Simulating Hot QCD with a Small Chemical Potential

hep-lat/0204010

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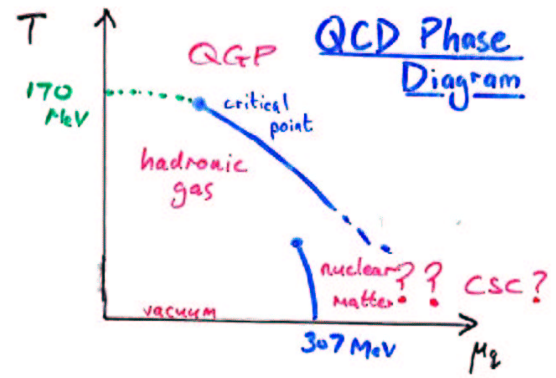
(Bielefeld - Swansea collaboration)

Cymro-German?

QCD Phase Diagram



Simulating QCD away from $\mu = 0$ is difficult because invariance under time reversal is broken

$t \leftrightarrow -t \Leftrightarrow ix_4 \leftrightarrow -ix_4$

$\Rightarrow$ Euclidean functional measure $e^{-S/\hbar}$ is complex

eg. for QCD with N_f flavors $\det^{N_f} M^*(\mu) = \det^{N_f} M(-\mu)$

"Sign Problem"

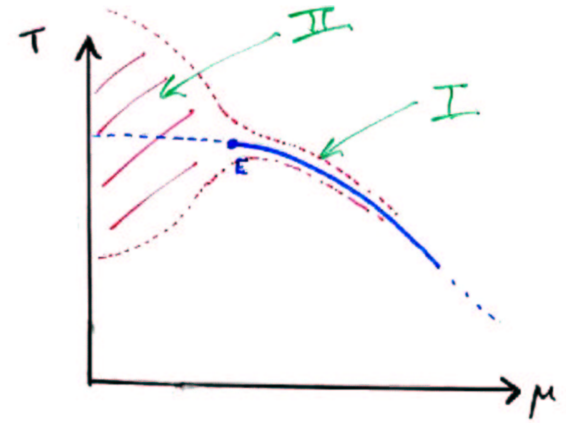
Formal solution via Reweighting:

$$\langle O \rangle = \frac{1}{Z(\beta, m, \mu)} \langle\langle O \rangle\rangle$$

$$= \frac{1}{Z} \int DU \left\{ O \left[\frac{\det M(\mu)}{\det M(0)} \right]^{N_f} e^{-\Delta S_g} \right\} \det^{N_f} M(0) \, e^{-S_g(\beta_0)}$$

Problem is that $Z = \langle\langle \mathbb{1} \rangle\rangle \sim e^{-V}$

$\Rightarrow$ Accumulating sufficient statistics is exponentially difficult in thermodynamic limit...



Two Routes Into the Plane

(I) Along crossover/coexistence line equilibrium configurations should not differ too greatly, and overlap between (μ, β) and $(\mu+\Delta\mu, \beta+\Delta\beta)$ remains useful

⇒ Multi-parameter reweighting is unusually effective up to eg. $8^3\times 4$ ⇒ $T_E = 160(4)$ MeV, $\mu_E = 242(12)$ MeV — Fodor & Katz

(II) Analytic continuation via eg. evaluation of $\frac{d}{d\mu}$, $\frac{d^2}{d\mu^2}$ at $\mu=0$ — Gottlieb et al., Gavai & Gupta, QCDTARO

or simulation with imaginary μ — Hart, Laine, Philipsen; deForcrand, Philipsen

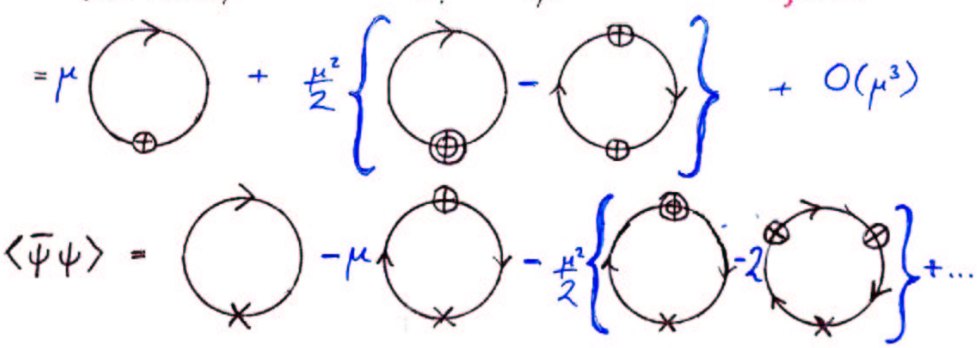
Should converge within a region bounded by endpoint

Our method is a hybrid of I and II:

we Taylor expand:

$$N_f \ln\left(\frac{\det M(\mu)}{\det M(0)}\right) = N_f \sum_{n=1}^{\infty} \frac{\mu^n}{n!} \frac{\partial^n \ln\det M(0)}{\partial\mu^n}$$

Reweighting factor



$\times = 1\!\!1$ $\quad \oplus = \frac{\partial M}{\partial\mu}$ $\quad \circledcirc = \frac{\partial^2 M}{\partial\mu^2}$

All terms can be estimated numerically using standard stochastic techniques

⇒ Not restricted to small volumes

⇒ Self-averaging might alleviate sign problem?

Note that even derivatives are real, odd derivatives pure imaginary

$$\mathrm{tr}\left(M^{-1}\frac{\partial^{n_1}M}{\partial\mu^{n_1}}M^{-1}\frac{\partial^{n_2}M}{\partial\mu^{n_2}}\ldots\right)^* = (-)^{n_1+n_2+\cdots}\,\mathrm{tr}\left(M^{-1}\frac{\partial^{n_1}M}{\partial\mu^{n_1}}M^{-1}\frac{\partial^{n_2}M}{\partial\mu^{n_2}}\ldots\right)$$

⇒ For a real observable eg. $\langle\bar\Psi\Psi\rangle$ (But NOT L...)

expect first non-vanishing correction at $O(\mu^2)$

In this study we calculate consistently to $O(\mu^2)$ with errors to real quantities $O(\mu^4)$

Hybrid Reweighting:

expansion of operator — expansion of reweighting factor

$$\langle O\rangle_{\beta,\mu} = \frac{\langle\langle (O_0 + O_1\mu + O_2\mu^2)\exp(R_1\mu + R_2\mu^2 - \Delta S_g)\rangle\rangle}{\langle \exp(R_1\mu + R_2\mu^2 - \Delta S_g)\rangle}$$

we implement this using 6–7 β values near $\beta_c(\mu=0)$

If $\langle O\rangle$ real then complex action effects enter through correlated fluctuations of O_1 and R_1

Consider an isovector chemical potential $\mu_I = \mu_u = -\mu_d$

⇒ $\det M_u \det M_d$ manifestly real

⇒ O_n and R_n vanish for all odd n

Can assess effect of complex phase by comparison of μ_q and μ_I

The simulation...

We use $N_f = 2$ flavors of p-4 improved staggered fermion coupled via fat links to Symanzik improved gluons...

Karsch, Laermann, Peikert

On a $16^3\times 4$ lattice: $\left(\Rightarrow \frac{1}{a} = 4T\right)$

in free field limit pressure $p_F \approx 0.6\, p_{SB}$

interaction measure $\frac{\varepsilon_F - 3p_F}{T^4} \approx 1.3$

Expect dramatic improvements at $N_\tau = 6$

A quark chemical potential is introduced by multiplying each temporal link by $e^{\pm\mu a}$

⇒ $\frac{\mu}{T}$ constant as β varies

We have studied quark masses $ma = 0.1, 0.2$

⇒ $\frac{m}{T}$ constant as β varies

At T_c these correspond to $m_q \approx 70\,\text{MeV}, 140\,\text{MeV}$

Simulations consumed $O(3)$ APEmille months ($O(10^{17})$ ops.) at UW Swansea

A Simple Test: Reweighting in Quark Mass m

In all cases pseudocritical point identified by location of susceptibility peak

Peak in Polyakov line susceptibility grows as m↗...

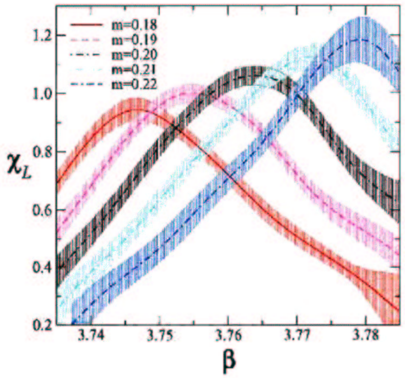


Figure 1: Quark mass dependence of χ_L as a function of β at $m_0 = 0.2$

... whereas peak in chiral susceptibility grows as m↘

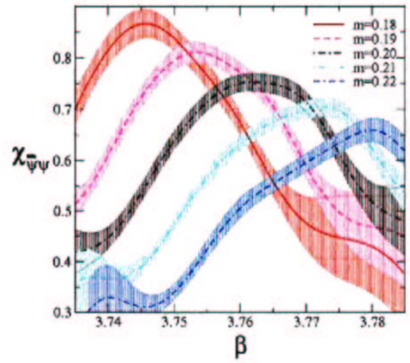


Figure 2: Quark mass dependence of $\chi_{\bar\psi\psi}$ as a function of β at $m_0 = 0.2$

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N.B. $\chi_O = \langle O^2\rangle - \langle O\rangle^2$

$$\left.\frac{\partial \chi}{\partial \beta}\right|_{\beta_c} = 0$$

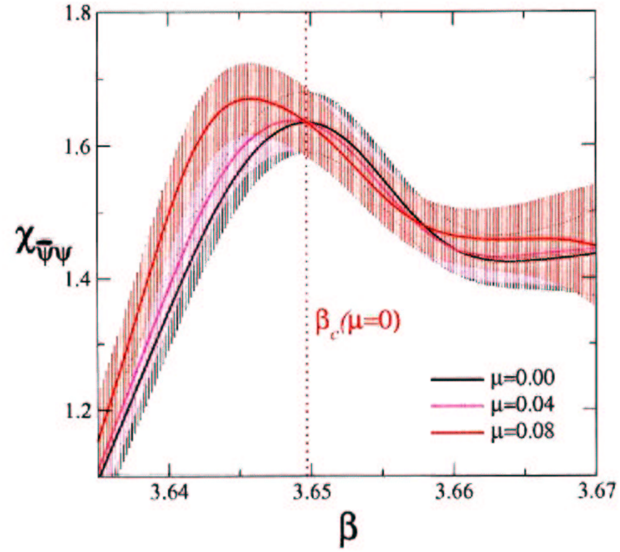

Figure 3: $\chi_{\bar\psi\psi}(\beta)$ for various μ at $m = 0.1$

Reweighting in μ

Position of susceptibility peak moves to smaller β as μ↗

$$\Rightarrow \quad T_c(\mu) < T_c(\mu=0)$$

in accordance with Clausius-Clapeyron equation

$$\left.\frac{\partial T_c}{\partial \mu}\right|_V = -\frac{\Delta N}{\Delta S} < 0$$

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The Polyakov line responds differently to positive and negative μ

Anti-quarks screen a $\mathbf{3}$ charge more effectively than quarks

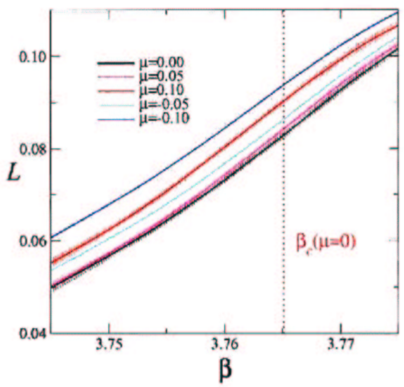
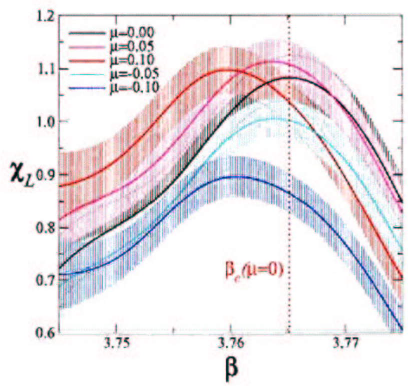


Figure 4: Polyakov line $L(\beta)$ for positive and negative μ at $m = 0.2$



The screening also weakens the susceptibility peak

Figure 5: Polyakov susceptibility $\chi_L(\beta)$ for positive and negative μ at $m = 0.2$

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But the peak shift $\Delta\beta(\mu)$ is $O(\mu^2)$ and hence the same for $\pm\mu$

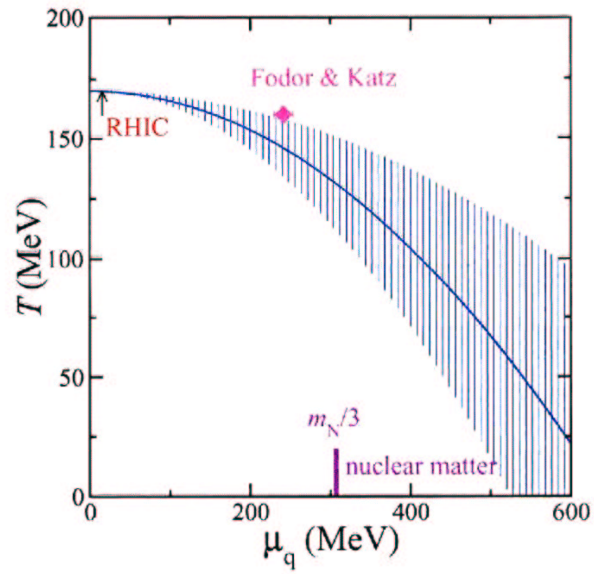

Figure 6: Estimated phase transition line extrapolated to $T = 0$

We find $\dfrac{d^2\beta_c}{d\mu^2} \approx -1.1$ with no significant variation with quark mass m

Estimates using $\chi_{\bar\psi\psi}$ and χ_L at $m=0.2$ are consistent

Convert to physical units using

$$\frac{d^2T_c}{d\mu_q^2} = \frac{-1}{N_\tau^2 T_c}\frac{d^2\beta_c}{d\mu^2} \Bigg/ \underbrace{\left(a\frac{d\beta}{da}\right)}_{\text{lattice } \beta\text{-fn.}}$$

$a\dfrac{d\beta}{da} = -2.08(43)$ Karsch, Laermann, Peikert $\Rightarrow$ $\boxed{T_c\left(\dfrac{d^2T_c}{d\mu_q^2}\right) = -0.14(6)}$ for $m=0.1$

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The discrepancy from $T_c(\mu=0)$ at RHIC is small

Comparison with Fodor & Katz

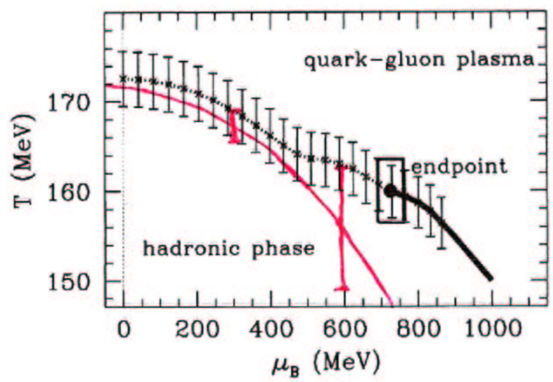

Figure 7: Phase transition line due to Fodor and Katz hep-lat/0106002

and with chemical freezeout in ion collisions

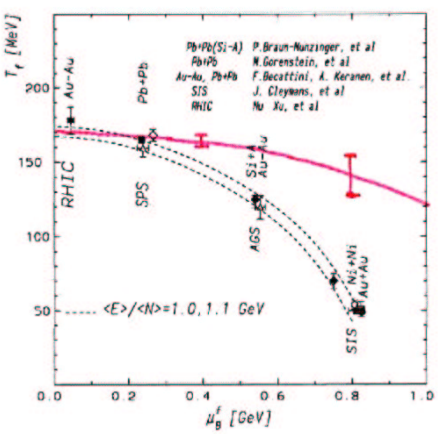

Figure 8: Chemical freezeout compilation due to Redlich **NPA698** (2002) 94

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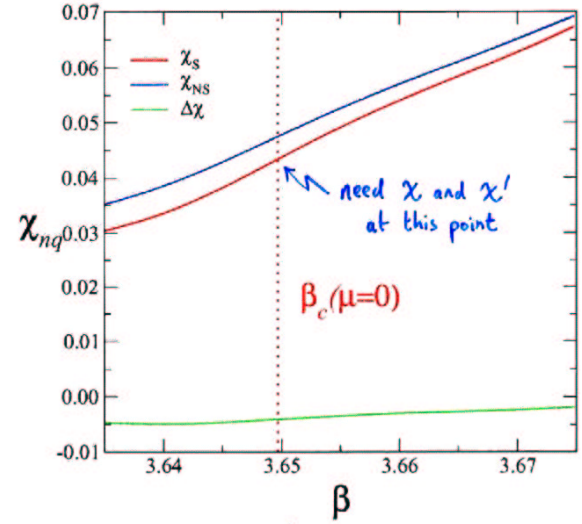


Figure 9: Quark number susceptibilities $\chi_S(\beta)$, $\chi_{NS}(\beta)$ at $m = 0.1$

Equation of State: Three Stages

Variation of Pressure

(i) $$\left.\frac{\partial p}{\partial \mu}\right|_T = \frac{T}{V}\frac{\partial \ln Z}{\partial \mu} = n_q$$ quark number density (vanishes at $\mu=0$)

$$\left.\frac{\partial^2 p}{\partial \mu^2}\right|_T = \frac{\partial n_q}{\partial \mu} = \chi_s$$ quark number susceptibility

$$\Rightarrow\Rightarrow \quad T_c^2 \frac{\partial^2 (P/T_c^4)}{\partial \mu_q^2} = \begin{matrix} 0.69 & (m=0.1) \\ 0.48 & (m=0.2) \end{matrix}$$

RHIC: $$P(\mu/T \approx 0.1) - p(\mu=0) \approx 0.01 p$$

$$\frac{n_q}{T^3}\left(\frac{\mu}{T} \approx 0.1\right) = \begin{matrix} 0.7 & (m=0.1) \\ 0.5 & (m=0.2) \end{matrix} \Rightarrow$$ 6-10% nuclear matter

Variation of Energy density: estimate from conformal anomaly

$$\frac{\varepsilon-3p}{T^4} = -\frac{1}{VT^3}\, a\frac{\partial \ln Z}{\partial a} \approx -\frac{1}{VT^3}\, a\frac{\partial\beta}{\partial a}\,\frac{\partial \ln Z}{\partial \beta}$$

$$\Rightarrow \frac{\partial^2(\varepsilon-3p)}{\partial\mu^2} \approx -a\frac{\partial\beta}{\partial a}\,\frac{\partial \chi_s}{\partial\beta}$$

$$\Rightarrow\Rightarrow T_c^2\frac{\partial^2(\varepsilon/T_c^4)}{\partial\mu_q^2} \approx 10$$

RHIC $\varepsilon(\mu/T\approx 0.1) - \varepsilon(\mu=0) \approx 0.01\,\varepsilon$

(ii) Line of constant pressure/energy density

$$\frac{dT}{d(\mu^2)} = \underbrace{-\frac{\partial(p/T^4)}{\partial(\mu^2)}}_{\text{we just calculated}} \Big/ \Big(\underbrace{\frac{\partial(p/T^4)}{\partial T} + \frac{4p}{T^5}}_{\text{available from } p(T) \text{ calculation using integral method}}\Big)$$

(iii) Combine with our estimate for $d^2T_c/d\mu^2$ to get variation of p, ε along phase transition line

Errors are large!

$$p(T_c(\mu),\mu) - p(T_c(0),0) = \mu^2T_c^2 \times 0.12(11)$$

$$\varepsilon(T_c(\mu),\mu) - \varepsilon(T_c(0),0) = \mu^2T_c^2 \times (0.7\pm 2.2)$$

No evidence for variation along the line ...

The Sign Problem

Write $\det M(\mu) = |\det M|\, e^{i\theta}$

$$\Rightarrow \theta = \mu\frac{N_f}{4}\,\mathrm{Im}\Big[\bigcirc\Big] + O(\mu^3)$$

$$= \mu\frac{N_f}{4}\, V\, \mathrm{Im}\Big[\frac{n_q}{T}\Big]$$

$\Rightarrow \langle\theta\rangle = 0$ because n_q is real

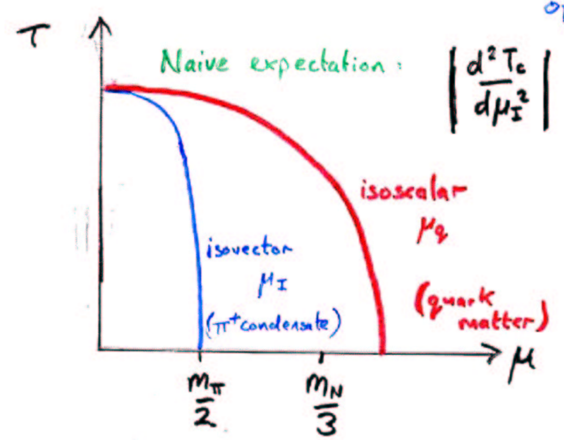
Phase fluctuations give an "average sign" $\langle\cos\theta\rangle$ which must remain $O(1)$ for simulation to be effective (figure)

Find $\langle\cos\theta\rangle \searrow$ as $m\searrow$ and/or $T\searrow$

N.B. should explore different # of noise vectors

Can also probe sign fluctuations via comparison of μ vs. μ_I

Naive expectation: $\left|\frac{d^2T_c}{d\mu_I^2}\right| \gg \left|\frac{d^2T_c}{d\mu_q^2}\right|$



Our data does not exhibit this, (figure) because $m_\pi \sim m_N$

$\Rightarrow$ Need to go closer to chiral limit

Average Sign

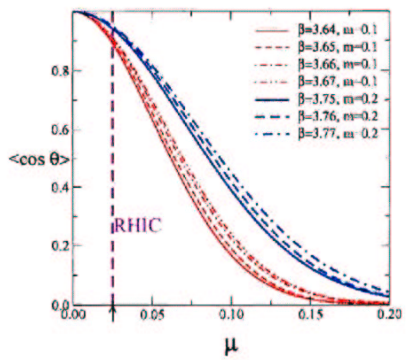
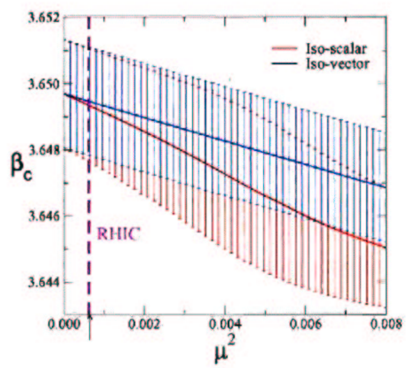


Figure 10: Average determinant phase as a function of μ for various β, m



Comparison of μ_L and μ_I response

Figure 11: Comparison of isovector and isoscalar critical curves

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The Sign Problem Revisited (2 Color QCD)

For $N = 1$ adjoint flavor

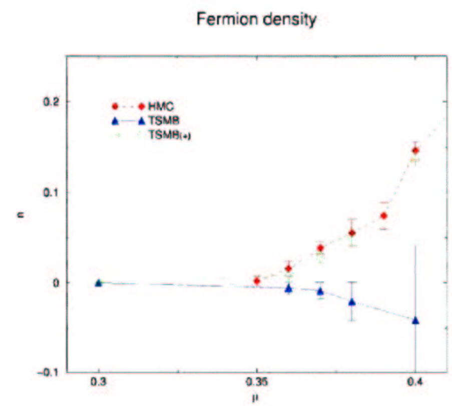
- χPT not expected to hold (no Goldstone baryons)
- simplest local diquark is superconducting

$$qq^i_{sc} = \frac{1}{2}\left[\chi^{tr} t^i \chi + \bar{\chi} t^i \bar{\chi}^{tr}\right] \in \mathbf{3} \text{ of SU(2)}$$

à la Georgi-Glashow

- det$M(\mu)$ is real but not positive definite – use Multi-Bosonic algorithm and reweighting

[SJH,Montvay,Scorzato,Skullerud]



n_B vs. μ for $\beta = 2.0$, $m = 0.1$ on $4^3 \times 8$.
Average sign $\langle \text{sgn(det)} \rangle = 0.30(4)$ at $\mu = 0.38$

World's most expensive simulation of the vacuum?

We have made progress:

LGT is now probing RHIC physics

Our value for $\frac{d^2 T_c(\mu)}{d\mu^2}$ is consistent with what's known,

and seems to be insensitive to quark mass m

BUT

some questions need further study

- What is the interplay between $\langle \cos\theta \rangle$ and radius of convergence of expansion?
- Does self-averaging help? Can we beat exact reweighting?
- What happens as $m \to 0$? Can we ever say anything about the critical point?