Nuclear Lattice Simulations using Chiral Effective Theory

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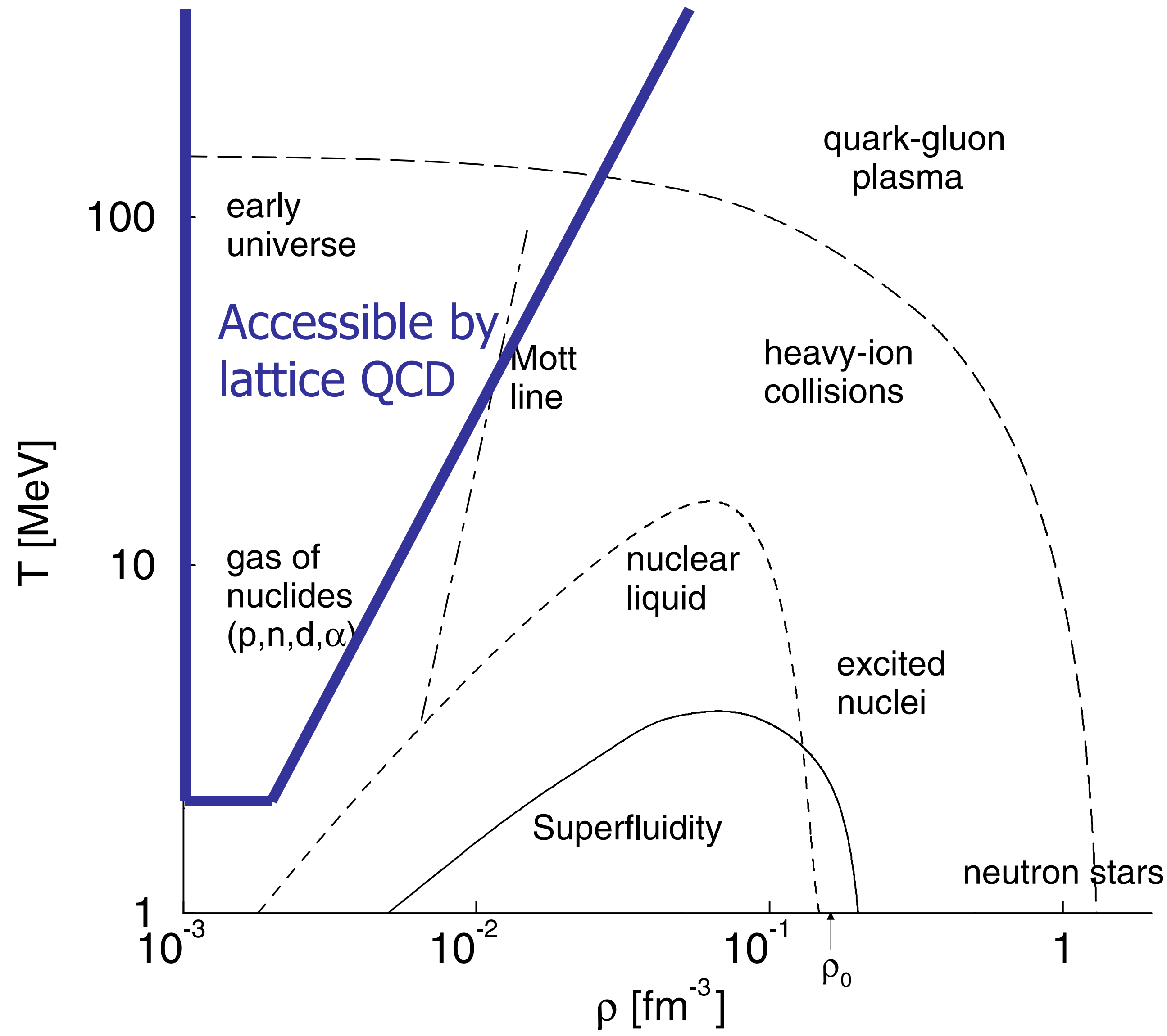
Nuclear Lattice Collaboration

Outline

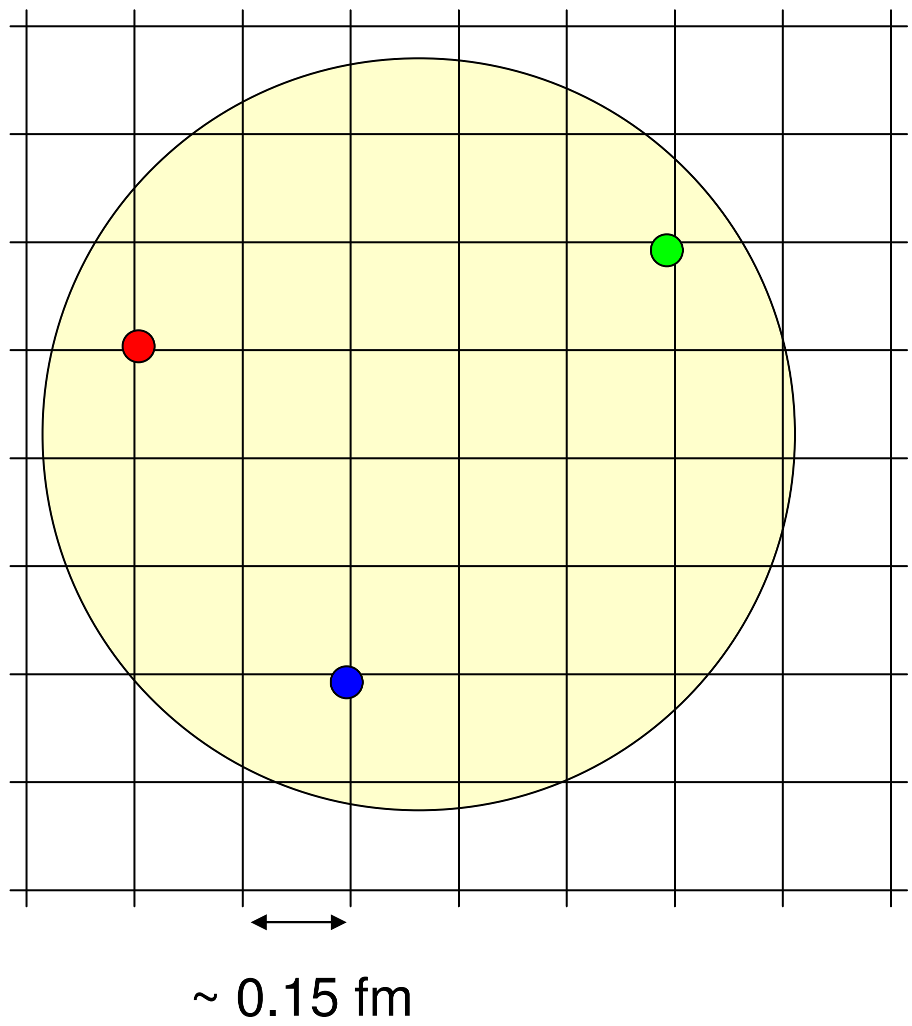
1. Why nuclear lattice simulations?
2. Chiral effective theory and lattice methods
3. Numerical challenges
4. Operator coefficients
5. Determinant zone expansion
6. Results and directions



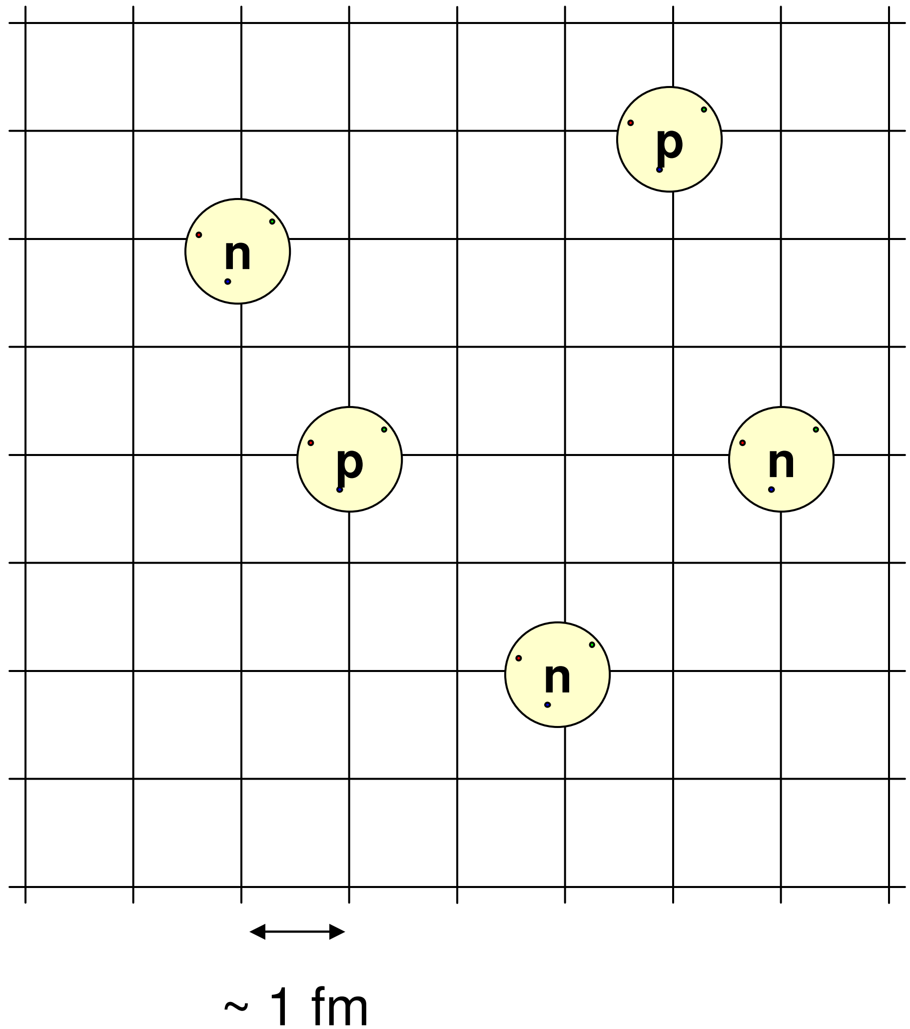
Ropke and Schell, Prog. Part. Nucl. Phys. 42, 53 (1999)

Why do nuclear lattice simulations?

Nucleon in lattice QCD



Nucleons as point particles on lattice



Nuclear Lattice Simulations

Numerous studies of ground state properties of few nucleon systems using potential models together with variational and/or Green's function Monte Carlo

[Wiringa and Pieper, PRL 89 (2002)182501; Carlson and Schiavilla, Rev. Mod. Phys. 70 (1998) 743; etc.]

Also studies of the liquid-gas transition using classical lattice gas models

[Ray, Shamanna, and Kuo, PLB 392 (1997) 7]

First study of quantum many body effects in infinite nuclear matter on the lattice (quantum hadrodynamics on momentum lattice)

[Brockmann and Frank, PRL 68 (1992) 1830]

First study on spatial lattice at finite temperature

[Müller, Koonin, Seki, and van Kolck, PRC 61 (2000) 044320]

In the continuum language,

$$H = K + V_c + V_\sigma$$

$$K = -\tfrac{1}{2m_N} \sum_{\sigma\tau} \int d^3\vec{x}\, \psi^\dagger_{\sigma\tau}(\vec{x}) \vec{\nabla}^2 \psi_{\sigma\tau}(\vec{x})$$

$$V_c =$$

$$\tfrac{1}{2}\sum_{\sigma\tau\sigma'\tau'}\int d^3\vec{x}\int d^3\vec{x}'\psi^{\dagger}_{\sigma\tau}(\vec{x})\psi^{\dagger}_{\sigma'\tau'}(\vec{x}')V_c(\vec{x}-\vec{x}')\psi_{\sigma'\tau'}(\vec{x}')\psi_{\sigma\tau}(\vec{x})$$

$$V_\sigma = \tfrac{1}{2}\sum_{\xi\tau\xi'\tau'\kappa\lambda\kappa'\lambda'}\int d^3\vec{x}\int d^3\vec{x}'\begin{bmatrix}\psi^{\dagger}_{\xi\tau}(\vec{x})\psi^{\dagger}_{\xi'\tau'}(\vec{x}')V_\sigma(\vec{x}-\vec{x}') \\ \vec{\sigma}_{\xi\tau\kappa\lambda}\cdot\vec{\sigma}_{\xi'\tau'\kappa'\lambda'}\psi_{\kappa'\lambda'}(\vec{x}')\psi_{\kappa\lambda}(\vec{x})\end{bmatrix}$$

$\psi^{\dagger}_{\sigma\tau}$ creates a nucleon of spin σ, isospin τ

$\vec{\sigma}_{\xi\tau\kappa\lambda}$ elements of generalized Pauli spin-isospin matrix

$$V_c(\vec{x}-\vec{x}') = V_c^{(0)}\delta(\vec{x}-\vec{x}') + V_c^{(2)}\vec{\nabla}^2\delta(\vec{x}-\vec{x}')$$
$$V_\sigma(\vec{x}-\vec{x}') = V_\sigma^{(0)}\delta(\vec{x}-\vec{x}') + V_\sigma^{(2)}\vec{\nabla}^2\delta(\vec{x}-\vec{x}')$$

Used Hubbard-Stratonovitch transformation (introduces an auxiliary boson field) to put fermion interactions in quadratic form,

$$\overline{\psi}M(\phi)\psi$$

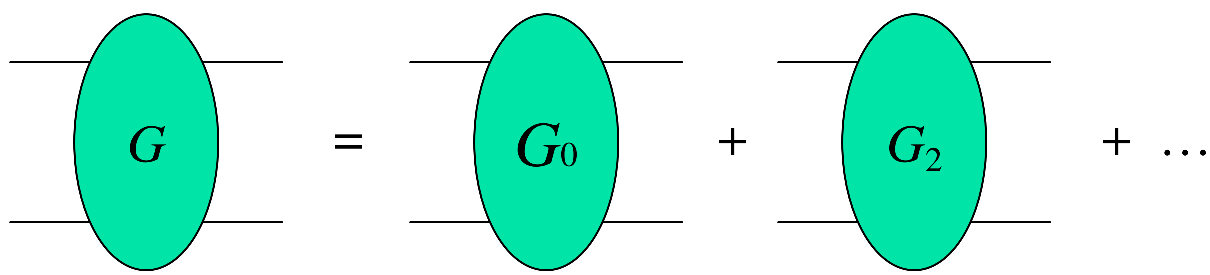
Studied phase transition from uncorrelated Fermi gas to clustered phase. Calculated saturation curve for a $4^3 \times L_t$ lattice with a = 1.84 fm.

Simulations with Chiral Effective Theory

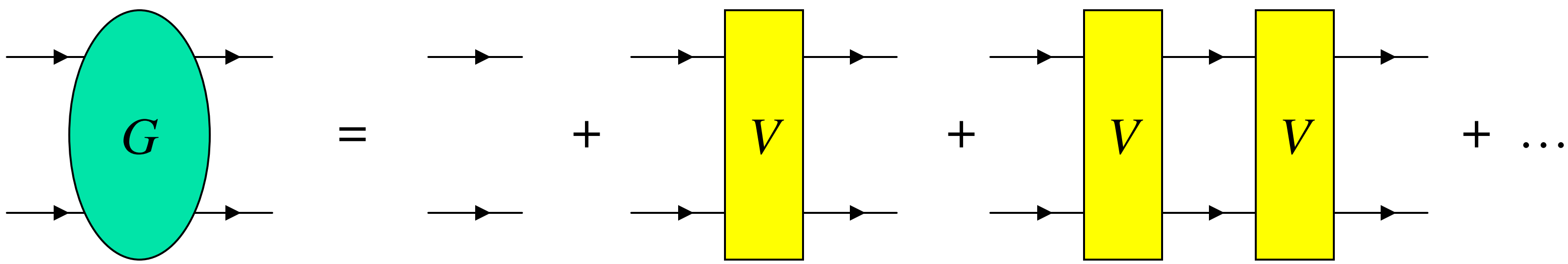
Non-perturbative lattice simulations of effective field theory of low energy pions and nucleons.

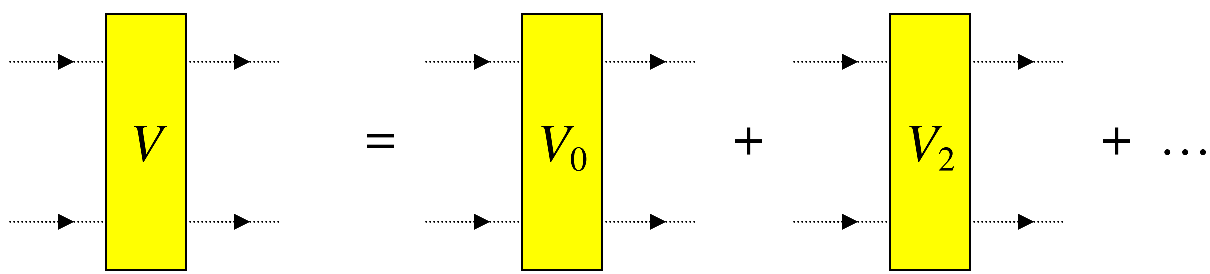
Non-perturbative effective field theory?... but isn't effective field theory based upon an expansion?

For pions the expansion is simple

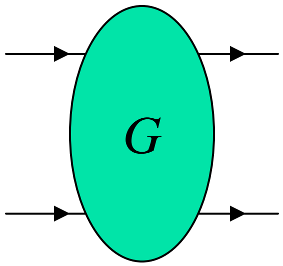


For nucleons we must take care of infrared singularities
[Weinberg, PLB 251 (1990) 288, NPB 363 (1991) 3]

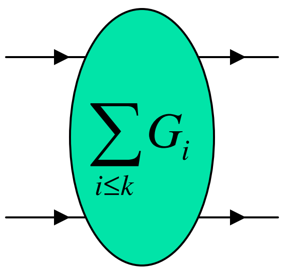




We will iterate "everything"



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



$$= \frac{\int D\pi DND\overline{N}\; G(\pi, N, \overline{N})e^{-\sum_{i \le k} S_i[\pi,N,\overline{N}]}}{\int D\pi DND\overline{N}\; e^{-\sum_{i \le k} S_i[\pi,N,\overline{N}]}}$$

A complete summation of all diagrams involving interaction terms with order $\leq\ k$

We use a low energy cutoff 150 ~ 300 MeV. The renormalization group flow to low energies tells us that the contribution of higher-dimensional operators are suppressed by powers of

$$\frac{\Lambda_{\text{cutoff}}}{\Lambda_{\text{high-energy}}}$$

The characteristic high-energy scale is set by heavy particle masses which we integrate out of the low energy theory or, equivalently, the chiral symmetry breaking scale (~1 GeV)

Our method:

$$N = \begin{bmatrix} p \\ n \end{bmatrix} \otimes \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix}$$

Following Weinberg [PLB 251 (1990) 288; NPB 363 (1991) 3], we write the most general local Lagrangian involving pions and low-energy nucleons

$$D \equiv 1 + \pi_i{}^2 / F_\pi^2$$

$$S = S_{\pi\pi} + S_{\overline{N}N} + S_{\pi\overline{N}N} + S_{\overline{N}N\overline{N}N} + S_{\pi\pi\overline{N}N} + \cdots$$

$$S_{\pi\pi} = \int d^3\vec{r}dr_4 \left[\tfrac{D^{-2}}{2} \left(\tfrac{\partial \pi_i}{\partial r_4} \right)^2 + \tfrac{D^{-2}}{2} \left(\vec{\nabla} \pi_i \right)^2 + \tfrac{D^{-1}}{2} m_\pi^2 \pi_i{}^2 \right]$$

$$S_{\overline{N}N} = \int d^3\vec{r}dr_4 \left[N^\dagger \tfrac{\partial N}{\partial r_4} - N^\dagger \tfrac{\vec{\nabla}^2 N}{2m_N} + (m_N - \mu) N^\dagger N \right]$$

$$S_{\pi \bar{N} N} = \int d^3\vec{r}\, dr_4 \left[D^{-1} g_A F_\pi^{-1} N^\dagger \left(\tau_i \vec{\sigma} \cdot \vec{\nabla} \pi_i \right) N \right]$$

$$S_{\bar{N} N \bar{N} N} = \int d^3\vec{r}\, dr_4 \left[\tfrac{1}{2} C_s N^\dagger N N^\dagger N + \tfrac{1}{2} C_t N^\dagger \vec{\sigma} N \cdot N^\dagger \vec{\sigma} N \right]$$

$$S_{\pi\pi \bar{N} N} = \int d^3\vec{r}\, dr_4 \left[i D^{-1} g_A F_\pi^{-2} N^\dagger \tau_i \left(\varepsilon_{ijk} \pi_j \tfrac{\partial \pi_k}{\partial r_4} \right) N \right]$$

Weinberg power counting:

$$\Delta = \#\partial + \tfrac{\# f}{2} - 2$$

We use Hubbard-Stratonovitch transformation for the *NN* contact interaction.

We start with neutron matter – just neutrons and neutral pions

Operator coefficients

Neutron-neutron contact interaction coefficient determined by s-wave zero-temperature scattering phase shifts on the lattice

Two possibilities:

Luscher's formula [Luscher, NPB 354 (1991) 531]

Solve lattice Schrodinger equation and find asymptotic wavefunctions of scattering states

If we ignore pion exchange (i.e., only bubble diagrams), we expect C ~ a

As expected we see significant cutoff dependence

a^{-1} (MeV)	C (MeV^{-2})
150	-0.40E-4
200	-0.35E-4
250	-0.31E-4
300	-0.29E-4

Numerical challenges

Good news… sign/phase problem is not bad at all

Problems occur only for temperatures less that about 1 MeV

Far better situation when compared with finite density lattice QCD

Why?

Physics answers– nucleons and pions give a simpler representation of the essential physics in the hadronic phase

Algorithmic answer – nucleons are much heavier than up and down quarks

The determinant of the one-body nucleon interaction matrix is not positive**

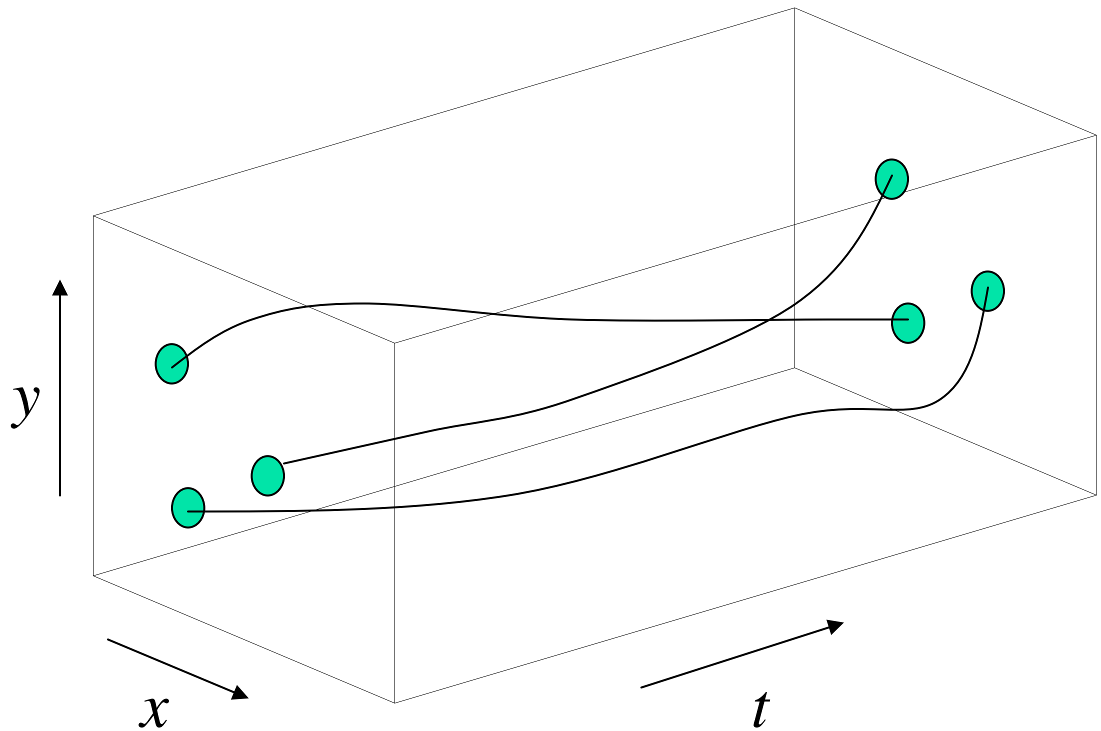
Although the phase is not oscillating much, there is a phase and to calculate it one needs to use LU decomposition

Numerical complexity for LU decomposition scales as the dimension of the matrix to the third power – slows down as L^{12} where L is the length of the system

**Except in special cases similar to attractive Hubbard model due to up-down spin symmetry [Chen and Kaplan, hep-lat/0308016]

Determinant zone expansion

Worldlines in finite temperature simulation:



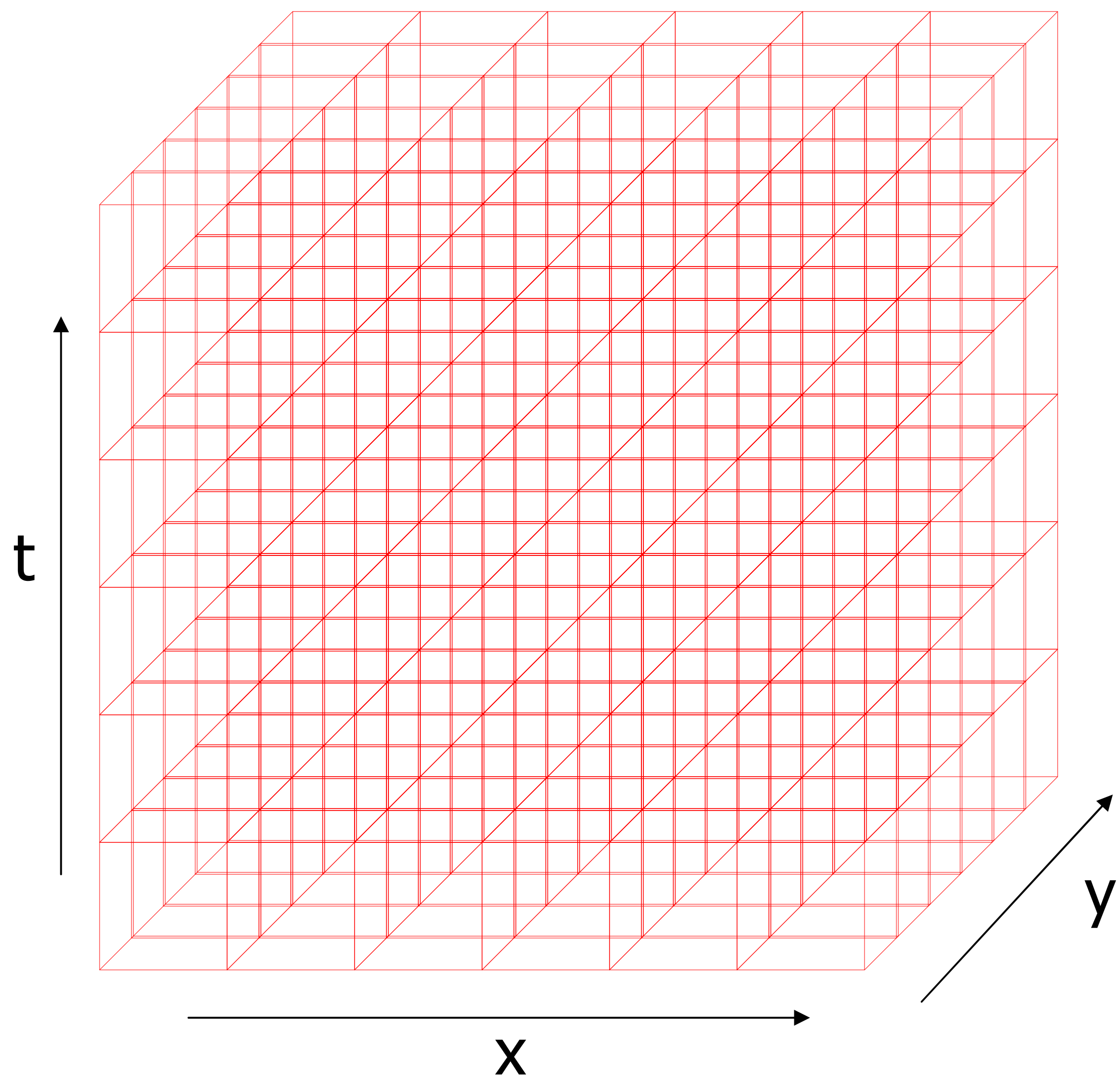
Let h be the spatial hopping parameter, and let β be the inverse temperature (imaginary time)

For a given fermion worldline we expect ~ βh total hops to the left and ~ βh hops to the right.

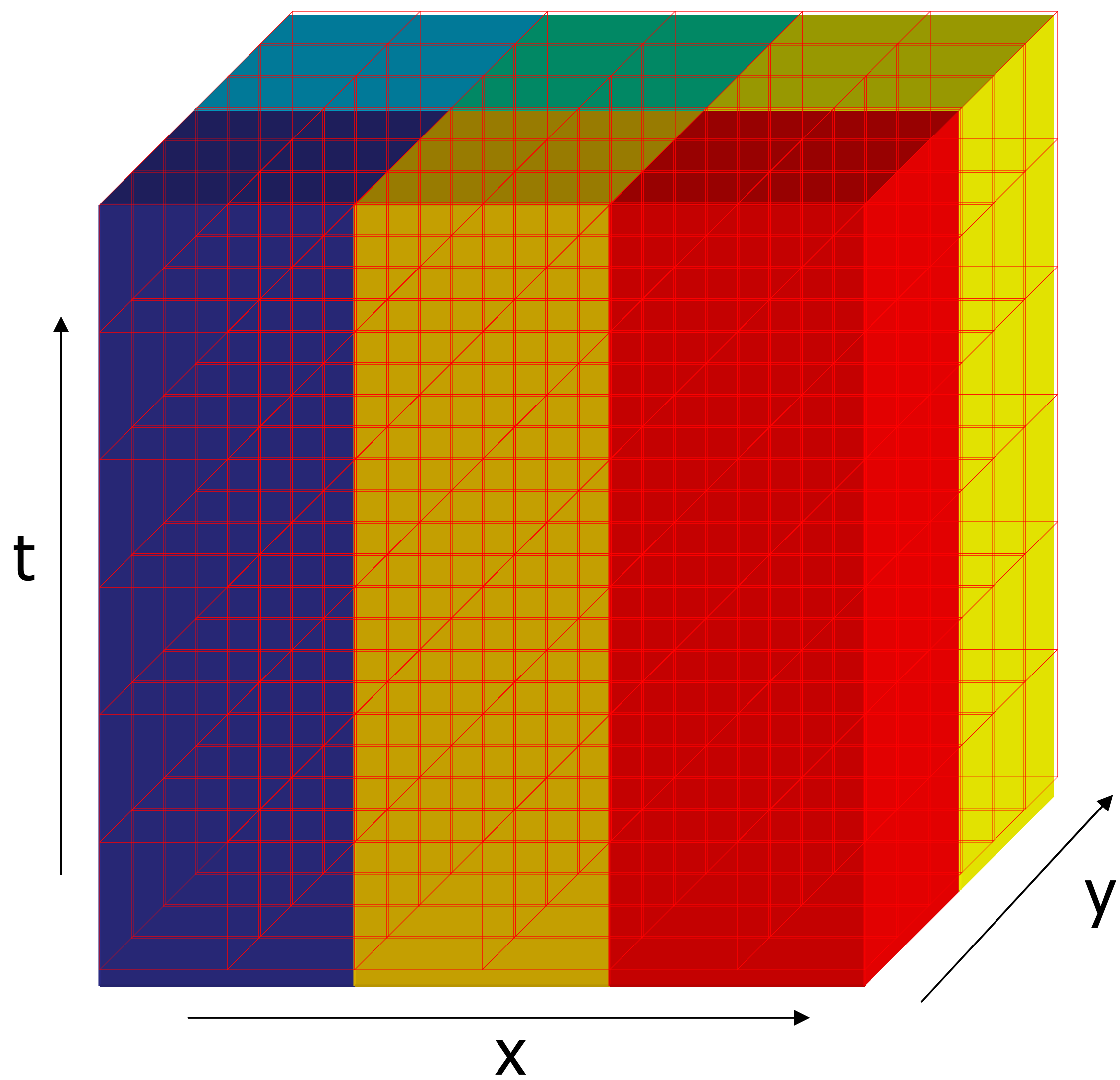
Equivalent to a random walk with $2\beta h$ steps. The average net displacement is therefore

$$l \sim \sqrt{\beta h}$$

Space-time lattice



Break up into spatial zones



If the zone size is much larger than the localization length

$$l \sim \sqrt{\beta h}$$

then neglecting fermion hopping across the zone boundaries is a relatively small effect. We can then expand in the zone boundary hopping term.

Let M be the nucleon matrix on the Euclidean lattice for given pion background field and Hubbard-Stratonovitch field. Let M_0 be the corresponding matrix with spatial hopping across zone boundaries eliminated.

We can use a trace log expansion for the determinant

$$M = M_0 + M_E$$

$$\det M = \det M_0 \exp\left[\sum_{p=1,2,\ldots} \frac{(-1)^{p-1}}{p} \mathrm{tr}\left[(M_0^{-1} M_E)^p\right]\right]$$

Using the second order approximation speeds up the calculation of determinants using LU decomposition by a factor of $10^5 - 10^7$ times for typical simulations with errors $\sim 1\%$.

[D.L. and I. Ipsen, nucl-th/0308052, to appear in PRC]

Sample configurations (neutron matter)

$$L^3 \times L_t = 4^3 \times 6,\ \rho = 0.57\,\rho_{\text{nucl}}$$

$$\Lambda = 150\ \text{MeV}, T = 37.5\ \text{MeV}$$

configuration	1	2	3
R	0.538	0.523	0.534
$\log(\det(M))$	16.473+0.367i	18.119+0.448i	18.261-0.181i
$\log(\Delta_0)$	12.170+0.381i	13.793+0.490i	14.006+0.208i
$\log(\Delta_2)$	16.496+0.369i	18.179+0.448i	18.284-0.180i
$\log(\Delta_4)$	16.496+0.366i	18.133+0.447i	18.286-0.181i
$\log(\Delta_6)$	16.466+0.367i	18.115+0.448i	18.255-0.181i
$\log(\Delta_8)$	16.474+0.367i	18.120+0.448i	18.262-0.181i

$$L^3 \times L_t = 4^3 \times 6,\ \rho = 1.67\,\rho_{\mathrm{nucl}}$$
$$\Lambda = 150\ \mathrm{MeV}, T = 37.5\ \mathrm{MeV}$$

configuration	1	2	3
R	0.520	0.478	0.536
log(det(M))	70.635+0.412i	76.176+0.710i	73.483-0.158i
log(Δ_0)	64.800+0.441i	71.001+0.799i	67.850-0.181i
log(Δ_2)	70.953+0.412i	76.393+0.701i	73.792-0.154i
log(Δ_4)	70.603+0.411i	76.161+0.711i	73.448-0.158i
log(Δ_6)	70.639+0.412i	76.178+0.710i	73.489-0.157i
log(Δ_8)	70.634+0.412i	76.176+0.710i	73.482-0.158i

$$L^3 \times L_t = 6^3 \times (6, 9, 12)$$

$$\Lambda = 150\ \mathrm{MeV}$$

temperature	37.5 MeV	25.0 MeV	18.8 MeV
R	0.5122	0.6742	0.7631
$\log(\det(M))$	$65.801-0.725i$	$37.691-1.593i$	$16.002+0.054i$
$\log(\Delta_0)$	$51.399-0.789i$	$20.765-1.575i$	$4.100+0.203i$
$\log(\Delta_2)$	$66.003-0.722i$	$36.257-1.654i$	$11.759+0.086i$
$\log(\Delta_4)$	$65.829-0.724i$	$38.087-1.580i$	$15.939+0.034i$
$\log(\Delta_6)$	$65.793-0.725i$	$37.653-1.592i$	$16.312+0.048i$
$\log(\Delta_8)$	$65.803-0.725i$	$37.678-1.594i$	$16.011+0.058i$

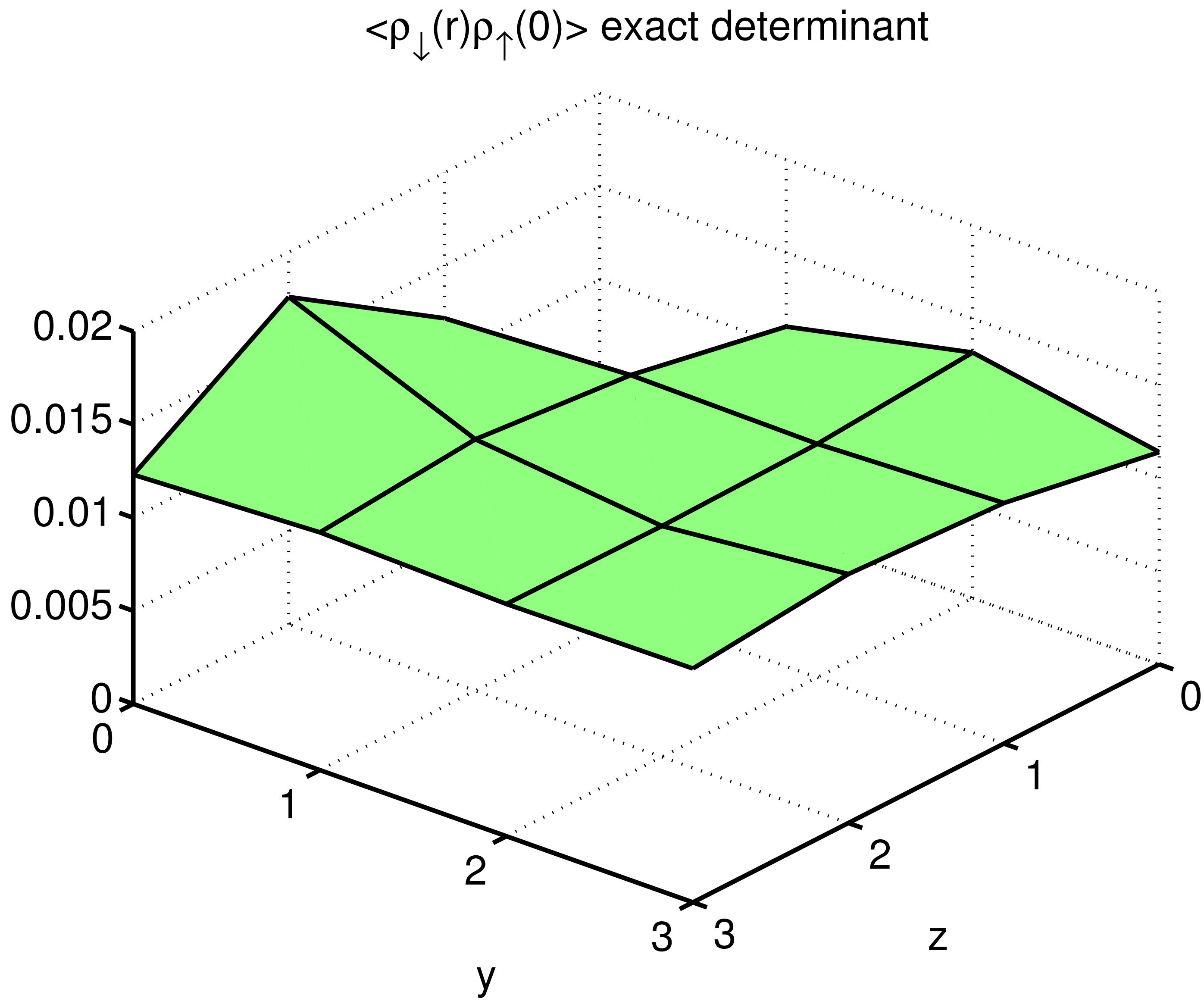
$$L^3 \times L_t = 6^3 \times 6$$

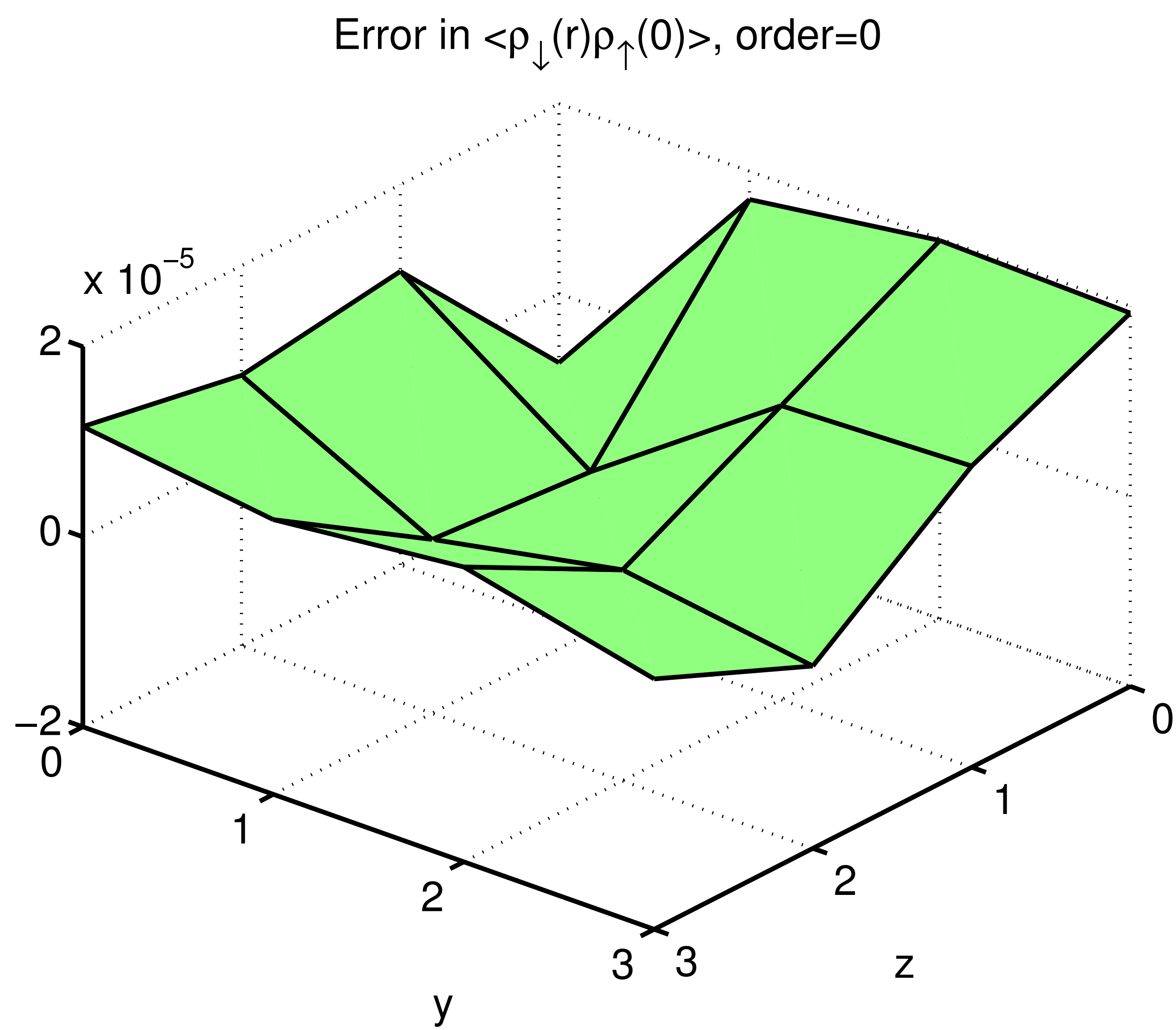
$$\Lambda = 150\ \mathrm{MeV}, T = 37.5\ \mathrm{MeV}$$

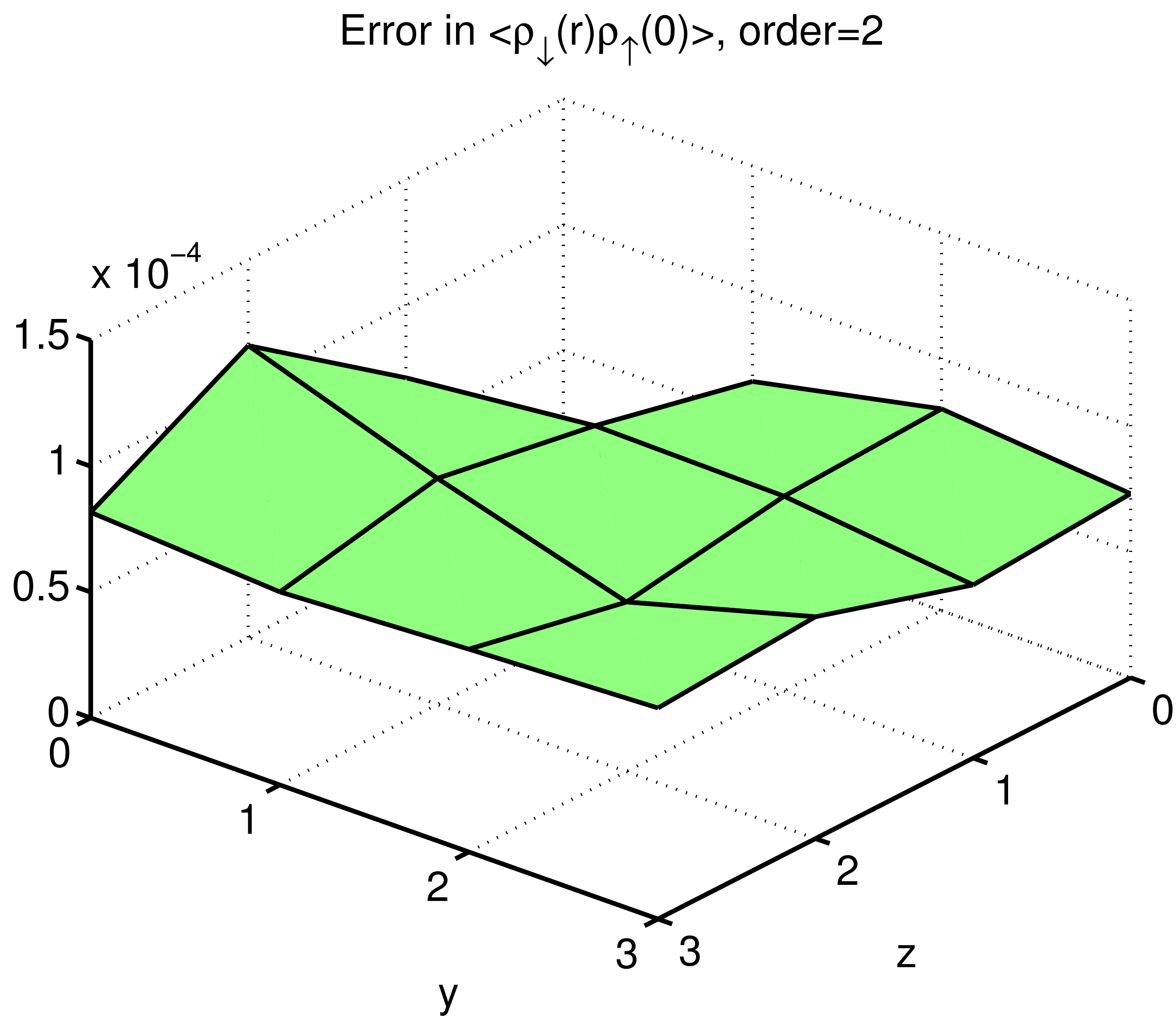
zone	[1,1,1]	[2,2,2]	[3,3,3]
R	0.5122	0.3013	0.3014
$\log(\det(M))$	65.801-0.725i	65.801-0.725i	65.801-0.725i
$\log(\Delta_0)$	51.399-0.789i	58.659-0.754i	61.047-0.772i
$\log(\Delta_2)$	66.003-0.722i	65.857-0.723i	65.832-0.723i
$\log(\Delta_4)$	65.829-0.724i	65.802-0.725i	65.801-0.725i
$\log(\Delta_6)$	65.793-0.725i	65.801-0.725i	65.801-0.725i
$\log(\Delta_8)$	65.803-0.725i	65.801-0.725i	65.801-0.725i

The error in the logarithm of the determinant seems to be the roughly the same for different configurations… observables could be more accurate since overall normalization is irrelevant

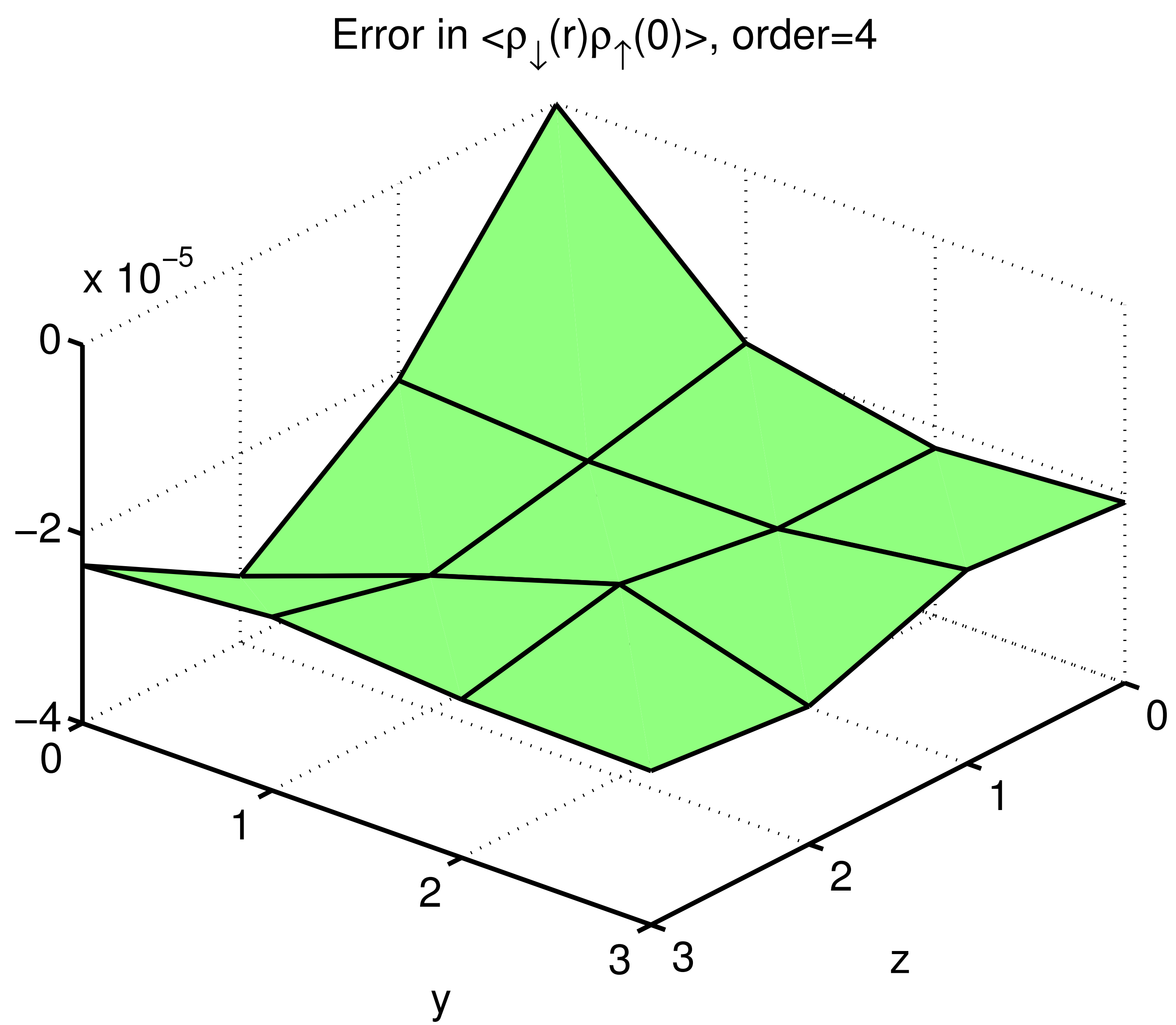
We compute the density-density correlation function for pure neutron matter and look at errors in the zone determinant expansion


$<\rho_{\downarrow}(r)\rho_{\uparrow}(0)>$ exact determinant
0.02
0.015
0.01
0.005
0
0
1
2
3
y
0
1
2
3
z


Error in <ρ↓(r)ρ↑(0)>, order=0
x 10^−5
2
0
−2
0
1
2
3
y
0
1
2
3
z

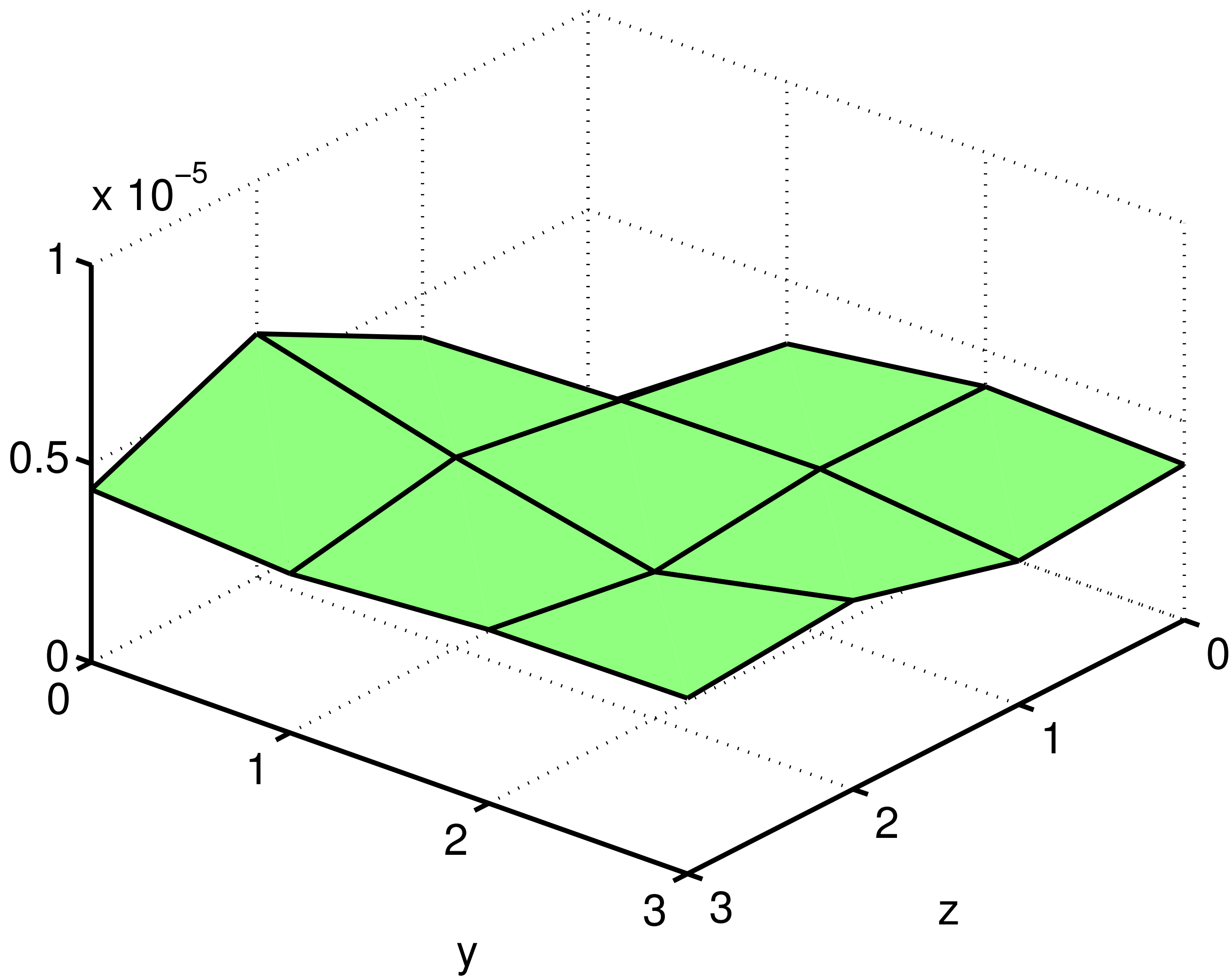


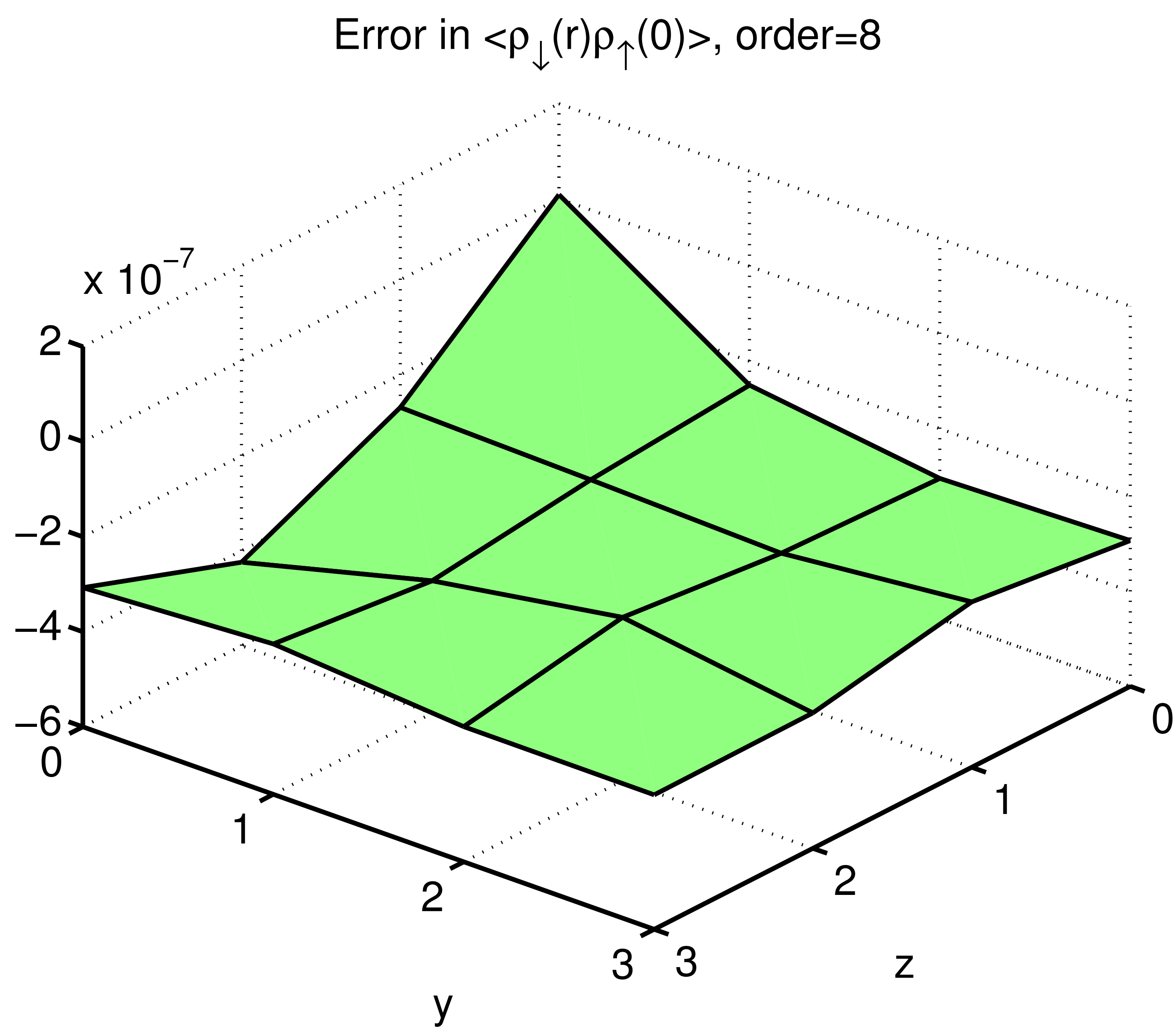
Error in <ρ↓(r)ρ↑(0)>, order=2
x 10^−4
1.5
1
0.5
0
0
1
2
3
y
0
1
2
3
z



Error in <ρ↓(r)ρ↑(0)>, order=4
x 10^−5
0
−2
−4
0
1
2
3
y
0
1
2
3
z

Error in $<\rho_{\downarrow}(r)\rho_{\uparrow}(0)>$, order=6





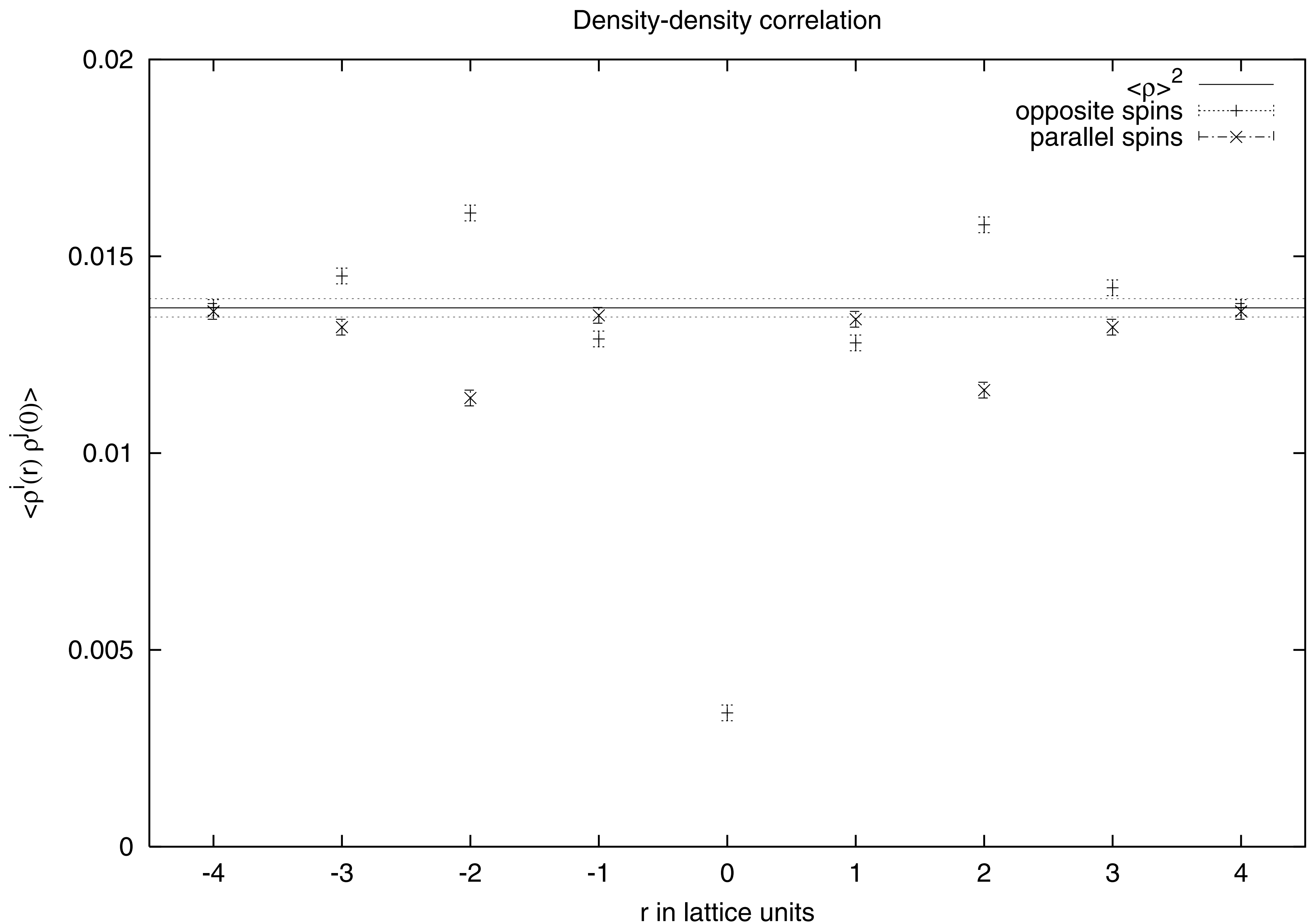
Error in <ρ↓(r)ρ↑(0)>, order=8
x 10^−7
2
0
−2
−4
−6
0
1
2
3
y
0
1
2
3
z

Using the second order approximation speeds up the calculation of determinants using LU decomposition by a factor of $10^5 - 10^7$ times for typical simulations with errors $\sim 1\%$.

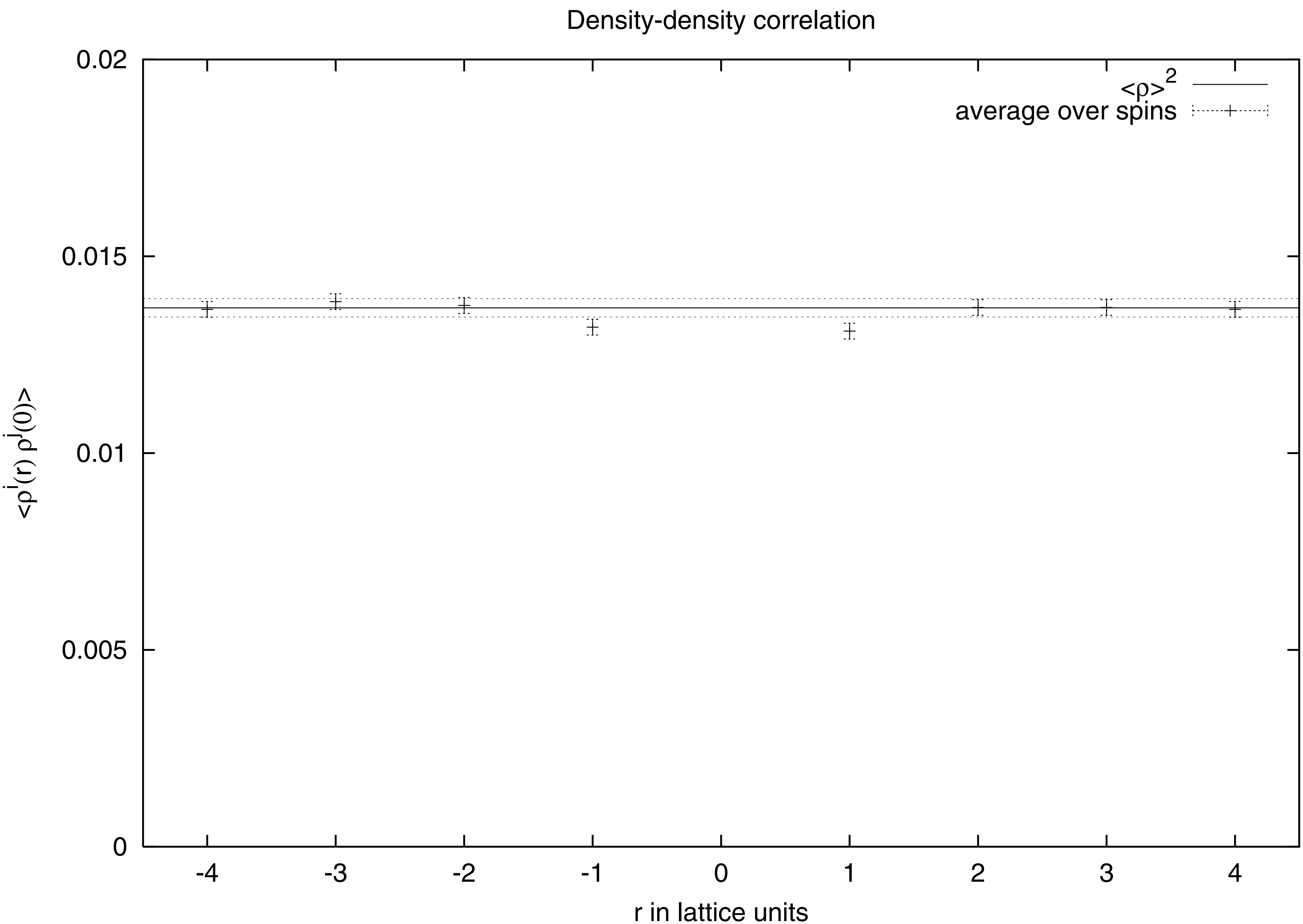
We compute the density-density correlation function for pure neutron matter on a $8^3 \times 6$ lattice at

$$T = 37.5\,\text{MeV}, \quad a^{-1} = 150\,\text{MeV}, \quad \mu = 800\,\text{MeV}$$

$$\rho \sim 0.62\rho_{\text{nucl}}$$



Density-density correlation
0.02
0.015
0.01
0.005
0
$<\rho^i(r)\, \rho^j(0)>$
-4
-3
-2
-1
0
1
2
3
4
r in lattice units
$<\rho>^2$
opposite spins
parallel spins



Density-density correlation
$<\rho>^2$
average over spins
0.02
0.015
0.01
0.005
0
-4
-3
-2
-1
0
1
2
3
4
r in lattice units
$<\rho^i(r)\ \rho^j(0)>$

Directions (near future – hopefully some this week at the INT)

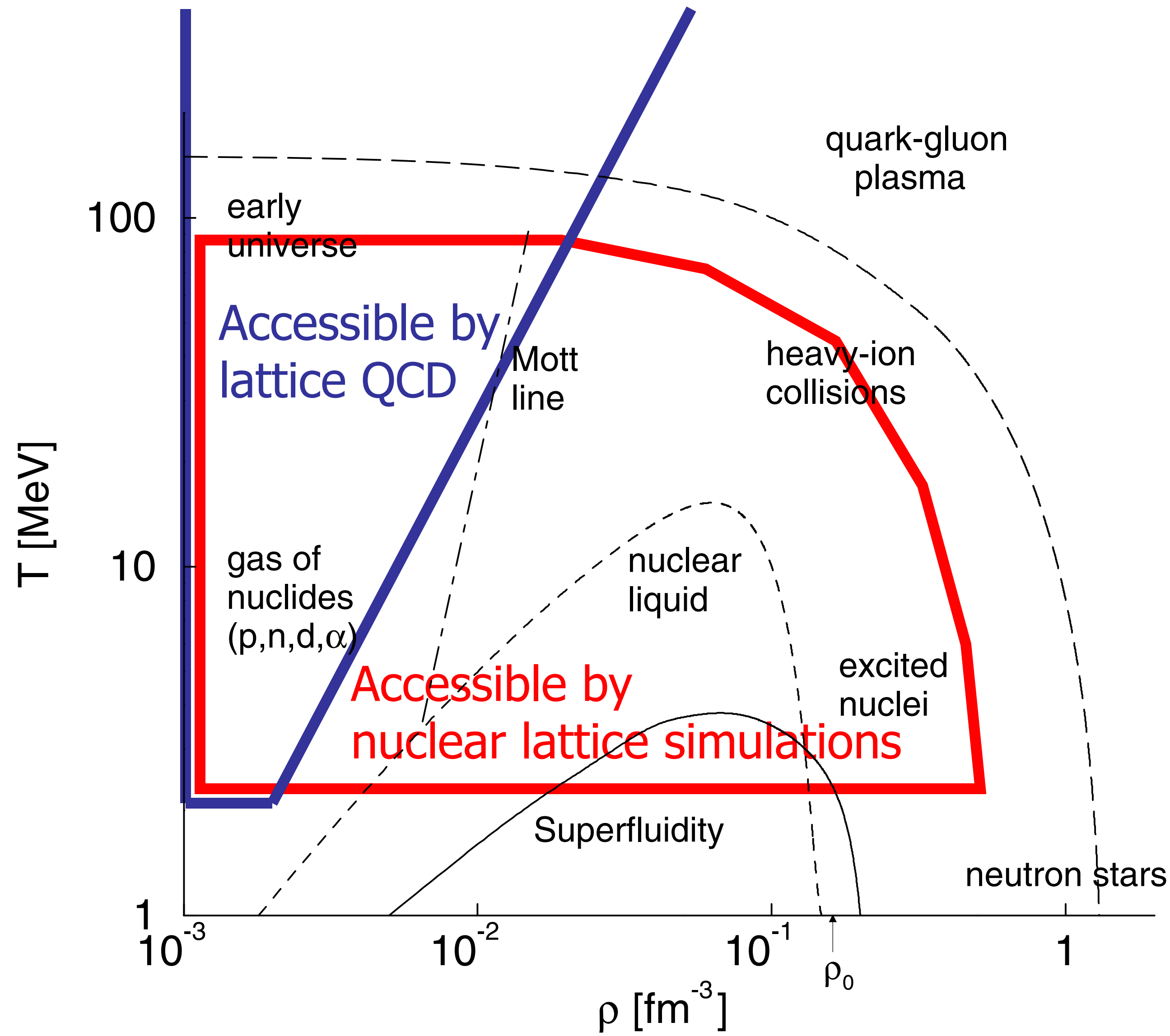
1. Calculations of E/A as a function of temperature and density

2. Show that physical observables are cutoff independent

3. Measure Fermi surface and occupation numbers for momentum modes

4. Equation of state – measuring pressure using local chemical potentials

5. Include protons and charged pions



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