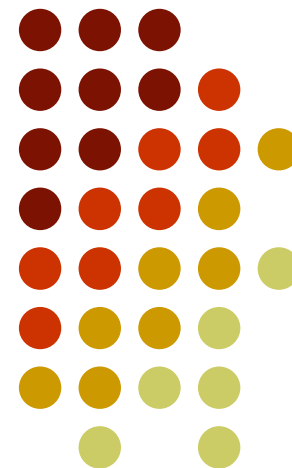


Lattice QCD at finite density using the canonical approach

Andrei Alexandru

with

Manfried Faber, Ivan Horvath, Keh-Fei Liu, Anyi Li

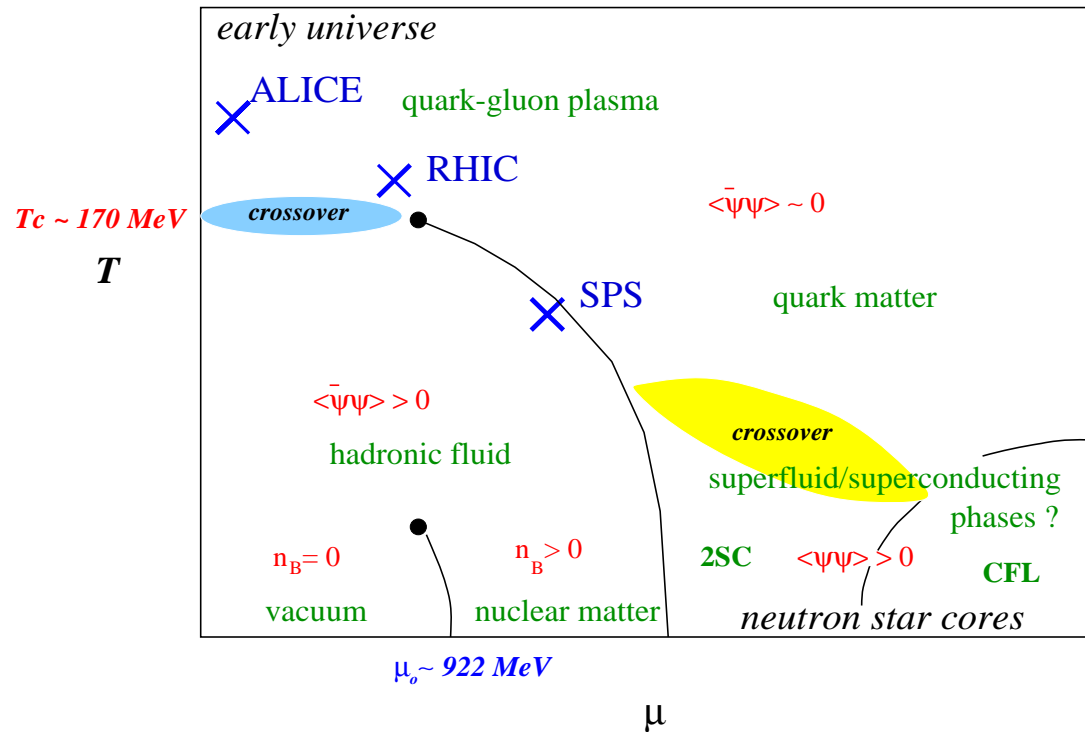


Outline

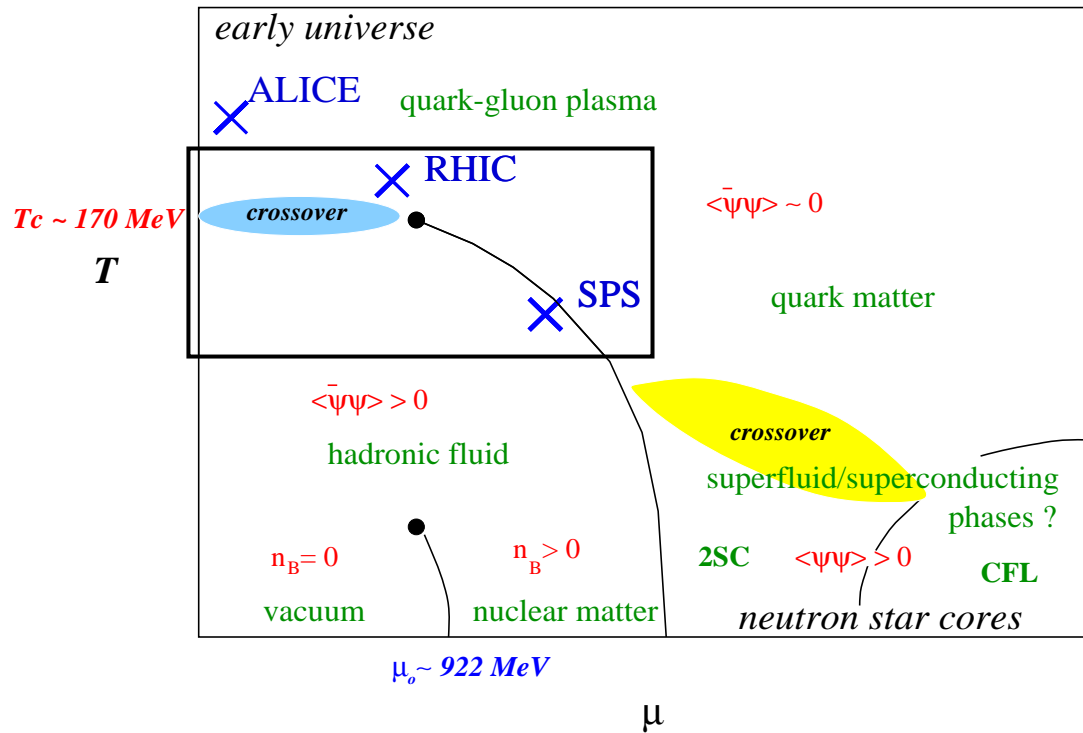


- Canonical partition function
- Method I: exact determinant calculation
- Results
- Method II: estimator for determinant calculation
- Outlook

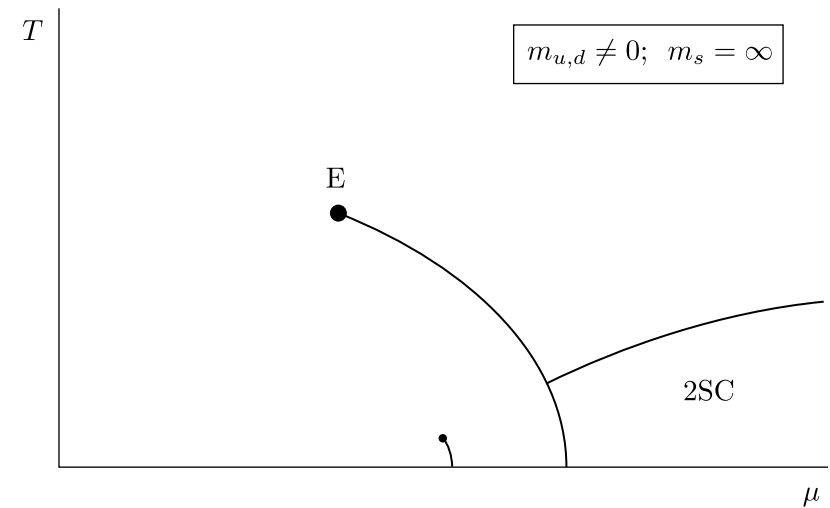
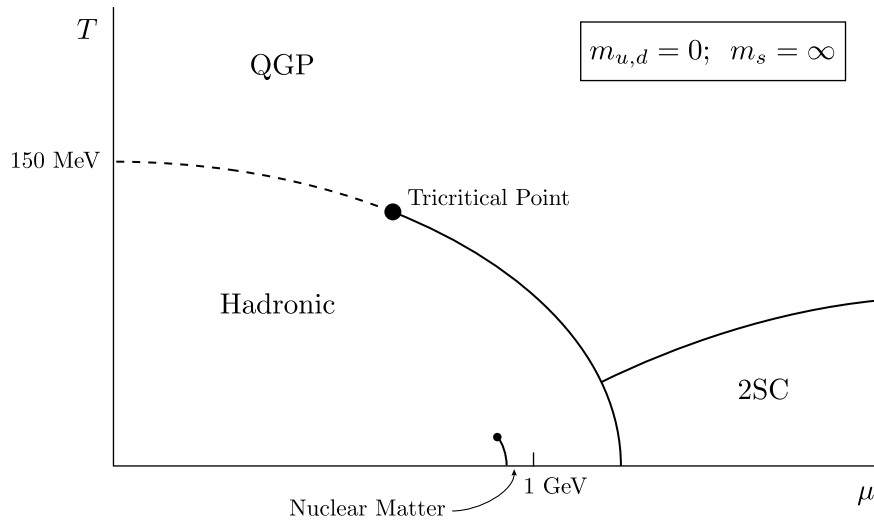
Real QCD – expected phase diagram



Region of interest for our simulations



2 flavors QCD – Phase diagram





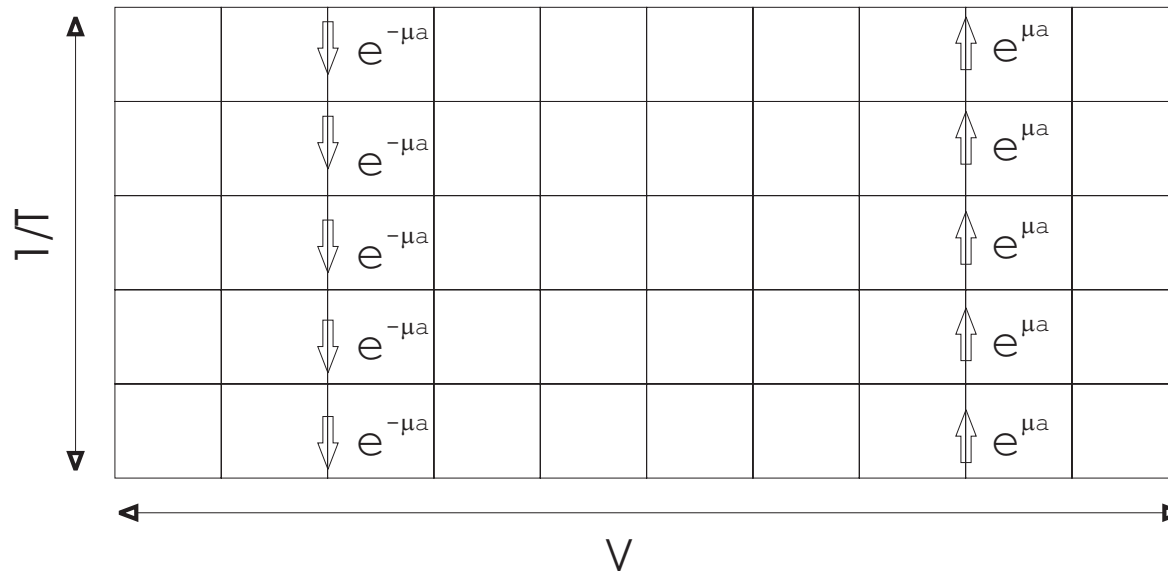
Canonical partition function

- Grand canonical partition function
- Canonical partition function from fugacity expansion
- Discrete vs continuous Fourier transform



Grand canonical partition function

$$Z_{GC}(V, \mu, T) = \int D U D \bar{\psi} D \psi e^{-S_G[U] - S_F[\mu; U, \bar{\psi}, \psi]} = \int D U e^{-S_G[U]} \det M[\mu; U]^2$$

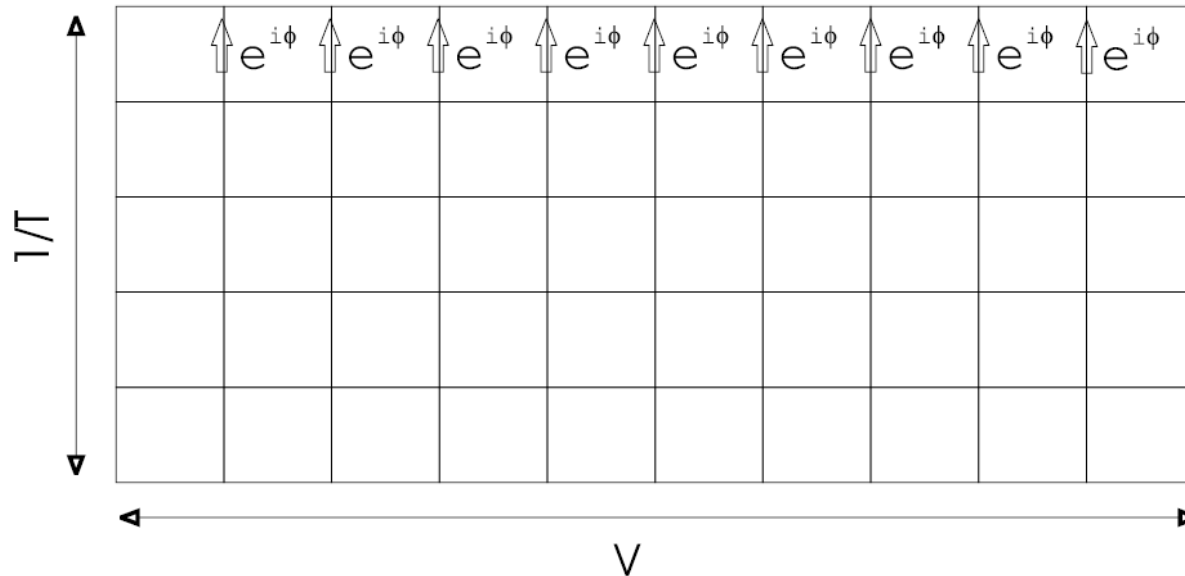


$$S_F[\mu; U, \bar{\psi}, \psi] = \bar{\psi} M[\mu; U] \psi$$

$$U_4 \rightarrow U_4 e^{-\mu a}$$



Canonical partition function



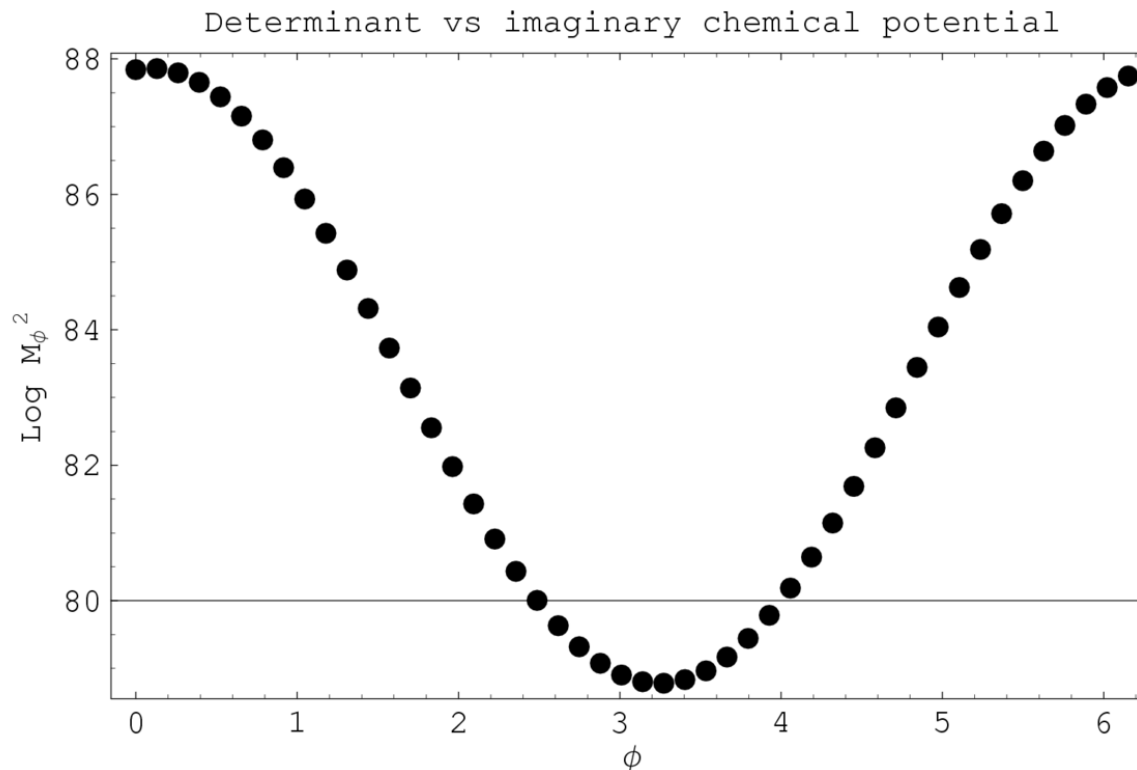
Using the fugacity expansion $Z_{GC}(V, \mu, T) = \sum_{n=-4V}^{n=4V} Z_C(V, n, T) e^{\frac{\mu}{T}n}$ we get

$$Z_C(V, n, T) = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-in\phi} Z_{GC}(V, \mu = i\phi T, T)$$

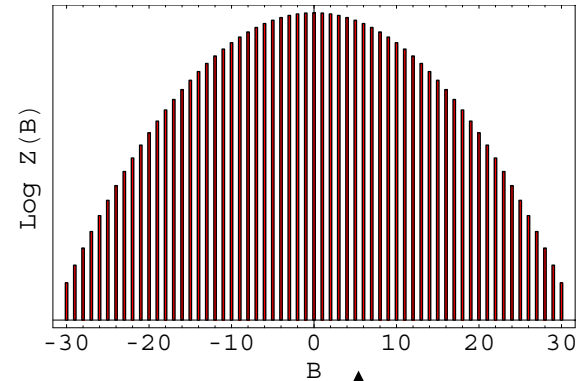
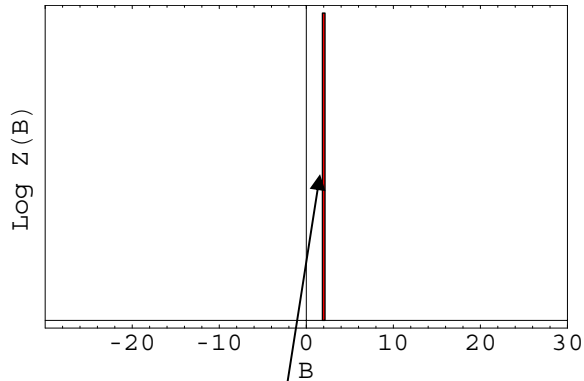
Canonical partition function



$$Z_C(V, n, T) = \int DU e^{-S_G[U]} \det_n M^2(U)$$



Projected determinant



$$\det_n M^2(U) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-in\varphi} \det M^2(U, \mu = i\varphi T)$$

Projected determinant

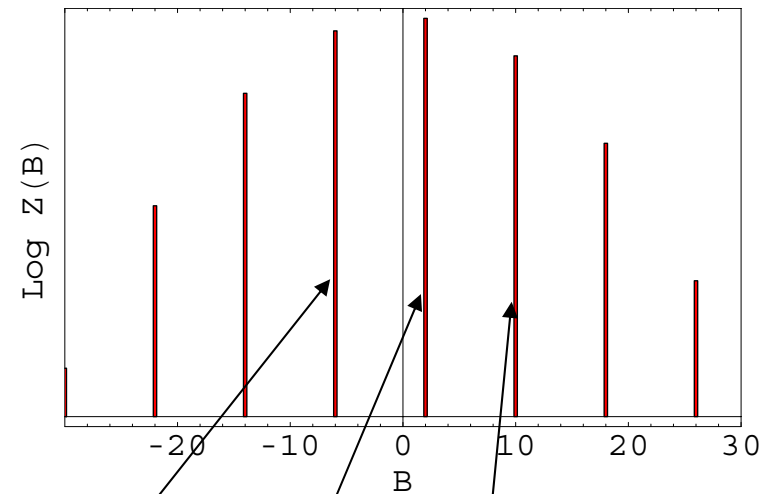
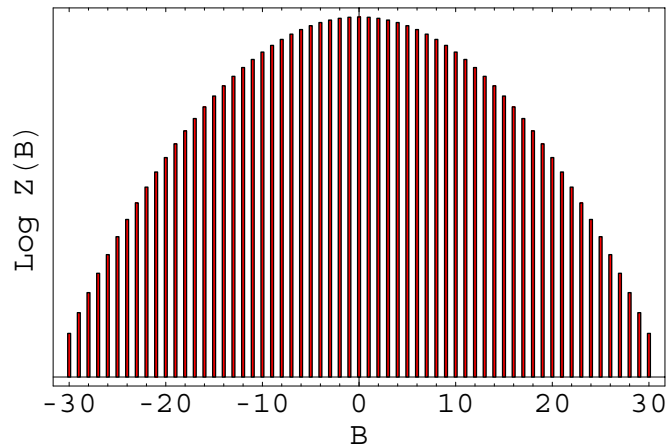


$$\det_n M^2(U) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-in\varphi} \det M^2(U, \mu = i\varphi T)$$



$$\det'_n M^2(U) = \frac{1}{N} \sum_{j=0}^{N-1} e^{-in\varphi_j} \det M^2(U, \mu = i\varphi_j T), \quad \varphi_j = \frac{2\pi}{N} j$$

Projected determinant

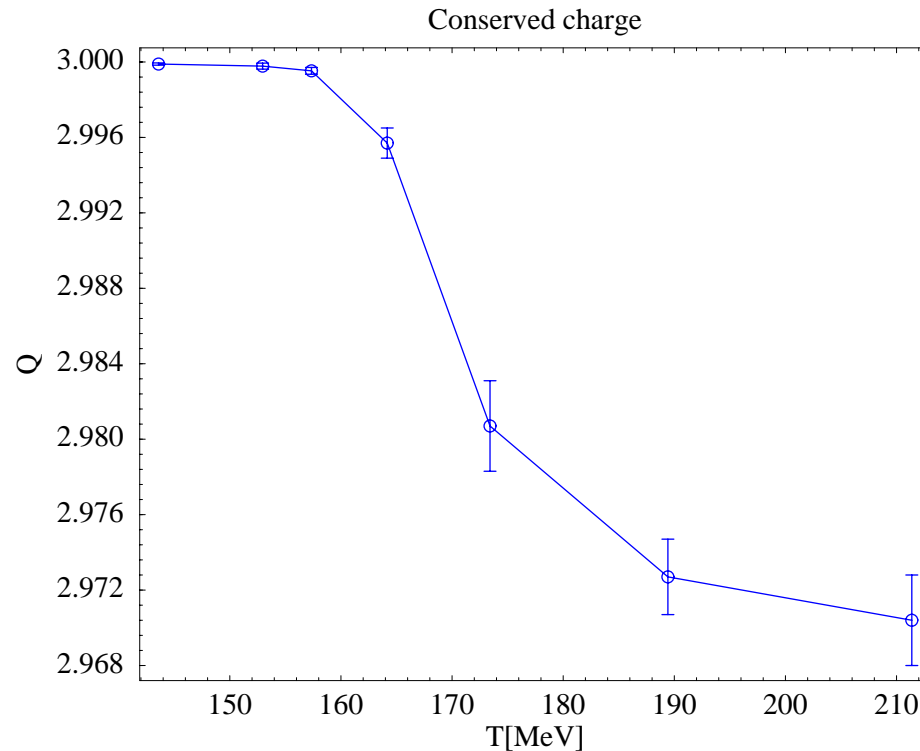


$$\det'_n M^2 = \frac{1}{N} \sum_{j=0}^{N-1} e^{-in\varphi_j} \det M_{\varphi_j}^2 = \dots + \det_{n-N} M^2 + \det_n M^2 + \det_{n+N} M^2 + \dots$$

Sector mixing



$$\langle Q \rangle_{Z_C(n)} = \frac{\sum_m (n + mN) Z_C(n + mN)}{\sum_m Z_C(n + mN)}$$





Canonical partition function

$$Z_C(V, n, T) = \int DU e^{-S_G[U]} \det'_n M^2(U)$$

$$\det'_n M^2(U) = \frac{1}{N} \sum_{j=0}^{N-1} e^{-in\varphi_j} \det M^2(U, \mu = i\varphi_j T)$$



Algorithm

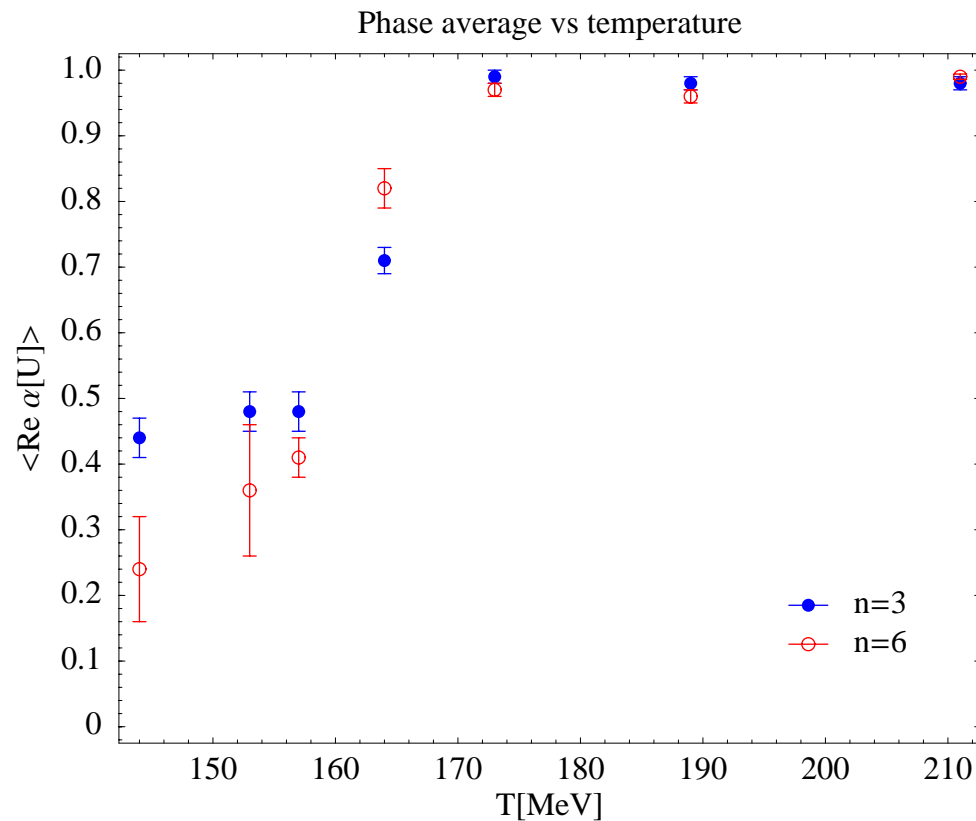
$$\begin{aligned}
 Z_C(V, n, T) &= \int DU e^{-S_G(U)} \det_n M^2(U) = \\
 &\int DU e^{-S_G(U)} \underbrace{|\operatorname{Re} \det_n M^2(U)|}_{\text{Standard HMC}} \underbrace{\frac{\det_n M^2(U)}{|\operatorname{Re} \det_n M^2(U)|}}_{\text{Phase}} \\
 &\quad \downarrow \\
 &\int DU e^{-S_G(U)} \underbrace{\det M^2(U, 0)}_{\text{Standard HMC}} \underbrace{\frac{|\operatorname{Re} \det_n M^2(U)|}{\det M^2(U, 0)}}_{\text{Accept/Reject}}
 \end{aligned}$$

complex

Sign problem



$$\alpha(U) = \frac{\det_n M(U)}{|\text{Redet}_n M(U)|} \quad \langle O \rangle_n = \frac{\langle O(U) \alpha(U) \rangle}{\langle \alpha(U) \rangle}$$





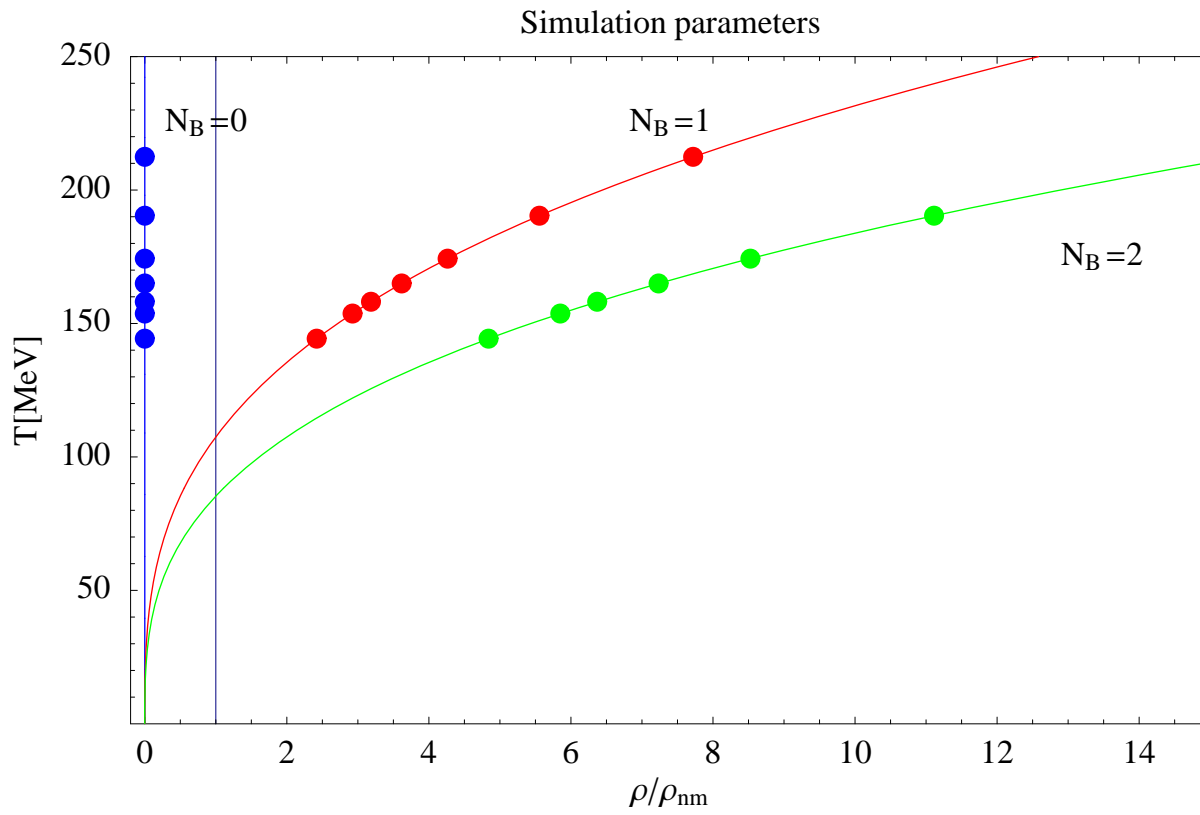
Simulation parameters

All runs are on a 4^4 lattice with Wilson fermions at $\kappa = 0.158$.

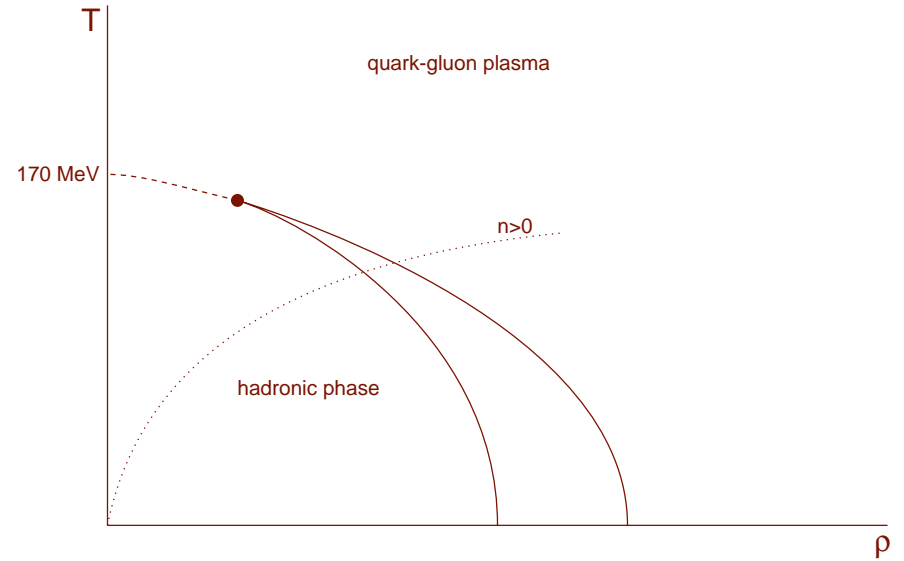
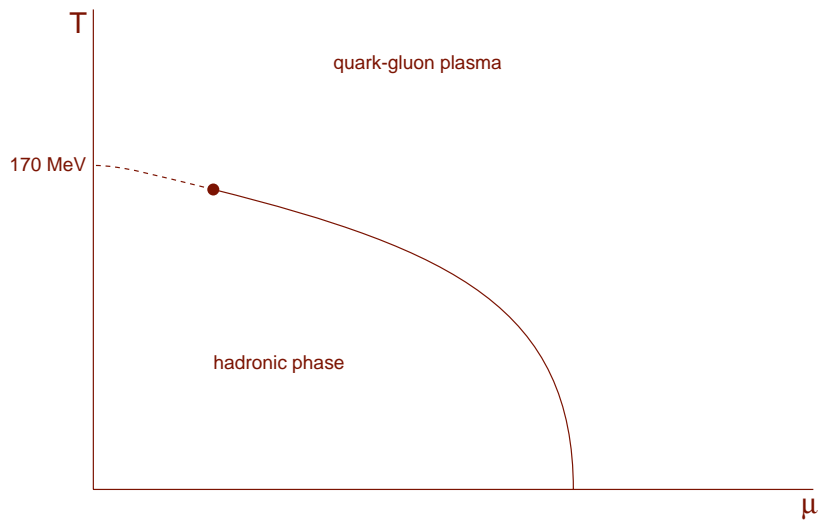
β	a(fm)	m_π (MeV)	$V^{-1}(fm^{-3})$	T(MeV)
5.00	0.343(2)	926(7)	0.387(7)	144(1)
5.10	0.322(4)	945(13)	0.468(17)	153(2)
5.15	0.313(3)	942(11)	0.510(15)	157(2)
5.20	0.300(1)	945(5)	0.579(6)	164(1)
5.25	0.284(5)	945(20)	0.682(36)	173(3)
5.30	0.260(1)	973(9)	0.889(10)	189(1)
5.35	0.233(2)	959(14)	1.235(32)	211(2)

We set $N=12$ and we run three sets of simulations: $k=0, 3$ and 6 .

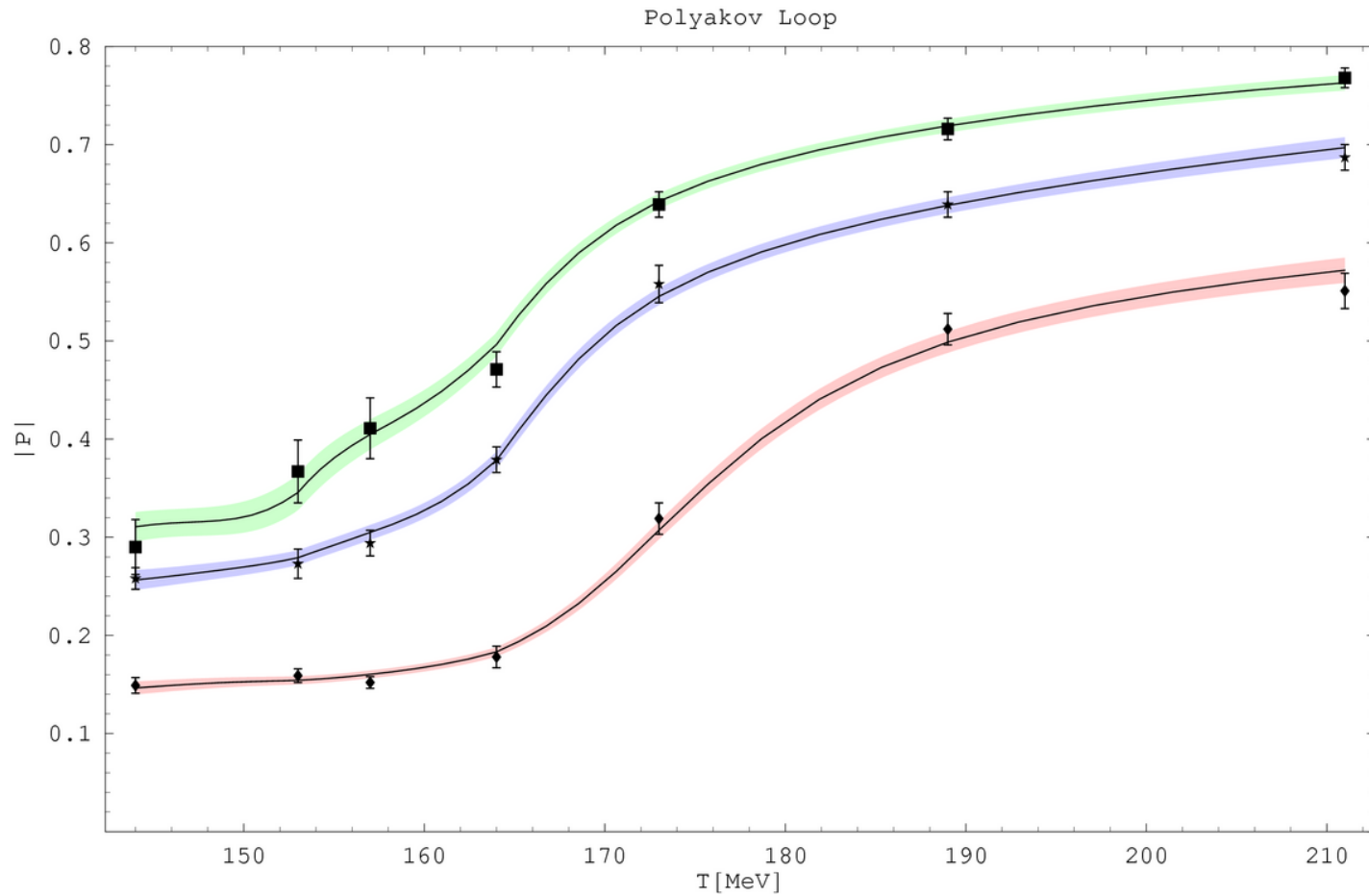
Run parameters



Phase diagram



Polyakov loop

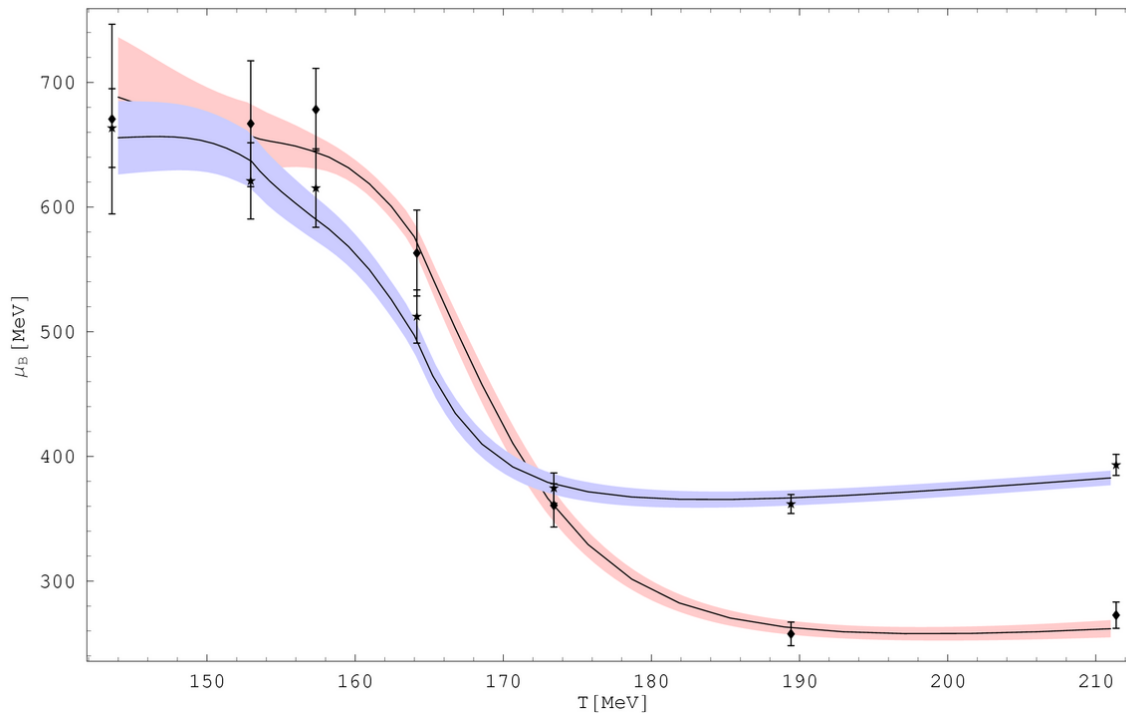


Chemical potential

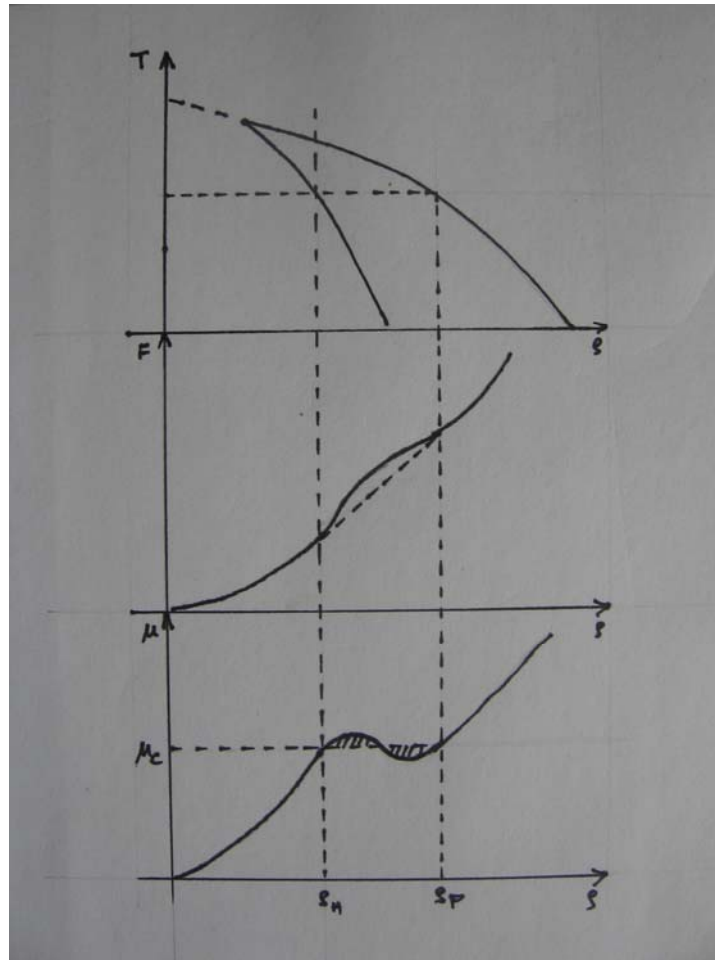


$$\mu_B = F(B+1) - F(B) = -\frac{1}{\beta} \ln \frac{Z_{B+1}}{Z_B} = -\frac{1}{\beta} \ln \langle e^{-i3\theta} \rangle_{3B}$$

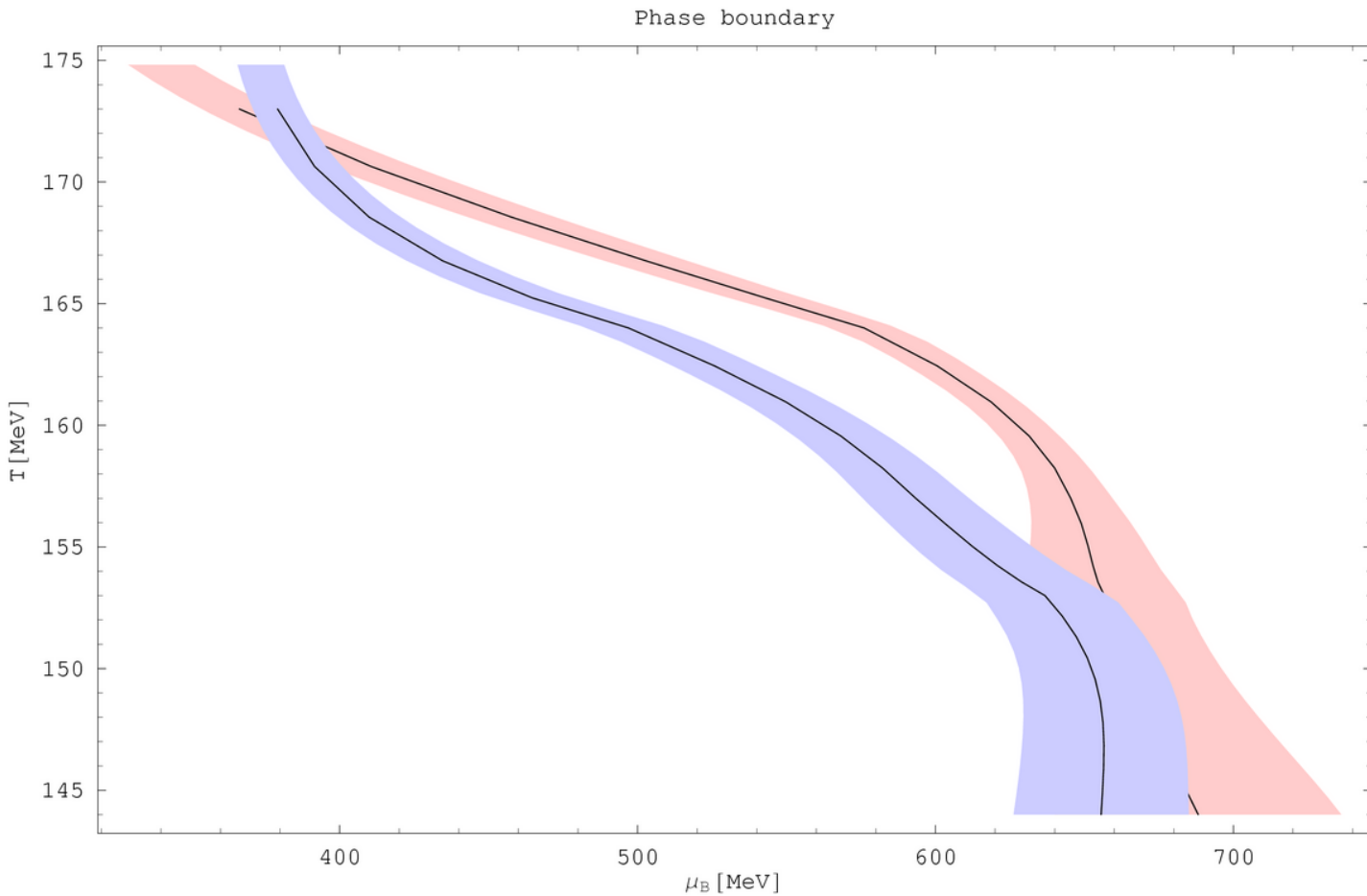
Baryon chemical potential



Maxwell construction



Phase transition line



Plans



- Increase volume from 4^4 to $6^3 \times 4$:
 - Physical volume is increase by a factor of 3.4 allowing finer steps in the density directions.
 - Computation time for the determinant increases by a factor of 38.
- Increase N to 60 to allow simulations with 10 baryons:
 - We need at least 3.4 more baryons to reach the same densities.
 - Kratochvila and de Forcrand work with 4 degenerate flavors suggest that 10 baryons would be enough to scan the coexistence region on a $6^3 \times 4$ lattice.
 - The simulation time increases by a factor of 5.
- Unfortunately the cost of such a simulations is at least 200 times more expensive: most of the increase comes from the poor scaling of the LU decomposition needed to compute the determinant exactly.

Algorithm -- estimator



$$\begin{aligned} Z_C(V, n, T) &= \int DU e^{-S_G(U)} \det'_n M^2(U) \\ &= \int DUD\xi e^{-S_G(U)} \det M^2(U) f_n(U, \xi) \end{aligned}$$

$$\int D\xi f_n(U, \xi) = \frac{\det'_n M^2(U)}{\det M^2(U)}$$



The updating process

$$\begin{aligned} Z_C(V, n, T) &= \int DUD\xi e^{-S_G(U)} \det M^2(U) f_n(U, \xi) \\ &= \int DUD\xi e^{-S_G(U)} \det M^2(U) |f_n(U, \xi)| \underbrace{\left| \frac{f_n(U, \xi)}{|f_n(U, \xi)|} \right|}_{\text{phase}} \end{aligned}$$

Simulation measure

$$(U, \xi) \xrightarrow{HMC + Acc / rej} (U', \xi) \xrightarrow{Acc / rej} (U', \xi')$$

The accept/reject steps are based on the ratios $\frac{|f_n(U', \xi)|}{|f_n(U, \xi)|}$ and $\frac{|f_n(U', \xi')|}{|f_n(U', \xi)|}$



Setting up the estimator

$$\det M = e^{\text{Tr} \ln M}$$

$$\langle g_1(\eta) \rangle = \text{Tr} \ln M, \quad P(g_1 = 0) = 0$$

$$\langle g_2(\eta) \rangle = \frac{1}{2} \text{Tr} \ln M, \quad P(g_2 = 0) = \frac{1}{2}$$

⋮

$$\langle g_k(\eta) \rangle = \frac{1}{k} \text{Tr} \ln M, \quad P(g_k = 0) = \frac{k-1}{k}$$

⋮

$$\text{Tr} \ln M = \int d\eta g(\eta)$$

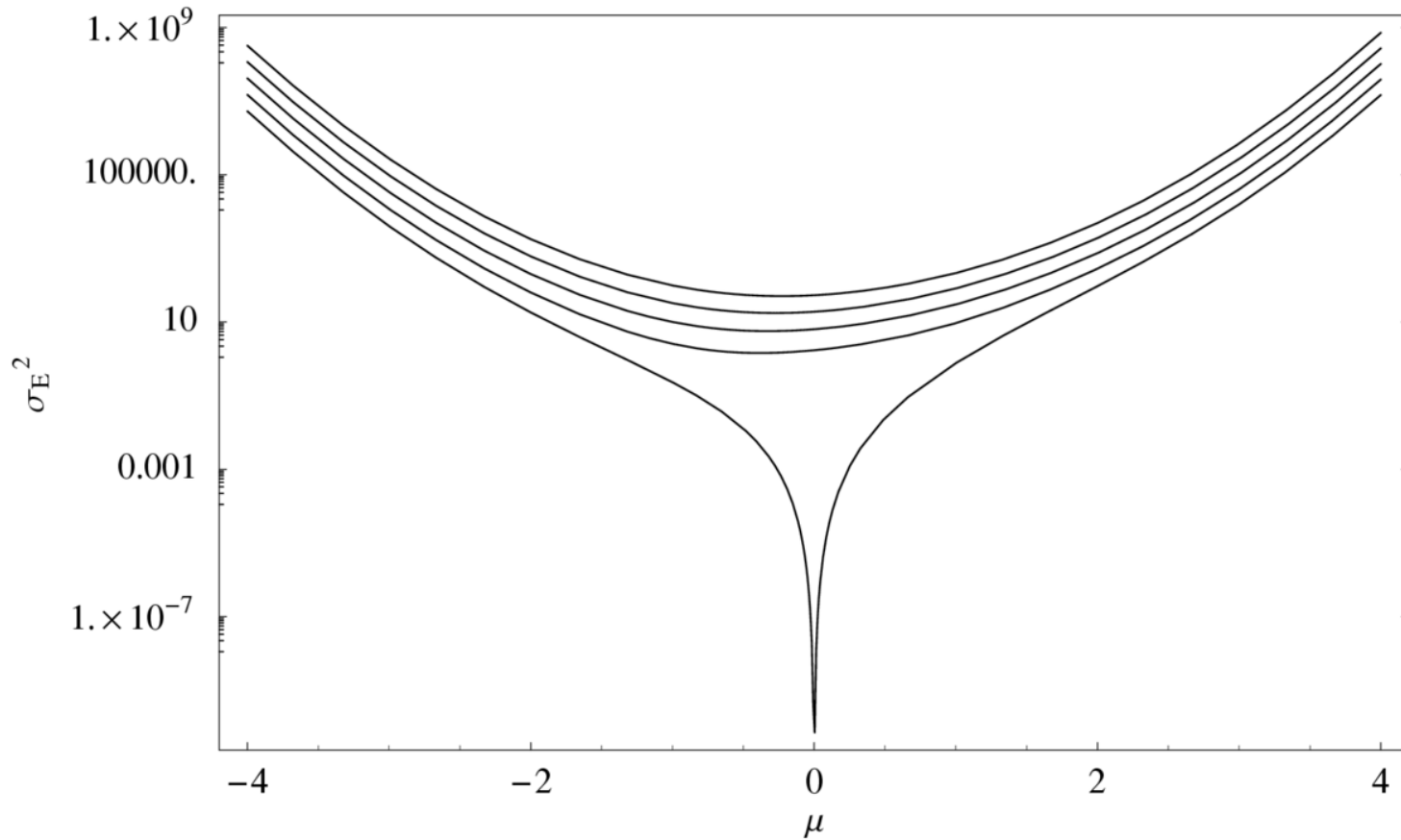
$$f(\eta_1, \eta_2, \dots) = 1 + g_1(\eta_1) + g_1(\eta_1)g_2(\eta_2) + g_1(\eta_1)g_2(\eta_2)g_3(\eta_3) + \dots$$

$$\langle f(\eta_1, \eta_2, \dots) \rangle = \det M$$

Variance



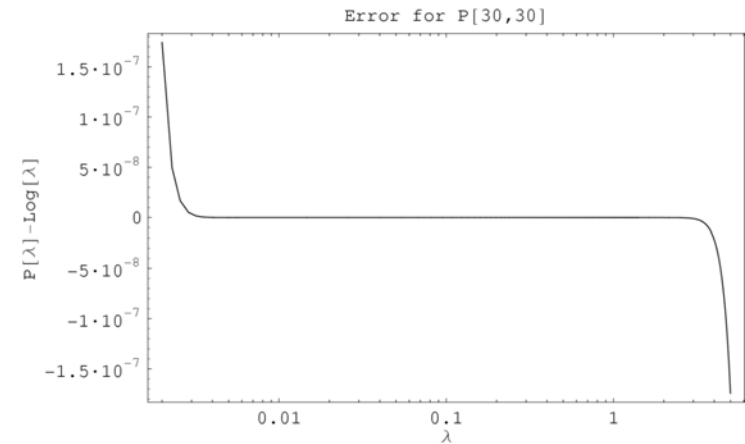
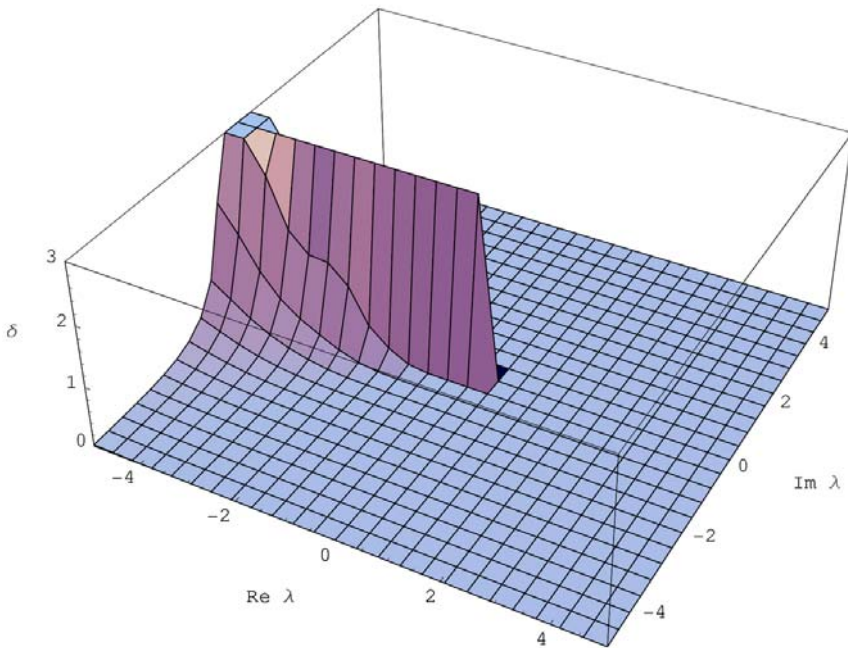
Estimator variance for $\sigma_x^2 = 0, 1, 2, 3$ and 4



Pade approximation



$$\ln \det M = \text{Tr} \ln M \cong b_0 \text{Tr} I + \sum_{k=1}^K \text{Tr} \frac{b_k}{c_k + M}$$



Trace improvement



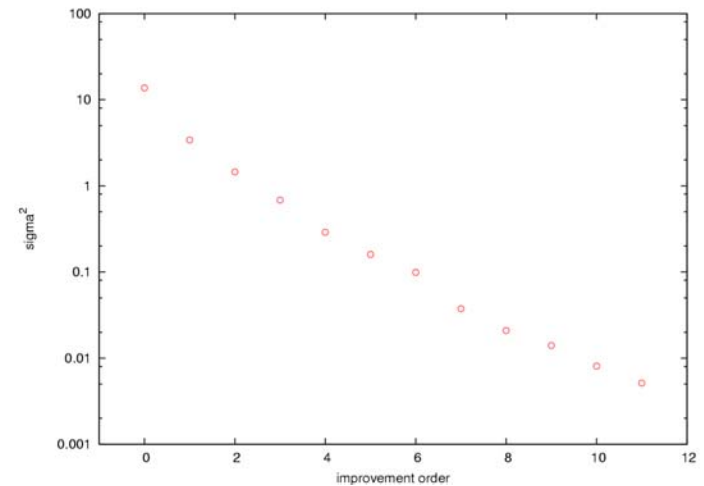
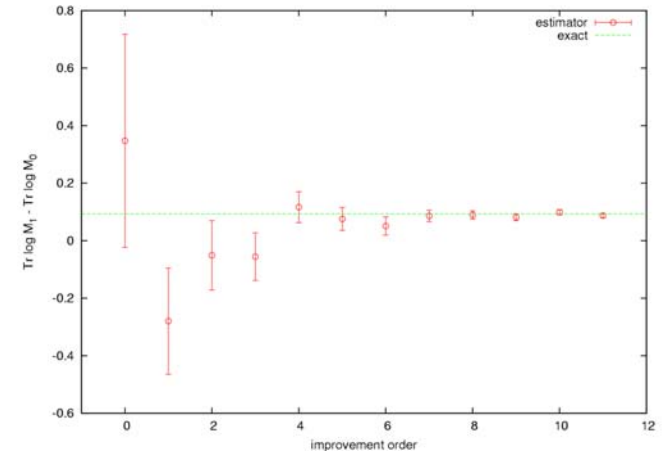
$$\text{Tr} \ln M = \int d\eta \eta^+ M \eta$$

$$\text{Tr} \ln M \cong b_0 \text{Tr} I + \sum_{k=1}^K \text{Tr} \frac{b_k}{c_k + M}$$

$$\text{Tr} \frac{1}{c + M} = \text{Tr} \left(\frac{1}{c + M} - \sum_i O_i \right)$$

$$\text{Tr} \frac{1}{c + M} = \frac{1}{1 + c} + \frac{\kappa}{(1 + c)^2} D + \frac{\kappa^2}{(1 + c)^3} D^2 + \dots$$

$$O_i = \frac{\kappa^i}{(1 + c)^{i+1}} \left(D^i - \frac{1}{\text{Tr} 1} \text{Tr} D^i \right)$$





Future plans

- Investigate possible problems:
 - Acceptance rates
 - Sign problem
 - Autocorrelation time
 - $Z(3)$ symmetry
- Scan the parameter space to determine optimum parameters.
- Determine how the algorithm scales with volume, temperature and baryon number.
- Determine phase boundary
- Move to smaller quark masses (use clover fermions)
- Use chiral fermions? (distant future)