Lattice QCD simulations using canonical ensemble

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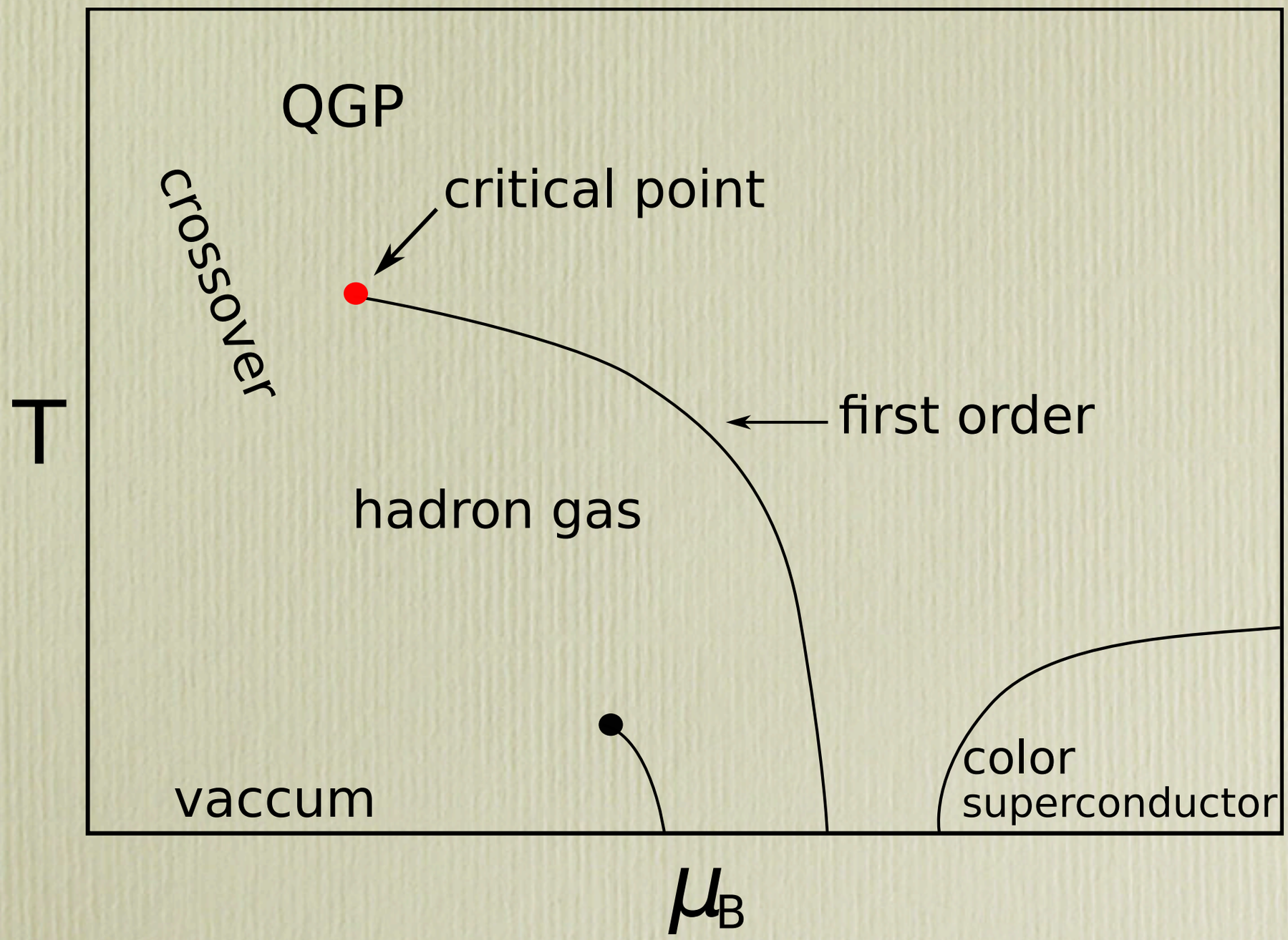
WASHINGTON, DC

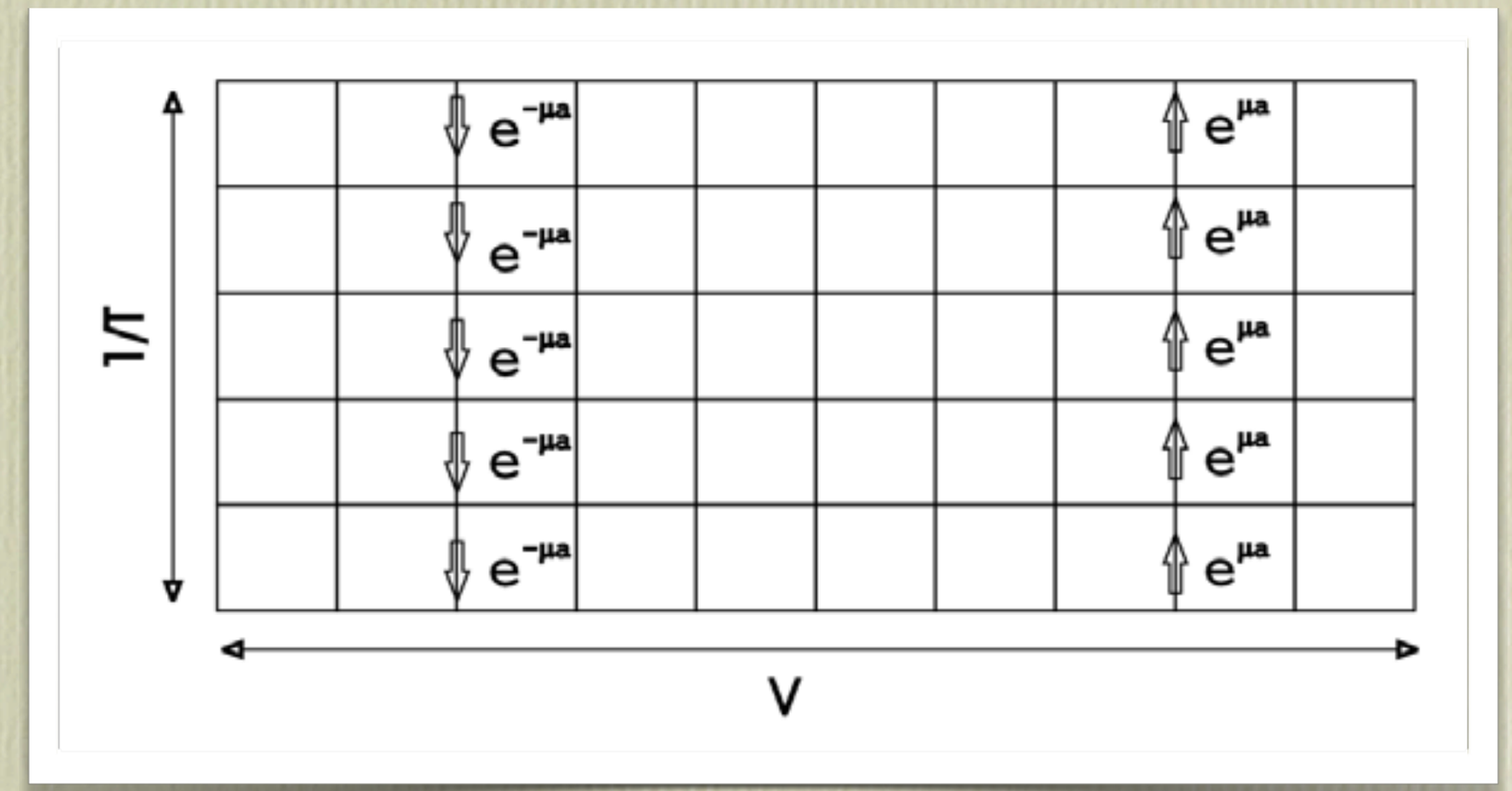
Outline

- Motivation
- Canonical partition function:
  - overlap problem
  - compression method for Wilson fermions
  - algorithm
- Numerical results: $N_f=4$ (benchmark), $N_f=3$

Expected QCD phase diagram



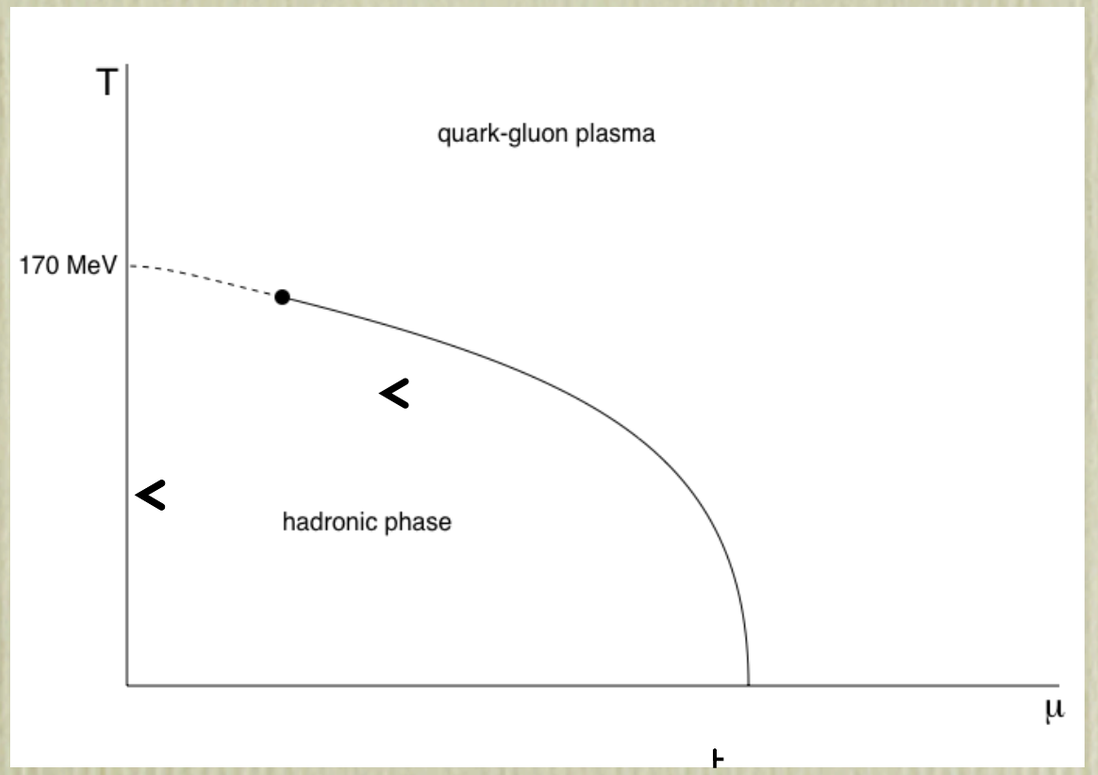
Grand canonical partition function

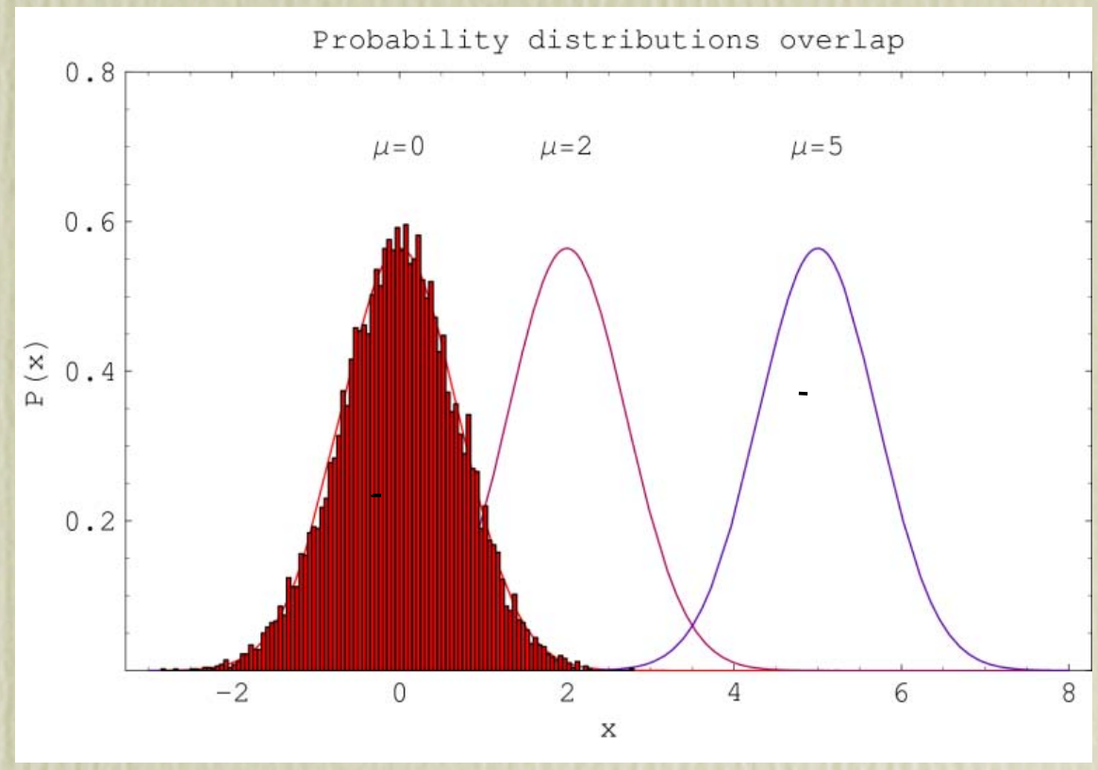


$$Z_{GC}(T,V,\mu) = \int \mathcal{D}U e^{-S_g(U)} \det M(U,\mu)^2$$

complex

Overlap problem

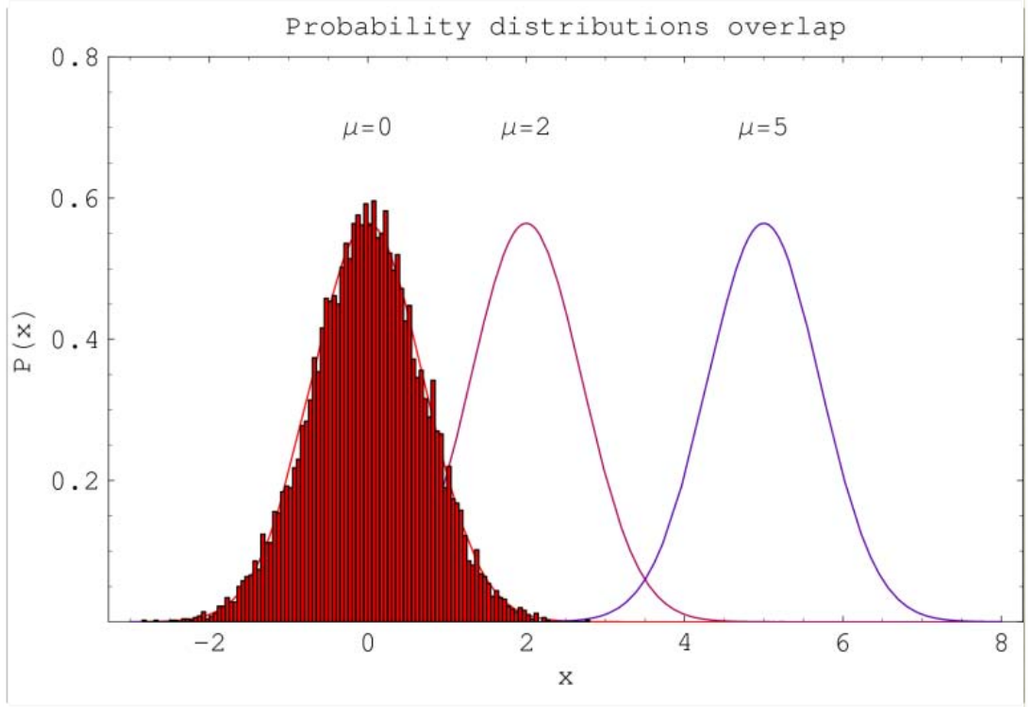


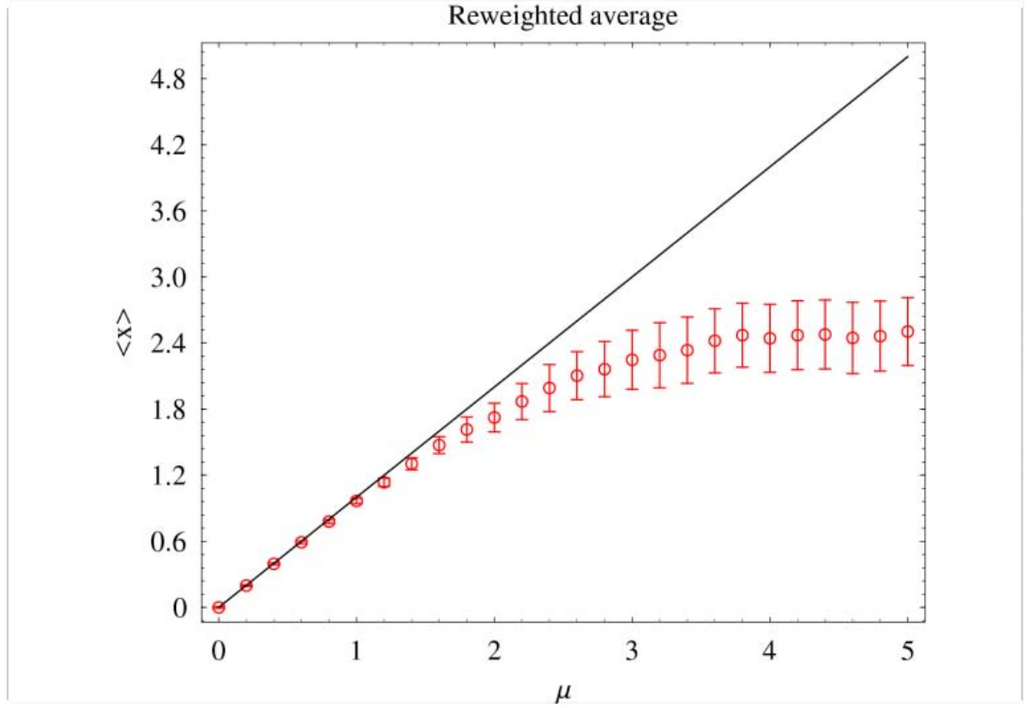


$$Z'_{GC}(T,V,\mu) = \int \mathcal{D}U e^{-S_g(U)} \det M(U,\mu=0)^2 \quad \alpha(U) = \frac{\det M(U,\mu)^2}{\det M(U,\mu=0)^2}$$

$$\langle O \rangle = \langle O\alpha \rangle' \,/\, \langle \alpha \rangle'$$

Overlap problem





$$P(x) \propto e^{-(x-\mu)^2}$$

$$\langle x \rangle = \frac{\left\langle x e^{x^2-(x-\mu)^2} \right\rangle'}{\left\langle e^{x^2-(x-\mu)^2} \right\rangle'}$$

Ising model

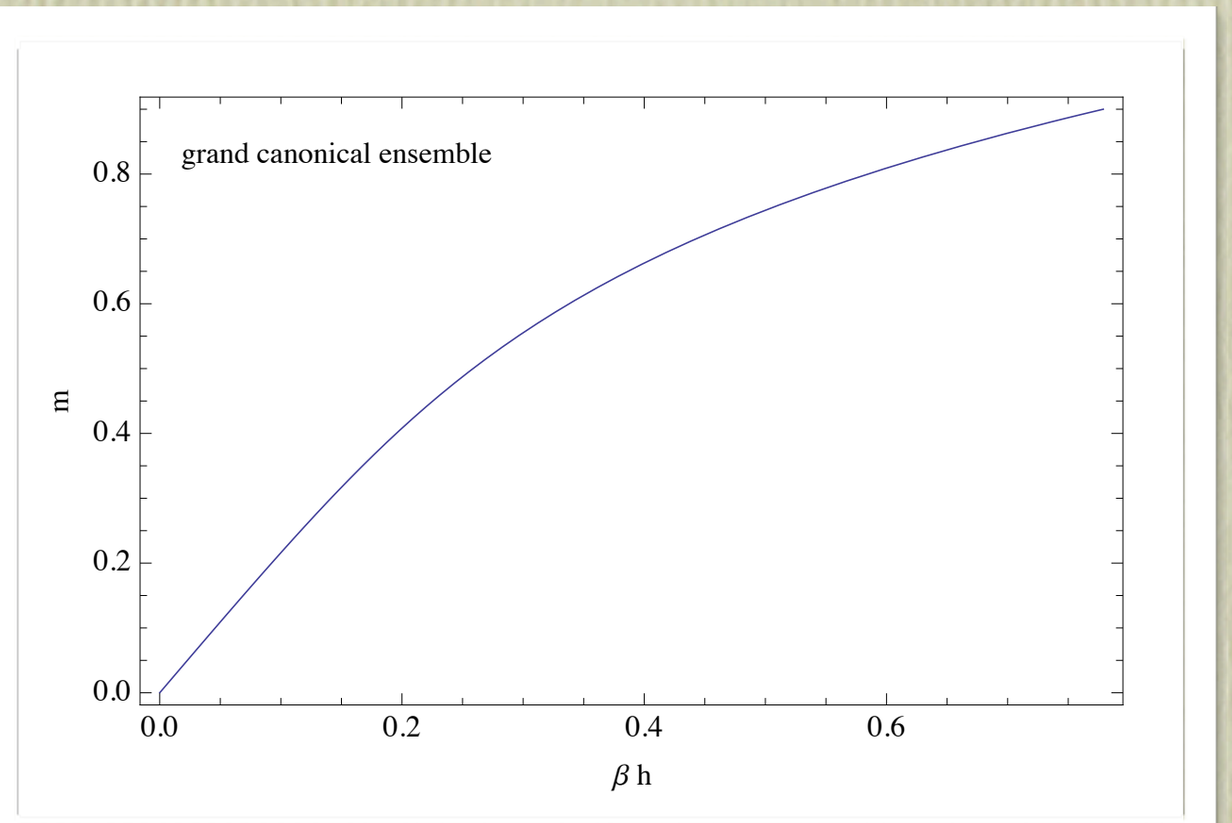
$$Z_{GC}(\beta J, \beta h) = \sum_{s} e^{\beta(J\sum_{\{ij\}} s_i s_j + h\sum_i s_i)}$$

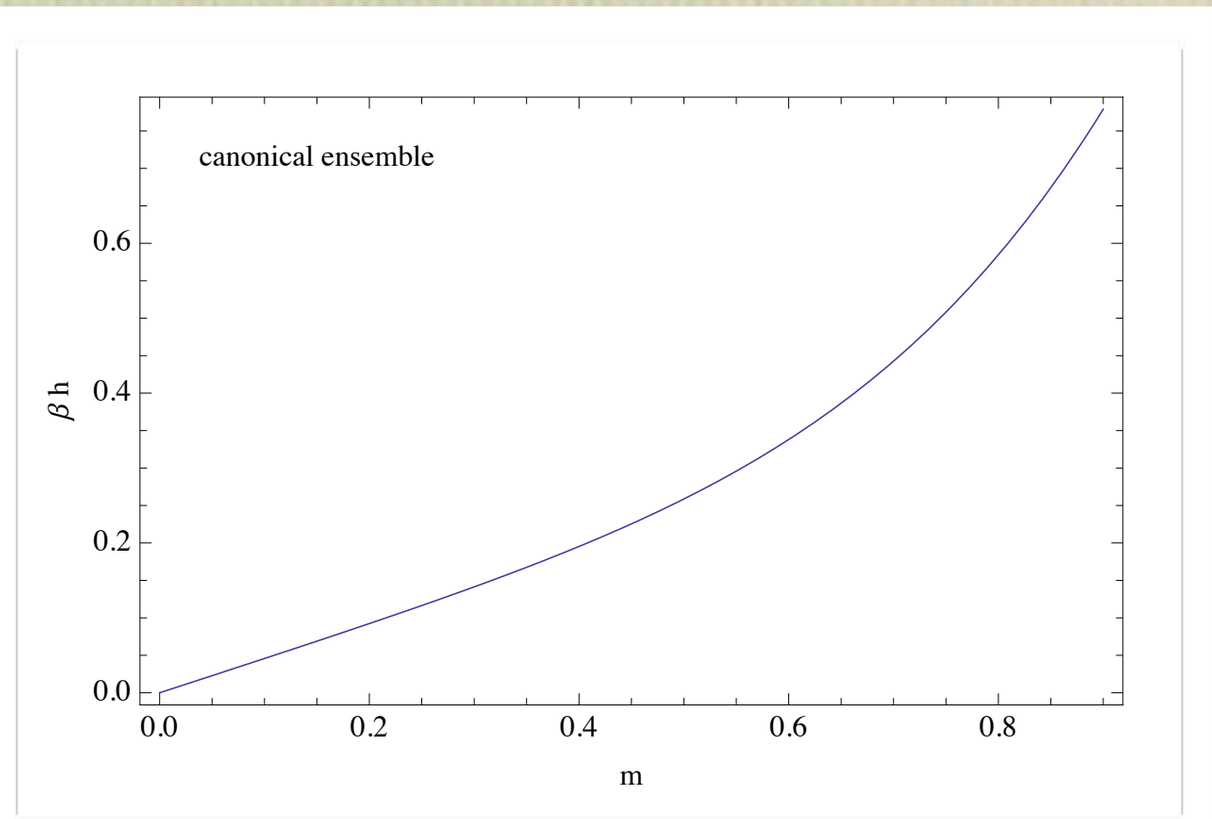
$$Z_C(\beta J, m) = \sum_{s} e^{\beta J \sum_{\{ij\}} s_i s_j}\, \delta(m - \sum_i s_i)$$

Using the spin flip symmetry

$$Z_C(\beta J, m) = \sum_{s} \underbrace{e^{\beta J \sum_{\{ij\}} s_i s_j}\, \frac{\delta(m - \sum_i s_i) + \delta(m + \sum_i s_i)}{2}}_{\text{canonical symmetric weight}}$$

Ising model

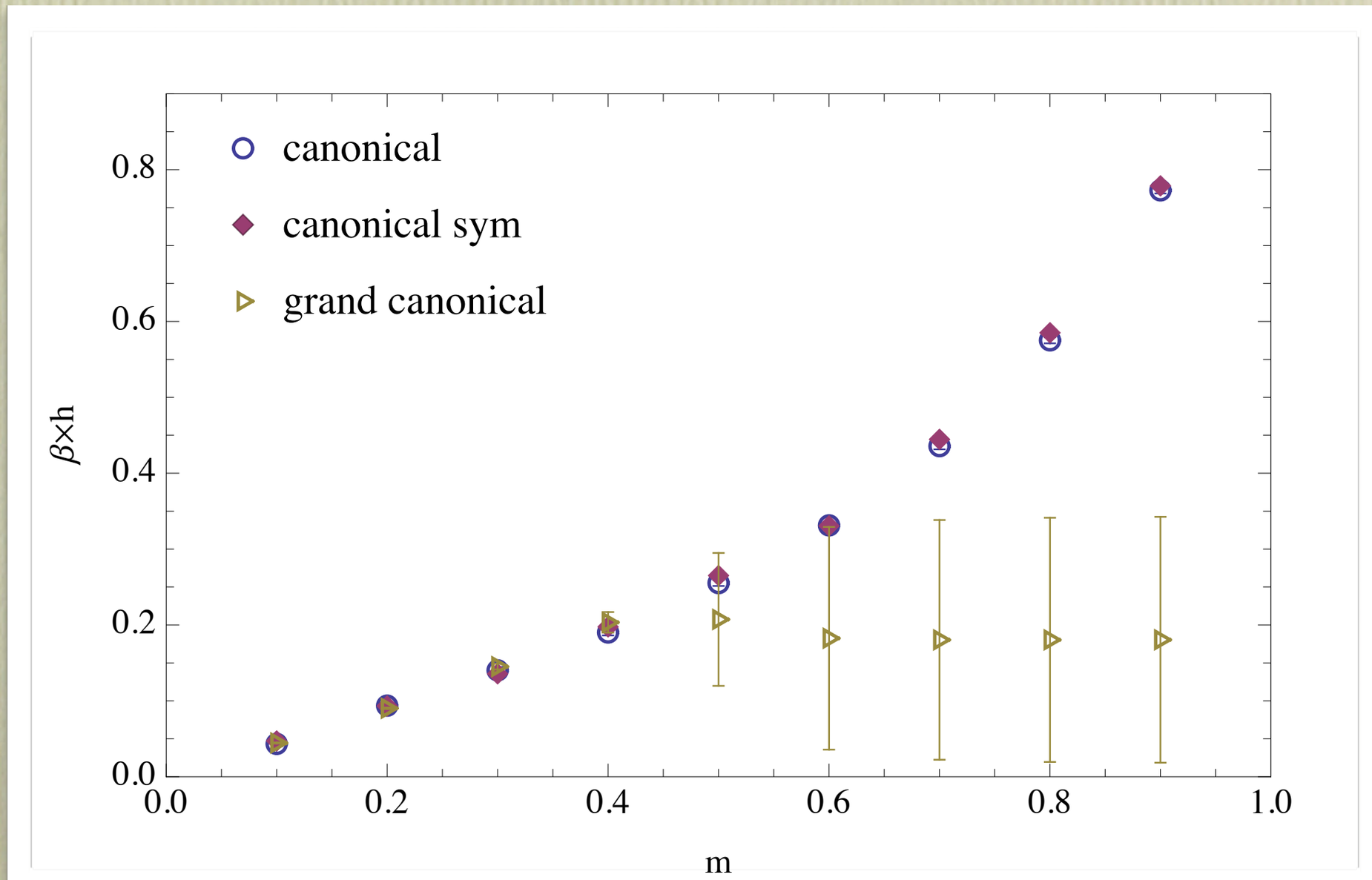




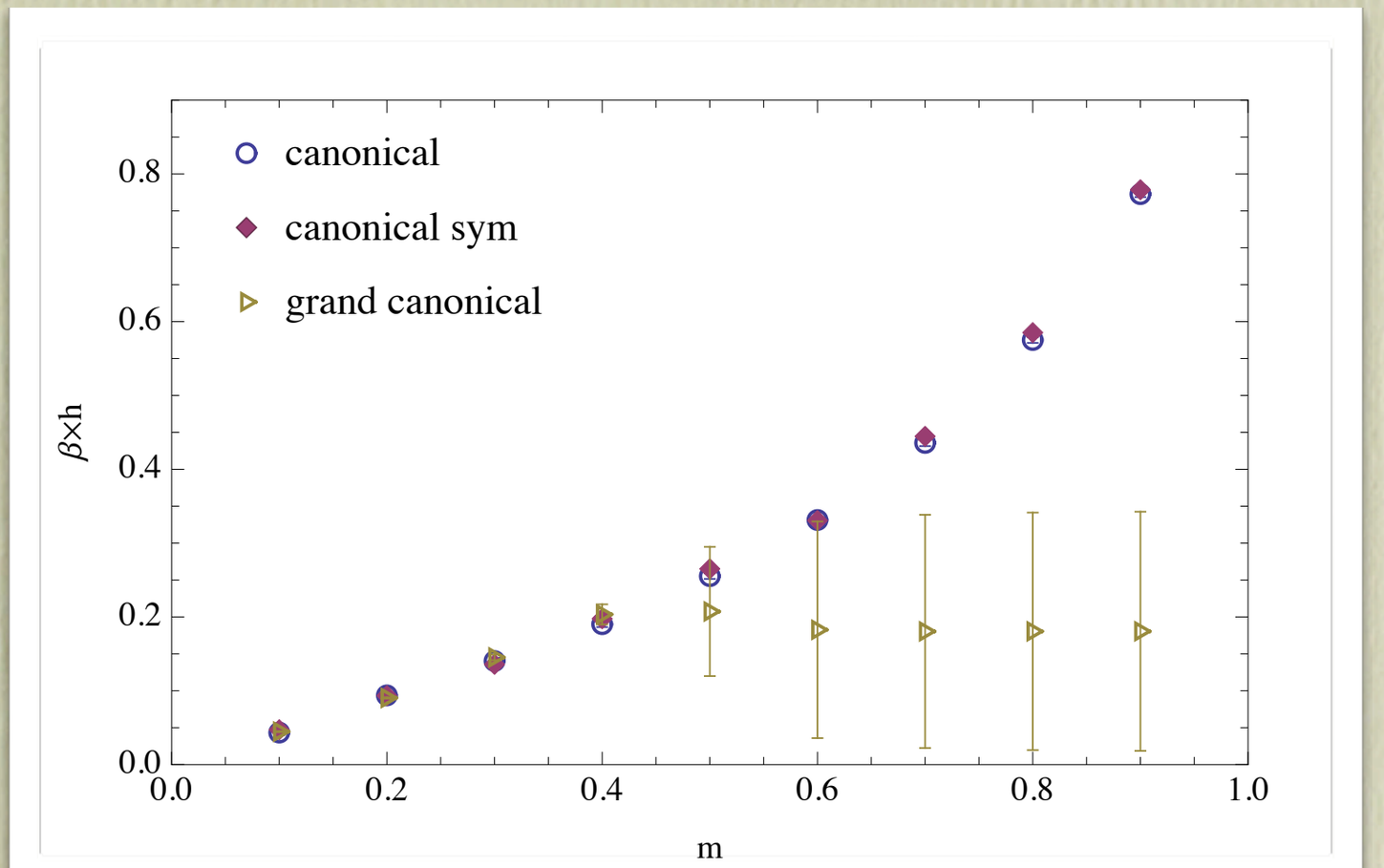
$$m(\beta h) = \left\langle \sum_i s_i \right\rangle_{Z_{GC}(\beta h)}$$

$$\beta h(m) = -\log \left\langle \frac{1}{m+1} \sum_i e^{\beta \delta V(i_1,\ldots,i_m;i)} \right\rangle_{Z_C(m)}$$

Ising model


canonical
canonical sym
grand canonical
0.8
0.6
0.4
0.2
0.0
β×h
0.0
0.2
0.4
0.6
0.8
1.0
m

Ising model


canonical
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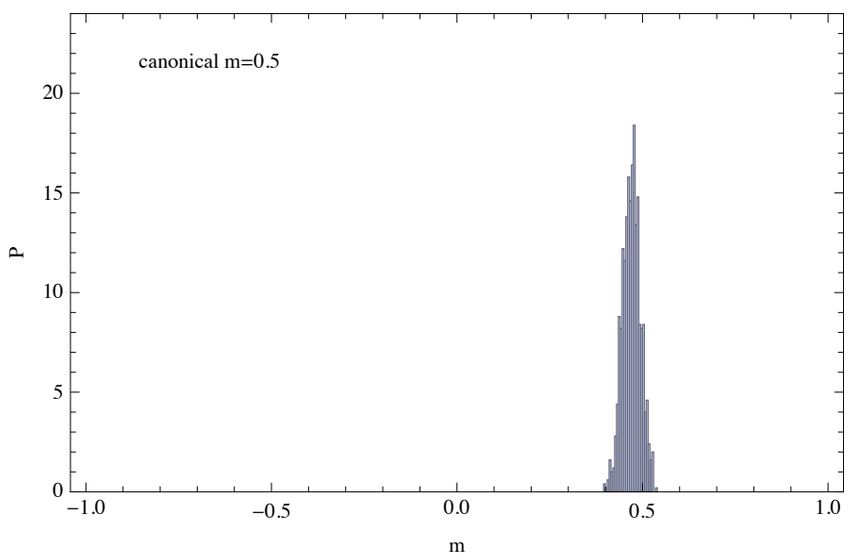
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20
15
10
5
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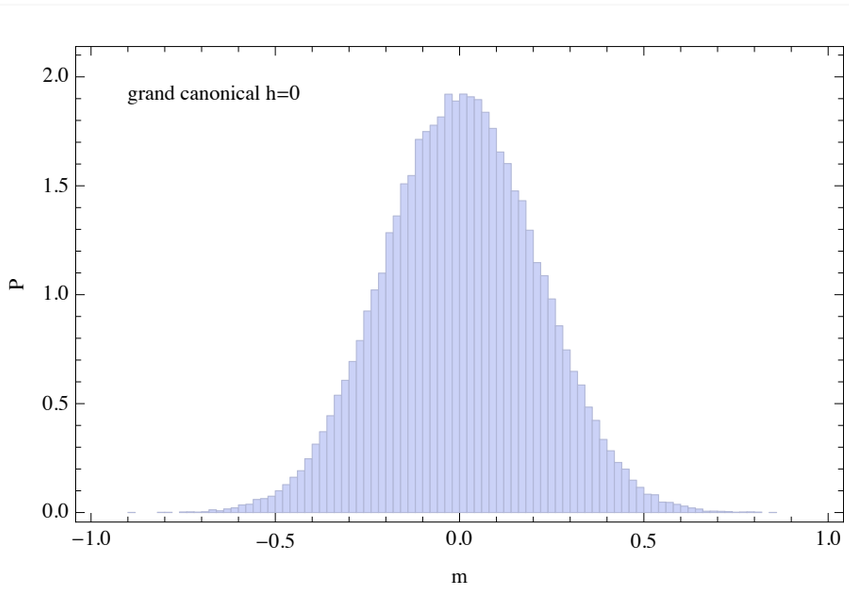
0.0
0.5
1.0
m


grand canonical h=0
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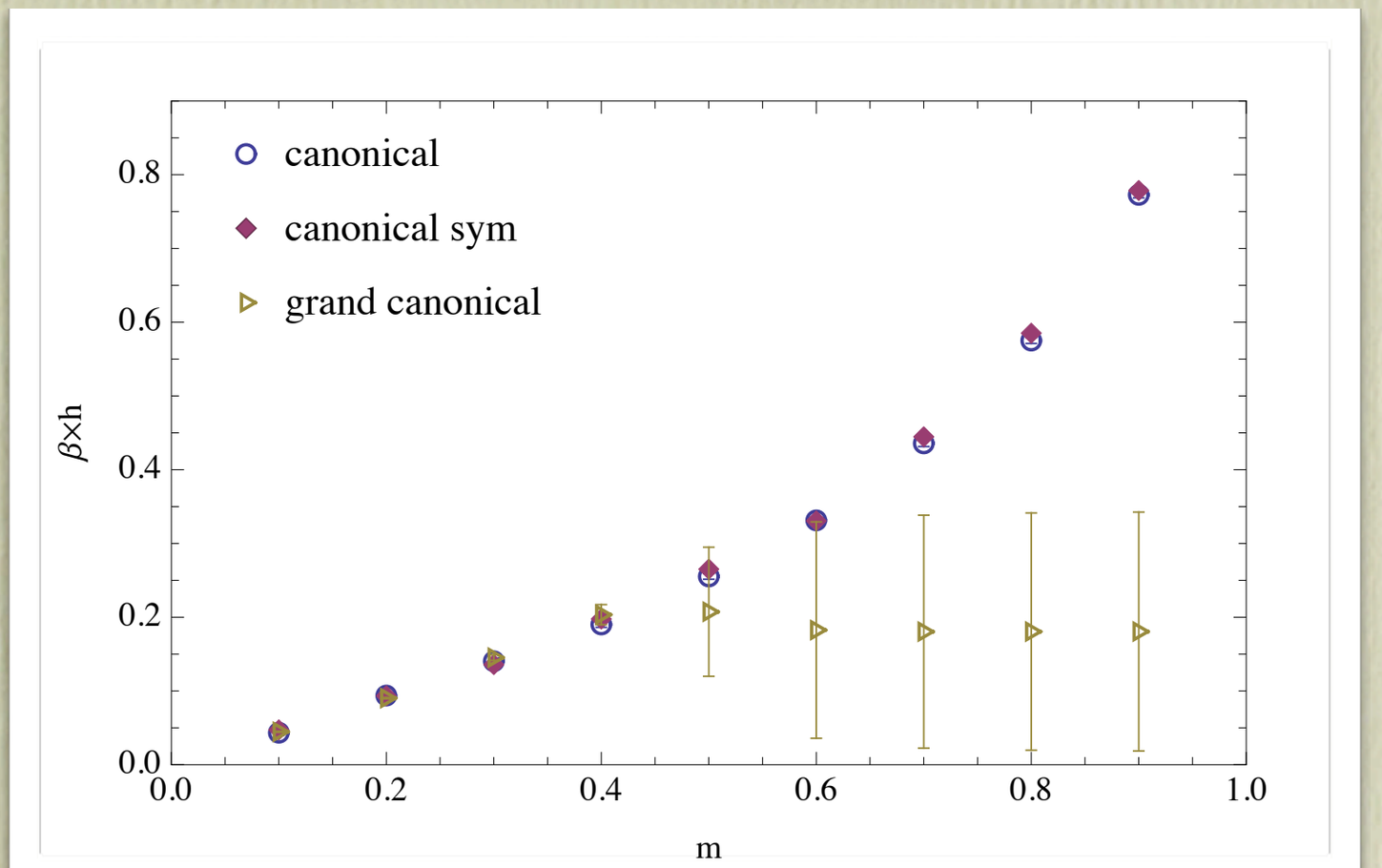
Ising model


canonical
canonical sym
grand canonical
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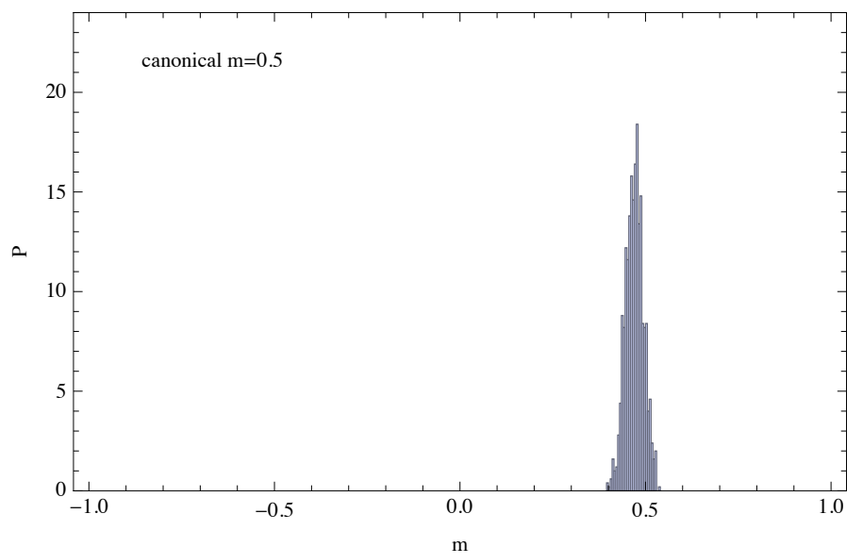
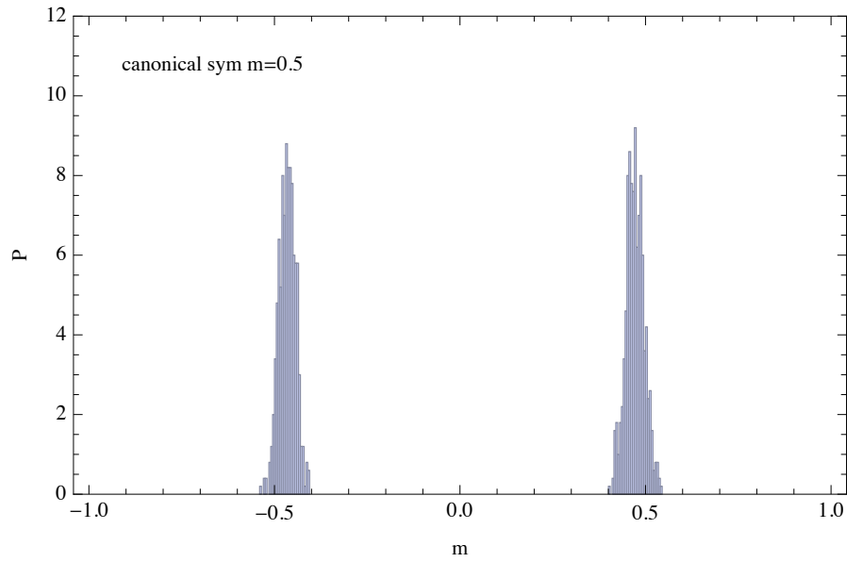
β×h
0.0
0.2
0.4
0.6
0.8
1.0
m


canonical m=0.5
20
15
10
5
0
P
−1.0
−0.5
0.0
0.5
1.0
m


canonical sym m=0.5
12
10
8
6
4
2
0
P
−1.0
−0.5
0.0
0.5
1.0
m

Canonical partition function

- Fugacity expansion in quark number

$$Z_{\mathrm{GC}}(T,V,\mu) = \sum_{n_q} (\underbrace{e^{\mu/T}}_{z})^{n_q} Z_{\mathrm{C}}(T,V,n_q)$$

- Canonical partition function as a Fourier transform at imaginary chemical potential

$$Z_{\mathrm{C}}(T,V,n_q) = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{\,-in_q\phi} Z_{\mathrm{GC}}(T,V,\mu = i\phi T)$$

Canonical partition function

- Canonical partition function

$$Z_C(T,V,k) = \int \mathcal{D}U e^{-S_g(U)} \det{}_k M(U)$$

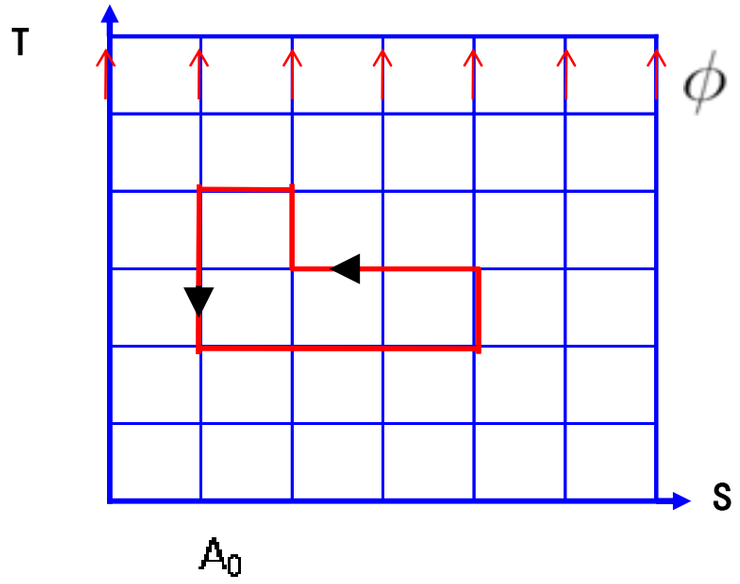
- Projected determinant

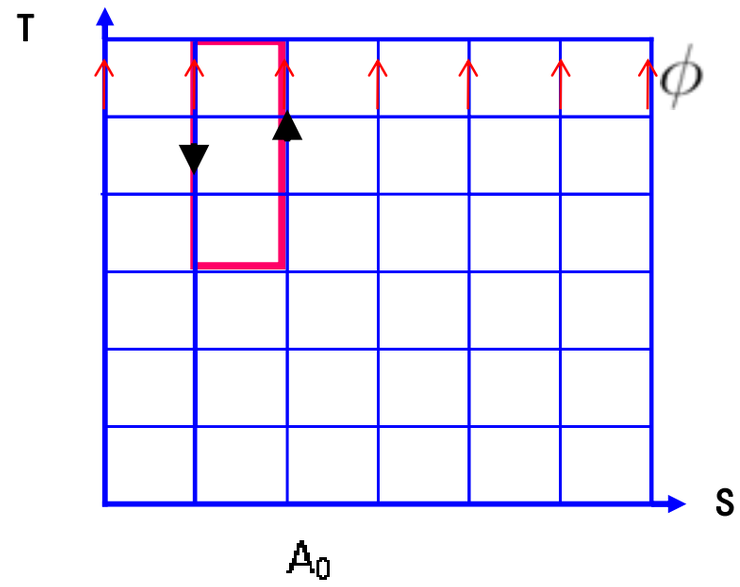
$$\det{}_k M(U) = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{-ik\phi} \det M(U,\phi)$$

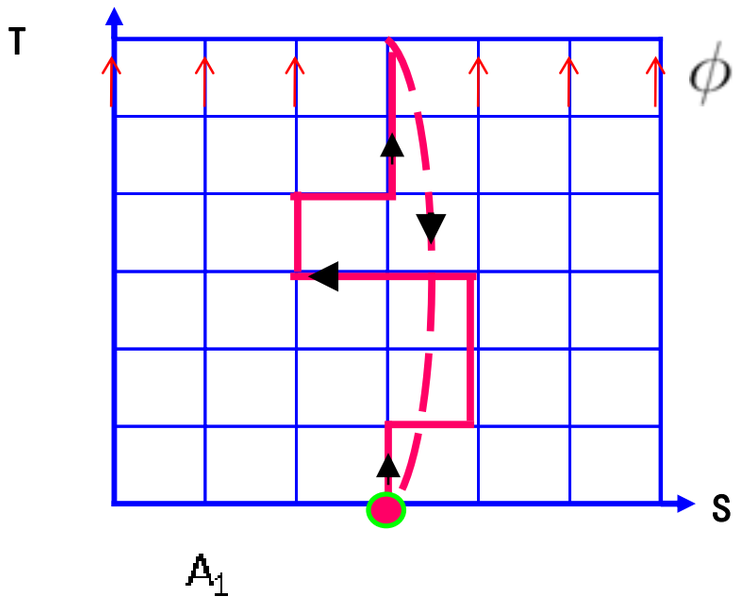
- Quark hopping matrix (Wilson type)

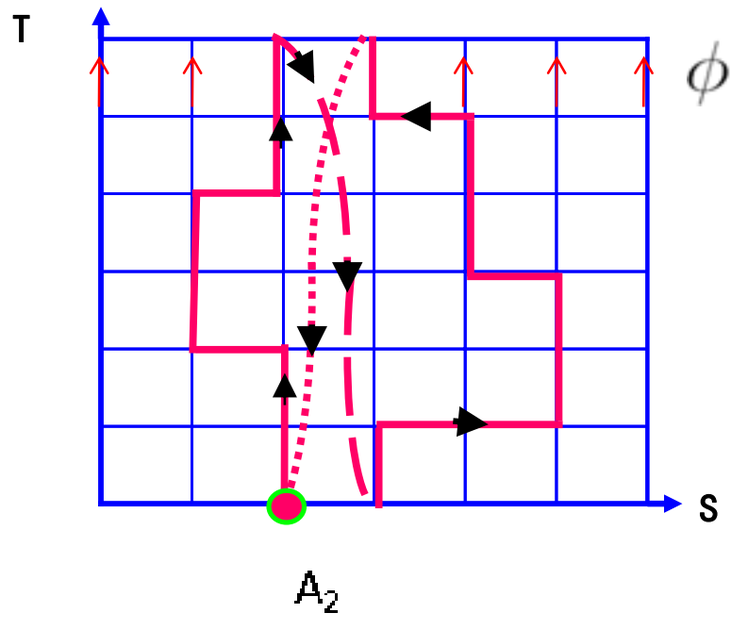
$$\begin{aligned} M_{x,y}(U,\phi) = \delta_{x,y} \quad &- \quad \kappa\delta_{x_4,N_t-1} e^{i\phi}(1+\gamma_4) U_4{}^\dagger(x-\hat{4})\ \delta_{x-\hat{4},y} \\ &- \quad \kappa\delta_{x_4,N_t-1} e^{-i\phi}(1-\gamma_4) U_4(x)\ \delta_{x+\hat{4},y} + \cdots \end{aligned}$$

Projected determinant









Compression method

- Using Schur complement techniques separate out the phase dependence in the determinant

$$\det M = \det \mathcal{Q} \cdot \det \left[e^{-\mu L_t/2} + T \cdot \mathcal{U} \cdot e^{+\mu L_t/2} \right]$$

- Once the eigenvalues of TU are known we can compute the determinant for any phase, hence any Fourier coefficient

$$\det M(\mu) = \det \mathcal{Q} \cdot e^{+\mu L_t \cdot 2N_c L_s^3} \prod_{i=1}^{4N_c L_s^3} (e^{-\mu L_t} + \lambda_i)$$

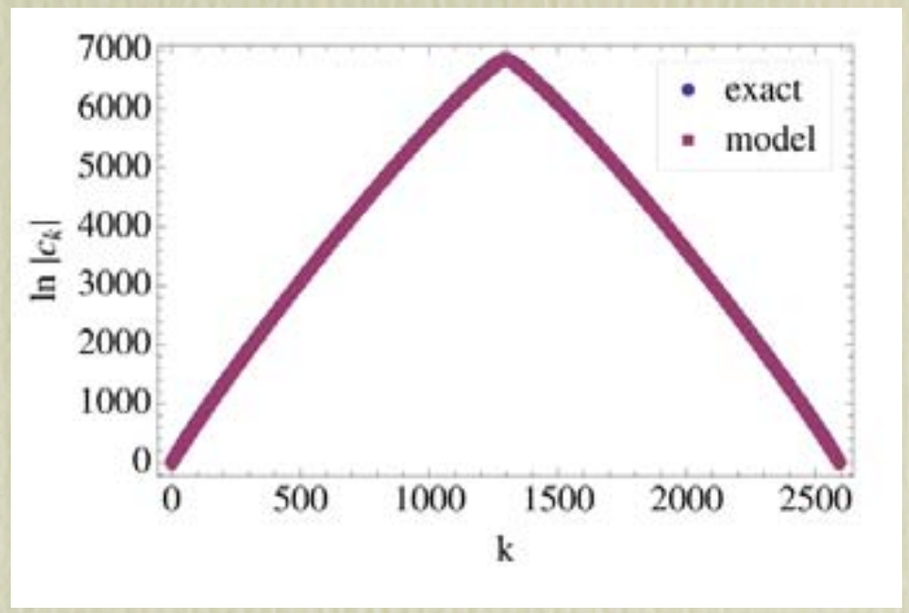
- The T and U matrices are N_t times smaller than M and the calculation is sped up considerably.

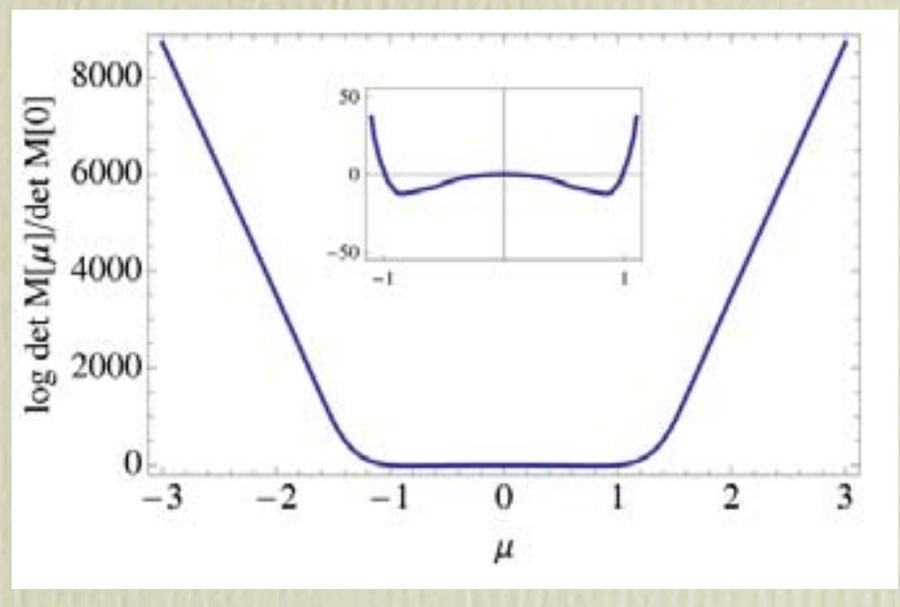
AA and U. Wenger, *Phys.Rev.* **D83** (2011) 034502, [arXiv:1009.2197].

K. Nagata and A. Nakamura, *Phys.Rev.* **D82** (2010) 094027, [arXiv:1009.2149].

Compression method

- compute projected determinants exactly
- compute them “fast”
- compute determinants for arbitrary chemical potential
- useful both for direct simulation and reweighting

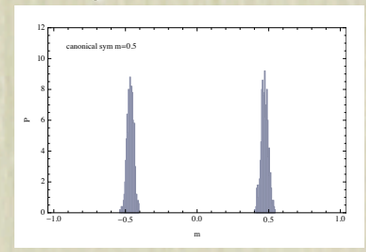


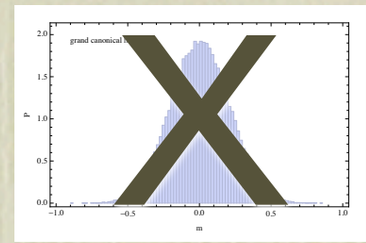


Sign problem

- The integrand is not real but using charge conjugation symmetry we can make it real

$$Z_C(T,V,k) = \int \mathcal{D}U e^{-S_g(U)} \mathrm{Re}\det{}_k M(U)$$





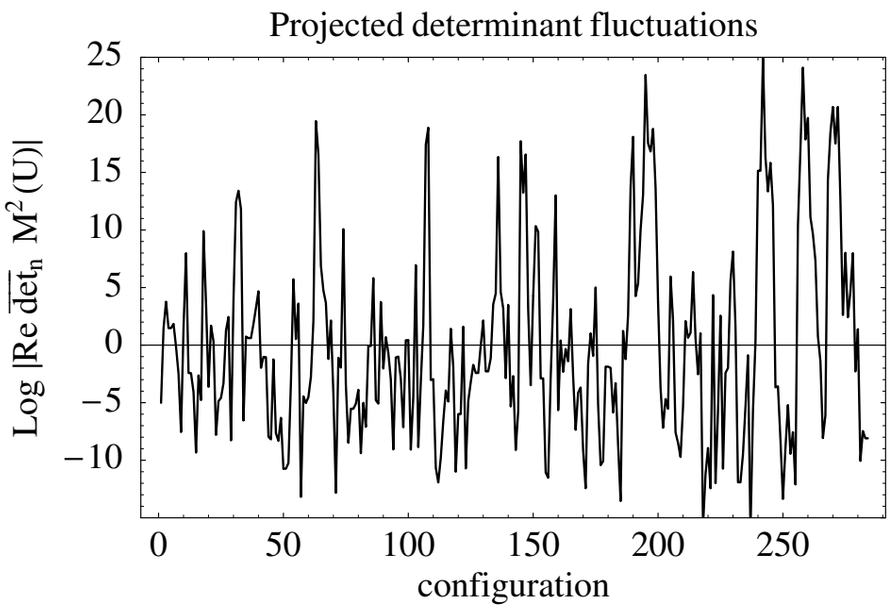
- However it isn't positive -- to simulate it we separate its sign

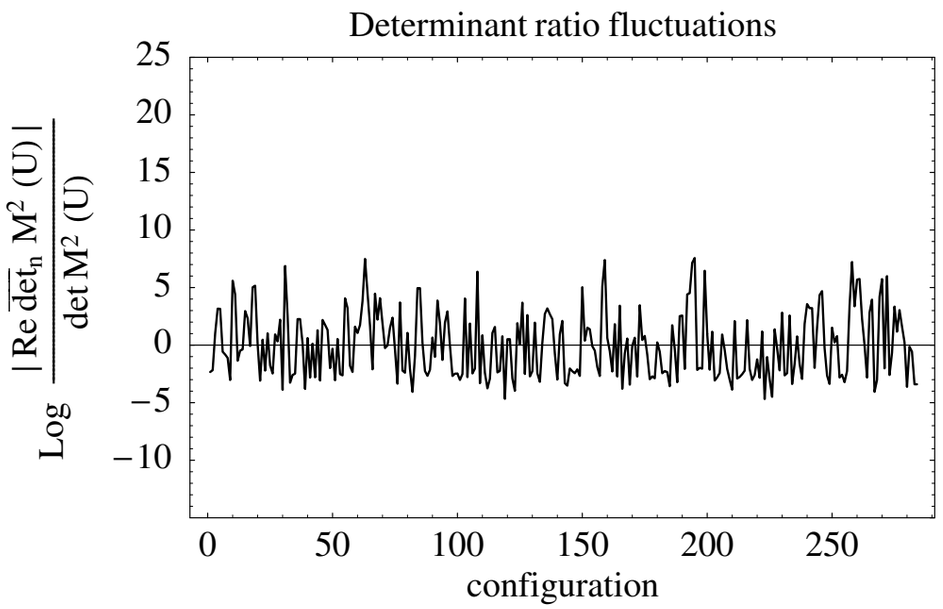
$$Z_C(T,V,k) = \int \mathcal{D}U e^{-S_g(U)} \left|\mathrm{Re}\det{}_k M(U)\right| \mathrm{sign}\,\mathrm{Re}\det{}_k M(U)$$

- To compute observables we need to re-introduce the sign

$$\langle O(U)\rangle = \frac{\langle O(U)\mathrm{sign}(U)\rangle_{||}}{\langle \mathrm{sign}(U)\rangle_{||}}$$

Simulation algorithm





$$Z_C(T,V,k) = \int \mathcal{D}U\, e^{-S_g(U)}\, |\mathrm{Re}\det{}_k M(U)|\, \mathrm{sign}\,\mathrm{Re}\det{}_k M(U)$$

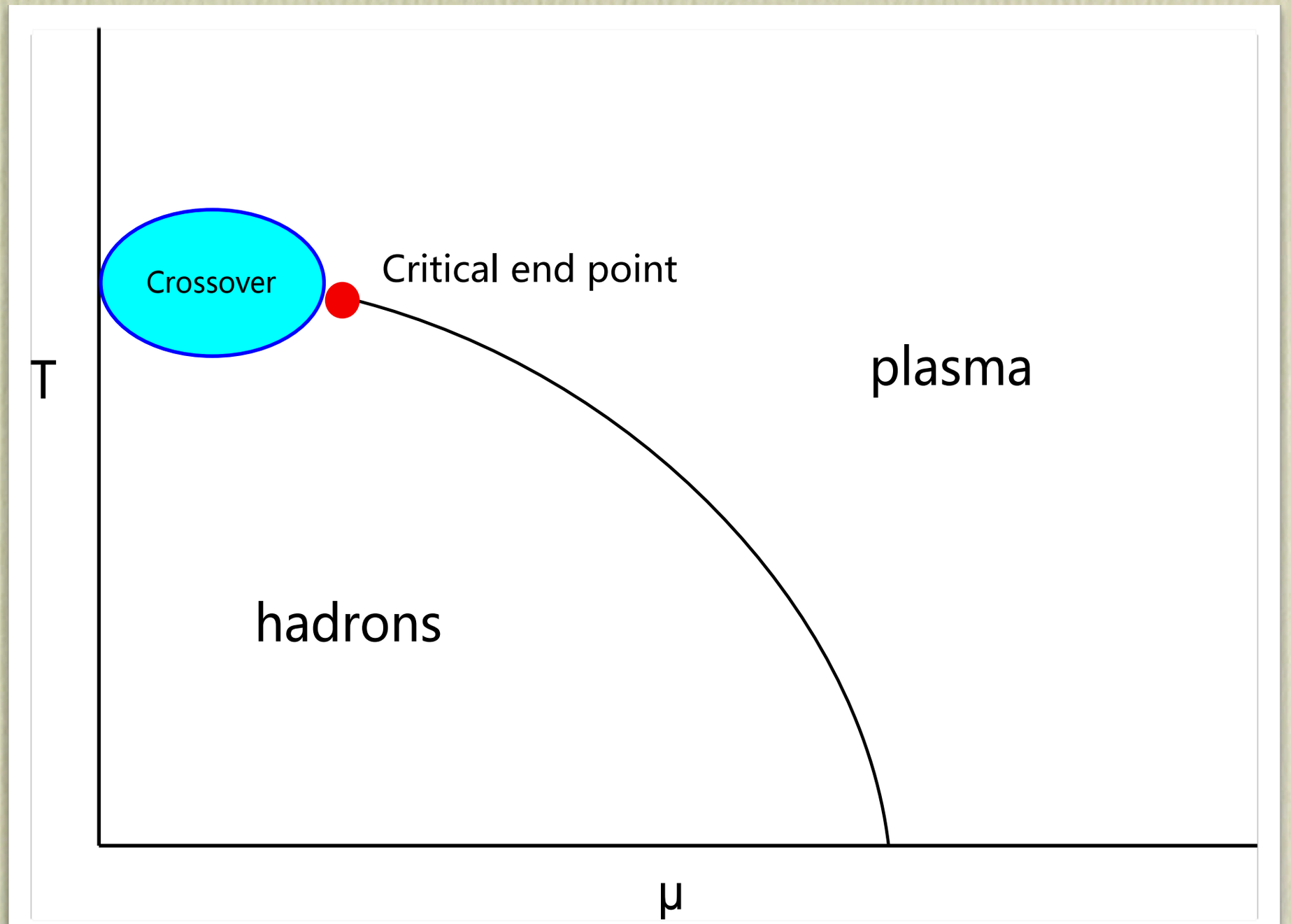
$$= \int \mathcal{D}U\, \underbrace{e^{-S_g(U)}\det M(U)}_{\mathrm{HMC}}\, \underbrace{\frac{|\mathrm{Re}\det{}_k M(U)|}{\det M(U)}}_{\mathrm{acc/rej}}\, \underbrace{\mathrm{sign}\,\mathrm{Re}\det{}_k M(U)}_{\mathrm{phase}}$$

AA, M. Faber, I. Horvath, and K.-F. Liu, *Phys.Rev.* **D72** (2005) 114513, [hep-lat/0507020].

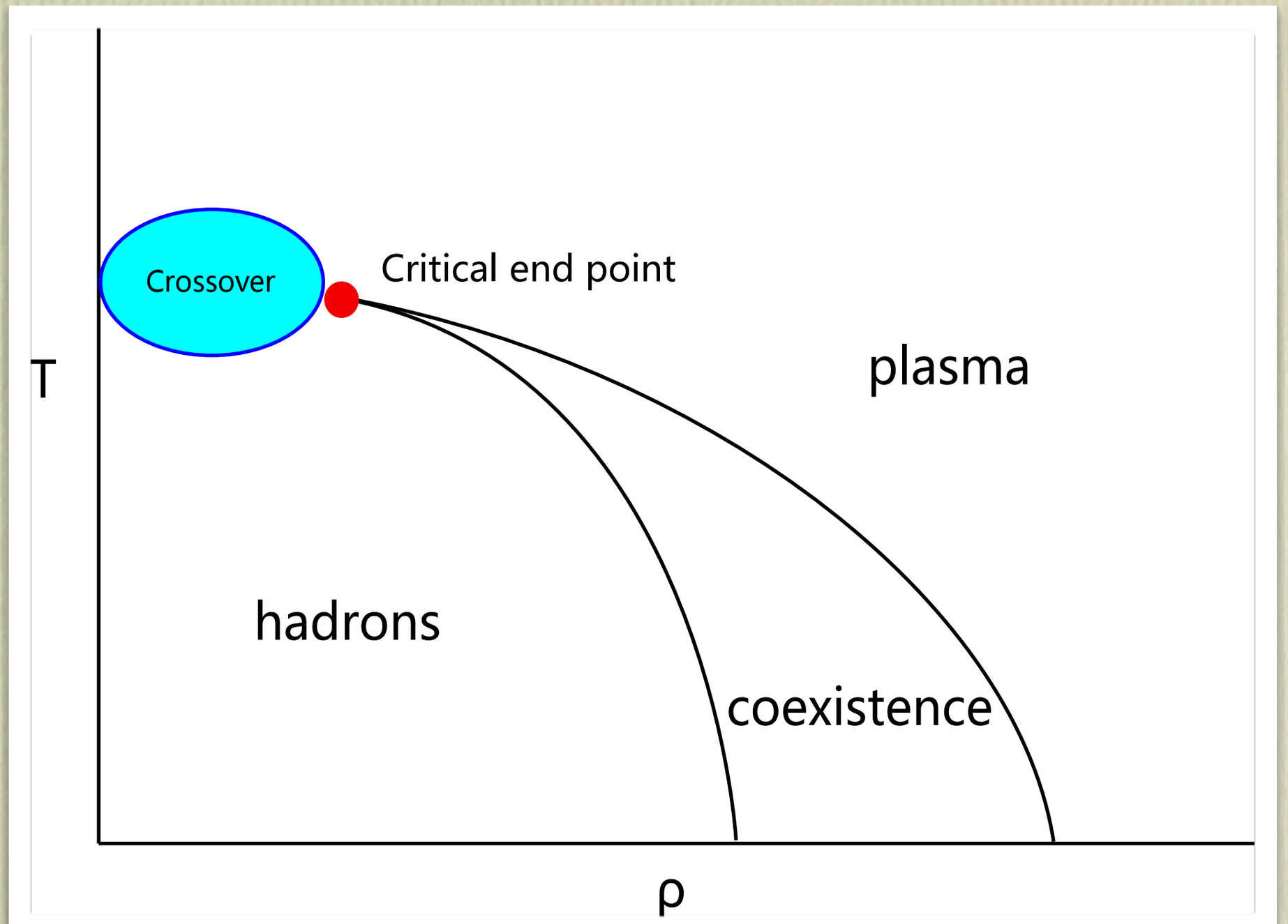
Algorithm features

- Our simulations use the projected determinant in generating the ensemble -- this should solve the overlap problem
- When sign fluctuations are under control the results should be reliable
- The simulations are computationally intensive since we need to evaluate the projected determinant for every accept/reject step

Phase diagram -- grand canonical approach



Phase diagram -- canonical approach

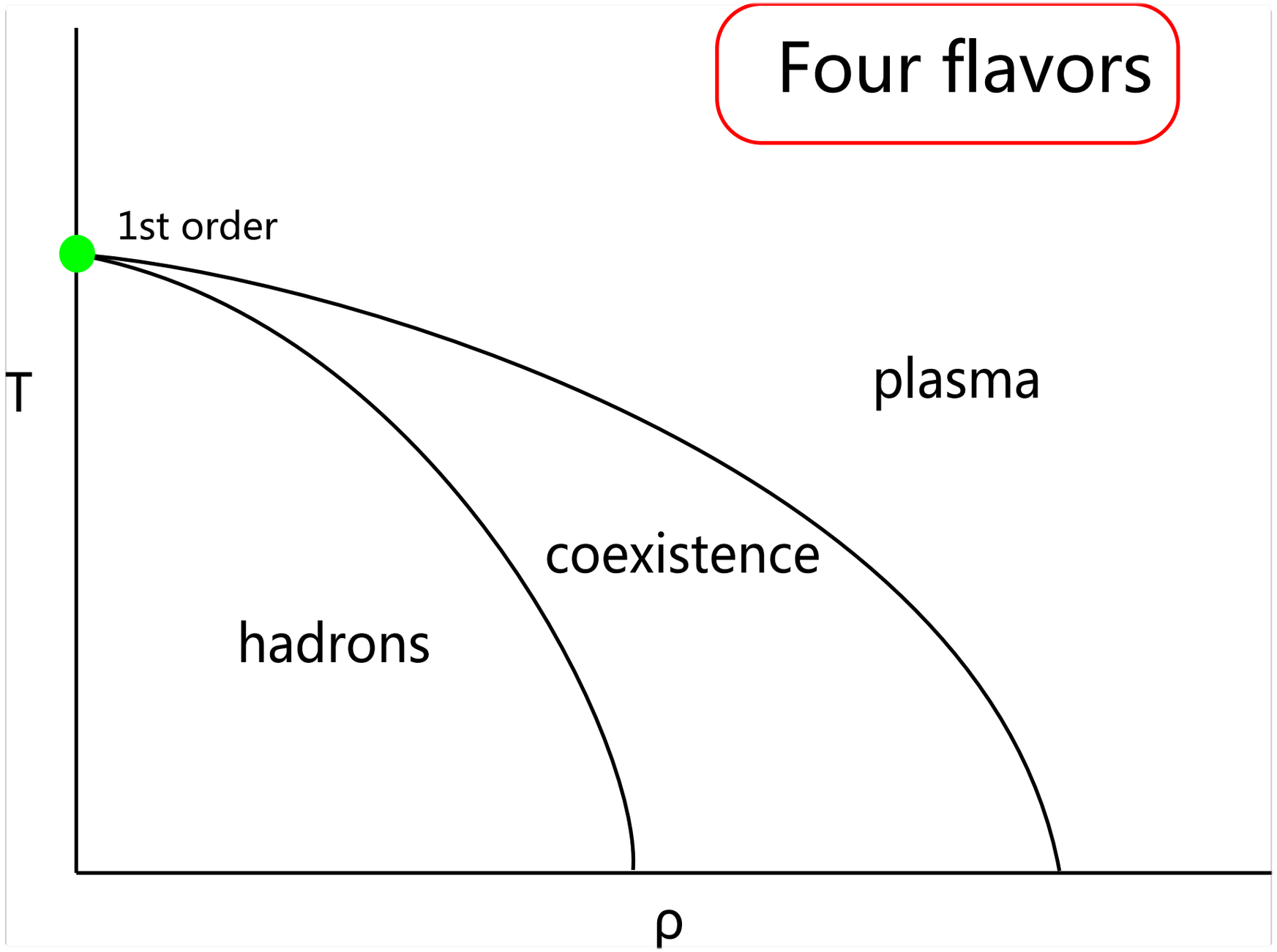


Numerical results

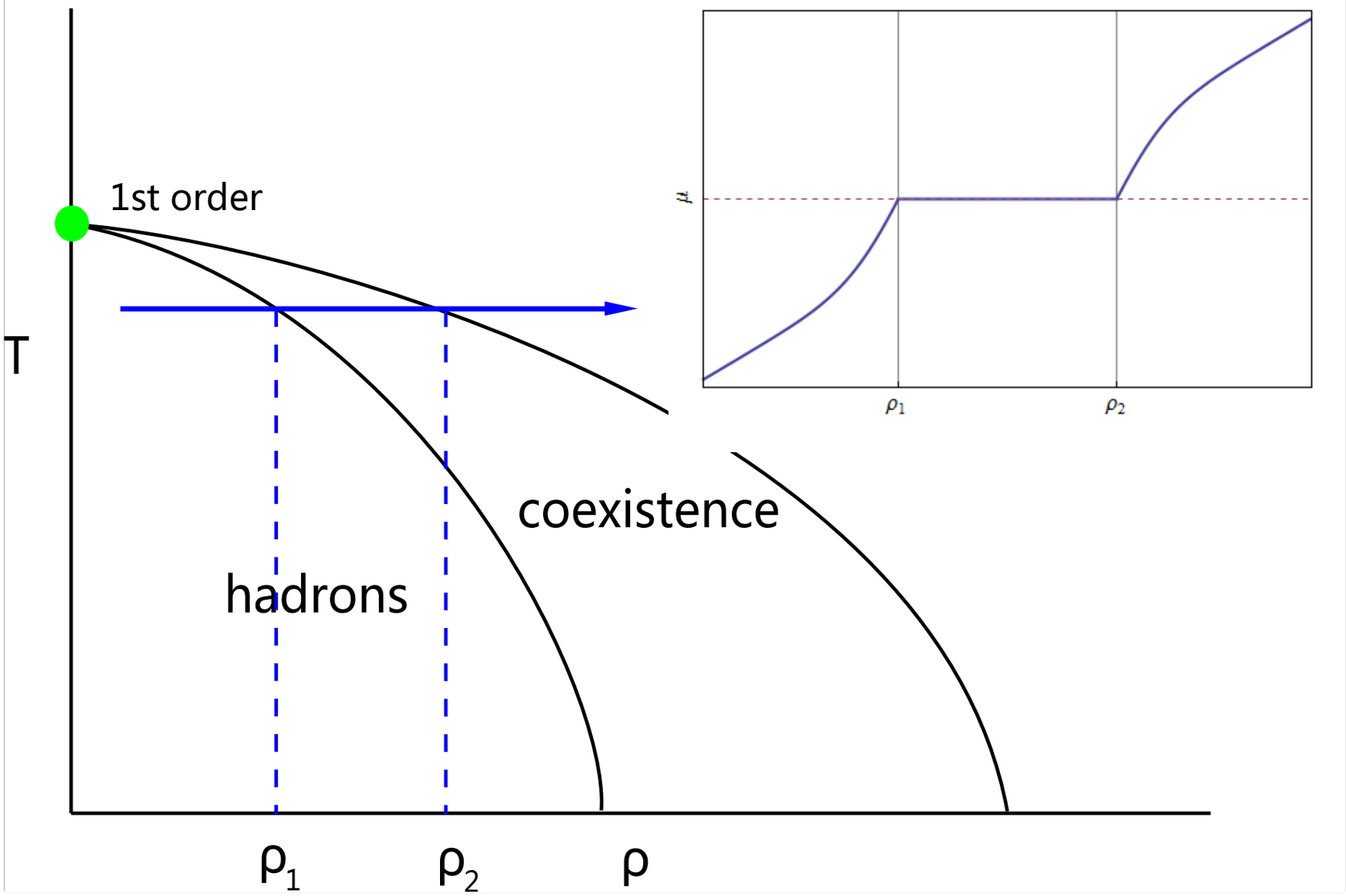
$N_f = 4$

A. Li, AA, K.-F. Liu, and X. Meng, *Phys.Rev.* **D82** (2010) 054502, [arXiv:1005.4158].

Schematic phase diagram

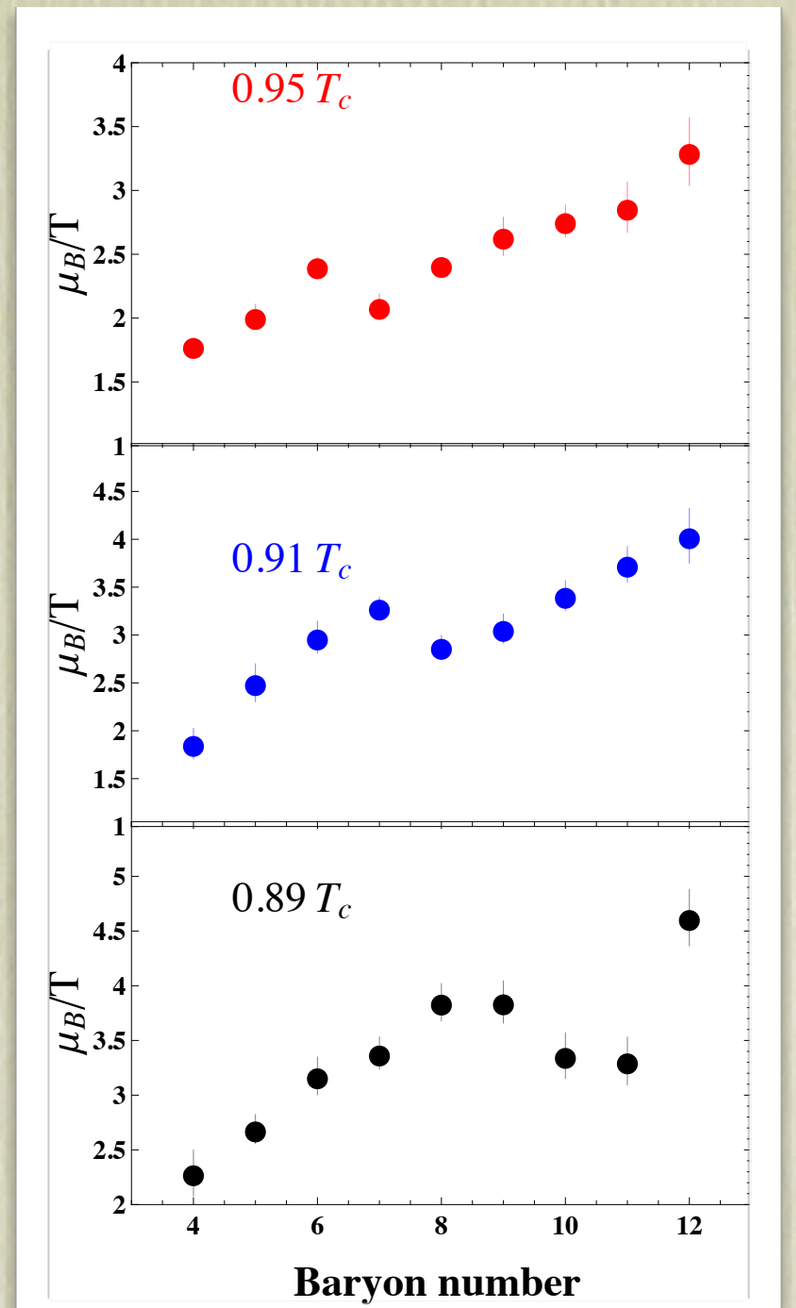


Scanning strategy



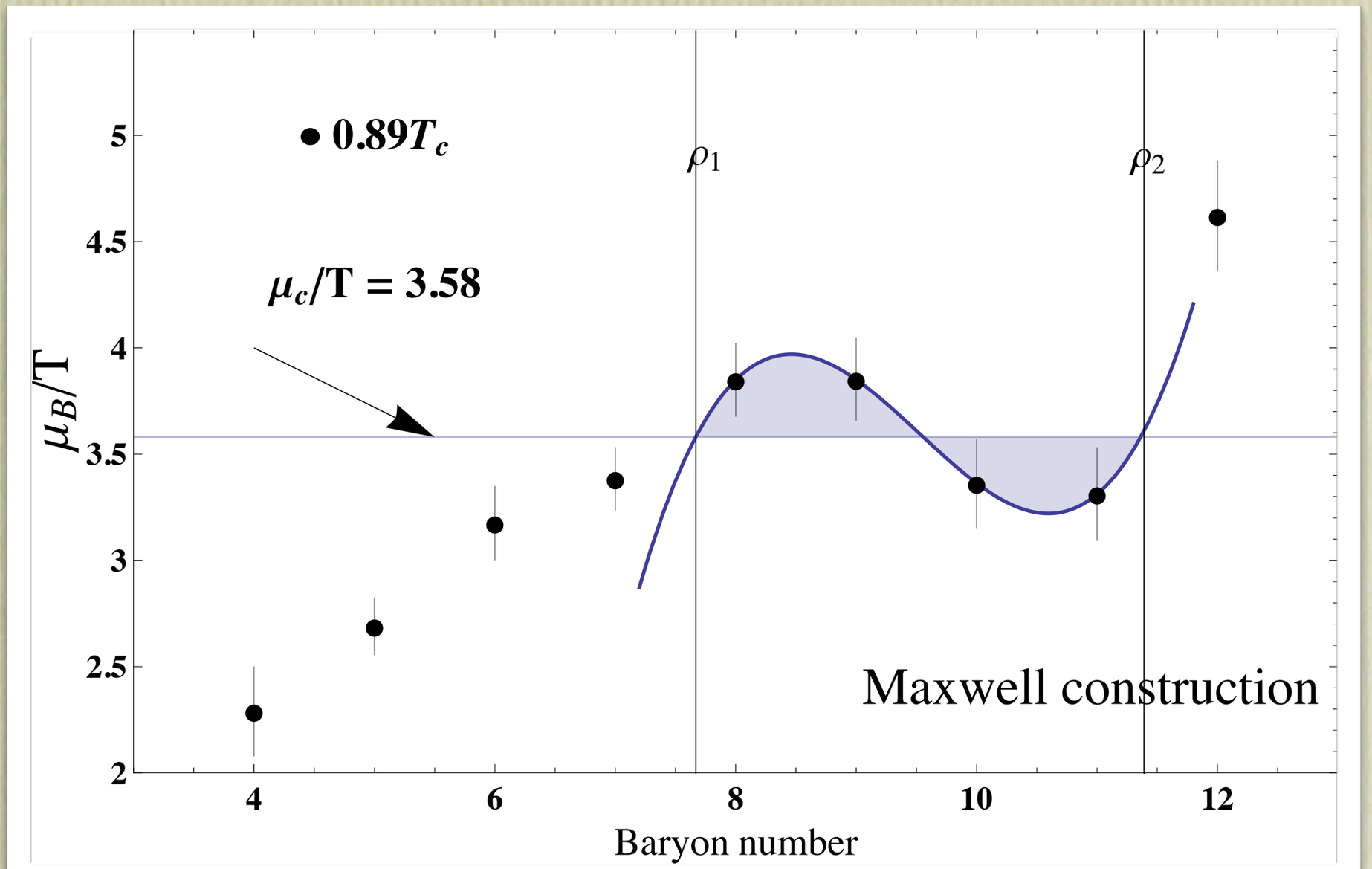
Baryon chemical potential

- In a finite volume the plateau turns into an “S-shape”
- The chemical potential is no longer increasing signaling an instability -- this is the signal for a first order transition
- Qualitatively, the signal follows the expectations:
  - it moves to larger chemical potential at smaller temperatures
  - it becomes more pronounced



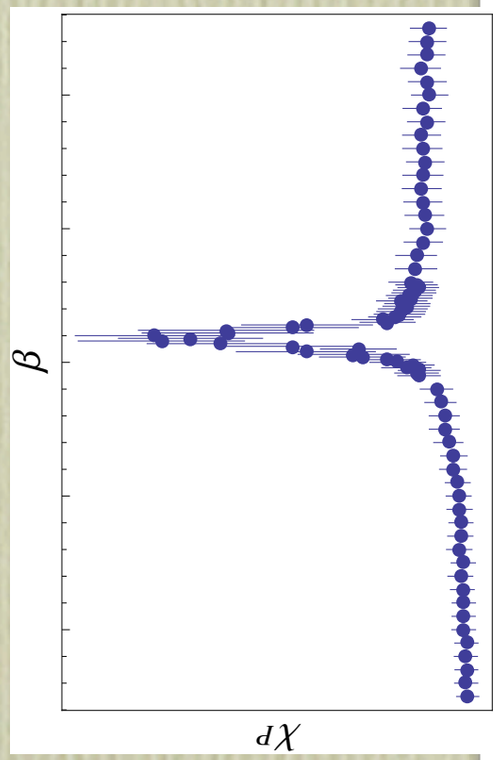
S. Takeda, Y. Kuramashi, and A. Ukawa, *Phys.Rev.* **D85** (2012) 096008, [arXiv:1111.6363].

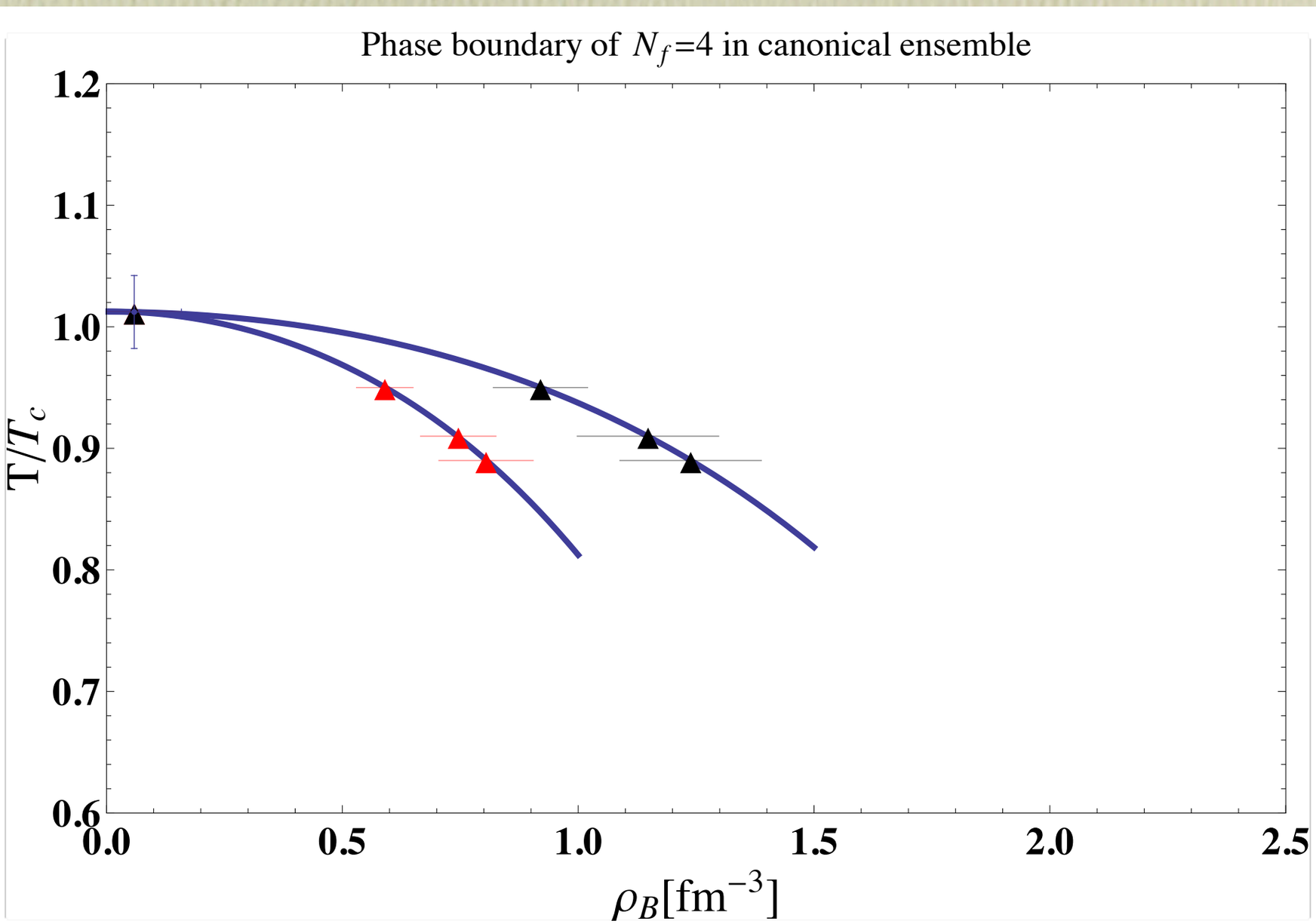
Maxwell construction



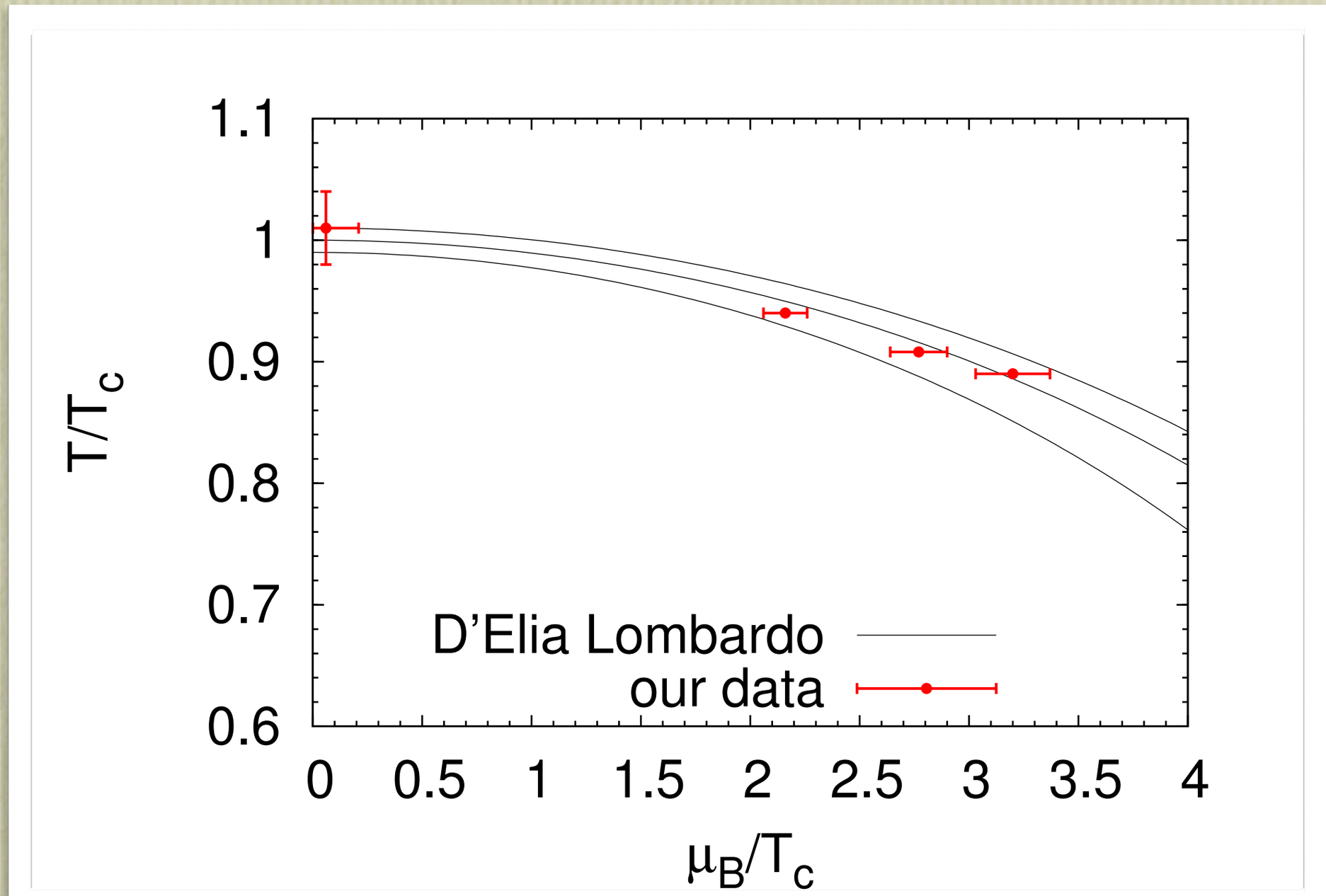
P. de Forcrand and S. Kratochvila, *Nucl.Phys.Proc.Suppl.* **153** (2006) 62–67,hep-lat/0602024.

Phase boundary





Critical chemical potential

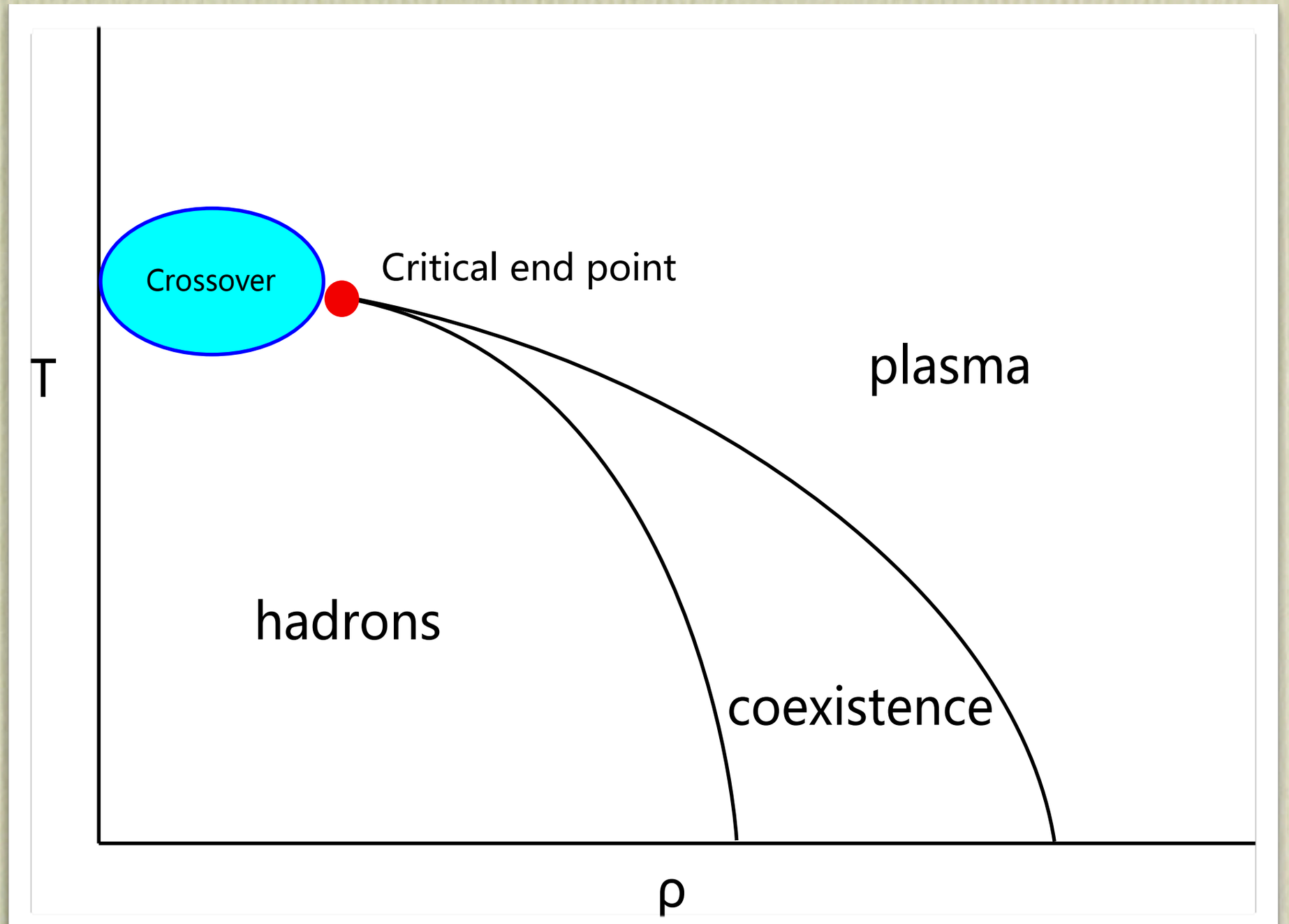


M. D'Elia and M.-P. Lombardo, *Phys. Rev.* **D67**, 014505 (2003), [arXiv:hep-lat/0209146]

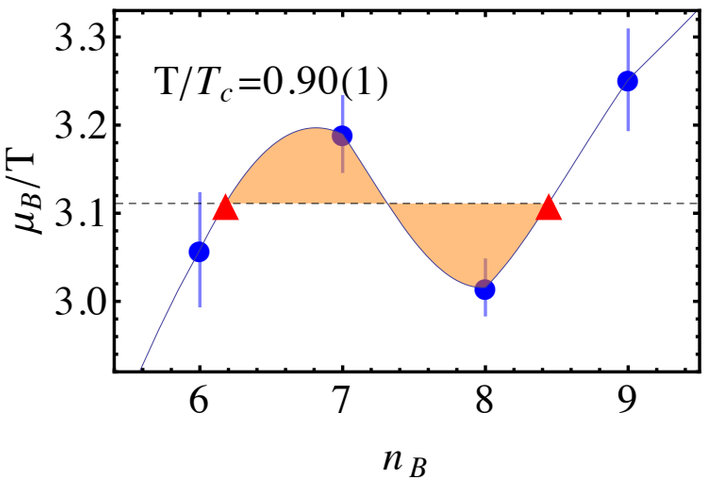
$N_f = 3$

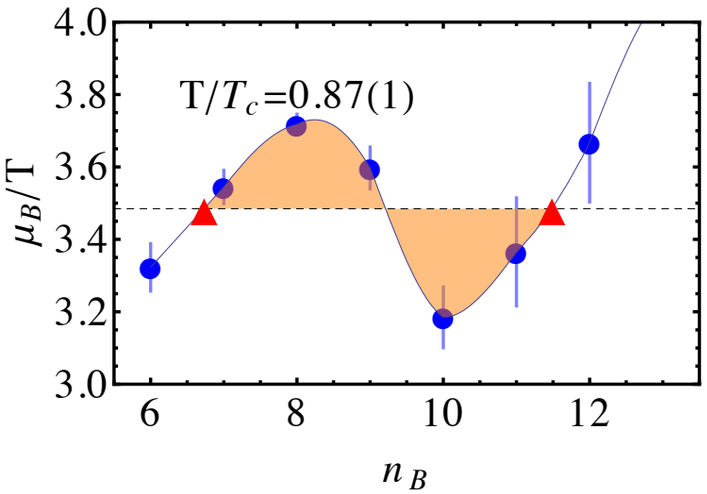
A. Li, AA, and K.-F. Liu, *Phys. Rev.* **D84** (2011) 071503 [arXiv:1103.3045].

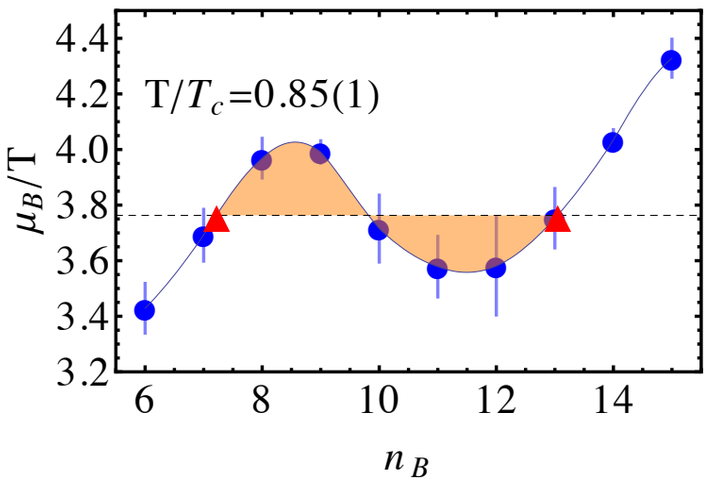
Schematic phase diagram



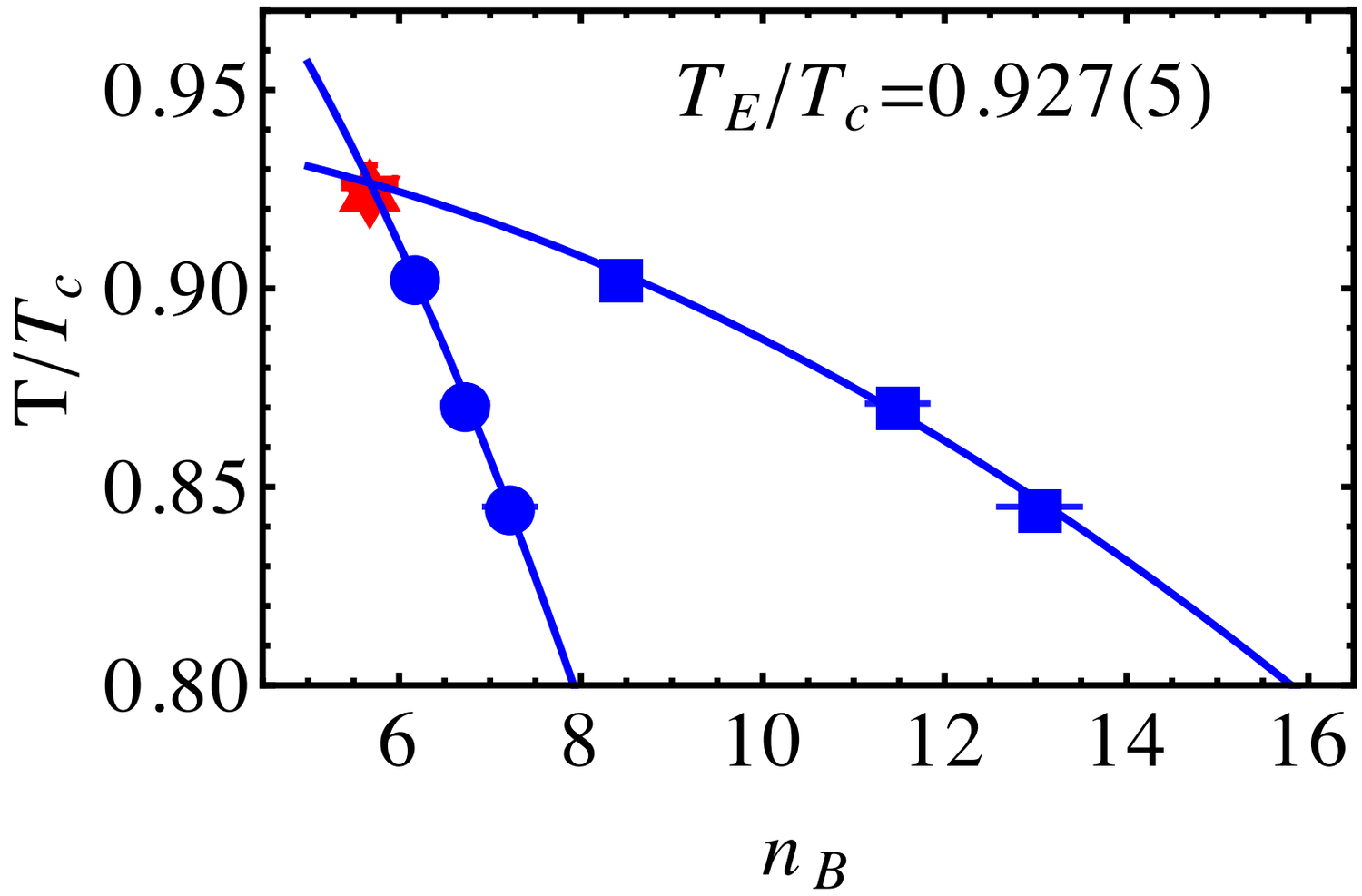
Baryon chemical potential



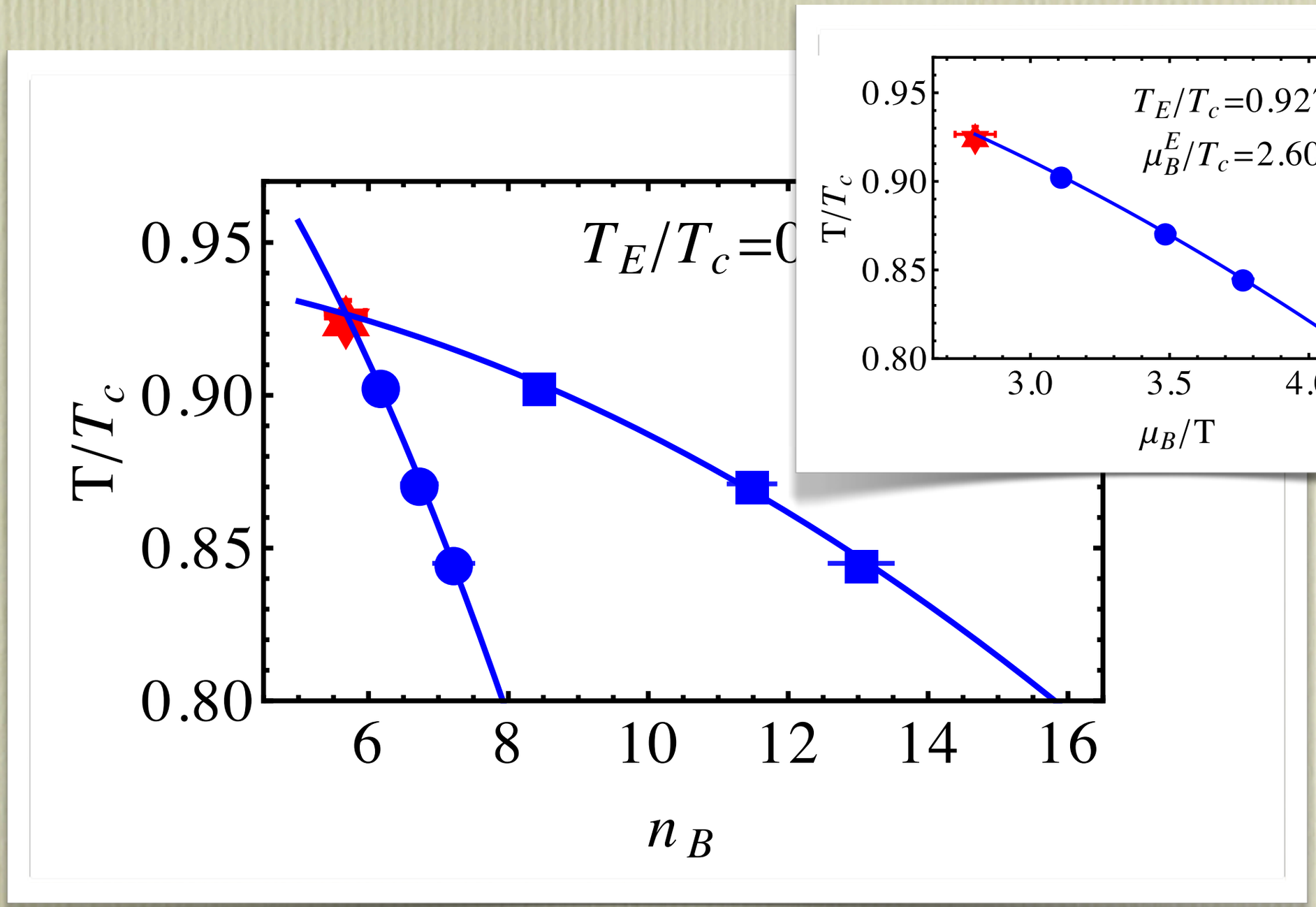




Phase boundary



Phase boundary



T_E/T_C=0.927(5) μ_B/T_C=2.60(8) for m_π=750MeV

Summary

- Using $N_f=4$ simulations we show that we can detect 1st order phase transitions by tracking the chemical potential as a function of baryon number

- In the $N_f=3$ case, at a pion mass of 750 MeV, we see a signal corresponding to a 1st order phase transition that disappears at $T=0.93\ T_C$ and $\mu_B/T_C=2.60$ – presumably the location of the critical point

- In $N_f=2$ simulations we don't see any clear signal for a transition for temperatures as low as $0.83\ T_C$ and densities as large as 6-7 nuclear matter density