, arXiv:1011.0312]

Results: the contact density

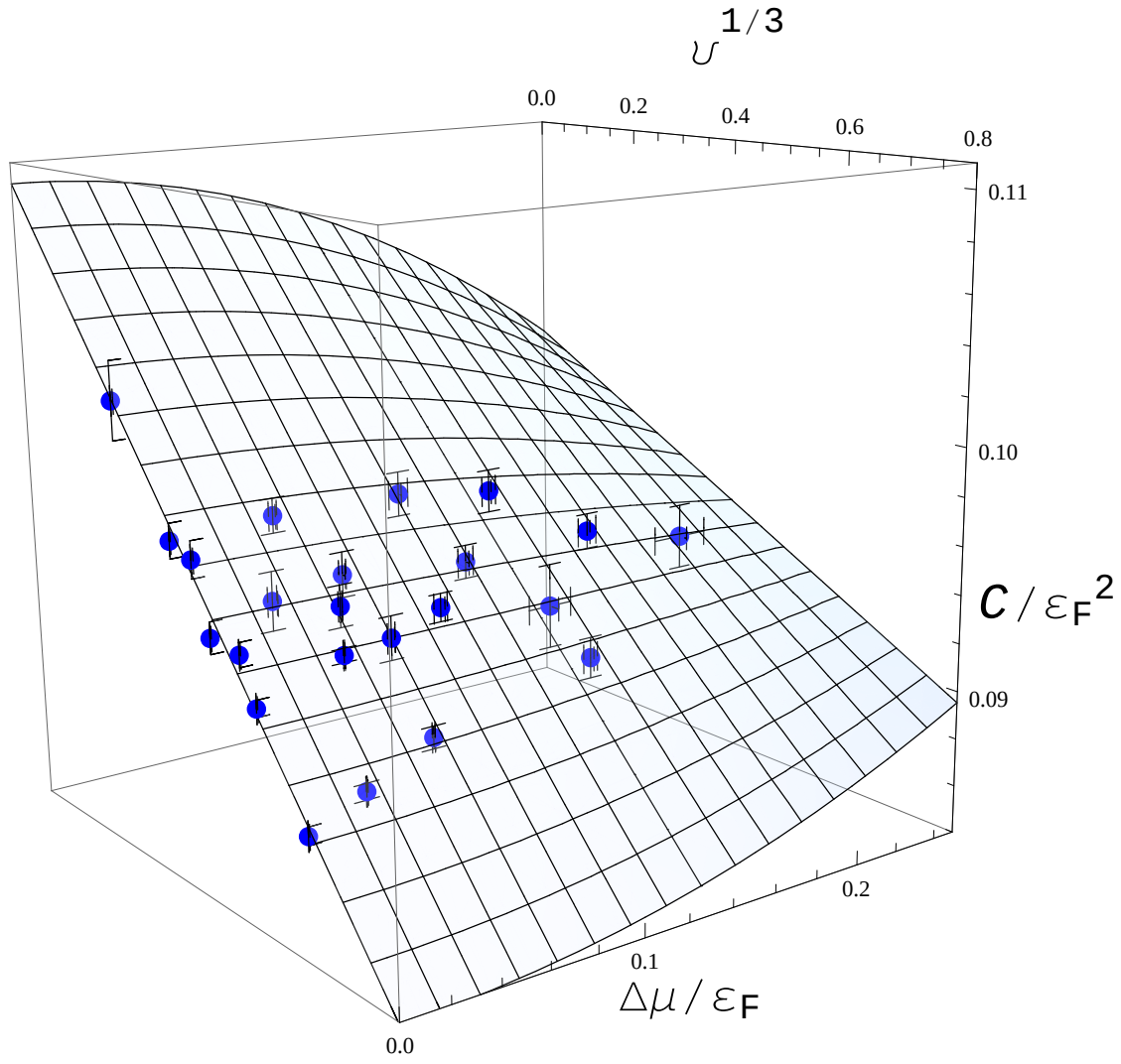
The contact density using only balanced data:



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

Results: the contact density

Surface fit of the contact density versus $\nu^{1/3}$ and h:



Outlook: temperatures beyond T_c

Problem: fixing the temperature for $T \neq T_c$

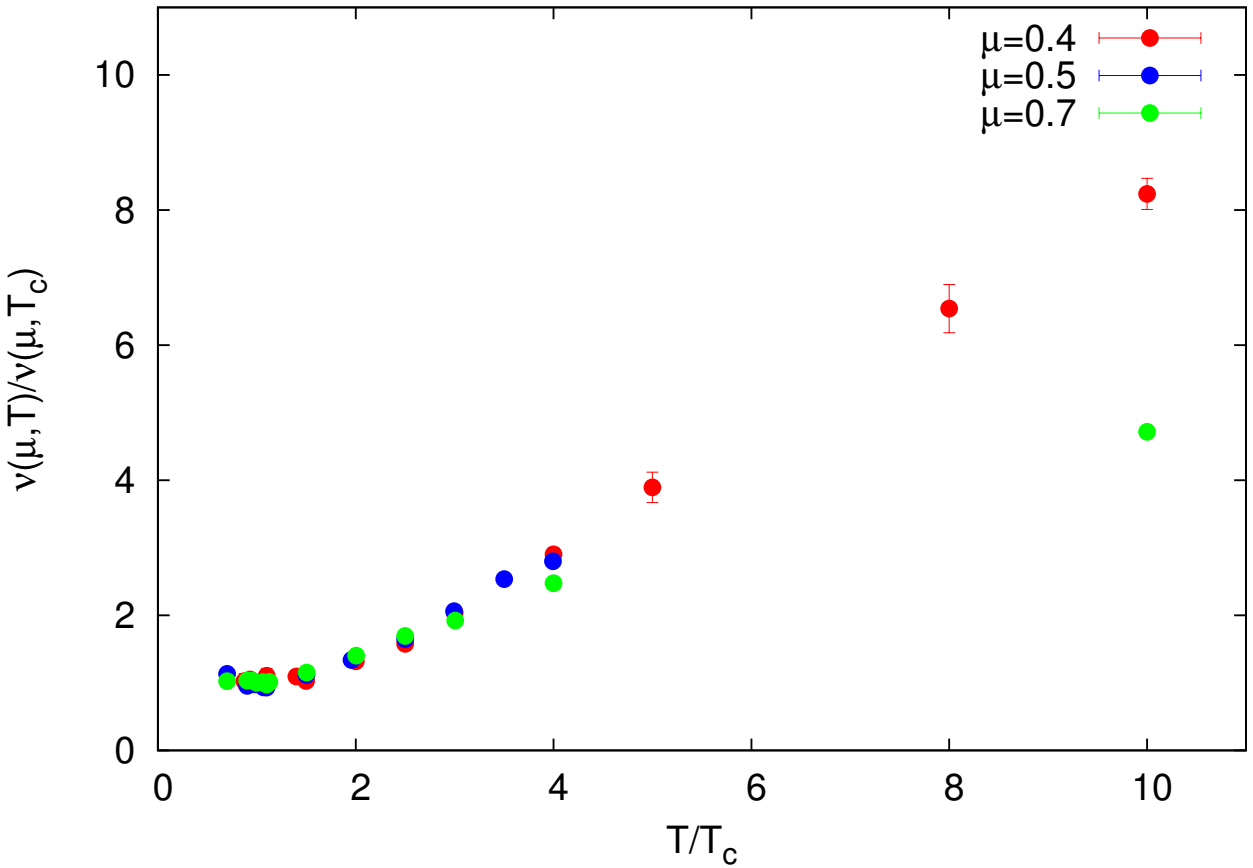
Setting the scale: set lattice spacing b to be independent of temperature $\Rightarrow b = b(\mu)$

$$\Rightarrow \frac{\nu(\mu, T)}{\nu(\mu, T_c)} = \frac{n(T)}{n(T_c)} \left(\frac{b(\mu, T)}{b(\mu, T_c)} \right)^3 = \frac{n(T)}{n(T_c)}$$

If the fix the lattice temperature ratio $T(\mu)/T_c(\mu)$ we will move towards the continuum limit along a line of fixed temperature.

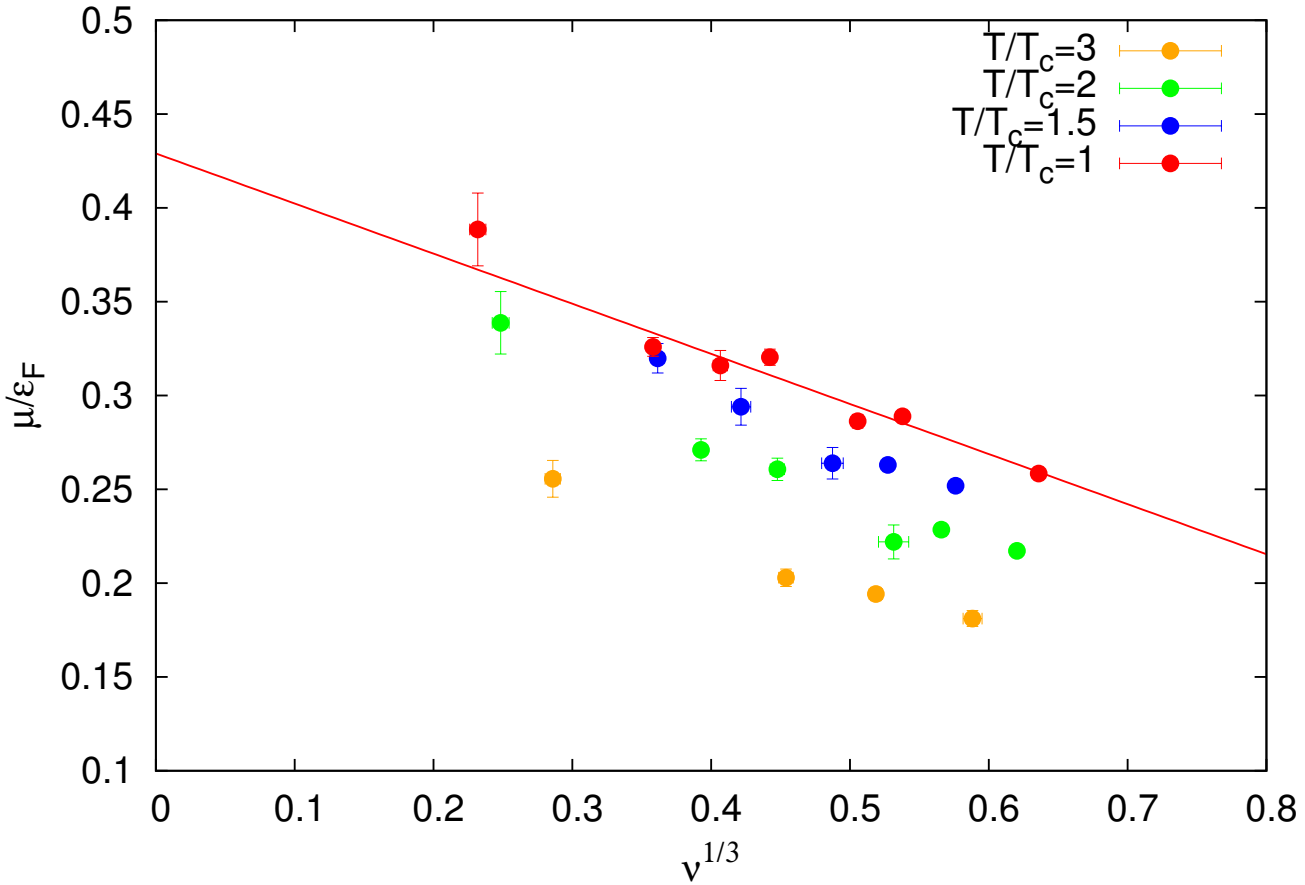
Outlook: temperatures beyond T_c

Works for $T/T_c \leq 4$ for sufficiently small μ:



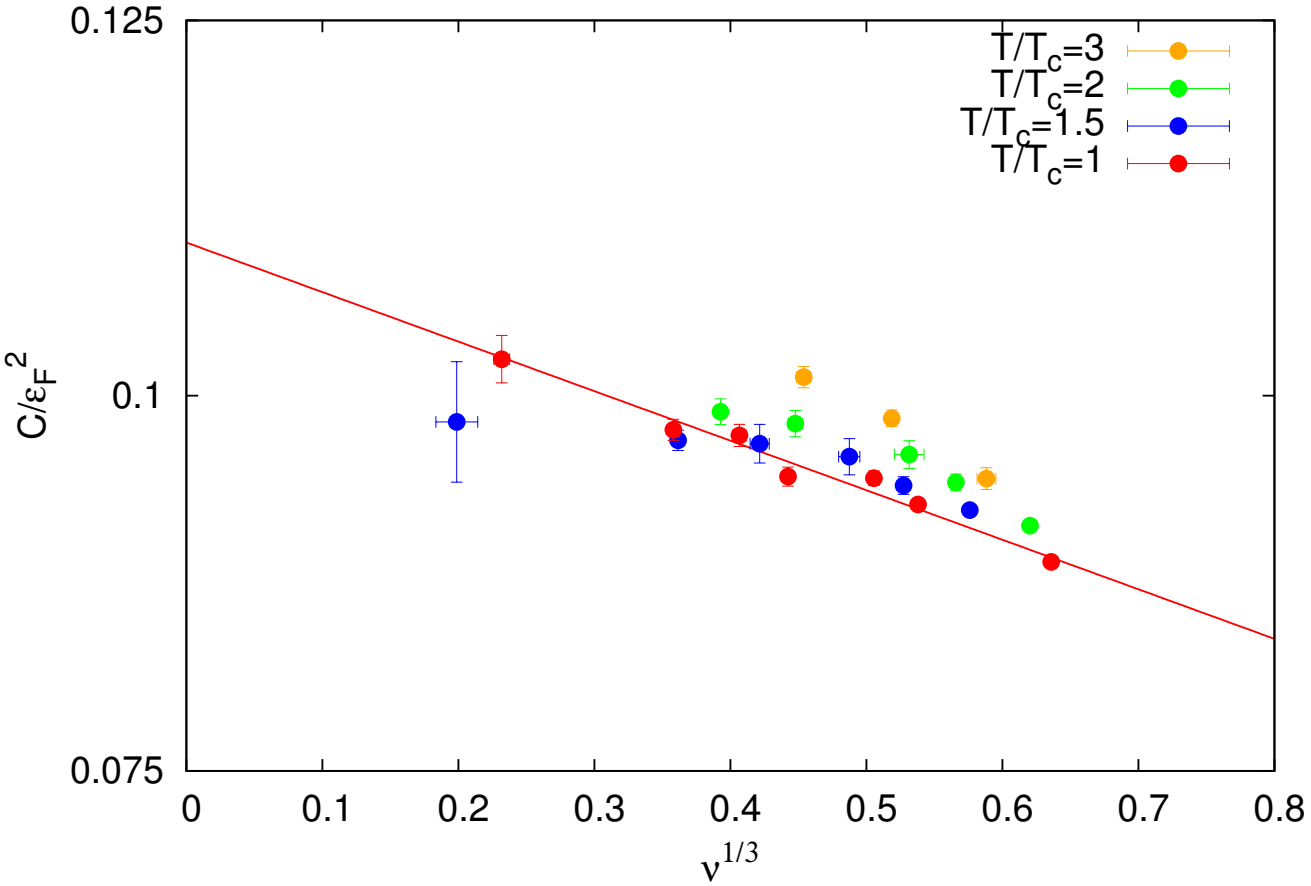
Outlook: temperatures beyond T_c

Preliminary results: temperature dependence of the chemical potential



Outlook: temperatures beyond T_c

Preliminary results: temperature dependence of the contact



Conclusions

- Lattice Field Theory is a useful tool for studying strongly interacting systems in condensed matter physics
- The DDMC algorithm can be applied to study the phase transition of the unitary Fermi gas
- Imbalanced case with the sign quenched method
- Results for T_c/ε_F, μ/ε_F, E/E_{FG} and $\mathcal{C}/\varepsilon_F^2$ for equal and unequal number of fermions in the two spin components
- Temperatures beyond T_c accessible

Thank you!