Lattice Simulations of Cold Dilute Neutron Matter

Dean Lee

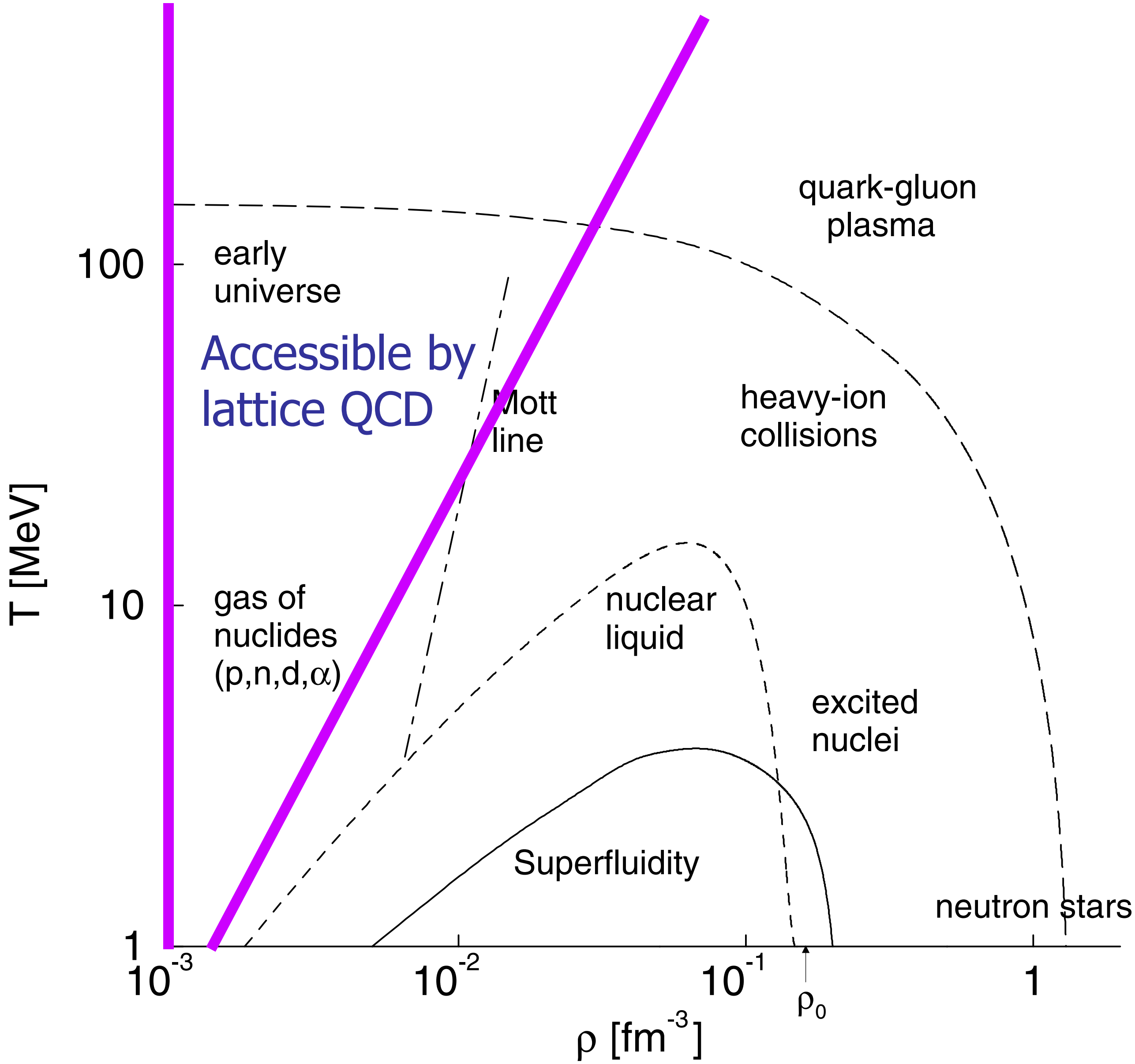
INT Workshop – Universal DF

Seattle - September 2005

Collaborator: T. Schäfer

Outline

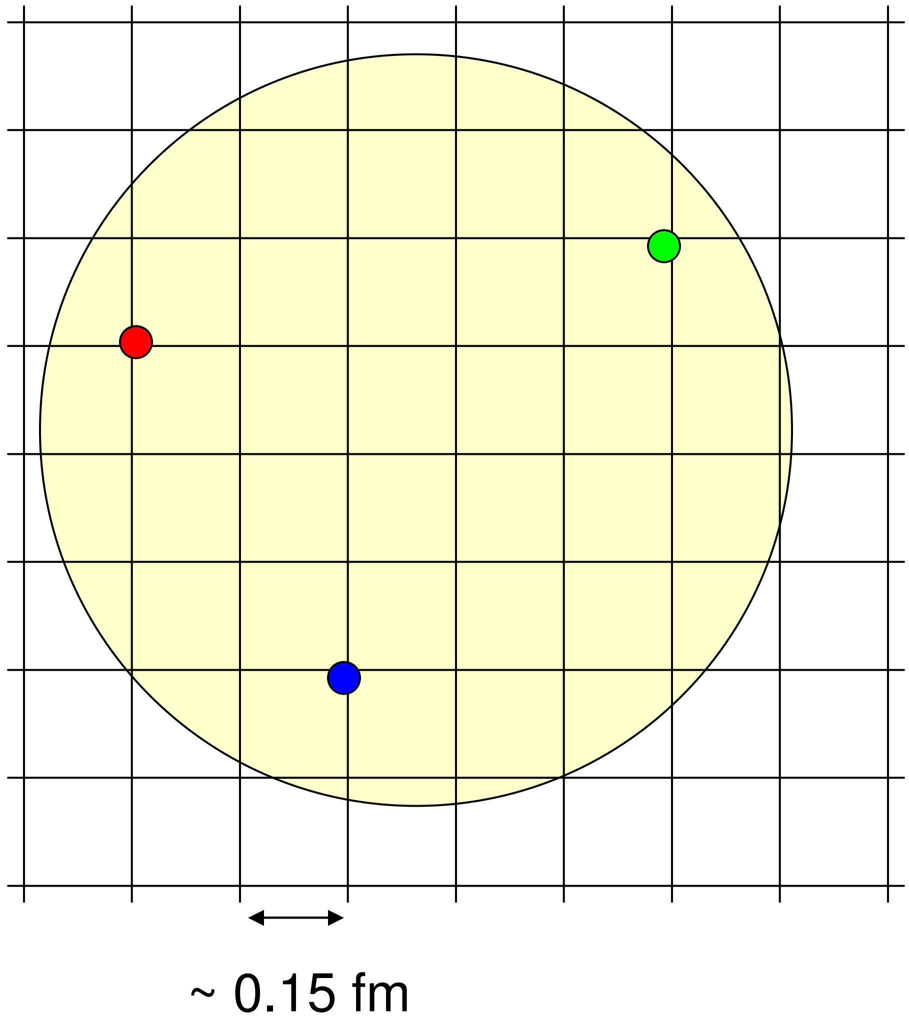
1. Lattice simulations with effective field theory
2. Neutron scattering and universality
3. A puzzle
4. High temperature/low density calculations
5. Virial coefficients
6. Unitary limit and scaling
7. Results in the unitary limit



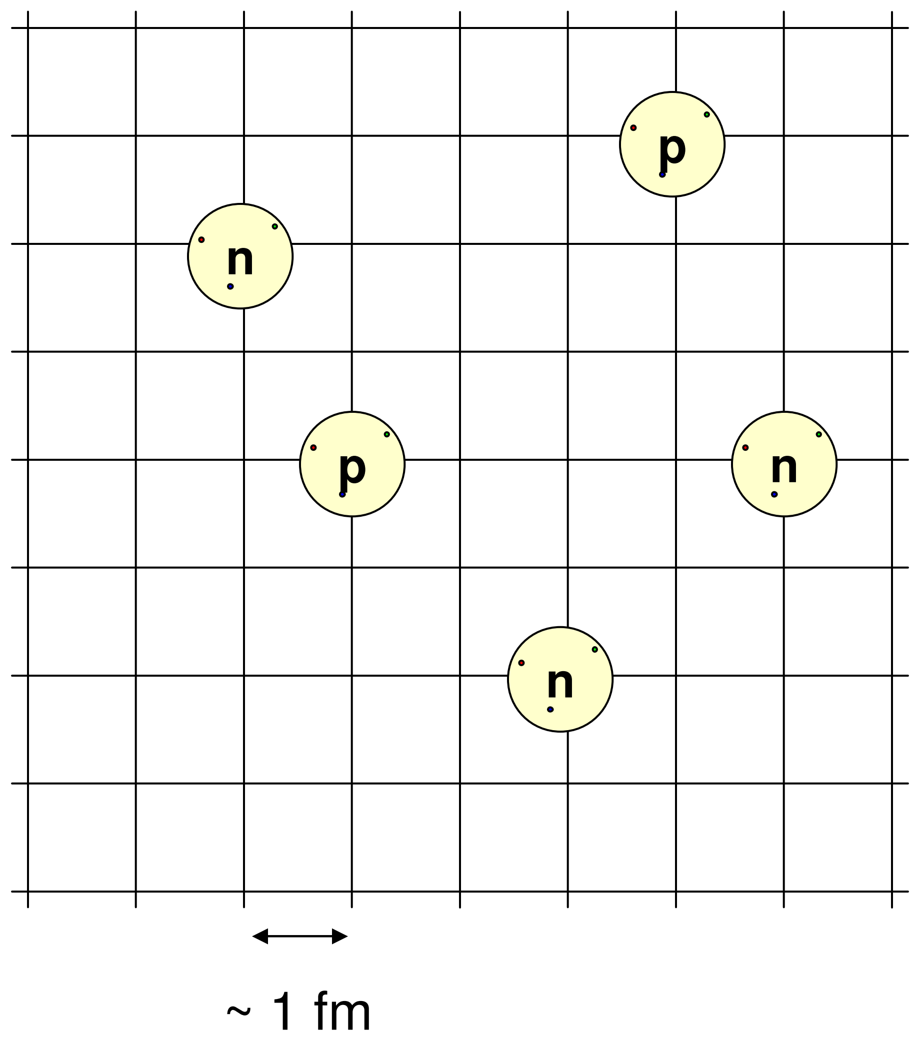
from Ropke and Schell, Prog. Part. Nucl. Phys. 42, 53 (1999)

Why do nuclear lattice simulations?

Nucleon in lattice QCD



Nucleons as point particles on lattice

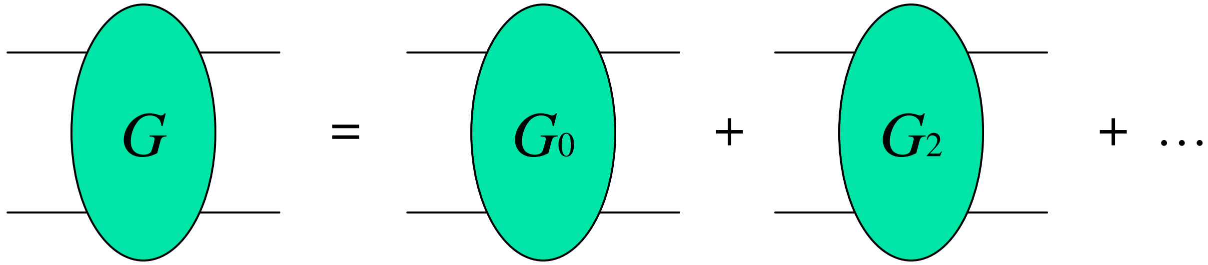


Simulations with Effective Field Theory

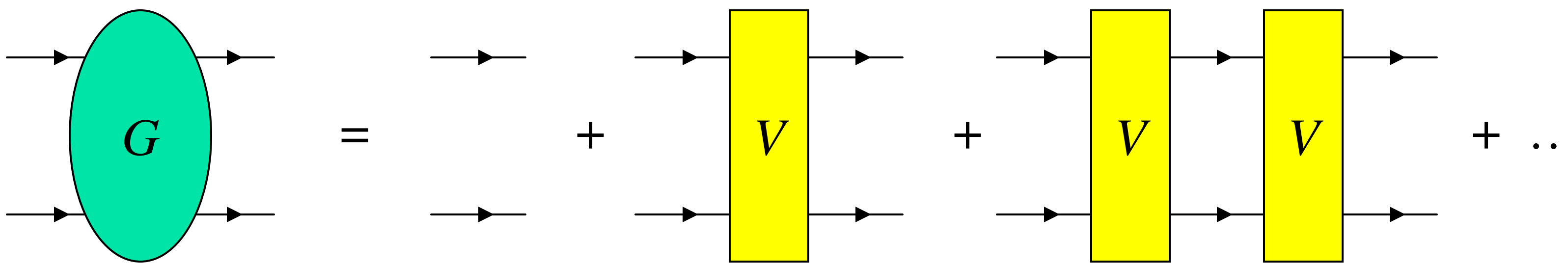
Non-perturbative lattice simulations of effective field theory of low energy pions and nucleons.

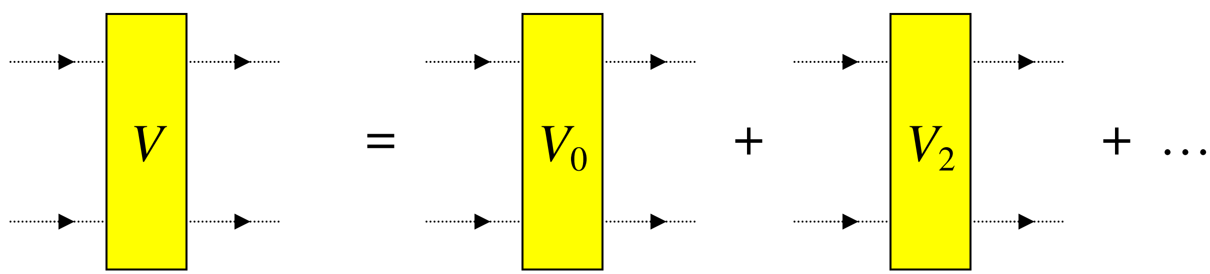
Non-perturbative effective field theory?... but isn't effective field theory based upon an expansion?

For pions the expansion is simple

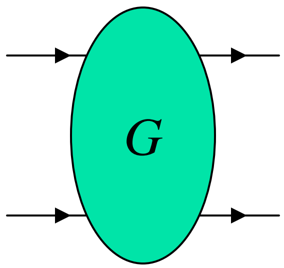


For nucleons we must take care of infrared singularities
[Weinberg, PLB 251 (1990) 288, NPB 363 (1991) 3]

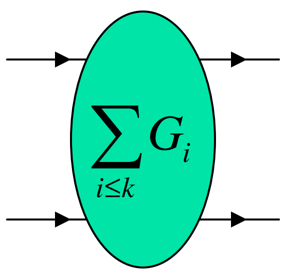




We will iterate "everything"



$$= \frac{\int D\pi DND\bar{N}\; G(\pi, N, \bar{N})\; e^{-S(\pi,N,\bar{N})}}{\int D\pi DND\bar{N}\; e^{-S(\pi,N,\bar{N})}}$$

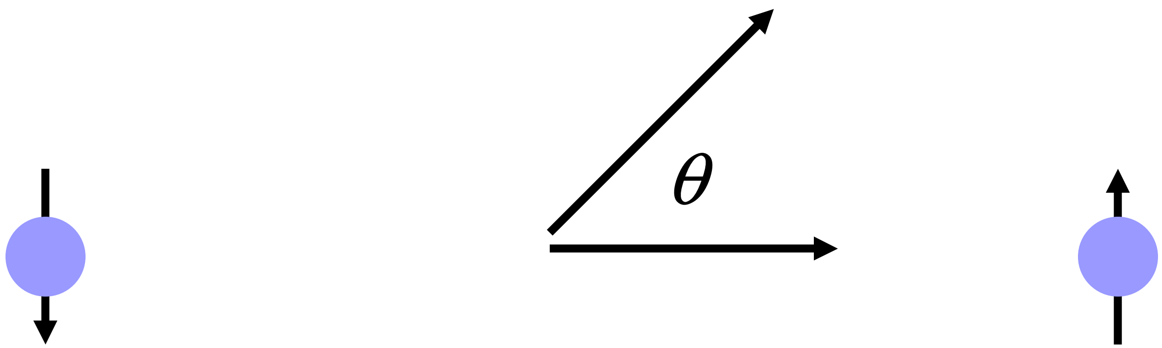


$$= \frac{\int D\pi DND\bar{N}\; G(\pi, N, \bar{N})\; e^{-\sum_{i\leq k} S_i(\pi,N,\bar{N})}}{\int D\pi DND\bar{N}\; e^{-\sum_{i\leq k} S_i(\pi,N,\bar{N})}}$$

A complete summation of all diagrams involving interaction terms with order $\leq k$. [D.L., Borasoy, Schäfer, PRC70 (2004) 014007]

Pure neutron matter

[D.L. and Schäfer, PRC72 (2005) 024006]



Incoming and scattered wave

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}', \mathbf{k})\frac{e^{i\mathbf{k}'\cdot\mathbf{r}}}{\mathbf{r}}$$

Partial wave decomposition

$$f(\mathbf{k}', \mathbf{k}) = \sum_{l=0}^{\infty} f_l(k) P_l(\cos\theta)$$

Phase shifts

$$f_l(k) = \frac{2l+1}{2ik}\left(e^{2i\delta_l(k)} - 1\right)$$

S-wave scattering dominant at lowest energies

$$f_0(k) = \frac{1}{k\cot\delta_0(k) - ik}$$

S-wave scattering length

$$a_{scatt} = - \lim_{k \to 0} \frac{\delta_0(k)}{k}$$

Effective range expansion

$$k \cot \delta_0(k) \approx -a_{scatt}^{-1} + \frac{1}{2} k^2 r_0$$

Neutron-neutron scattering length is –18 fm while the range is only 2.8 fm.

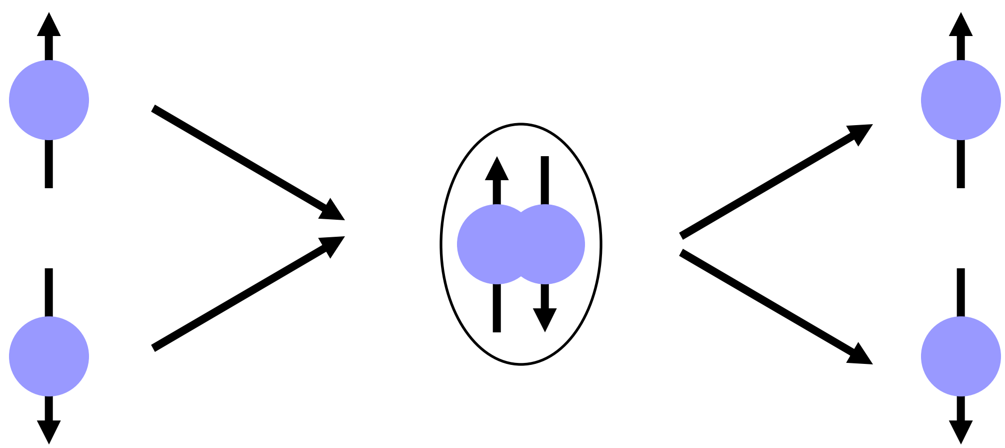
Theoretically interesting … for dilute neutron matter one is close to *unitary regime* or *universal scaling limit* where magnitude of scattering length $\to \infty$, range $\to 0$.

In this limit, no dimensionful parameters as $T \to 0$, and so we expect the energy per particle and superfluid gap to satisfy

$$\frac{E}{A} = \xi \frac{3}{5} \frac{k_F^2}{2m}, \quad \Delta = \zeta \frac{k_F^2}{2m}$$

Feshbach resonance

Experiments done with cold Li and K atoms, which can form diatomic molecules, Li_2 and K_2.



Tune energy of the diatomic molecule with external magnetic to produce a resonance near threshold. [O'Hara et. al., Science 298 (2002) 2179; Regal, Jin, PRL (2003) 230404; etc.]

For dilute neutron matter we have the effective Hamiltonian,

$$H = -\sum_i \int d^3x a_i^\dagger \frac{\nabla^2}{2m} a_i + C \int d^3x a_\downarrow^\dagger a_\uparrow^\dagger a_\uparrow a_\downarrow$$

On the lattice,

$$\begin{aligned} H - \mu N = & \sum_{\vec{n}_s, i} \left[(-\mu + \frac{3}{m}) a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s) \right] \\ & - \frac{1}{2m} \sum_{\vec{n}_s, l_s, i} \left[a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s + \hat{l}_s) + a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s - \hat{l}_s) \right] \\ & + C \sum_{\vec{n}_s} a_\downarrow^\dagger(\vec{n}_s) a_\uparrow^\dagger(\vec{n}_s) a_\uparrow(\vec{n}_s) a_\downarrow(\vec{n}_s) \end{aligned}$$

We use a Hubbard-Stratonovich transformation to rewrite the interaction as

$$\exp\left[-\frac{C}{2}(a_\uparrow^\dagger a_\uparrow + a_\downarrow^\dagger a_\downarrow)^2\right]$$

$$= \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + s\sqrt{-C}(a_\uparrow^\dagger a_\uparrow + a_\downarrow^\dagger a_\downarrow)\right]$$

We then integrate out the neutron field. The resulting action has no signs or phases, as the determinant of the matrix is positive semi-definite.

The matrix has the structure

$$M(s) = M_{\uparrow}(s) \oplus M_{\downarrow}(s)$$

$$M_{\uparrow}(s) = M_{\downarrow}(s)$$

$$\det M(s) = \left(\det M_{\uparrow}(s)\right)^2 \geq 0$$

So we can use standard pseudofermion methods with Hybrid Monte Carlo

$$\det M(s) = \left(\det M_{\uparrow}(s)\right)^2$$
$$\propto \int d\phi^* d\phi \ \exp\left[\left(M_{\uparrow}^{-1}(s)\phi\right)^{\dagger}\left(M_{\uparrow}^{-1}(s)\phi\right)\right]$$

Most computationally intensive step is conjugate gradient inversion

$$\left[M_{\uparrow}^{\dagger}(s)M_{\uparrow}(s)\right]v = b$$

Can be accelerated by diagonal preconditioning

$$\left[D^{-1}(s)M_{\uparrow}^{\dagger}(s)M_{\uparrow}(s)D^{-1}(s)\right]D(s)v = D^{-1}(s)b$$

where

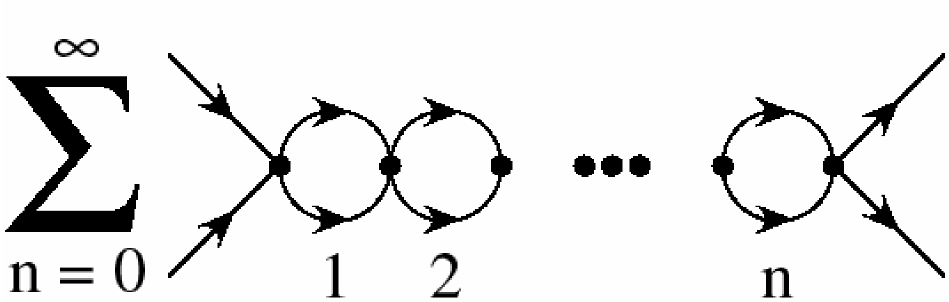
$$D(s) = \mathsf{diag}\left[M_{\uparrow}^{\dagger}(s)M_{\uparrow}(s)\right]$$

Operator coefficient on the lattice

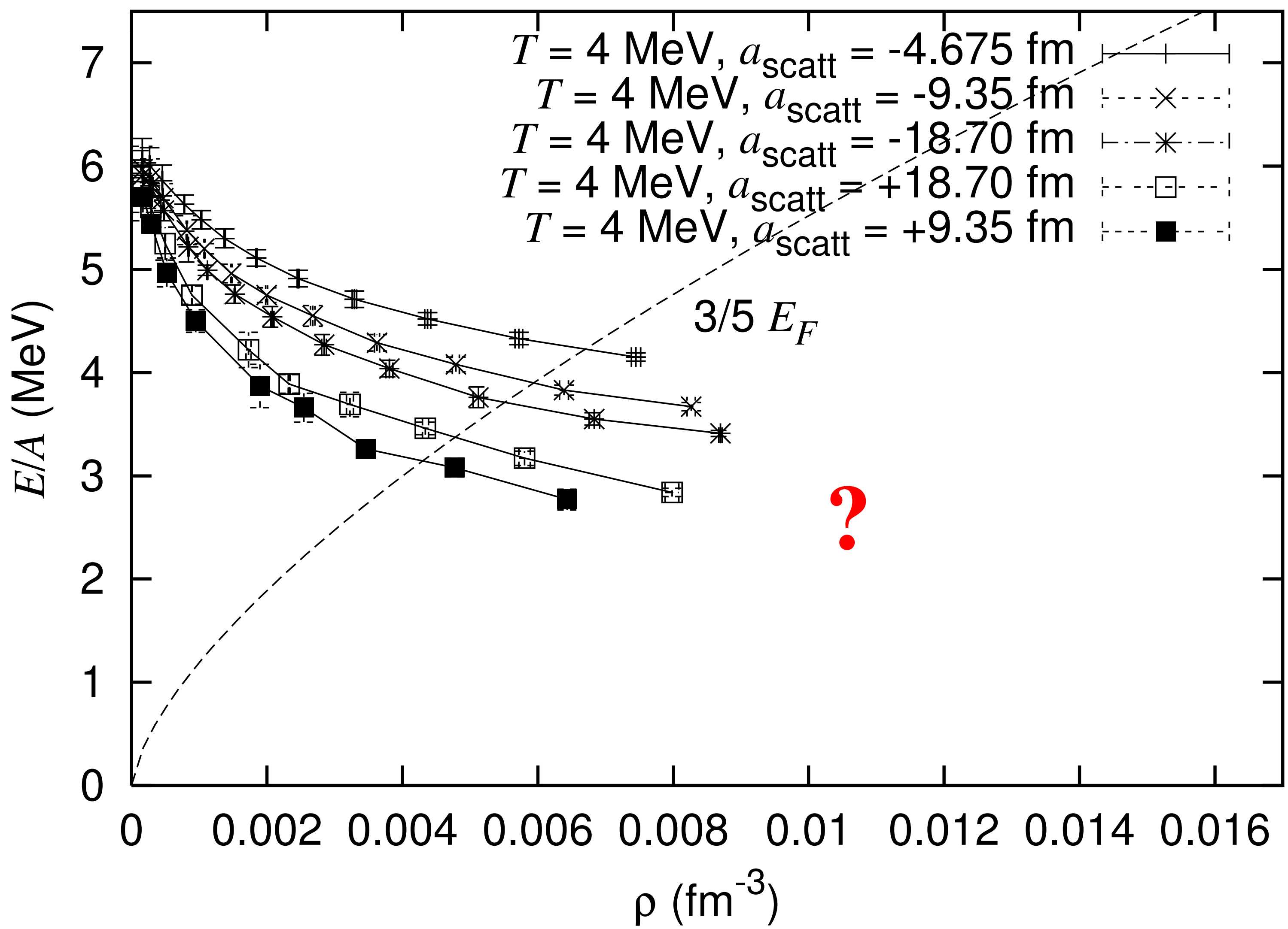
We use Lüscher's formula to set the operator coefficient C to give the physical s-wave scattering length for two-particle scattering.

$$E_0 = \frac{4\pi a_{scatt}}{mL^3}[1 - c_1 \frac{a_{scatt}}{L} + c_2 \frac{a_{scatt}^2}{L^2} + \cdots]$$

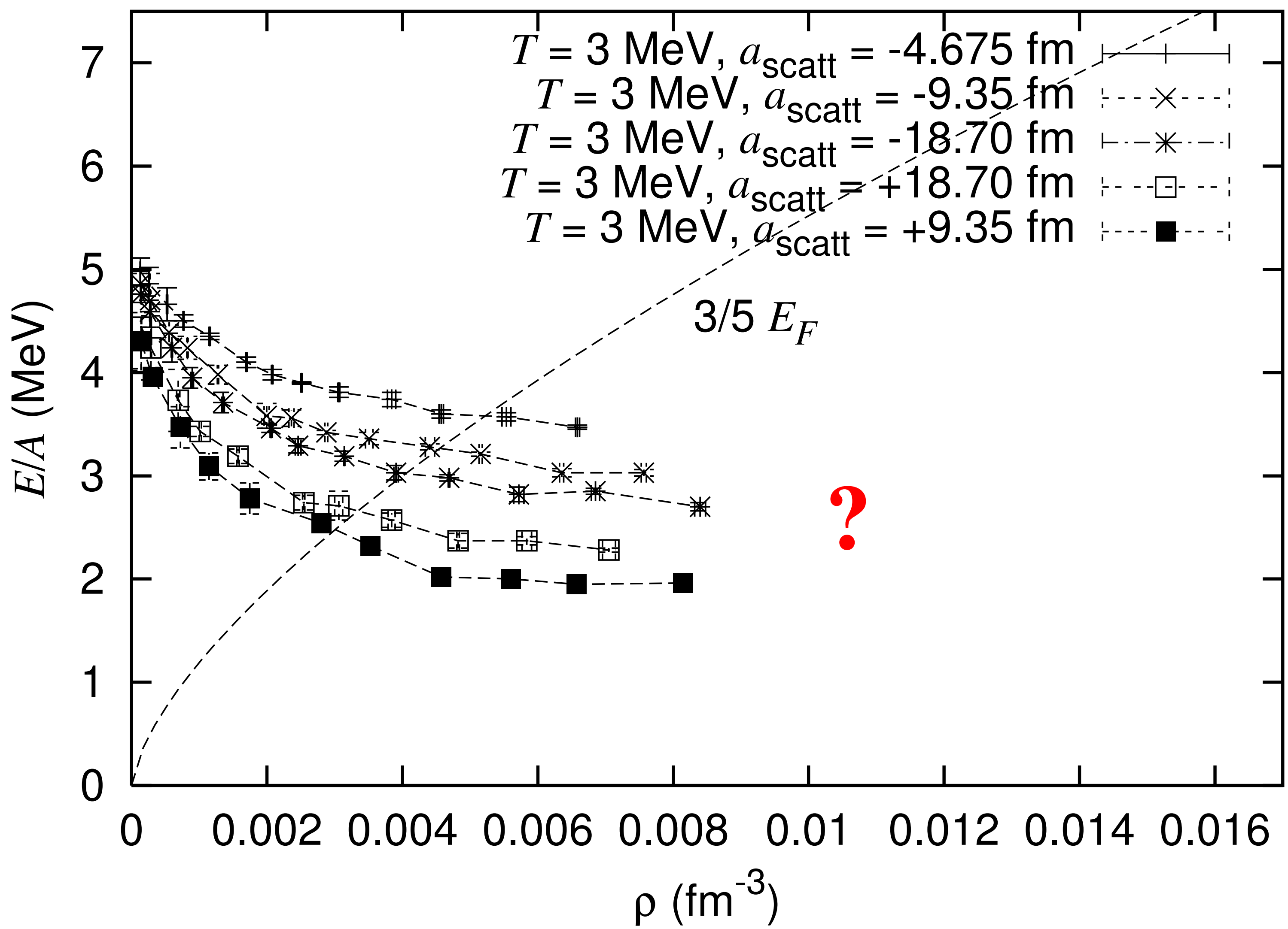
We sum the full set of bubble diagrams



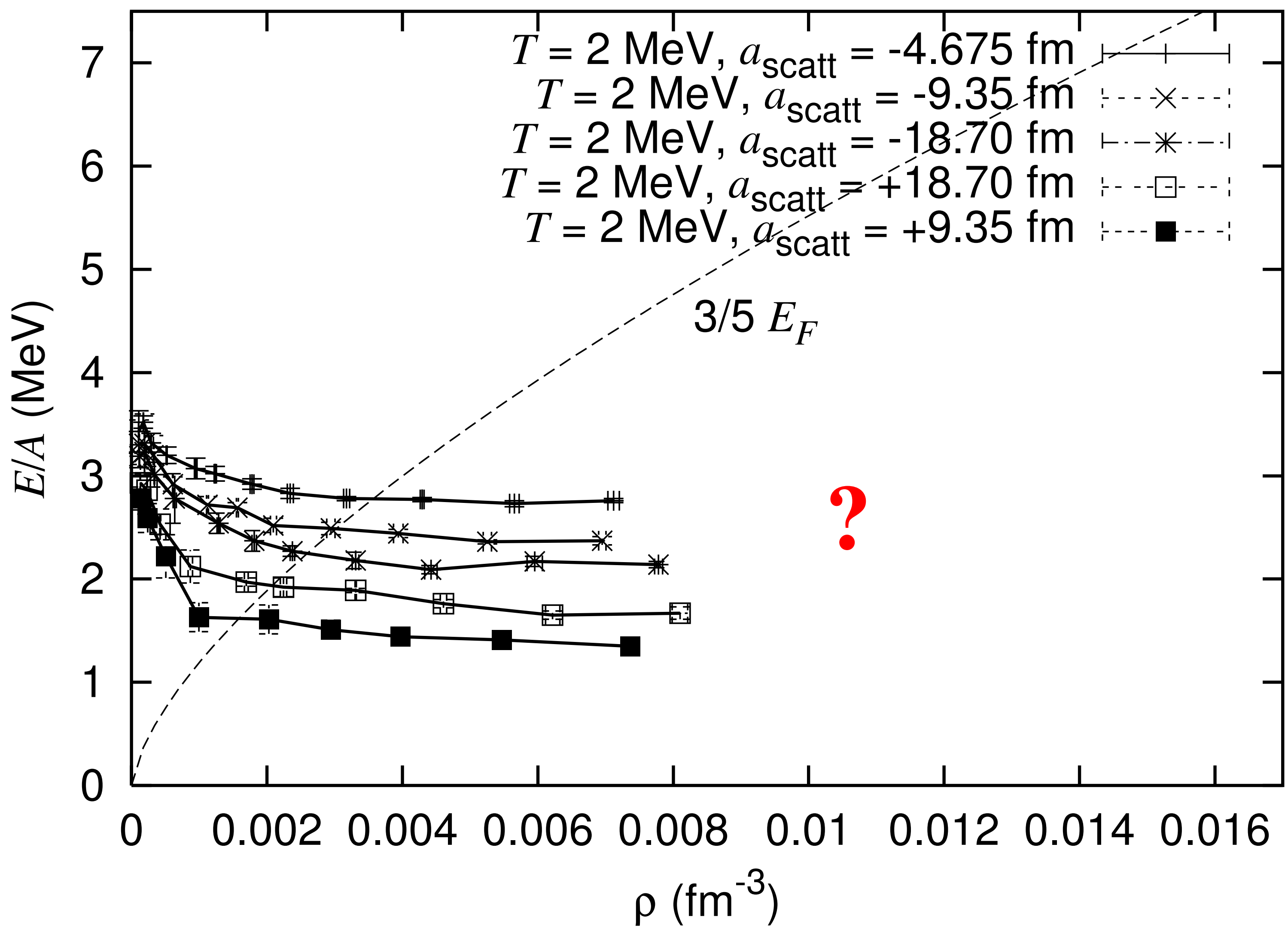
Energy per particle vs. density



Energy per particle vs. density



Energy per particle vs. density



Virial expansion

Expansion in fugacity,

$$z = e^{\beta\mu}$$

Thermal wavelength

$$\lambda_T = \sqrt{\frac{2\pi}{mk_BT}} = \left(\frac{2\pi}{m}\right)^{1/2} \beta^{1/2}$$

$$\frac{\ln Z_G}{V} = \frac{P}{k_BT} = \frac{2}{\lambda_T^3}\left[z + b_2(T)z^2 + \cdots\right]$$

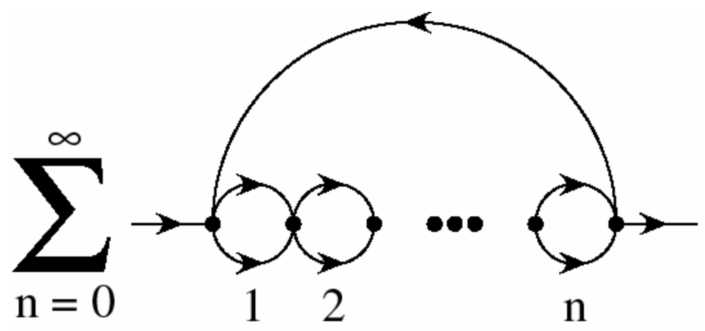
In the unitary regime (zero range and infinite scattering length)

$$b_2(T) \rightarrow \frac{3\sqrt{2}}{8} \approx 0.530$$

Second virial coefficient determined by two-particle interactions

High temperature/low density

At low densities we can compute the self-energy by summing bubble chain diagrams



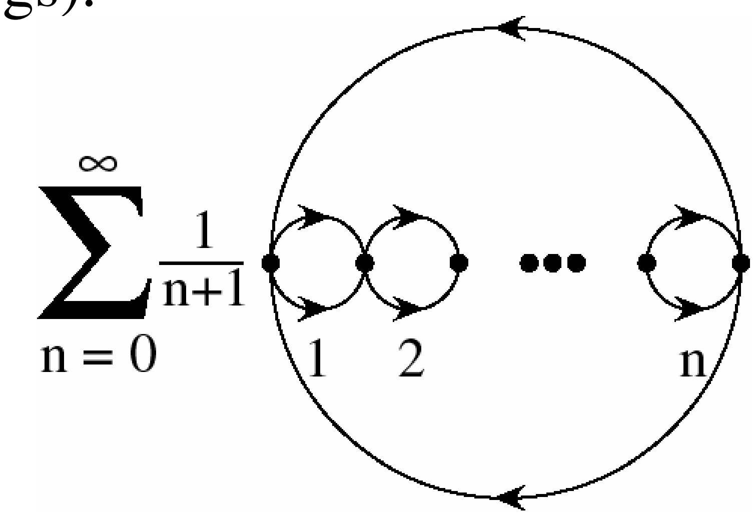
At $T = 0$, other diagrams are suppressed by factors of $k_F|a_{nn}|$. For $T > 0$, the thermal wavelength

$$\lambda_T = \sqrt{\frac{2\pi}{mT}}$$

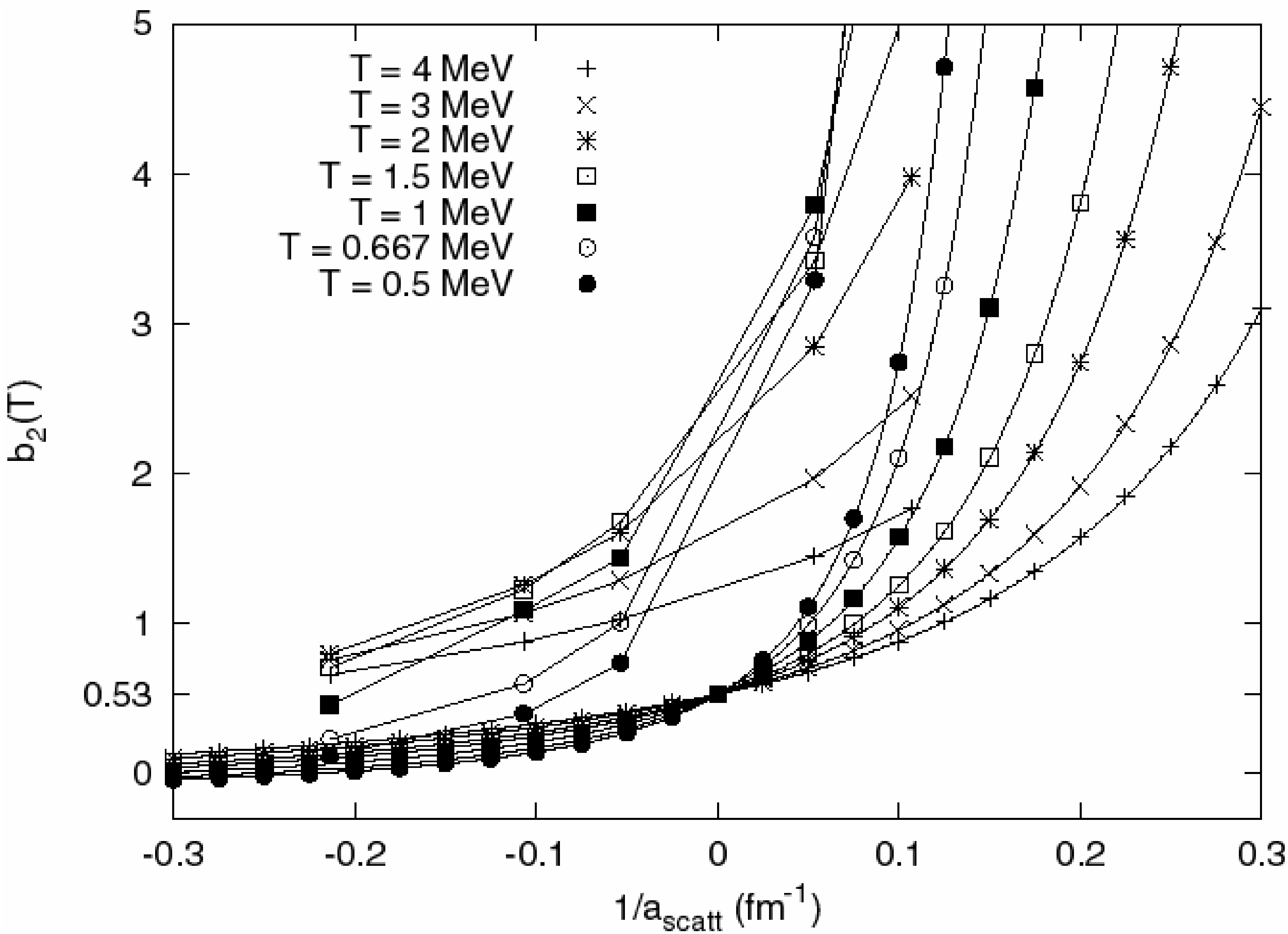
replaces the scattering length when it is the smaller of the two… comparable to expanding in fugacity

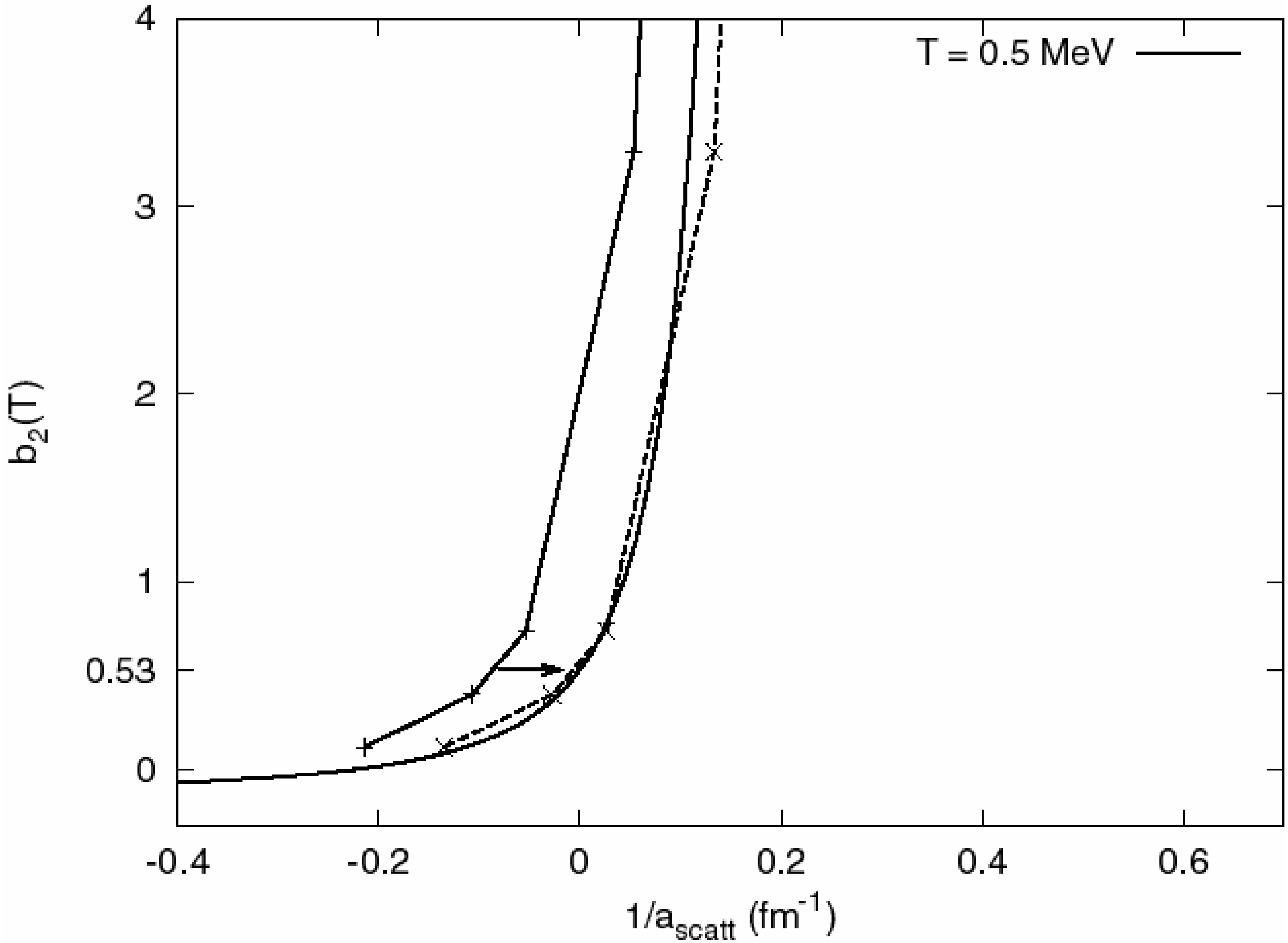
$$z = e^{\beta\mu}$$

Similarly we can compute the logarithm of the partition function (sum of connected diagrams with no external legs).



Lattice vs. continuum virial coefficients





T = 0.5 MeV
b_2(T)
1/a_scatt (fm^-1)
4
3
2
1
0.53
0
-0.4
-0.2
0
0.2
0.4
0.6

Fixing the problem…

Tune the operator coefficient to give the correct second virial coefficient at the given simulation temperature [D.L., Schäfer, nucl-th/0509017]

or

Use an improved lattice action [R. Thomson, D.L., work in progress]

Scaling limit (scattering length $\to \pm\infty$)

Hamiltonian lattice (temporal spacing = 0)

$$H - \mu N = \sum_{\vec{n}_s, i} \left[(-\mu + \frac{3}{m}) a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s) \right]$$

$$- \frac{1}{2m} \sum_{\vec{n}_s, l_s, i} \left[a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s + \hat{l}_s) + a_i^\dagger(\vec{n}_s) a_i(\vec{n}_s - \hat{l}_s) \right]$$

$$- \frac{\eta}{m} \sum_{\vec{n}_s} a_\downarrow^\dagger(\vec{n}_s) a_\uparrow^\dagger(\vec{n}_s) a_\uparrow(\vec{n}_s) a_\downarrow(\vec{n}_s)$$

$$\eta \simeq 3.96$$

Three-dimensional attractive Hubbard model with

$$U = -7.92t$$

We note that

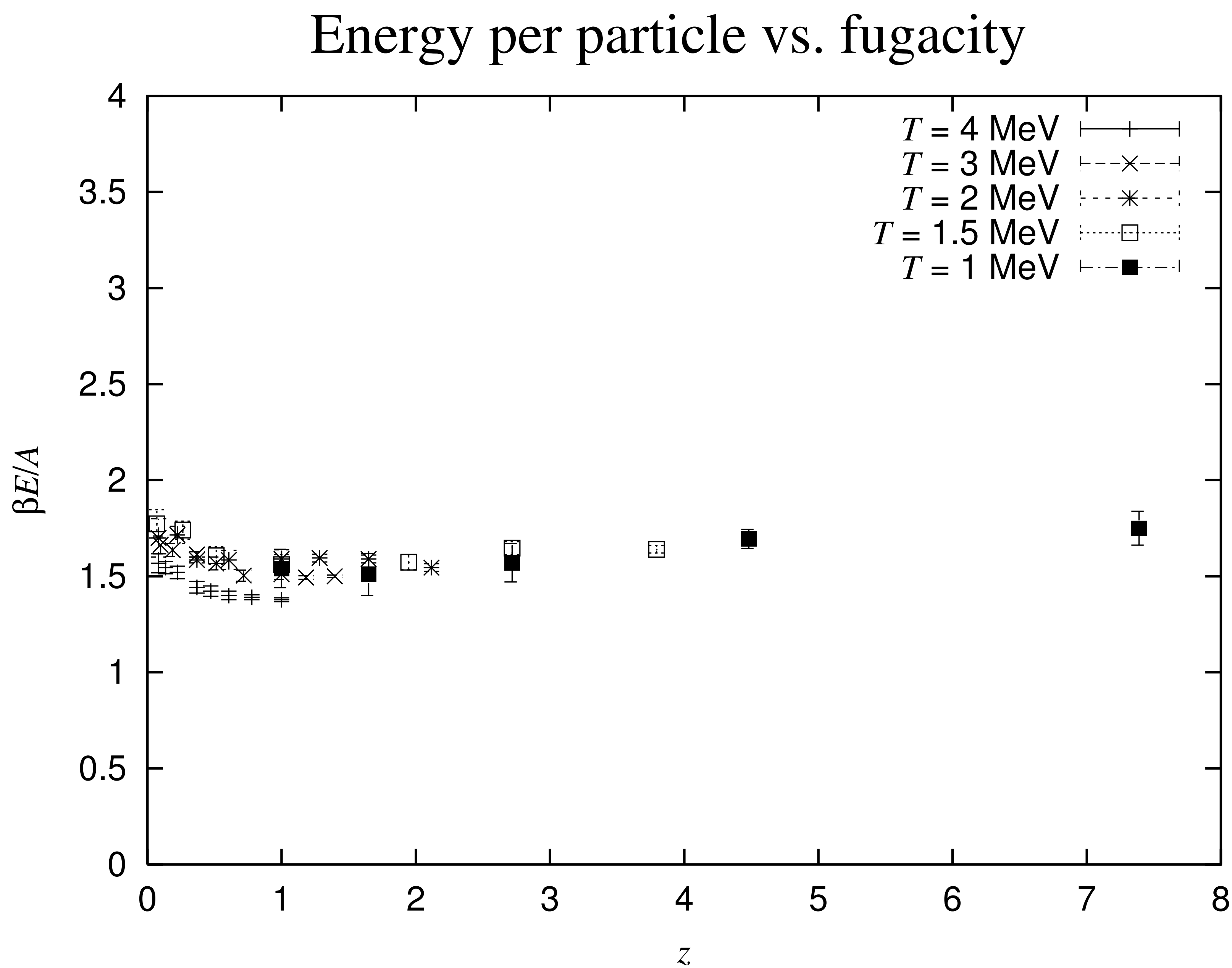
$$Z_G = Tr\left[-\beta\left(H - \mu N\right)\right]$$

is a function of only the two dimensionless quantities

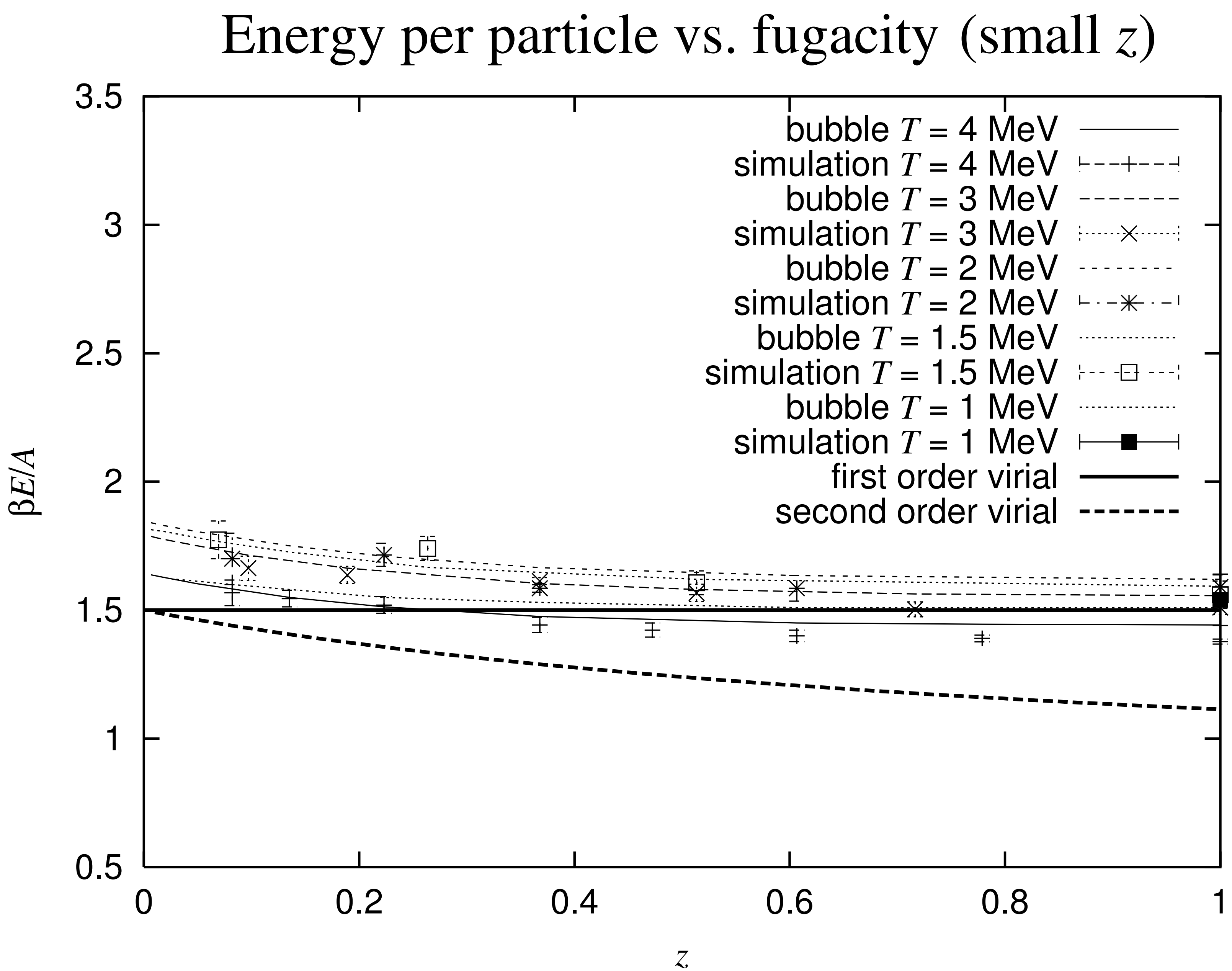
$$\frac{\beta}{2m} = \frac{1}{2m^{phys}T^{phys}a^2}$$

$$\beta\mu = \frac{\mu^{phys}}{T^{phys}}$$

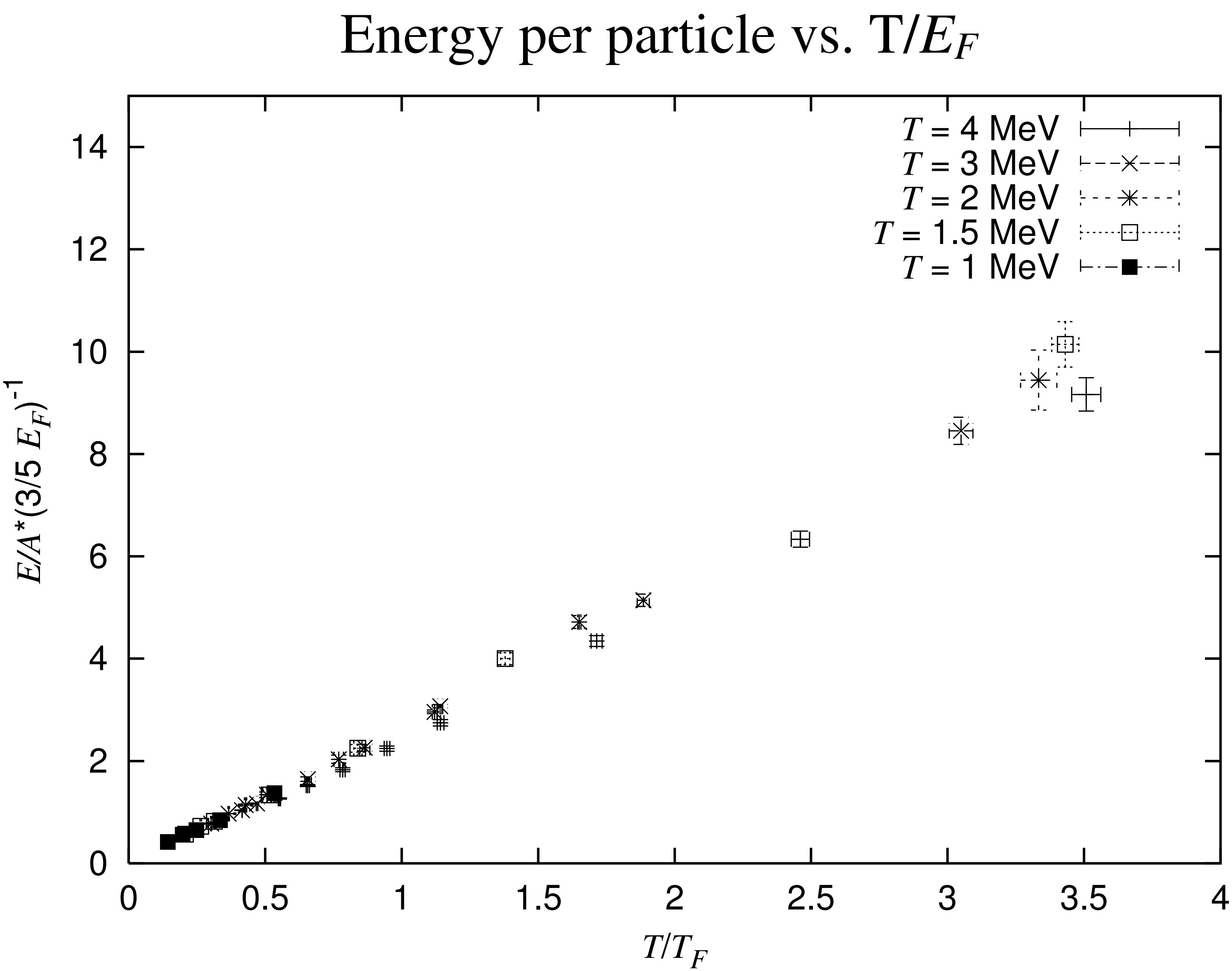
The dependence on the lattice spacing must drop out, so observables at different temperatures can be rescaled to a single universal function



Energy per particle vs. fugacity
T = 4 MeV
T = 3 MeV
T = 2 MeV
T = 1.5 MeV
T = 1 MeV
βE/A
z
0
0.5
1
1.5
2
2.5
3
3.5
4
0
1
2
3
4
5
6
7
8

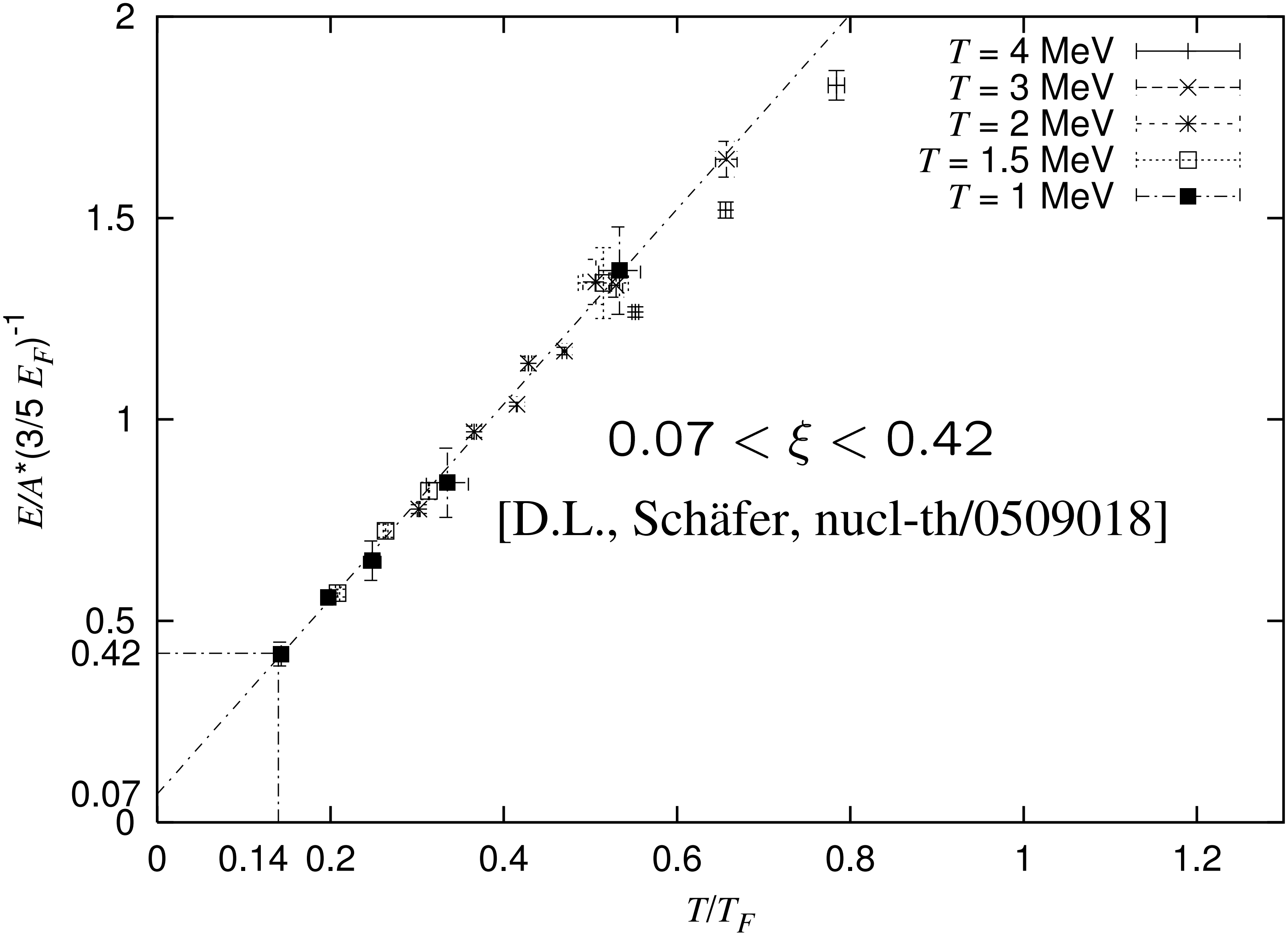


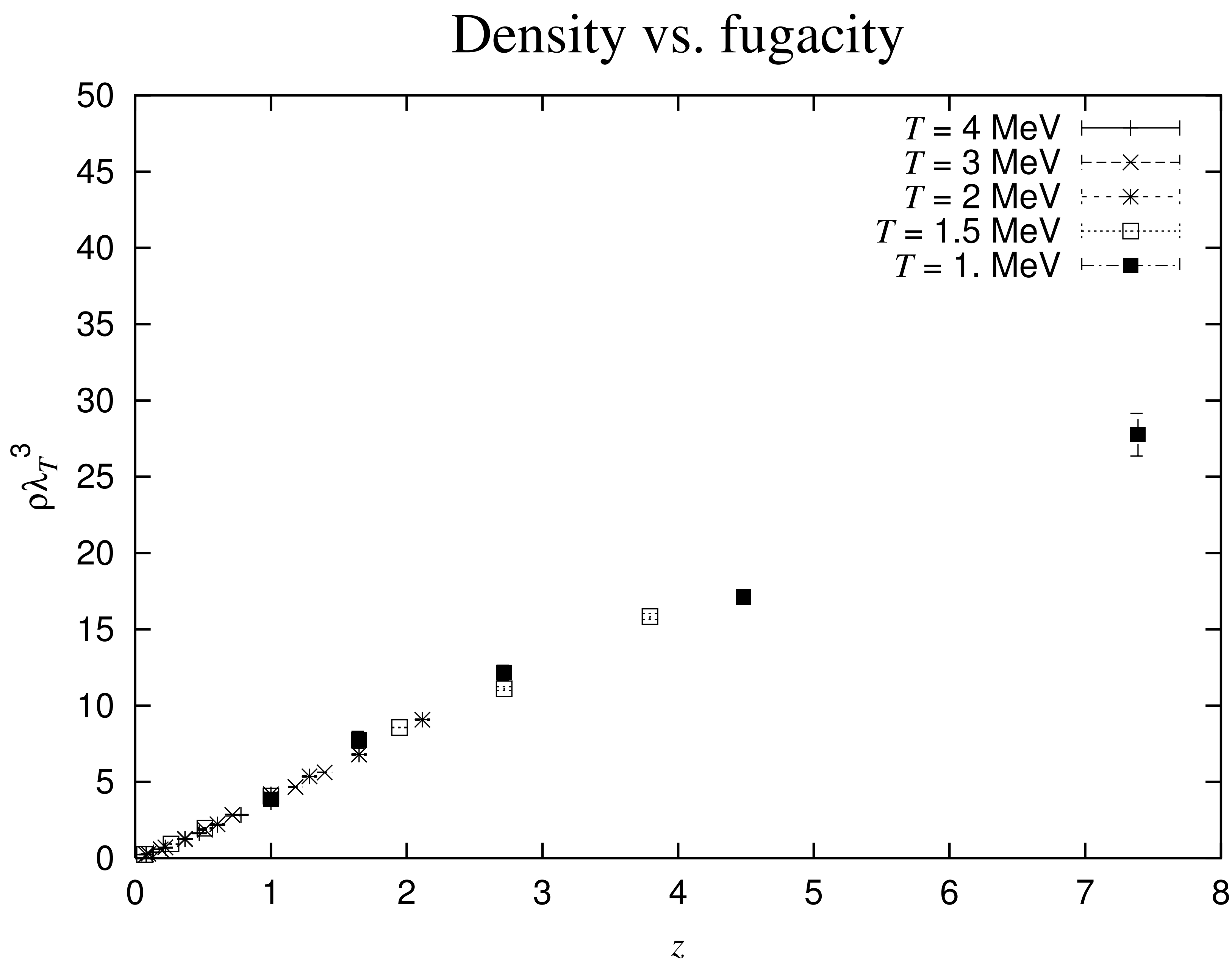
Energy per particle vs. fugacity (small z)
βE/A
z
3.5
3
2.5
2
1.5
1
0.5
0
0.2
0.4
0.6
0.8
1
bubble T = 4 MeV
simulation T = 4 MeV
bubble T = 3 MeV
simulation T = 3 MeV
bubble T = 2 MeV
simulation T = 2 MeV
bubble T = 1.5 MeV
simulation T = 1.5 MeV
bubble T = 1 MeV
simulation T = 1 MeV
first order virial
second order virial



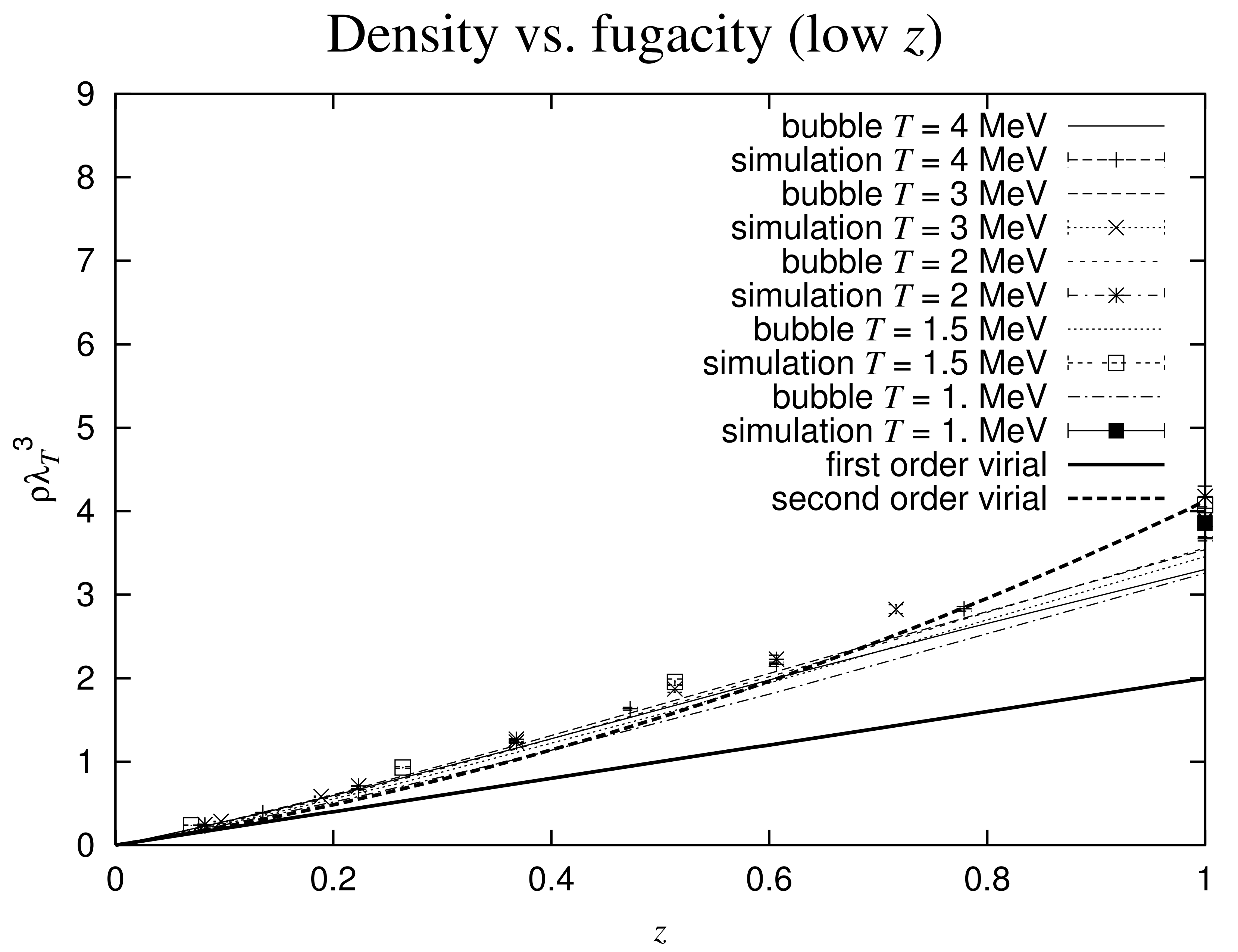
Energy per particle vs. T/E_F
T = 4 MeV
T = 3 MeV
T = 2 MeV
T = 1.5 MeV
T = 1 MeV
E/A*(3/5 E_F)$^{-1}$
T/T_F
0
2
4
6
8
10
12
14
0.5
1
1.5
2
2.5
3
3.5
4

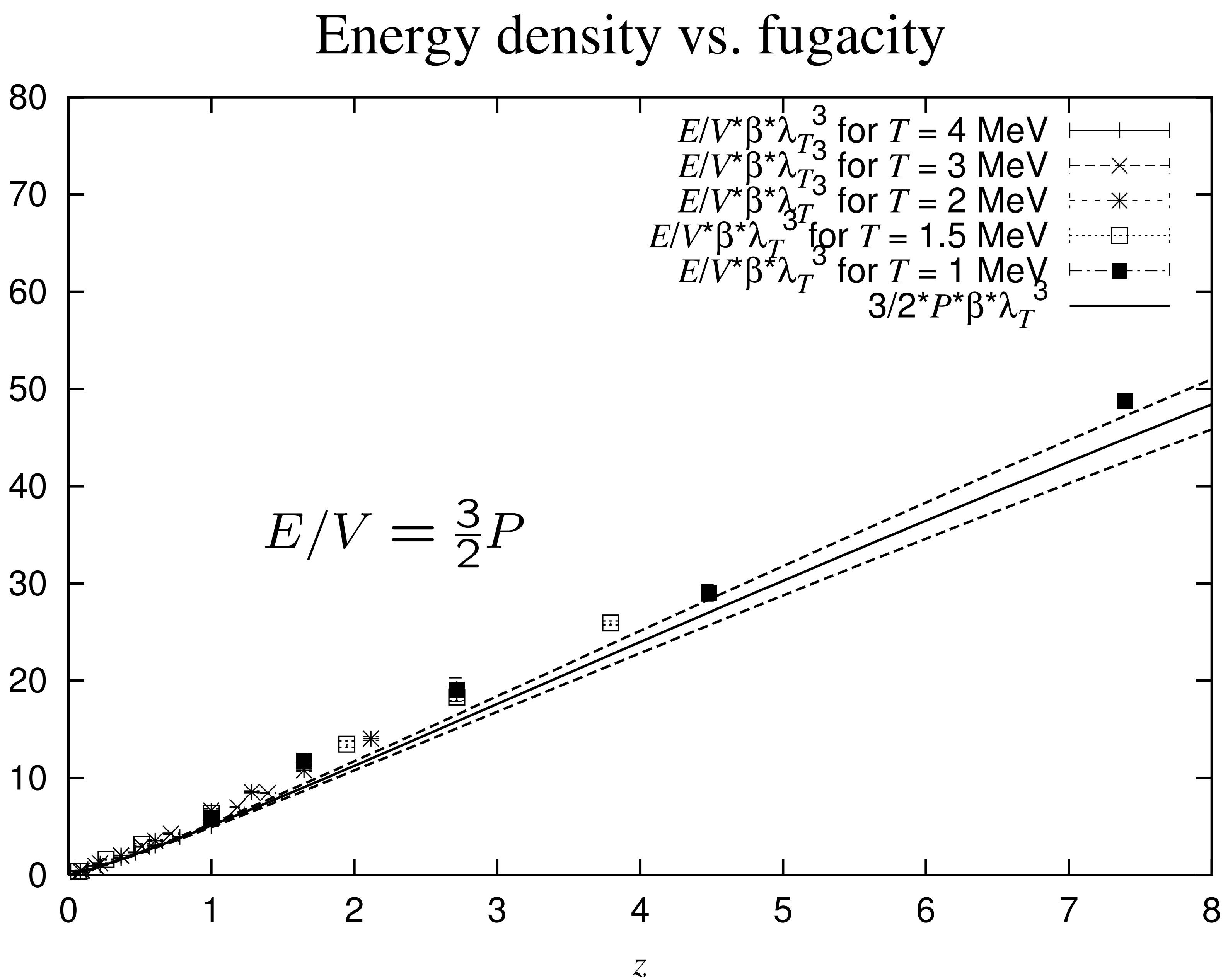
Energy per particle vs. T/E_F (low T)





Density vs. fugacity
T = 4 MeV
T = 3 MeV
T = 2 MeV
T = 1.5 MeV
T = 1. MeV
$\rho\lambda_T^3$
z
0
5
10
15
20
25
30
35
40
45
50
0
1
2
3
4
5
6
7
8

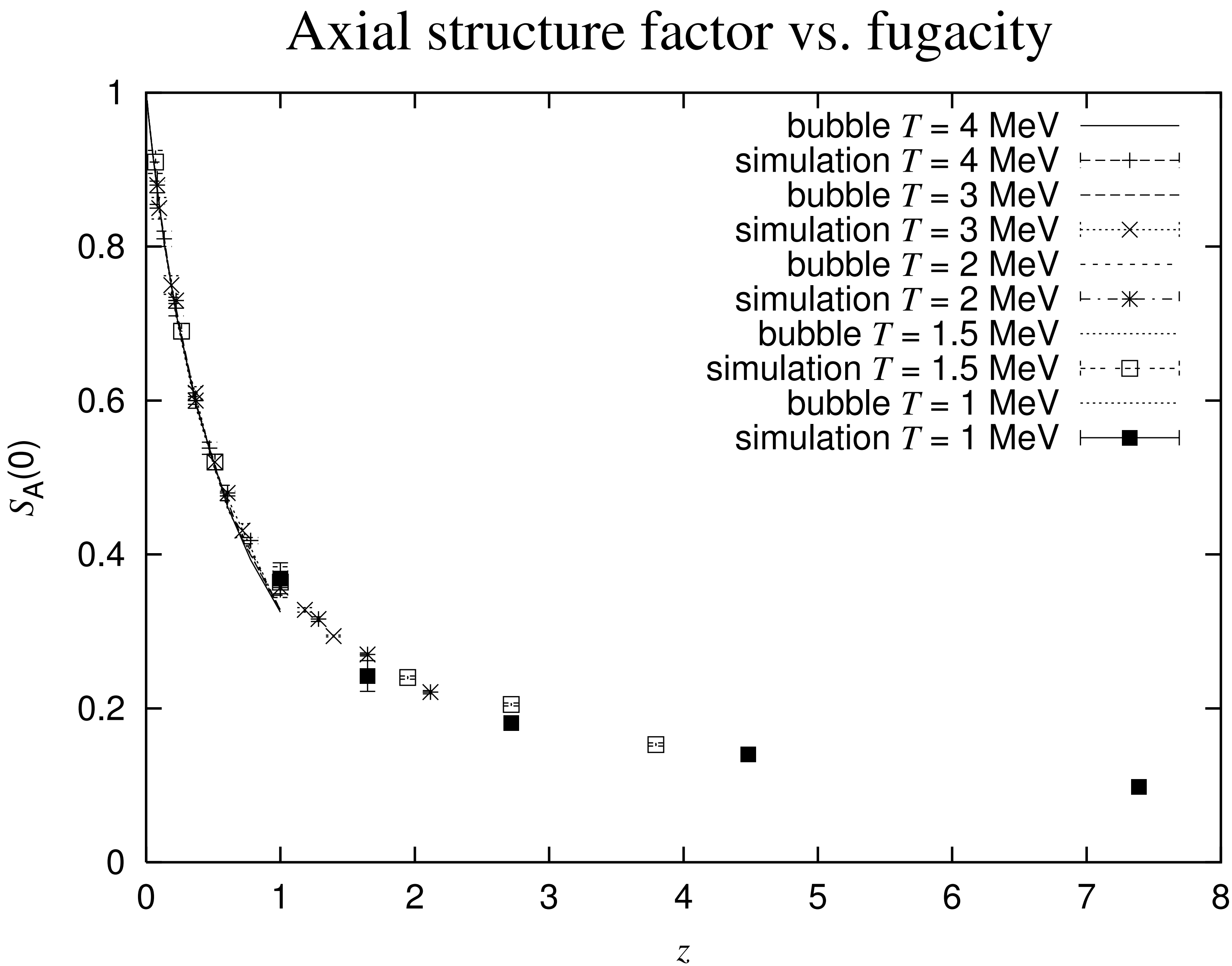

Density vs. fugacity (low z)
bubble T = 4 MeV
simulation T = 4 MeV
bubble T = 3 MeV
simulation T = 3 MeV
bubble T = 2 MeV
simulation T = 2 MeV
bubble T = 1.5 MeV
simulation T = 1.5 MeV
bubble T = 1. MeV
simulation T = 1. MeV
first order virial
second order virial
ρλ_T^3
z
0
1
2
3
4
5
6
7
8
9
0
0.2
0.4
0.6
0.8
1


Energy density vs. fugacity
$E/V*\beta*\lambda_T^3$ for T = 4 MeV
$E/V*\beta*\lambda_T^3$ for T = 3 MeV
$E/V*\beta*\lambda_T^3$ for T = 2 MeV
$E/V*\beta*\lambda_T^3$ for T = 1.5 MeV
$E/V*\beta*\lambda_T^3$ for T = 1 MeV
$3/2*P*\beta*\lambda_T^3$
$E/V = \frac{3}{2}P$
z
0
10
20
30
40
50
60
70
80
0
1
2
3
4
5
6
7
8

Axial structure factor
(or spin susceptibility)

$$S_A(0) = \frac{1}{\left\langle \hat{N} \right\rangle} \left\langle (\hat{N}_\uparrow - \hat{N}_\downarrow)(\hat{N}_\uparrow - \hat{N}_\downarrow) \right\rangle$$

measures spin correlation … decreases if neutrons form spin zero pairs



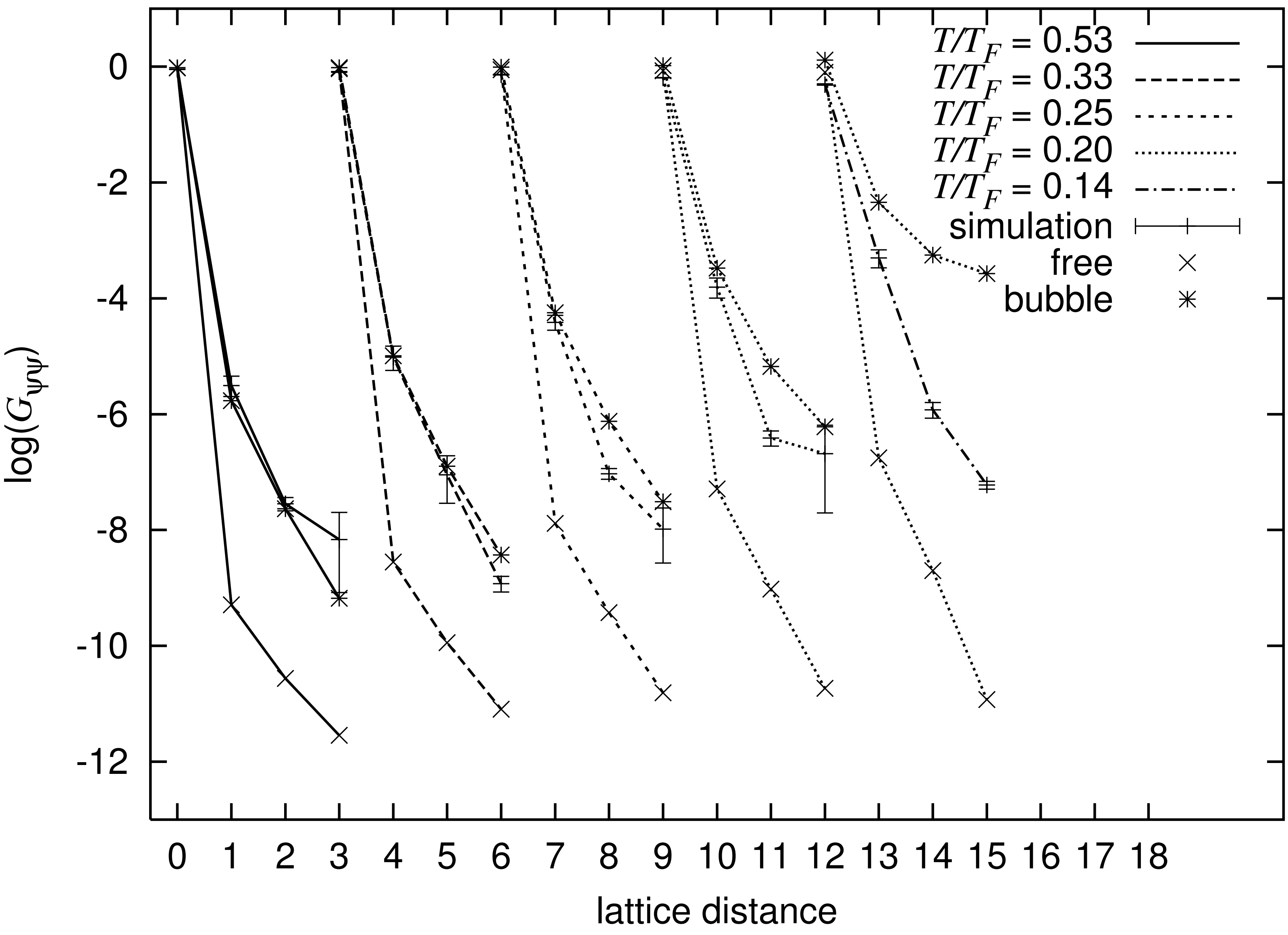
Axial structure factor vs. fugacity
bubble T = 4 MeV
simulation T = 4 MeV
bubble T = 3 MeV
simulation T = 3 MeV
bubble T = 2 MeV
simulation T = 2 MeV
bubble T = 1.5 MeV
simulation T = 1.5 MeV
bubble T = 1 MeV
simulation T = 1 MeV
$S_A(0)$
z
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5
6
7
8

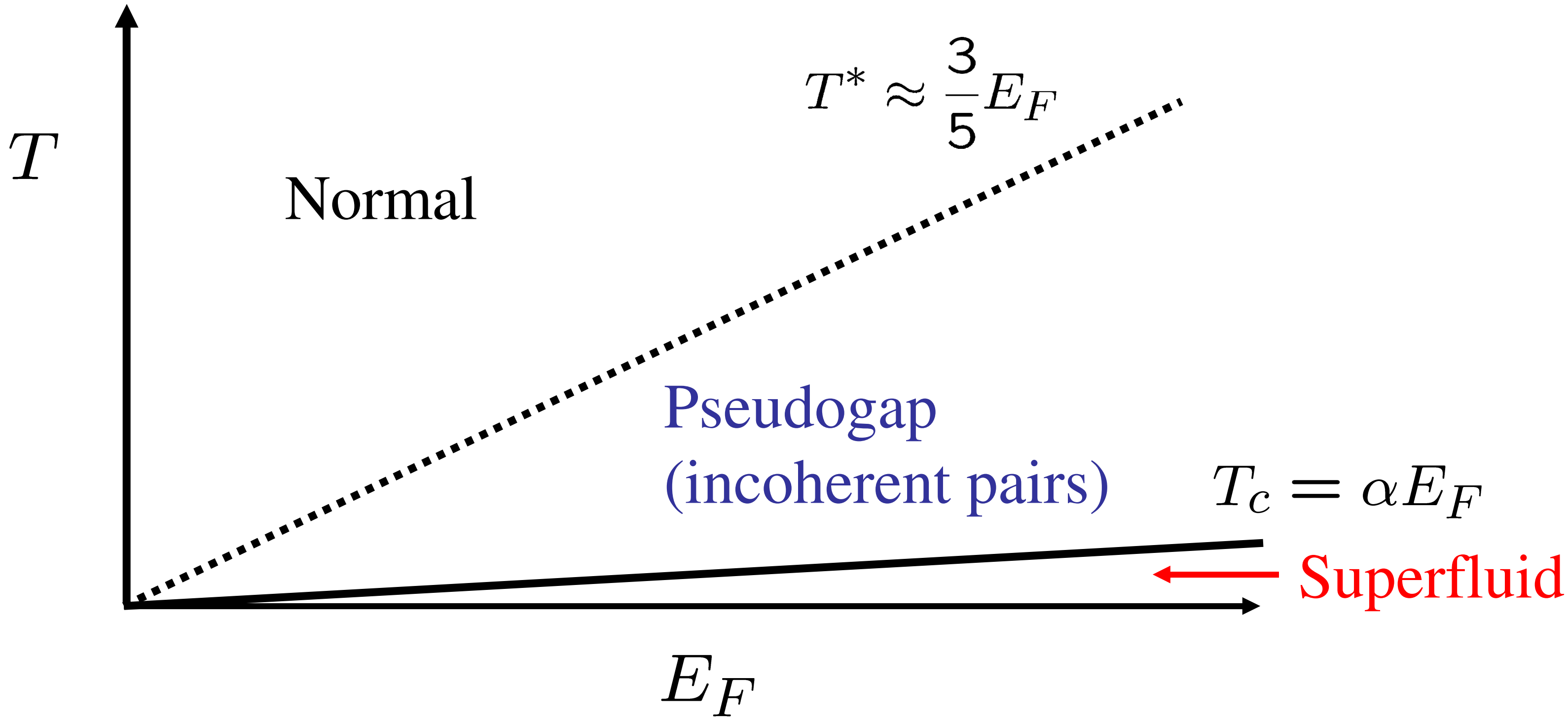
Dineutron correlator

$$\left\langle a_{\uparrow}(\vec{n}_s)a_{\downarrow}(\vec{n}_s)a_{\downarrow}^{\dagger}(0)a_{\uparrow}^{\dagger}(0)\right\rangle$$

Look for long range order and Bose condensate of dineutron pairs

Dineutron correlator vs. distance





$\alpha = 0.035(4)$ [Wingate, cond-mat/0502372]

$\alpha = 0.152(7)$ [Prokof'ev, Svistunov, preliminary]

$\alpha = 0.22(3)$ [Bulgac, Drut, Magierski, cond-mat/0505374]

$\alpha < 0.14$ [D.L., Schäfer, nucl-th/0509018]

Road map

1. Larger simulations of cold dilute neutron matter
2. Improved actions
3. Few body systems and three-body forces
4. Asymmetric nuclear matter without pions
5. Nuclear matter with pions