Finite density simulations via a canonical approach

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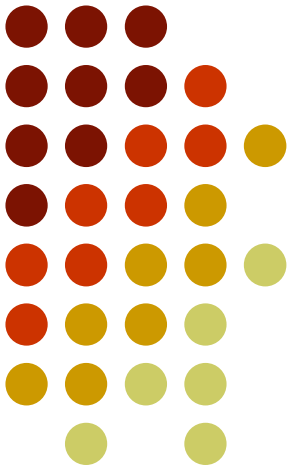
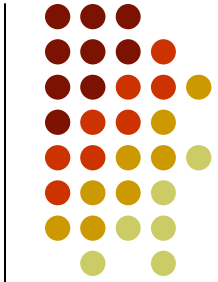
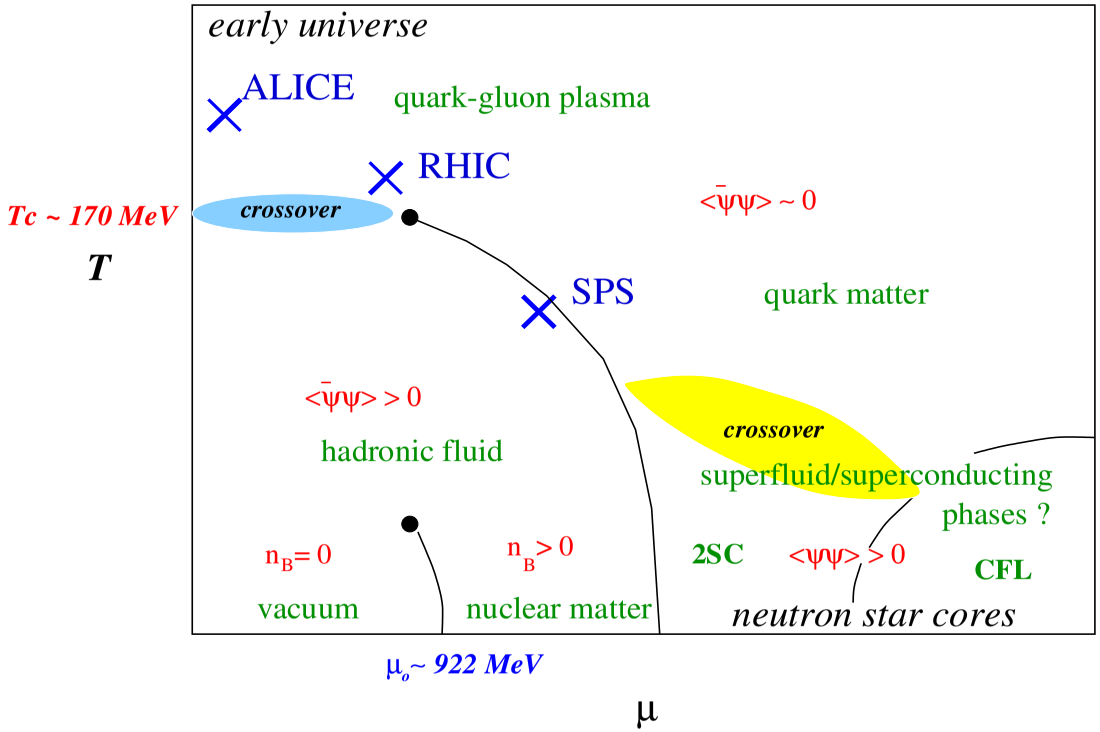


Outline

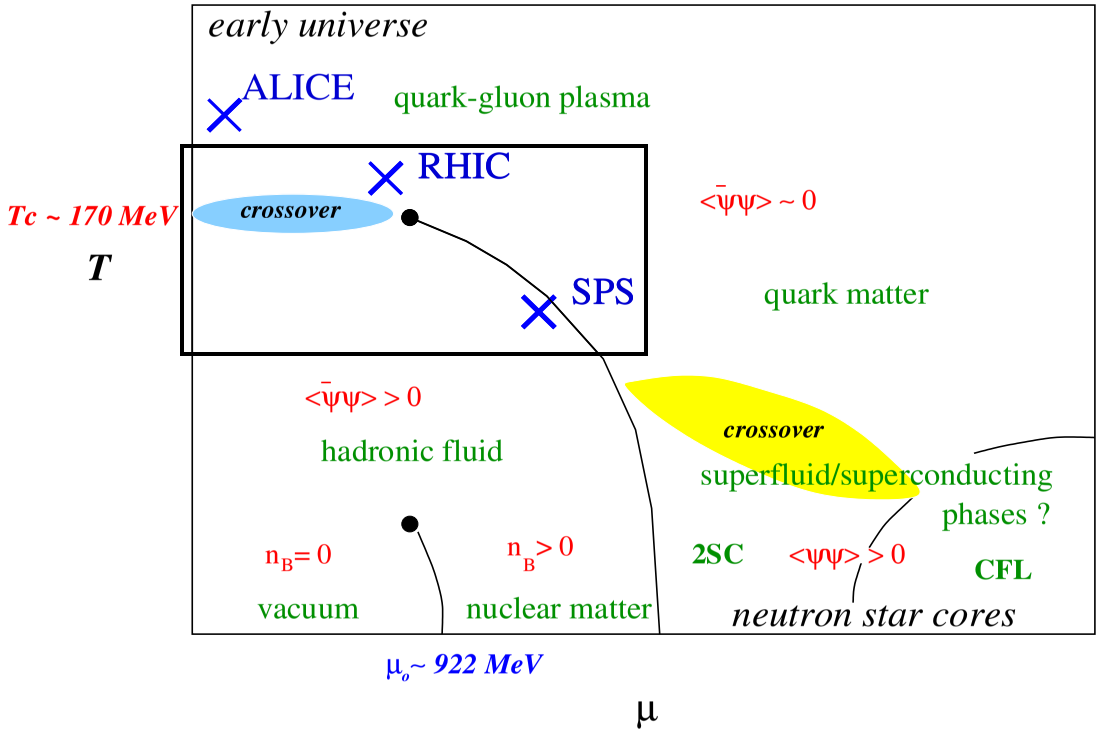


- Motivation
- Canonical partition function
- Method I: exact determinant calculation
- Results
- Method II: estimator for determinant calculation
- Outlook

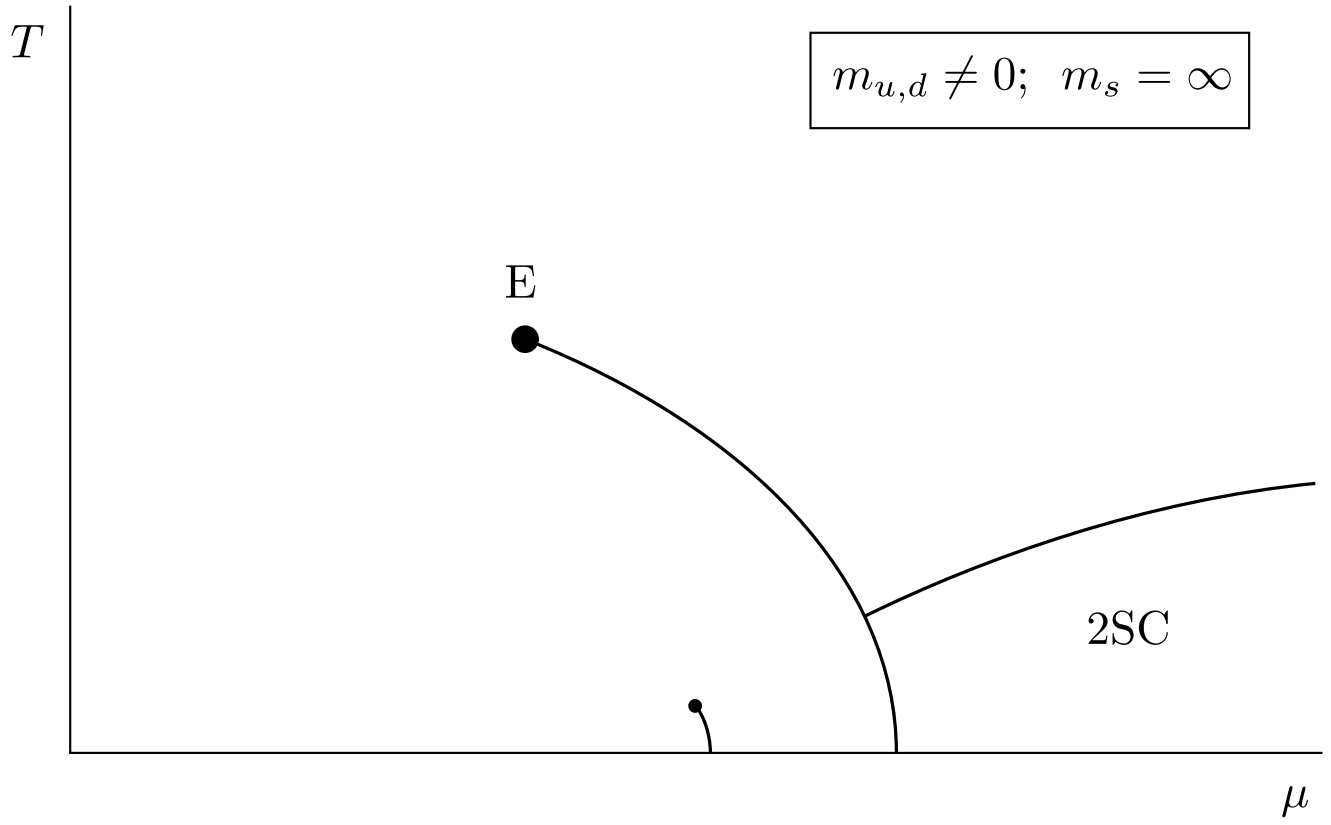
Real QCD – expected phase diagram



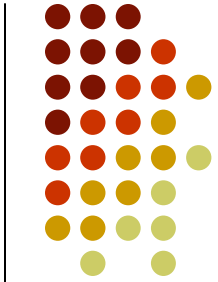
Region of interest for our simulations



2 flavors QCD – Phase diagram



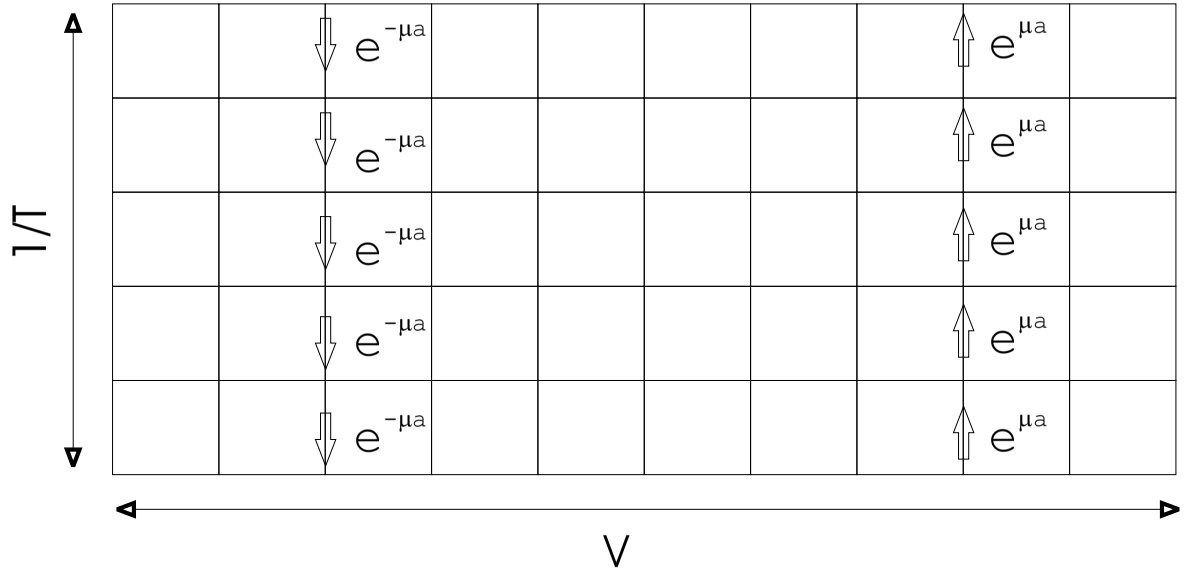
Canonical partition function



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

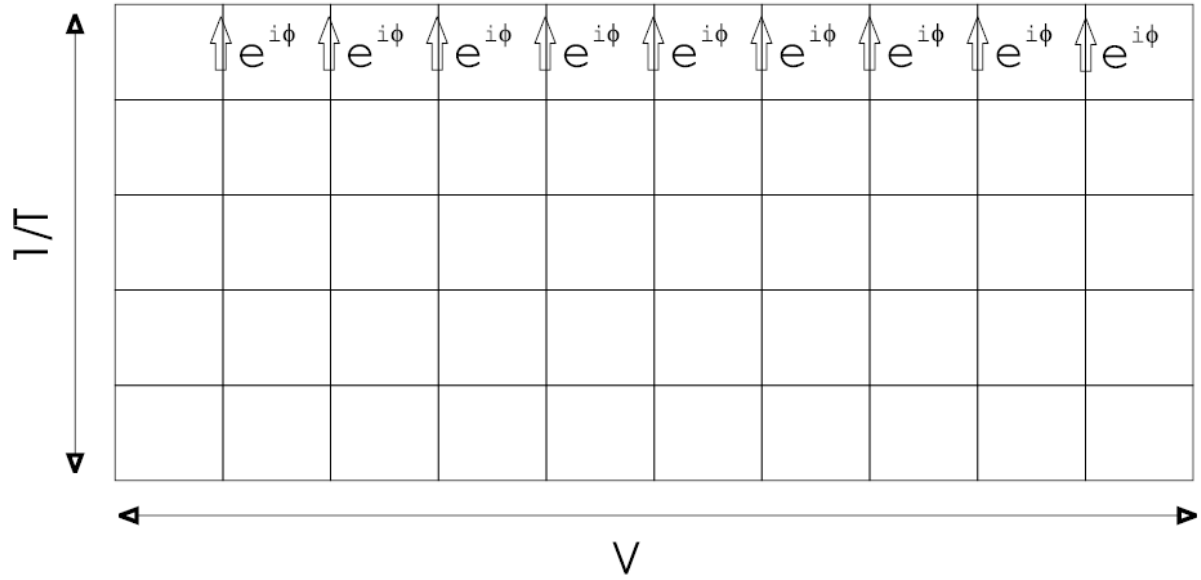
Grand canonical partition function

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



$$S_F[\mu;U,\overline{\psi},\psi] = \overline{\psi}\, M[\mu;U]\, \psi \qquad U_4 \rightarrow U_4 e^{-\mu a}$$

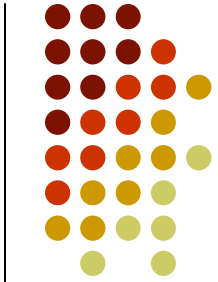
Canonical partition function



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

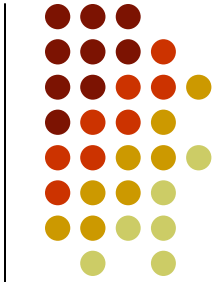
$$Z_C(V,n,T) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{-in\varphi} Z_{GC}(V,\mu = i\varphi T, T)$$

Canonical partition function



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

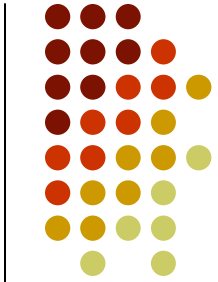
Projected determinant



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

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

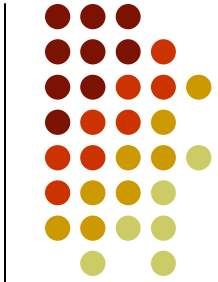
Canonical partition function



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

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

Algorithm



complex

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

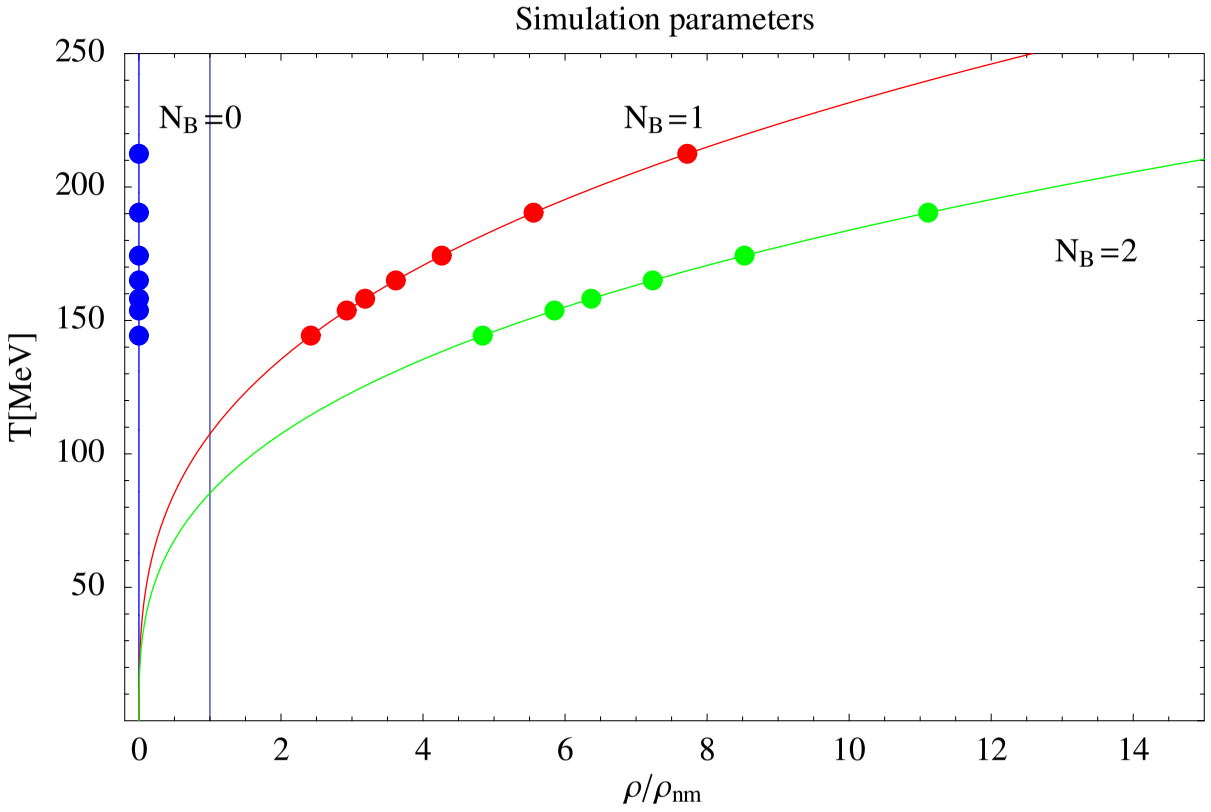
$$\int DU\ e^{-S_G(U)} \left|\mathrm{Re}\det{}_n M^2(U)\right| \frac{\det{}_n M^2(U)}{\left|\mathrm{Re}\det{}_n M^2(U)\right|}$$

Phase

$$\int DU\ e^{-S_G(U)} \det M^2(U,0) \frac{\left|\mathrm{Re}\det{}_n M^2(U)\right|}{\det M^2(U,0)}$$

Standard HMC Accept/Reject

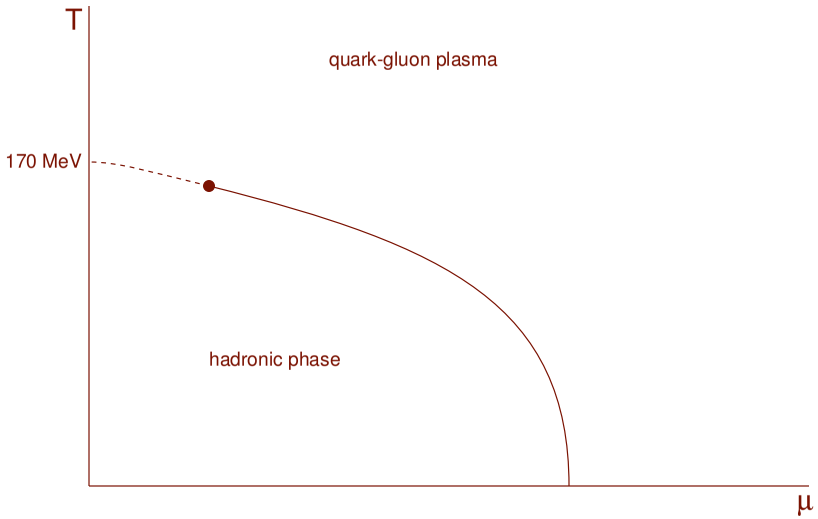
Run parameters

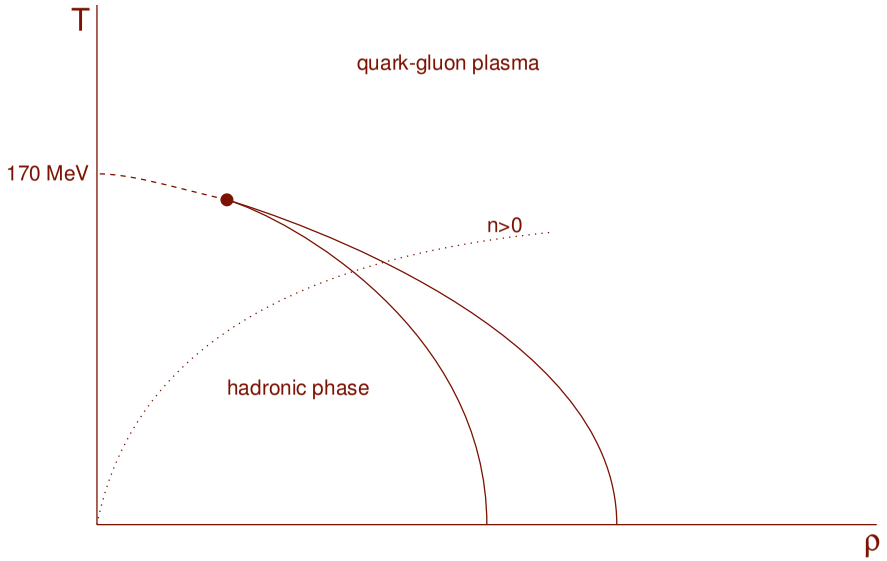


We use 4^4 lattices with pion mass around 950 MeV.

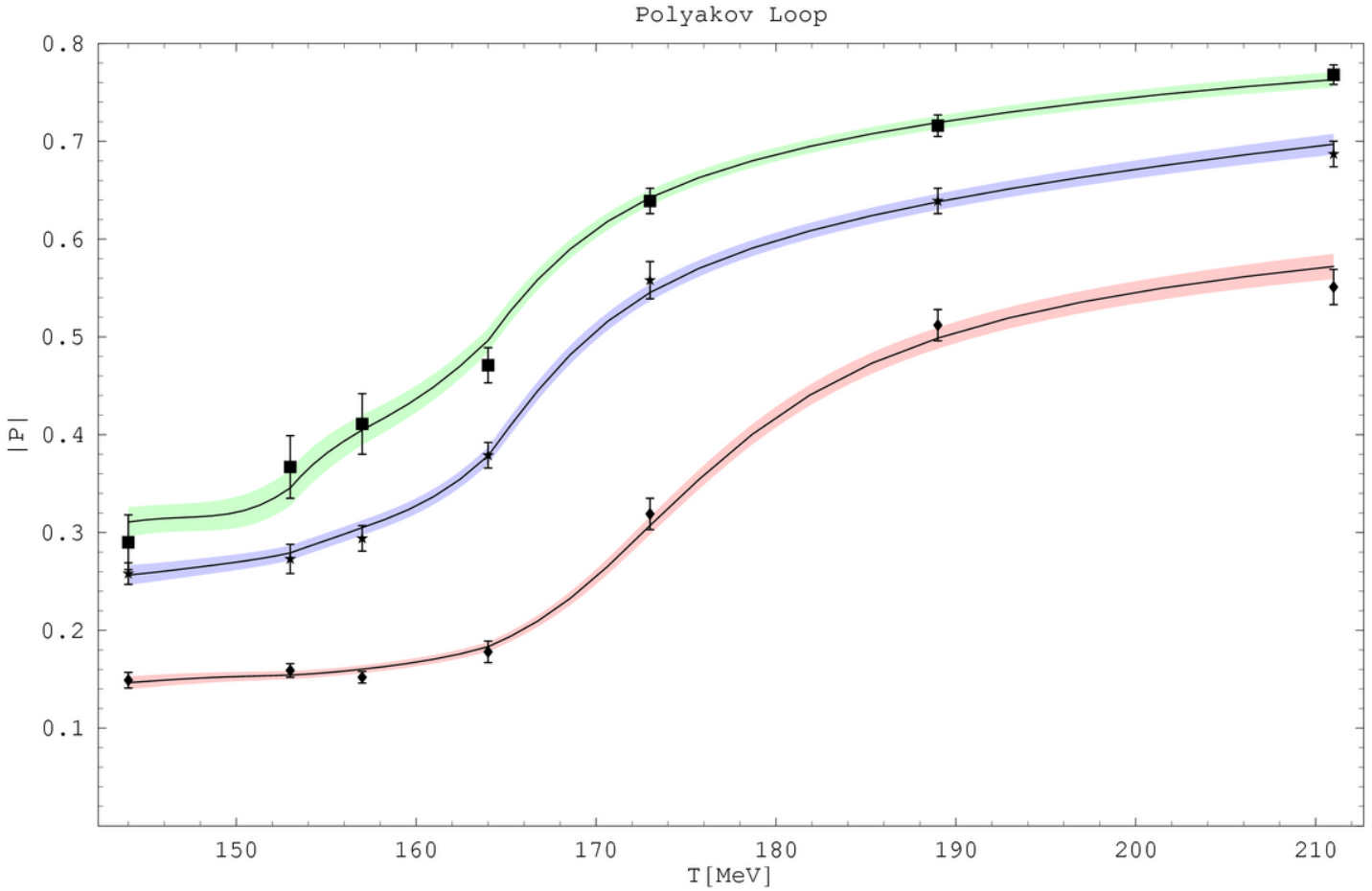
We set N=12 and we run three sets of simulations: k=0, 3 and 6.

Phase diagram



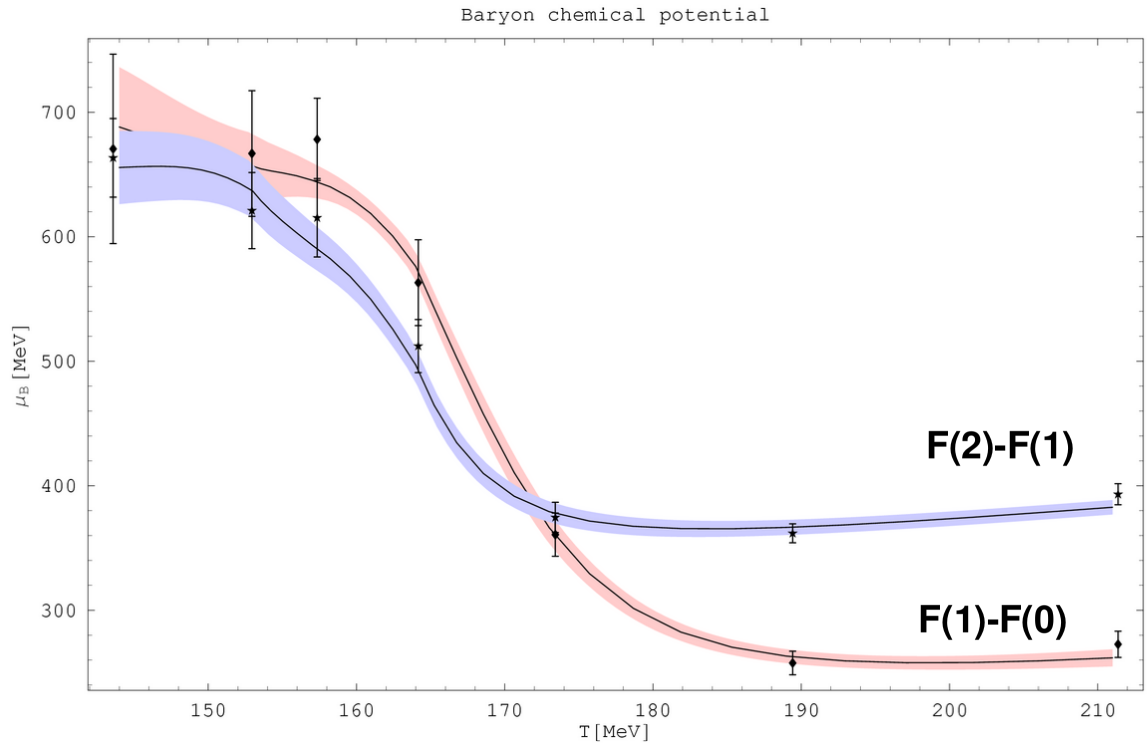


Polyakov loop

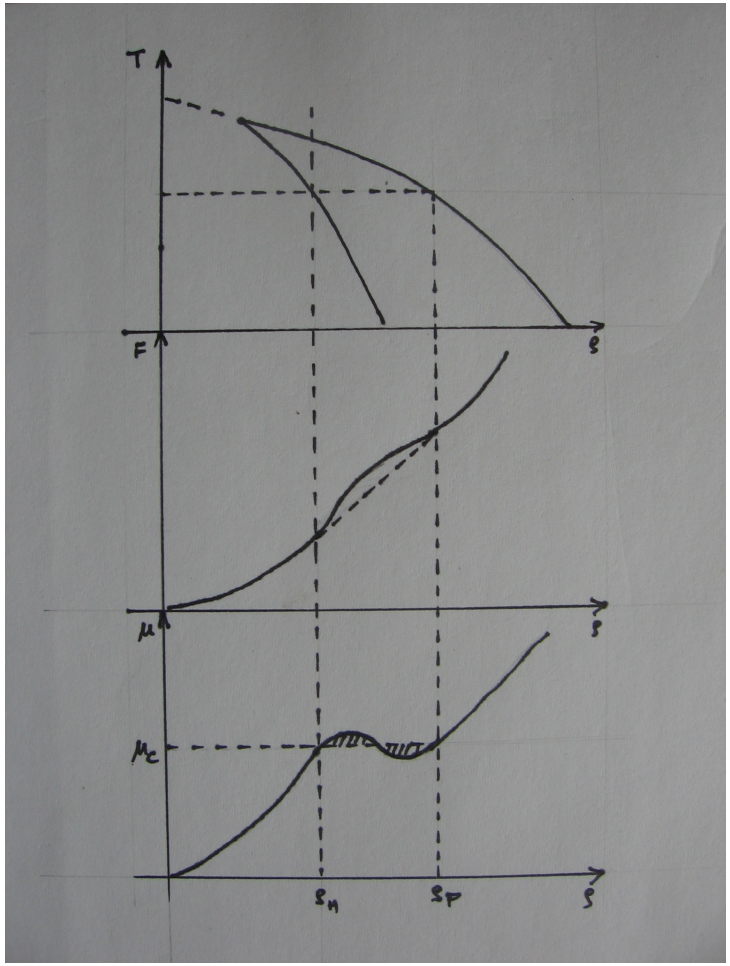


Chemical potential

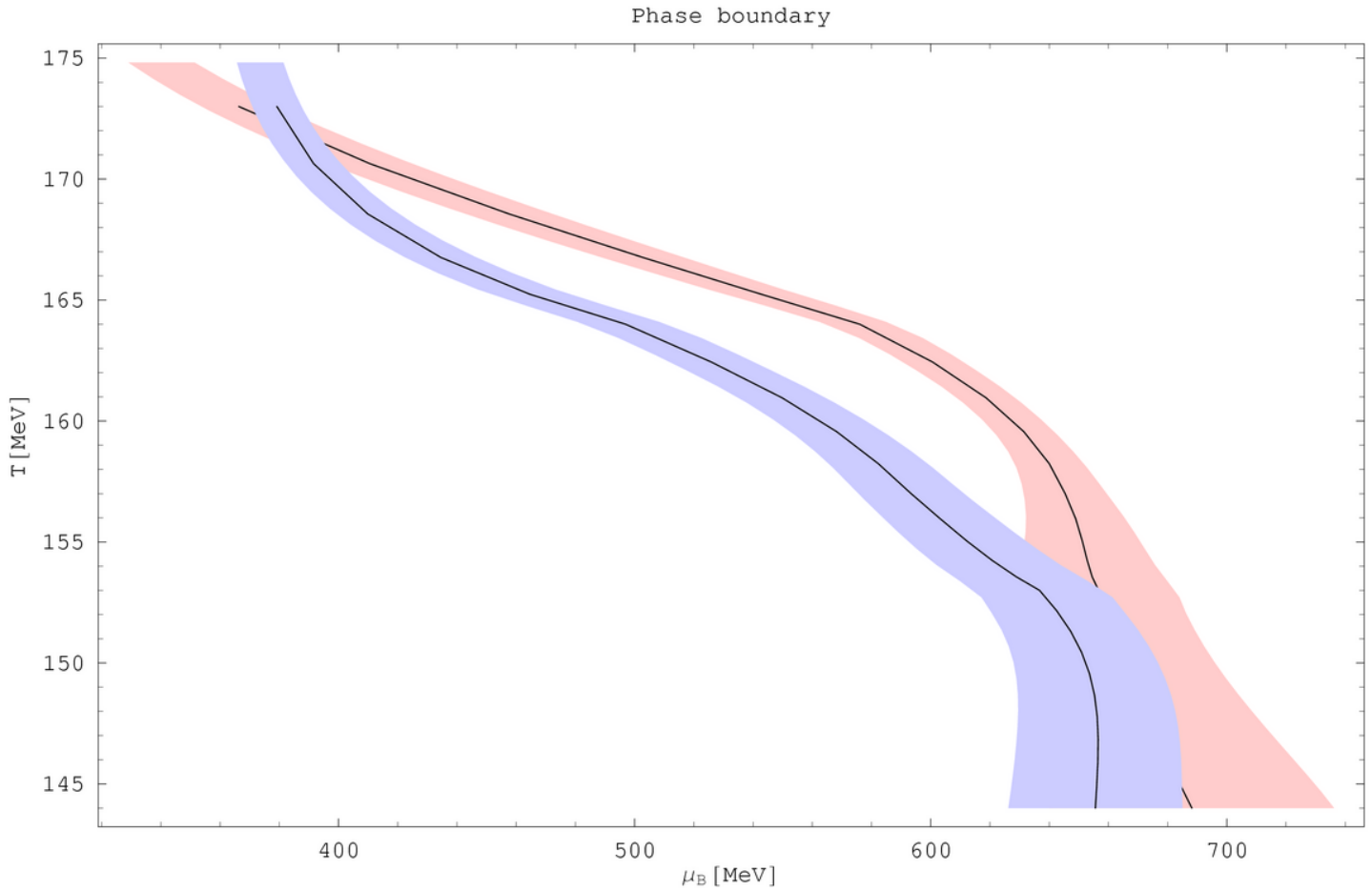
$$\mu_B = F(B+1) - F(B) = -\frac{1}{\beta}\ln\frac{Z_{B+1}}{Z_B} = -\frac{1}{\beta}\ln\left\langle e^{-i3\theta}\right\rangle_{3B}$$



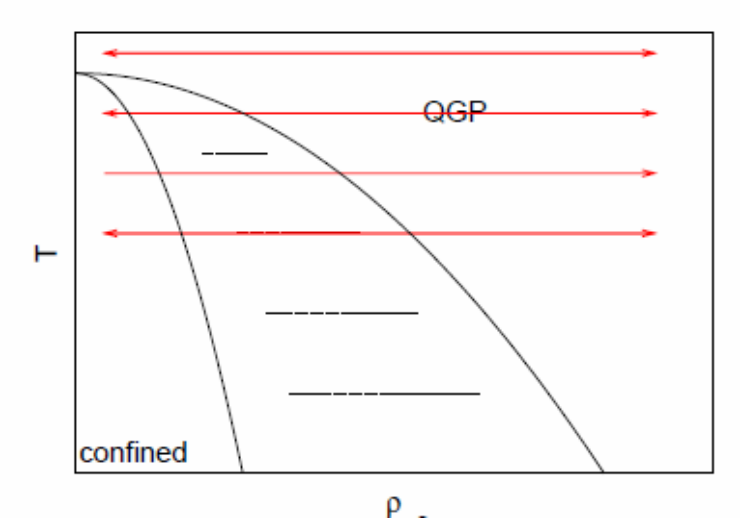
Maxwell construction

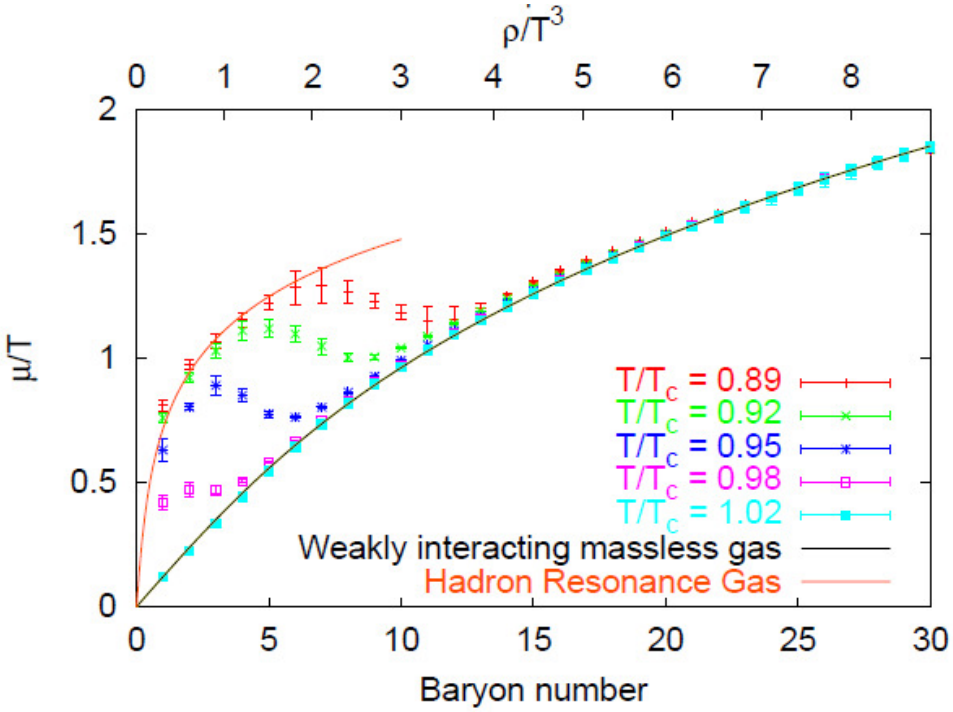


Phase boundary – a sketch

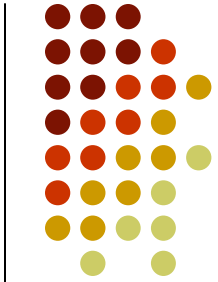


de Forcrand and Kratochvila



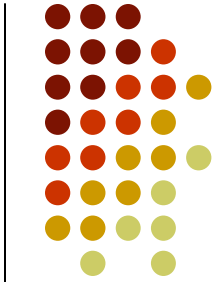


Plans



- Increase volume from 4^4 to 6^3x4:
  - 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 N=10 would be enough to scan the coexistence region on a 6^3x4 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

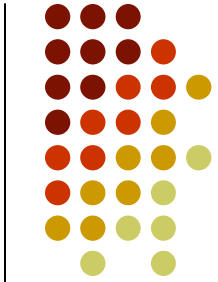


$$Z_C(V,n,T) = \int DU\ e^{-S_G(U)} \det{}'_n M^2(U)$$

$$= \int DUD\xi\ e^{-S_G(U)} \det M^2(U) f_n(U,\xi)$$

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

The updating process



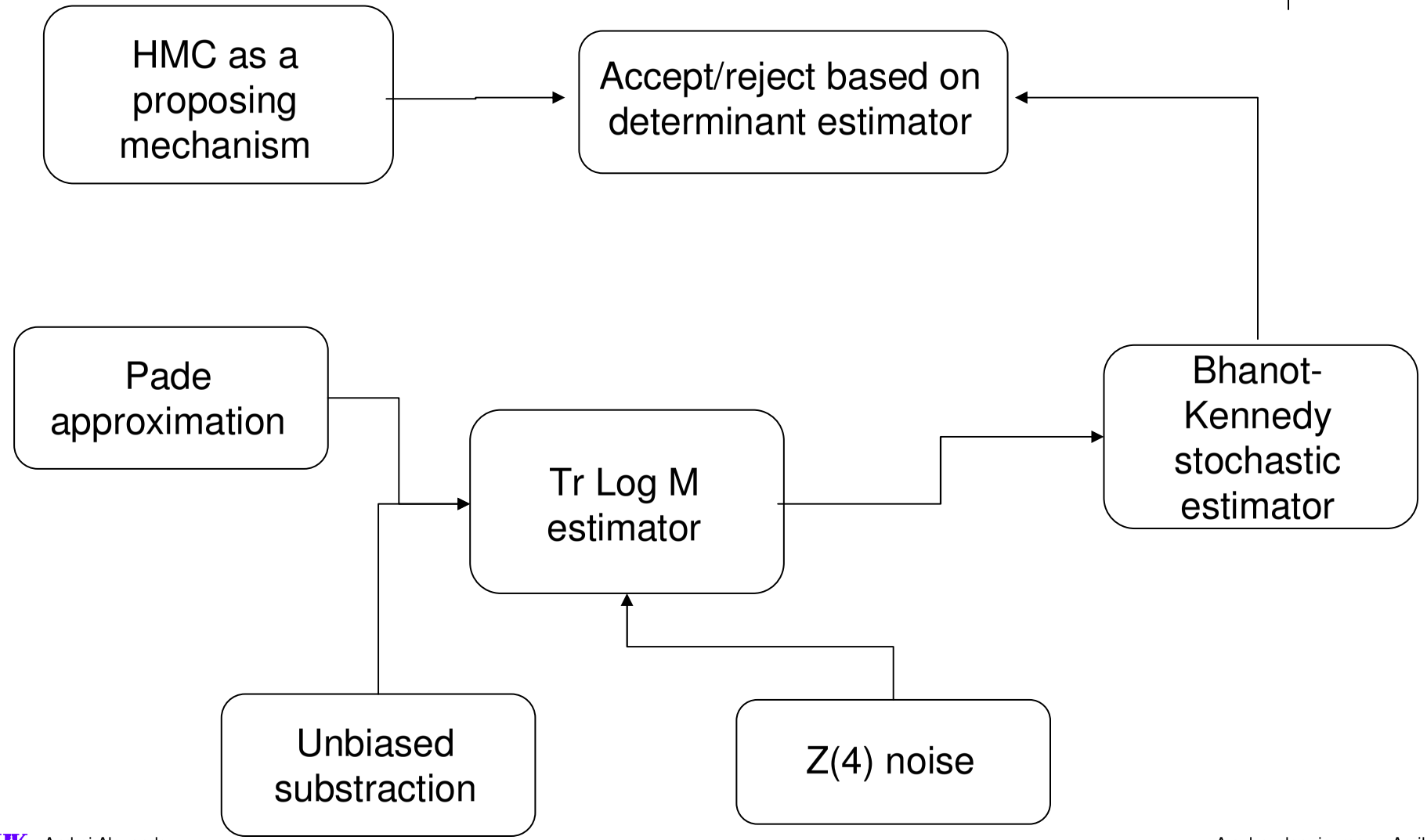
$$Z_C(V,n,T) = \int DUD\xi\, e^{-S_G(U)} \det M^2(U) f_n(U,\xi)$$

$$= \int DUD\xi\, \underbrace{e^{-S_G(U)} \det M^2(U) \mid f_n(U,\xi) \mid}_{\text{Simulation measure}} \underbrace{\frac{f_n(U,\xi)}{\mid f_n(U,\xi) \mid}}_{\text{phase}}$$

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

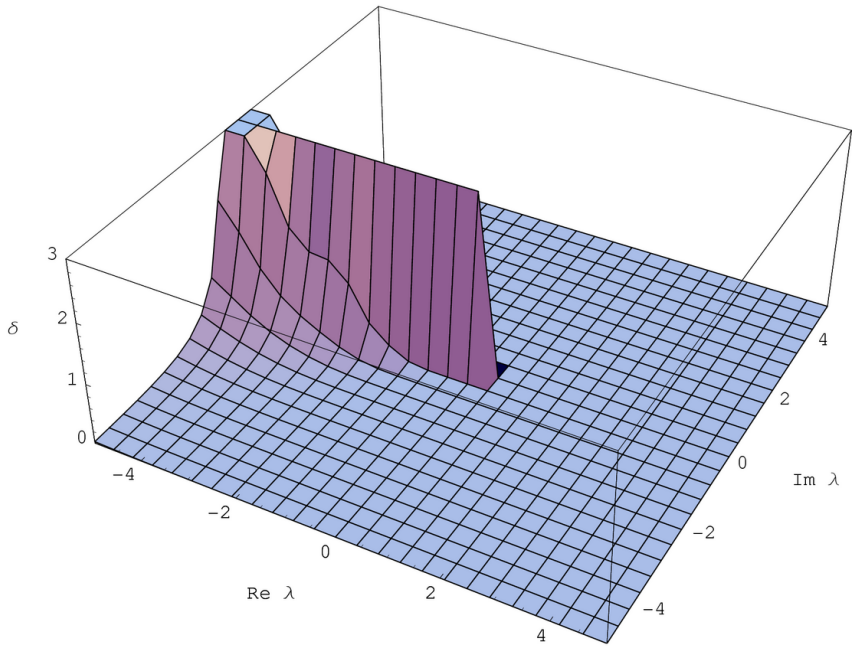
The accept/reject steps are based on the ratios $\frac{\mid f_n(U',\xi) \mid}{\mid f_n(U,\xi) \mid}$ and $\frac{\mid f_n(U',\xi') \mid}{\mid f_n(U',\xi) \mid}$.

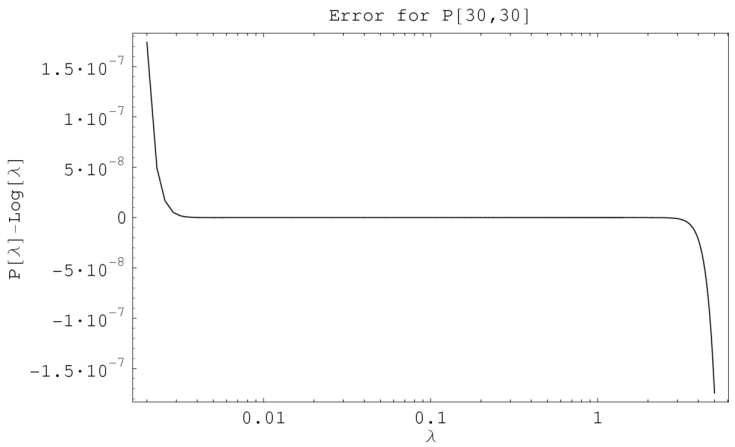
Building blocks



Pade approximation

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





Trace improvement

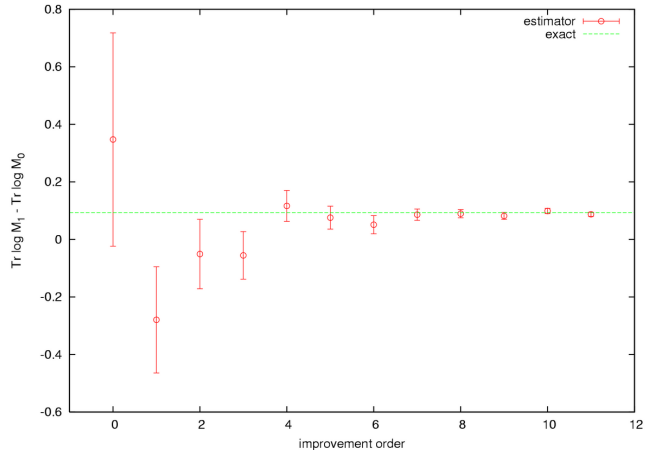
$$\mathrm{Tr}\ln M = \int d\eta\,\eta^{+} M \eta$$

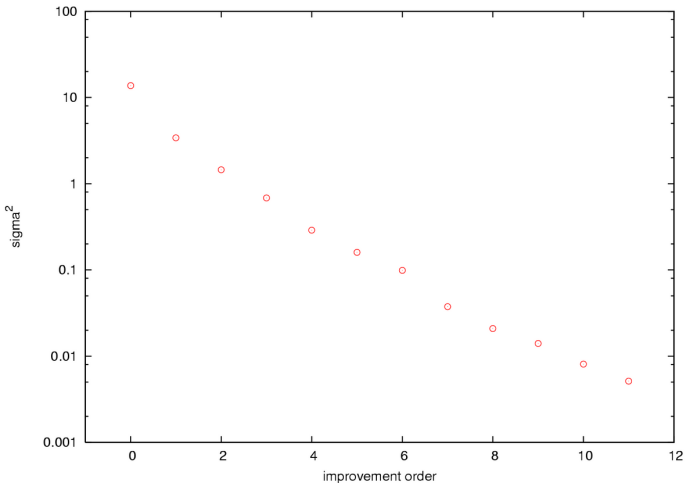
$$\mathrm{Tr}\ln M \cong b_0\,\mathrm{Tr}\,I + \sum_{k=1}^{K} \mathrm{Tr}\frac{b_k}{c_k + M}$$

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

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

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





Setting up the estimator

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

$$Tr \ln M = \int d\eta \; g(\eta)$$

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

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

$$\vdots$$

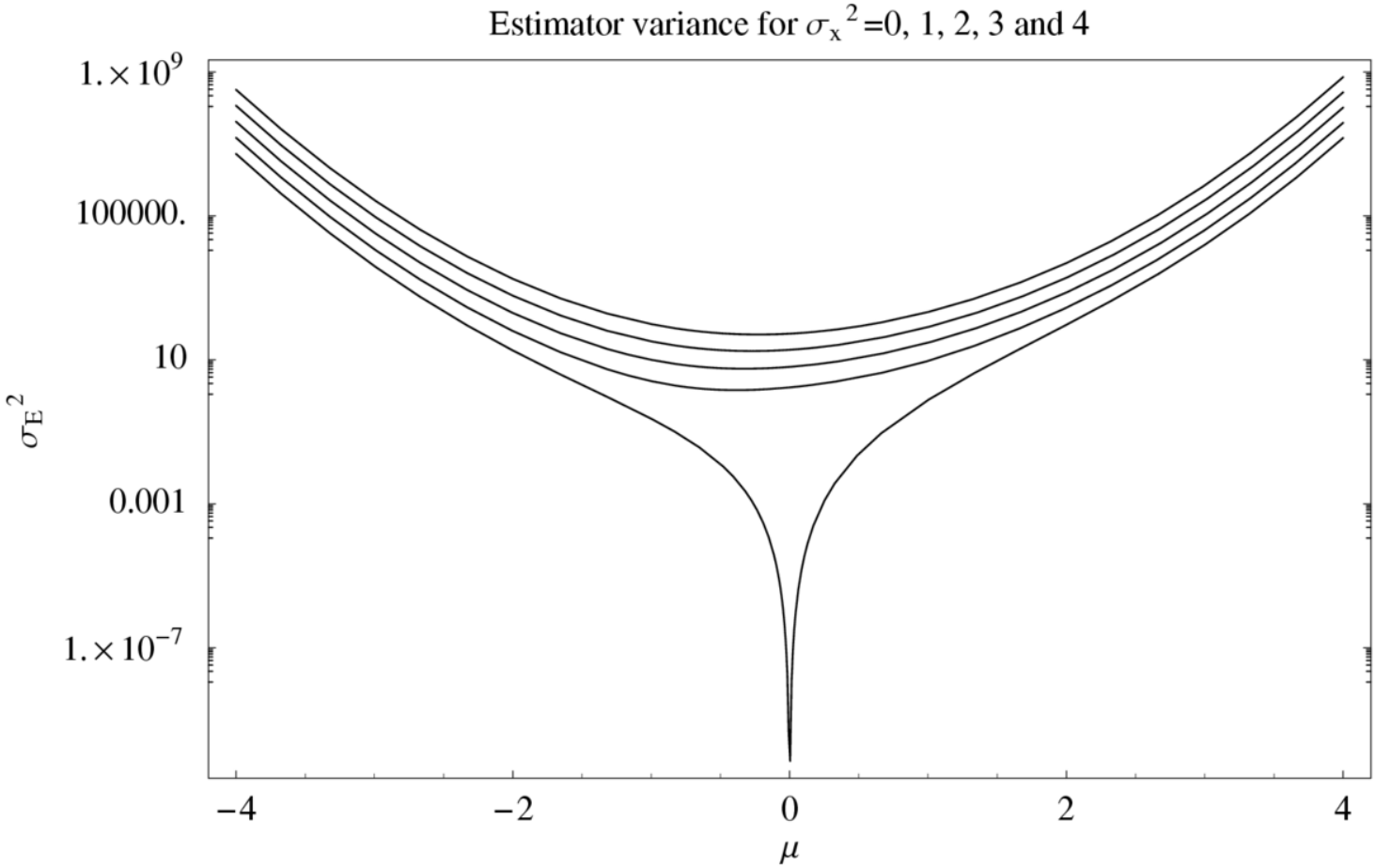
$$\langle g_k(\eta) \rangle = \frac{1}{k} Tr \ln M, \quad P(g_k = 0) = \frac{k-1}{k}$$

$$\vdots$$

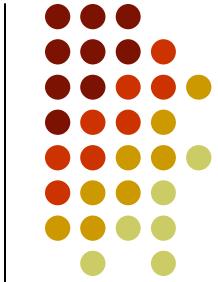
$$f(\eta_1, \eta_2, \ldots) = 1 + g_1(\eta_1) + g_1(\eta_1) g_2(\eta_2) + g_1(\eta_1) g_2(\eta_2) g_3(\eta_3) + \ldots$$

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

Variance

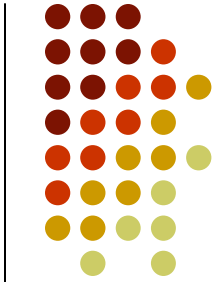

Estimator variance for σ_x^2=0, 1, 2, 3 and 4
$1.\times 10^9$
100000.
10
0.001
$1.\times 10^{-7}$
σ_E^2
−4
−2
0
2
4
μ

Near future



- Address technical issues:
  - 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.

Future plans



- Determine phase boundary
- Move to smaller quark masses (use clover fermions)
- Use chiral fermions (distant future)