Conundrums at Finite Density

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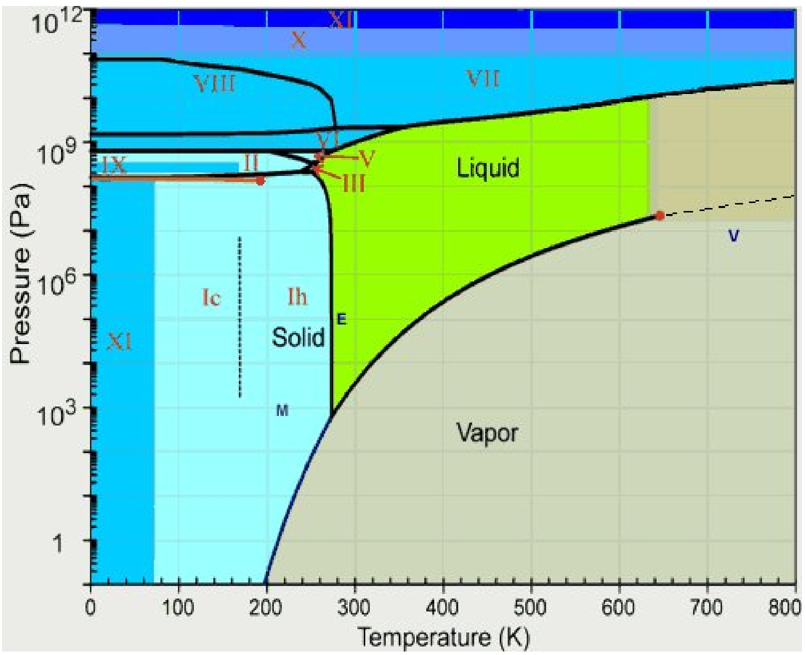
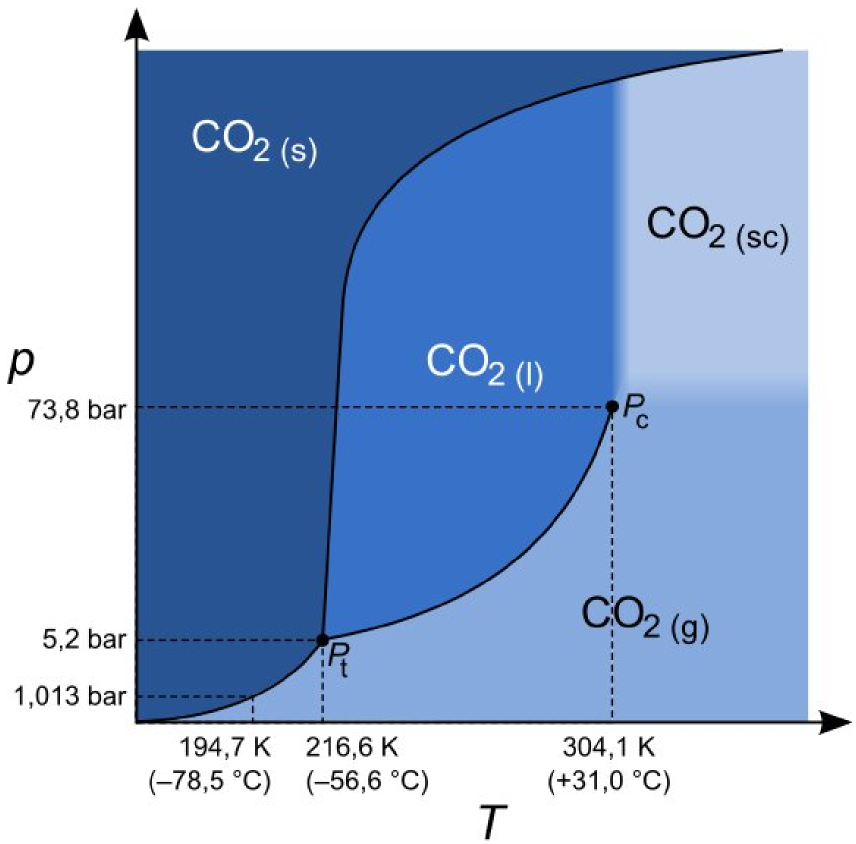
Critical Points : The meV Scale





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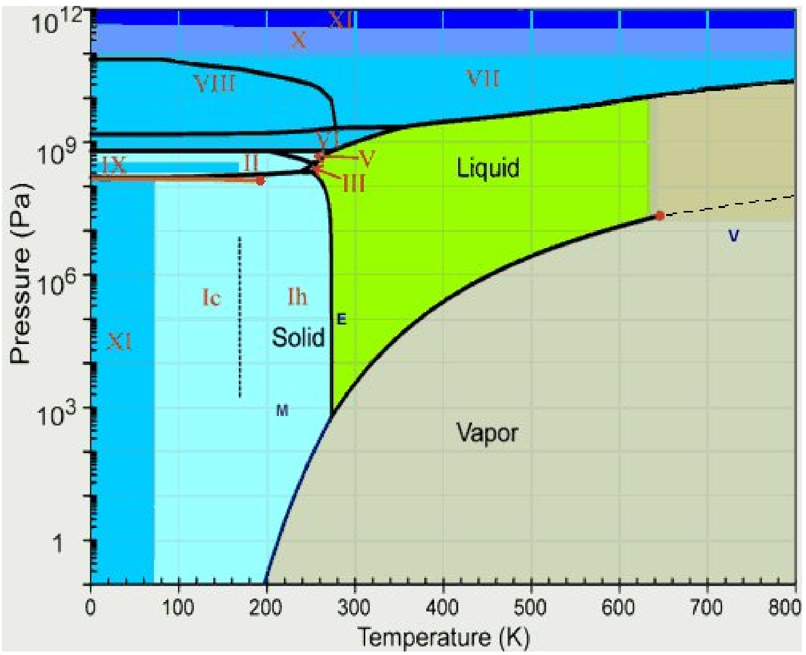

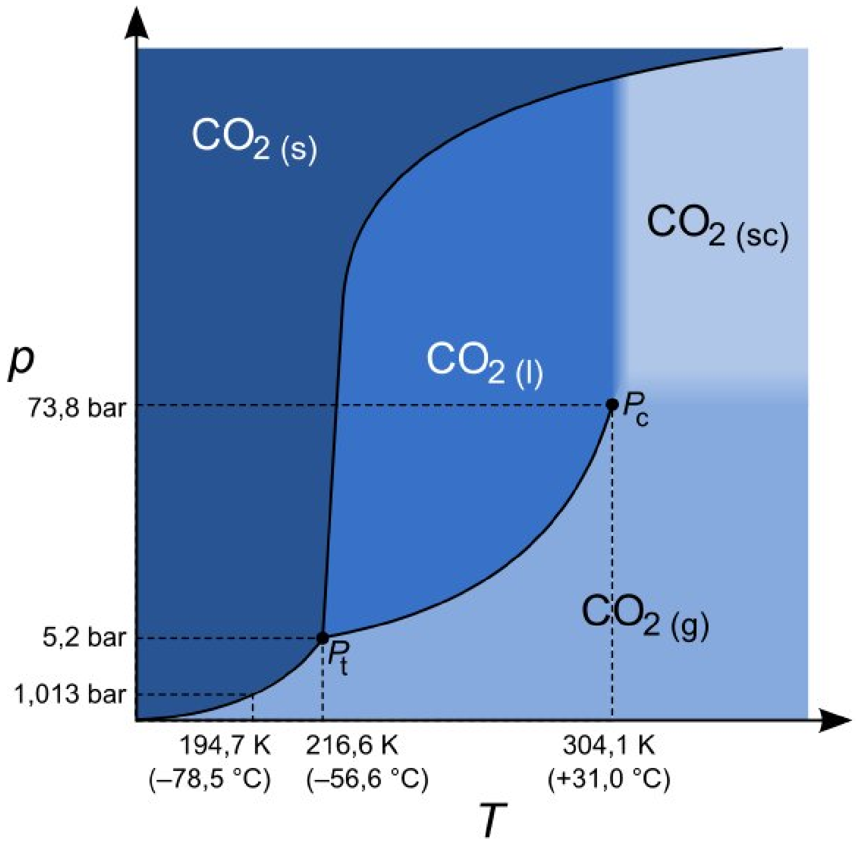

Using $\hbar = c = k = 1 \Longrightarrow 1.16 \times 10^4\ {}^\circ\mathrm{K} \equiv 1$ eV; $T^c_{CO_2}$=26 meV ↑

Picts from (http://www1.lsbu.ac.uk/ and Wikipedia)

Can Theory Predict the Phase Structure ?

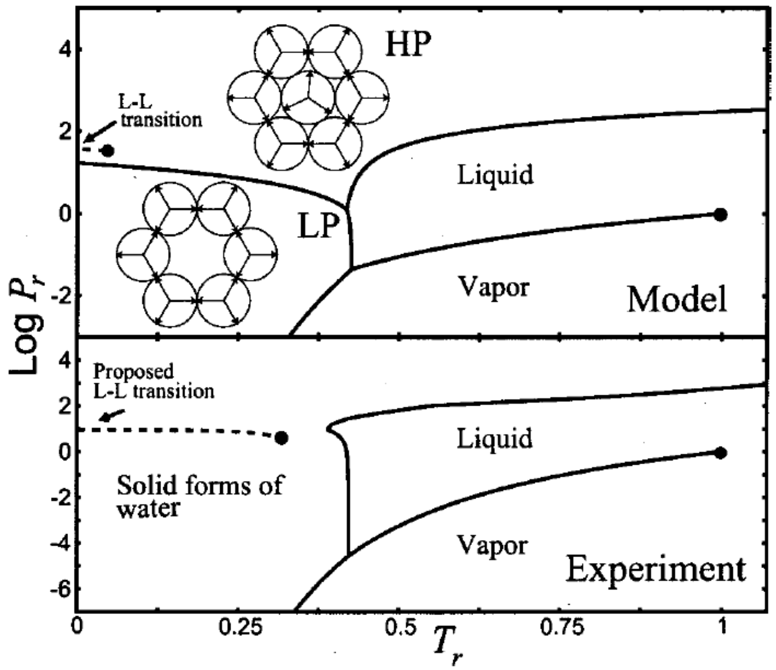

FIG. 4. Phase diagram of the model (top) compared to experiments (bottom) in pressure P_r vs temperature T_r. Unbroken curves are phase boundaries for the transitions discussed in the text. Dashed curves locate the metastable liquid–liquid (L–L) transition in the theory and a schematic of its proposed location in water (see Ref. 8). LP ice consists of open cages in which each molecule bonds to three neighbors. HP ice is identical to LP ice, except that it has an additional molecule in the center of each cage. For clarity, the solid–solid transitions in the experimental phase diagram of water are omitted. Parameters are given in Fig. 2.

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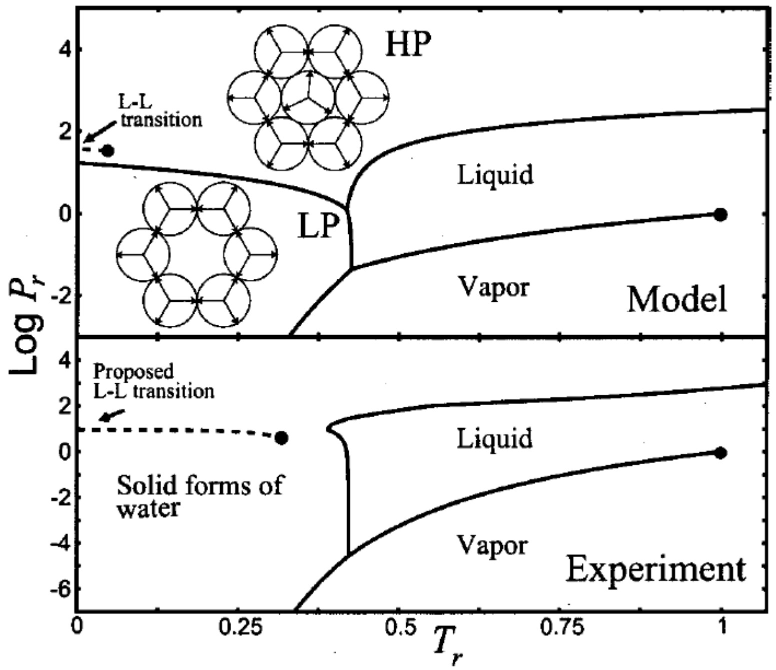

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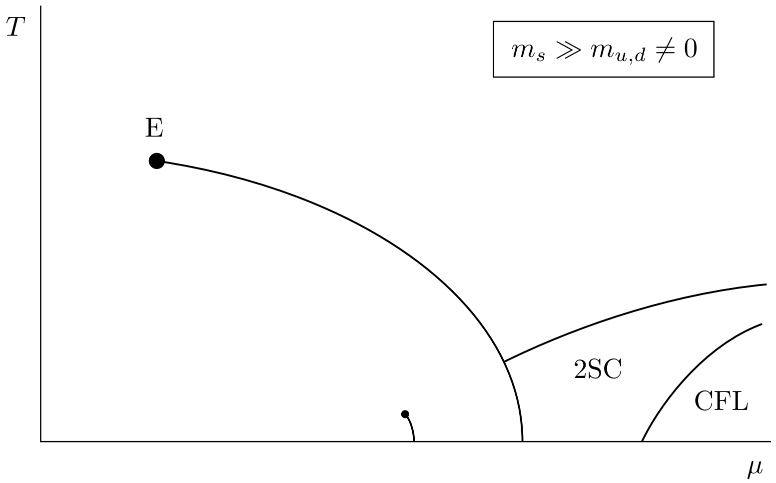
- *Ab initio:* Uses only laws of Statistical Mechanics and Quantum Mechanics. No empirical potentials used : Density functional methods.

- Nontrivial to extend to molecular interactions [Finney, J Mol Liqu 90(2001)303].

QCD Phase diagram

♠ A fundamental aspect – Critical Point in T-μ_B plane; Based on symmetries and models, expected QCD Phase Diagram



From Rajagopal-Wilczek Review, hep-ph/0011333

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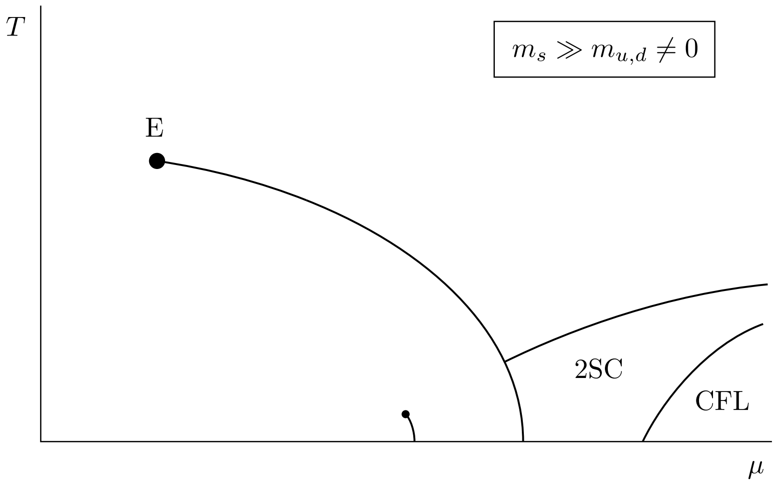

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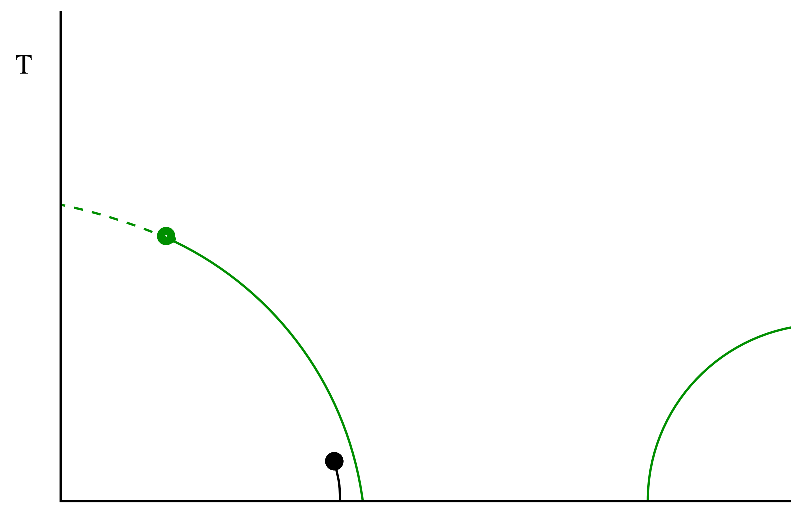

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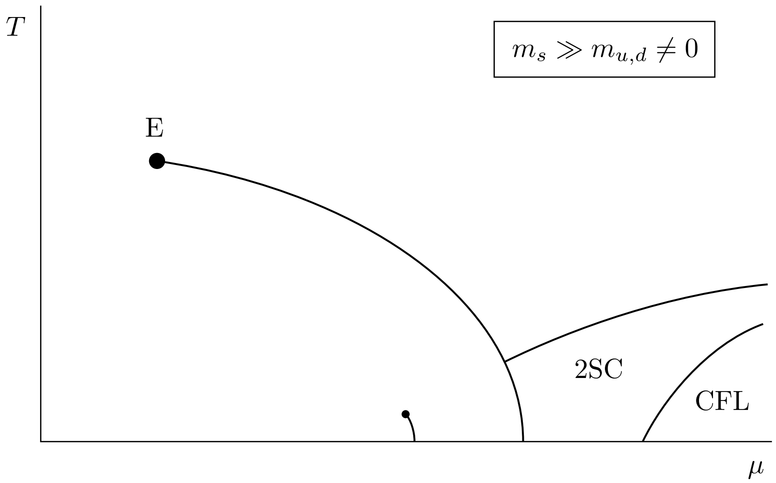

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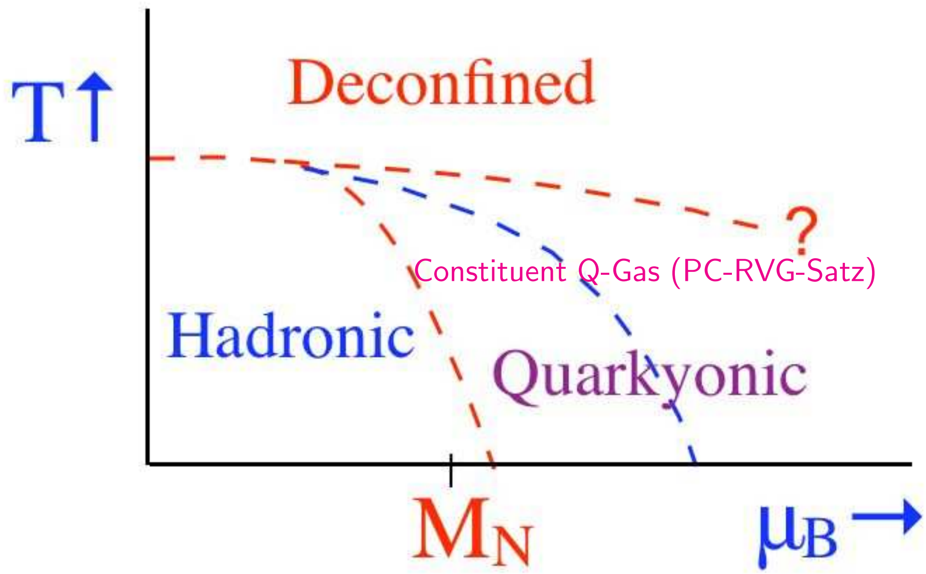

Putting QCD to Work

- QCD Partition Function : $Z_{QCD} = \mathrm{Tr}\ \exp[-(H_{QCD} - \mu_B N_B)/T]$.
- A first-principles calculation of $\epsilon(\mu, T)$ or $P(\mu, T)$ to look for phase transitions, Critical Point and many phases using the underlying theory QCD alone: NO free parameters and NO arbitrary assumptions.

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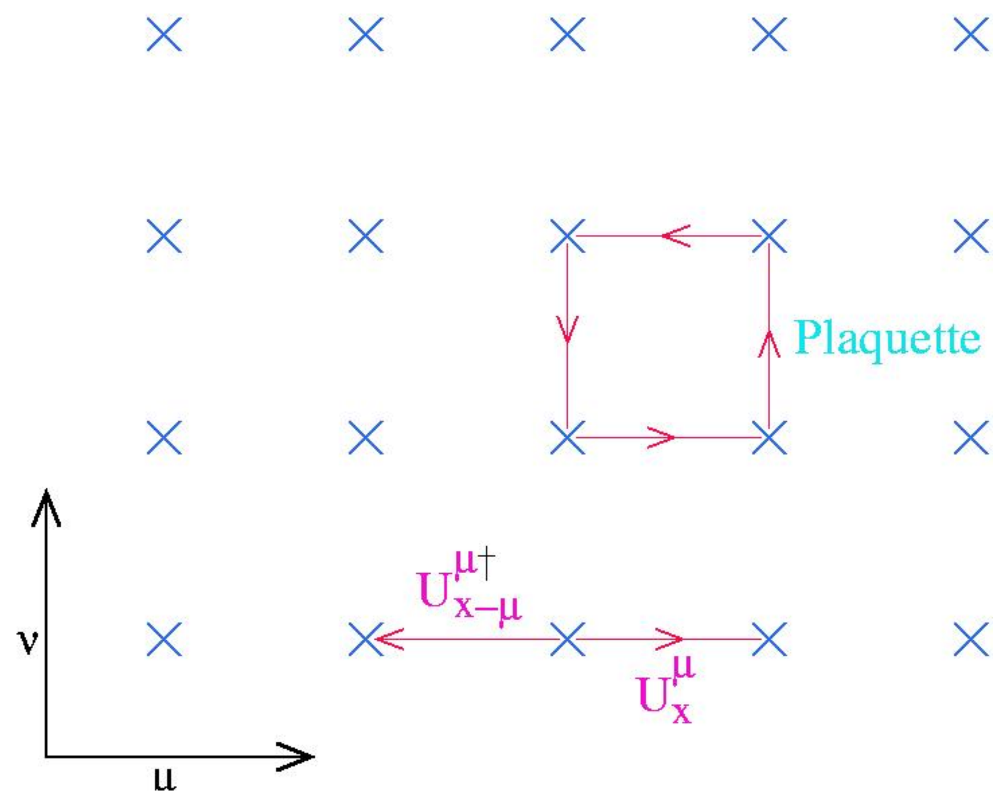
- Simpson integration trick : $\int\ dx\ F(x) = \lim_{\Delta x \to 0} \sum_i\ \Delta x\ F(x_i)$.
- Its analogue to perform functional integrations needs discretizing the space-time on which the fields are defined : Lattice Field Theory !

Basic Lattice QCD

- Discrete space-time : Lattice spacing a UV Cut-off.
- Quark fields $\psi(x)$, $\bar{\psi}(x)$ on lattice sites.
- Gluon Fields on links : $U_\mu(x)$



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- Quark fields $\psi(x)$, $\bar{\psi}(x)$ on lattice sites.
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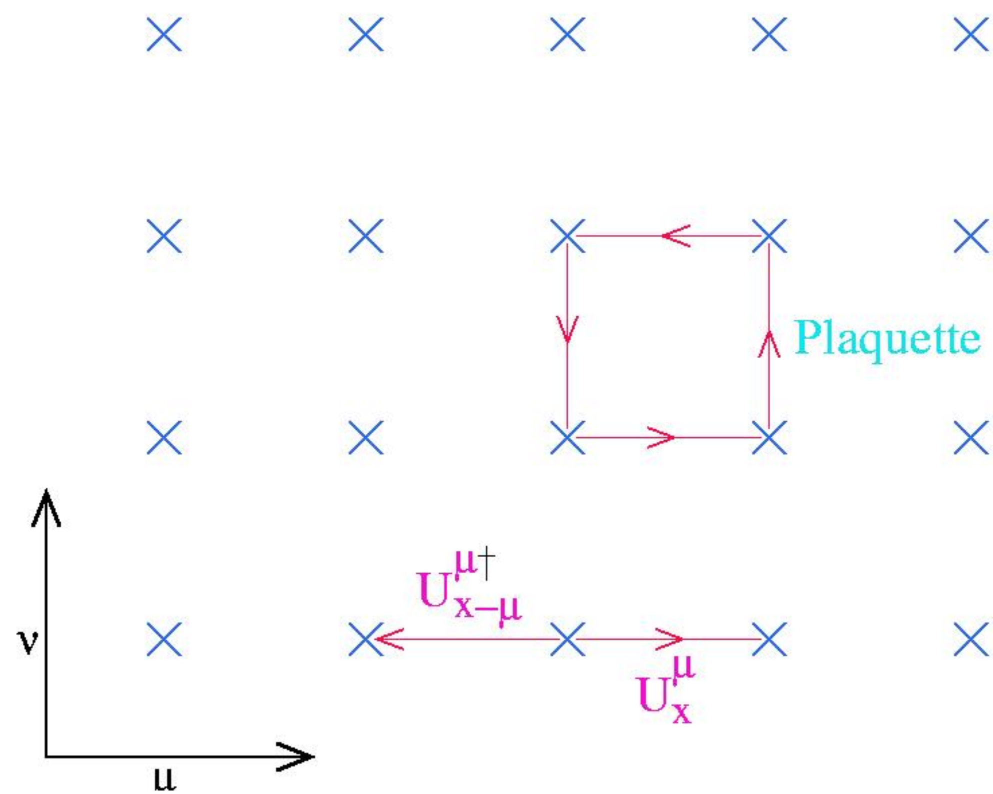
- Gauge invariance : Actions from Closed Wilson loops, e.g., plaquette.
- Fermion Actions : Staggered, Wilson, Overlap, Domain Wall..



The $\mu \neq 0$ problems : I. Divergences

♠ Well-known that no new divergences arise in field theories with nonzero temperature and/or density.

♢ So what are these divergences ? Are they lattice artifacts ? Are there any striking conceptual issues worth discussing ?

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♢ So what are these divergences ? Are they lattice artifacts ? Are there any striking conceptual issues worth discussing ?

♡ Recall that the naıvely discretized fermionic action is

$$S^F = \sum_{x,x'} \bar{\psi}(x) \left[\sum_{\mu=1}^{4} D^\mu(x,x') + ma\delta_{x,x'} \right] \psi(x'),$$

where

$$D^\mu(x,x') = \frac{1}{2}\gamma^\mu \left[U_x^\mu \delta_{x,x'-\hat{\mu}} - U_{x'}^{\mu\dagger} \delta_{x,x'+\hat{\mu}} \right].$$

♣ Easy to follow the canonical method to write a current conservation equation: $\sum_\mu \Delta_\mu J_\mu^{lat} = 0$, and obtain the conserved charge.

$\diamondsuit$ Conserved charge is the natural point-split for $N = \sum_x \bar{\psi}(x)\gamma^4[U_x^{4\dagger}\psi(x+\hat{4}) + U_x^4\psi(x-\hat{4})]/2$. Adding the chemical potential to the action above therefore amounts to weights $f(a\mu) = 1 + a\mu$ & $g(a\mu) = 1 - a\mu$ to forward and backward time links respectively.

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$\clubsuit$ This leads to μ-dependent a^{-2} divergences in energy density and quark number density even in the free theory!

$$\begin{aligned} \epsilon &= c_0 a^{-4} + c_1 \mu^2 a^{-2} + c_3 \mu^4 + c_4 \mu^2 T^2 + c_5 T^4 \\ n &= d_0 a^{-3} + d_1 \mu a^{-2} + d_3 \mu^3 + d_4 \mu T^2 + d_5 T^3. \end{aligned} \quad (1)$$

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♠ Subtracting off vacuum contribution at $T = 0 = \mu$, eliminates the leading divergence in each case but the μ-dependent divergence persists.

♡ Hasenfratz-Karsch (PLB 1983) & Kogut et al. (PRD 1983) proposed to modify the weights to $\exp(\pm a\mu)$ to obtain finite results while simultaneously Bilić-Gavai (EPJC 1984) showed $(1 \pm a\mu)/\sqrt{(}1 - a^2\mu^2)$ also lead to finite results.

$\diamondsuit$ Indeed, in general *any* set of functions f, g, satisfying $f(a\mu) \cdot g(a\mu) = 1$ with $f(0) = f'(0) = 1$ suffice (Gavai, PRD 1985).

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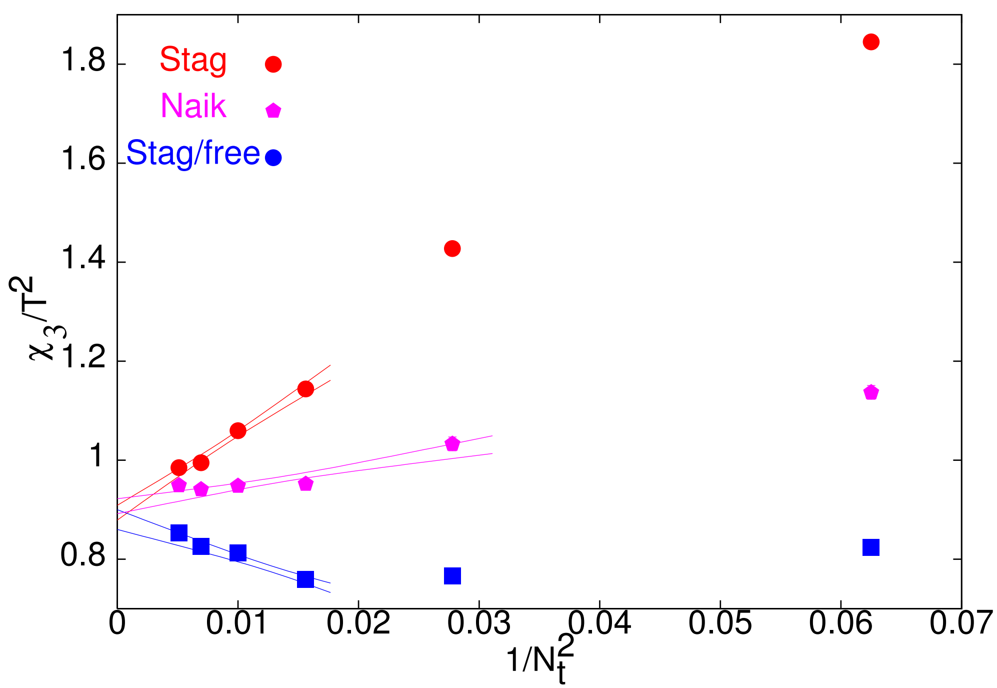
♡ Note that the analytical proof was *only* for free quarks & thus pert. theory. Numerical computations had to be performed to show that it worked for the non-perturbative interacting case as well (Gavai-Gupta PRD 67, 034501 (2003)) :



♢ Question : Why, and how, does lattice introduce this divergence? or Does it really ?

♣ It was argued [Hasenfratz-Karsch (PLB 1983)] that the divergence arises on the lattice due to the lack of a "formal" gauge symmetry: In continuum theory, μ term appears as a 4^{th} component of a constant gauge field. All the forms above restore this formal symmetry on lattice.

$$f(a\mu) \cdot g(a\mu) = 1 \Leftrightarrow F(a\mu) = \exp(\ln f(a\mu)). \tag{2}$$

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♣ Problem : With *any* of these functions above, one has **no** conserved charge anymore ! Alternatively $Z \neq \exp(-\beta[H - \mu N])$ on the lattice for them. Possible only in the continuum limit of $a \to 0$.

♣ One cannot define an *exact* canonical partition function on lattice from the Z defined this way.

Divergences exist in Continuum too

- It turns out that contrary to common belief, divergences are **NOT** a lattice artifact. The "formal gauge" symmetry has nothing to do with them.

- Indeed lattice regulator simply makes it easy to spot them. Using a momentum cut-off Λ in the continuum theory, one can show the presence of $\mu\Lambda^2$ terms in number density easily (Gavai-Sharma, 1406.0474).

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- The quark number density, or equivalently (1/3) the baryon number density, is defined as,

$$n = \frac{T}{V}\frac{\partial \ln \mathcal{Z}}{\partial \mu}\Big|_{T=\mathrm{fixed}} \tag{3}$$

with $\mathcal{Z}$ for free fermions given by

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \mathrm{e}^{\int_0^{1/\mathrm{T}} \mathrm{d}\tau \int \mathrm{d}^3\mathrm{x}\left[-\bar{\psi}(\gamma_\mu\partial_\mu + \mathrm{m} - \mu\gamma_4)\psi\right]}, \tag{4}$$

- Evaluating n in the momentum space, the expression for the number density is

$$n = \frac{2iT}{V} \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{(\omega_n - i\mu)}{p^2 + (\omega_n - i\mu)^2} \equiv \frac{2iT}{V} \int \frac{d^3p}{(2\pi)^3} \sum_{\omega_n} F(\omega_n, \mu, \vec{p}), \quad (5)$$

where $p^2 = p_1^2 + p_2^2 + p_3^2$ and $\omega_n = (2n+1)\pi T$. The gamma matrices are all Hermitian.

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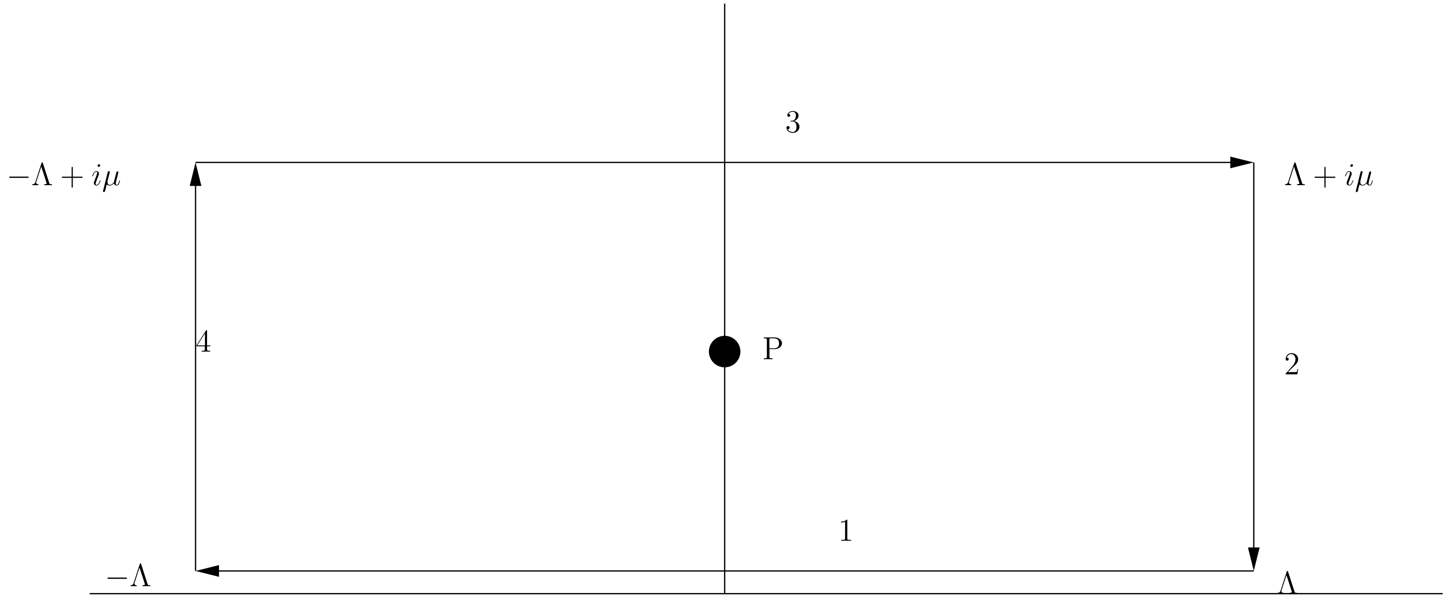
- In the usual contour method, the sum over n gets replaced as sum of integrals in the complex ω-plane:

$$n = \frac{2i}{\pi} \left[\oint_{Im\omega<0} \frac{F(\omega,\mu)d\omega}{\mathrm{e}^{\mathrm{i}\omega/\mathrm{T}} + 1} - \oint_{Im\omega>0} \frac{F(\omega,\mu)d\omega}{\mathrm{e}^{-\mathrm{i}\omega/\mathrm{T}} + 1} + \int_{-\infty}^{\infty} F(\omega,\mu)d\omega \right] . \quad (6)$$

- Introduce a cut-off Λ for all 4-momenta at $T = 0$ for a careful evaluation of the last term. Together with the subtracted (μ=0) contribution, one can rewrite in the complex ω-plane:



- The $\mu\Lambda^2$ terms arise from the arms 2 & 4 in figure above. (Gavai-Sharma, arXiv 1406.0474) :

$$\begin{aligned}\text{Sum of } 2+4 &= \int \frac{d^3p}{(2\pi)^3}\left(\int_2 + \int_4\right)\frac{d\omega}{\pi}\frac{\omega}{p^2+\omega^2} \\ &= -\frac{1}{2\pi}\int \frac{d^3p}{2\pi^3}\ln\left[\frac{p^2+(\Lambda+i\mu)^2}{p^2+(\Lambda-i\mu)^2}\right].\end{aligned}$$

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- One usually *assumes* this sum to cancel for $\mu \neq 0$ by setting Λ infinite. However, since $\Lambda \gg \mu$, expanding in μ/Λ, one finds the leading Λ^3 terms indeed cancel but there is a nonzero coefficient for the $\mu\Lambda^2$ term.

- Ignoring the contribution from the arms 2 & 4 amounts to a subtraction of the 'free theory divergence' in continuum !

- Why did this remain unnoticed, even in text books ?

- Often one uses T as the cut-off in analytic computations and does frequency sums on $\omega_n = (2\pi n + 1)T$ *first* [Kapusta-Gale Book].

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- The leading divergence term from the arms 2 & 4 do cancel. One needs to regulate the momentum integrals first to spot the sub-leading ones.
- Since these divergences exist in the continuum, and are simply subtracted for the free theory, one may follow the prescription of subtracting the free theory divergence by hand on Lattice as well.

Testing the idea

- In order to test whether the divergence is truly absent in simulations as well, one needs to take the continuum limit $a \to 0$ or equivalently $N_t \to \infty$ at fixed $T^{-1} = aN_t$.

- This was tested for quenched QCD. (Gavai-Sharma, 1406.0474). For $m/T_c = 0.1$, $N_t = 4$, 6, 8, 10 and 12 lattices were employed. On 50-100 independent configurations different susceptibilities were computed at $T/T_c = 1.25$, & 2.

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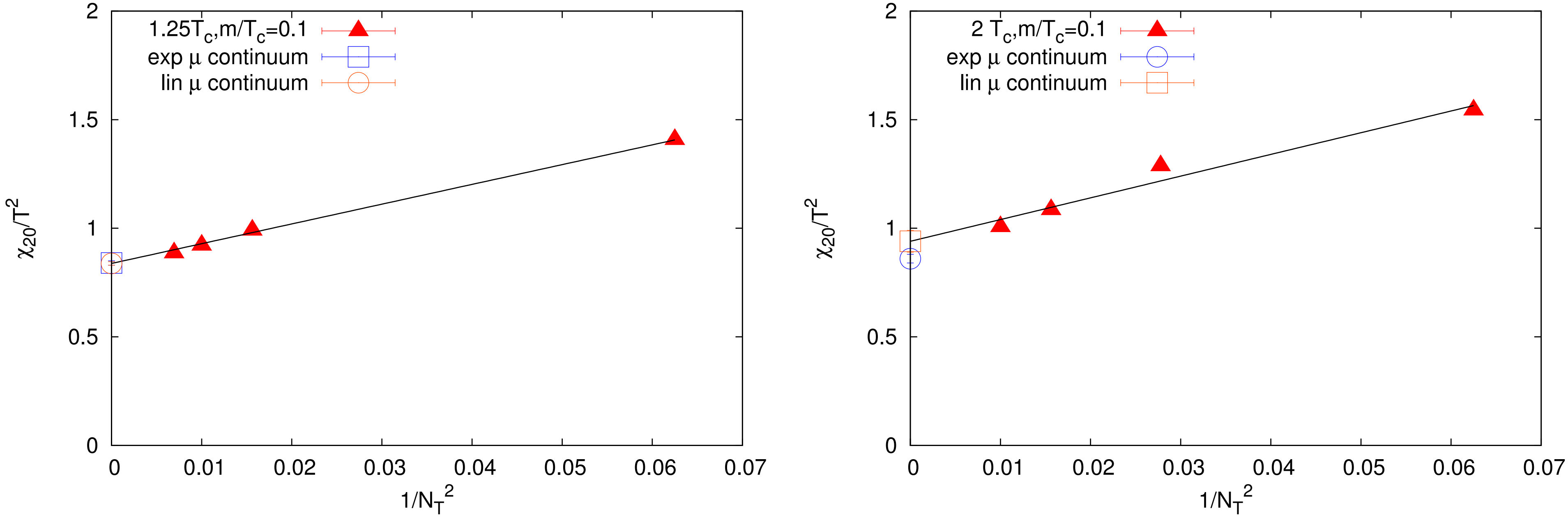
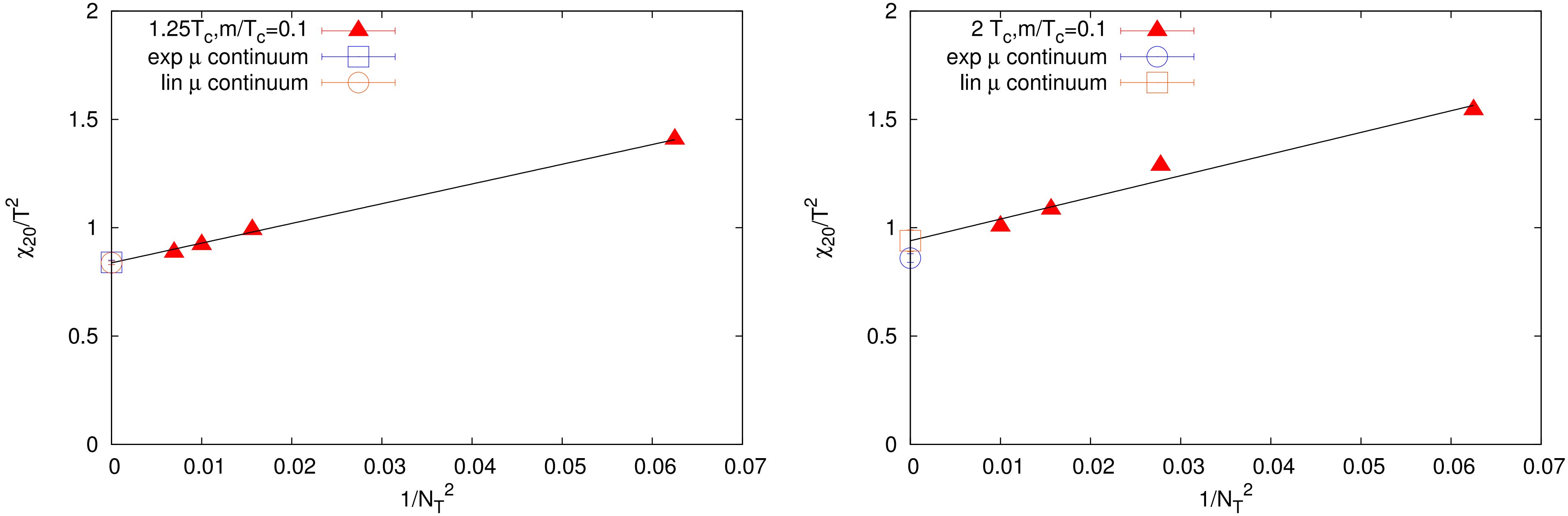
- $1/a^2$-term for free fermions on the corresponding $N^3 \times \infty$ lattice was subtracted from the computed values of the susceptibility.
- Expect χ_{20}/T^2 to behave as $\chi_{20}/T^2 = c_1(T) + c_2(T)N_T^2 + c_3(T)N_T^{-2} + \mathcal{O}(N_T^{-4})$.



- Absence of any quadratically divergent term is evident in the positive slope of the data. Logarithmic divergence cannot be ruled out with our limited N_t data.



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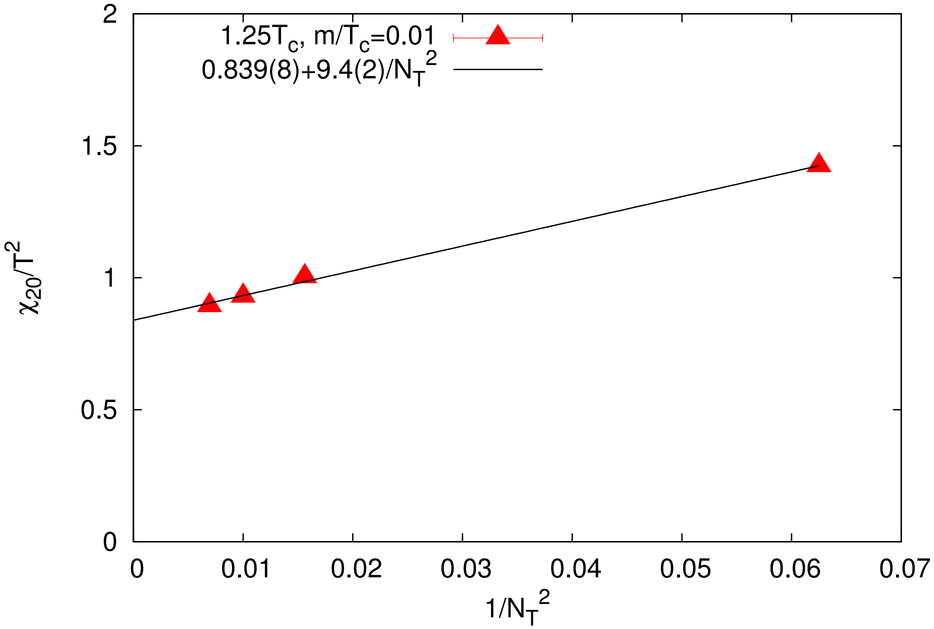
- Furthermore, the extrapolated continuum result coincides with the earlier result obtained with the $\exp(\pm a\mu)$ action (Swagato Mukherjee PRD 2006).

- Lowering the mass by a factor of 10 to $m/T_c = 0.01$ the exercise was repeated at a lower temperature on $T/T_c = 1.25$.



- Again no divergent term is evidently present in the slope of the data.

- Higher order susceptibility show similar finite result in continuum limit.

The $\mu \neq 0$ problem : II. Quark Type

- Mostly staggered quarks used in these simulations. Broken flavour and spin symmetry on lattice. Moreover, NO flavour singlet $U_A(1)$ symmetry or anomaly. Critical point needs $N_f = 2$ and anomaly to persist by T_c.

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- Introduction of μ a la "Formal" gauge symmetry by Bloch & Wettig (PRL 2006 & PRD2007).
- Unfortunately BW-prescription breaks chiral symmetry ! (Banerjee, Gavai & Sharma PRD 2008; PoS (Lattice 2008); PRD 2009) Furthermore, anomaly for it depends on μ unlike in continuum QCD (Gavai & Sharma PRD 2010).
- Good News : Action with Continuum-like (flavour & spin) symmetries for quarks at nonzero μ and T proposed. (Gavai & Sharma , arXiv : 1111.5944).

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- It was shown why this is physically the right thing to do. Using Domain Wall formalism, one discovers that such an action counts only the physical (wall) modes.
- Bad News (or is it?): Chirally invariant Overlap action with nonzero μ only in the linear form, i.e., with the divergence. Interestingly, even the exponential form leads to divergences in this case [Narayanan-Sharma JHEP 1110(2011)151].

The $\mu \neq 0$ problem : III. Complex Measure

Physical(thermal expectation) value of an observable $\mathcal{O}$ is

$$\langle \mathcal{O} \rangle = \int DU \, \left[\frac{\exp(-S_G) \ \mathrm{Det}^{N_f} \ M(m,\mu)}{\mathcal{Z}} \right] \mathcal{O},$$

where the QCD partition function $\mathcal{Z}$ is

$$\mathcal{Z} = \int DU \exp(-S_G) \ \mathrm{Det}^{N_f} \ M(m,\mu), \quad \text{with } \mathcal{Z} \ \text{ real } \& > 0,$$

and N_f is the number of quark flavours/types.

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Typically 8-9 million dimensional integral and M is million $\times$ million. Probabilistic methods are therefore used to evaluate $\langle \mathcal{O} \rangle$.

$\Longrightarrow$ Simulations can be done IF Det^{N_f} $M > 0$ for any set of $\{U\}$. However, Det M is a complex number for all $\mu \neq 0$: The Phase/sign problem

Lattice Approaches

Several Approaches proposed in the past two decades : None as satisfactory as the usual $T \neq 0$ simulations. Still scope for a good/great idea !

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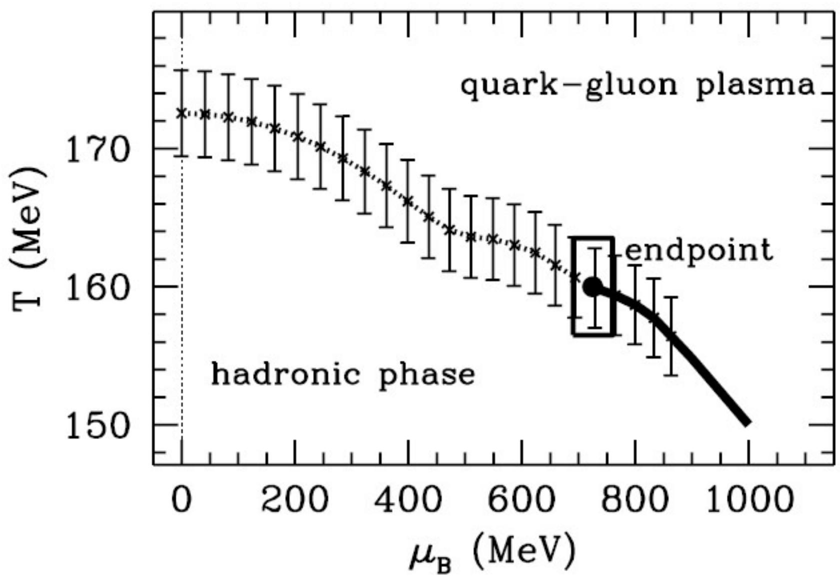
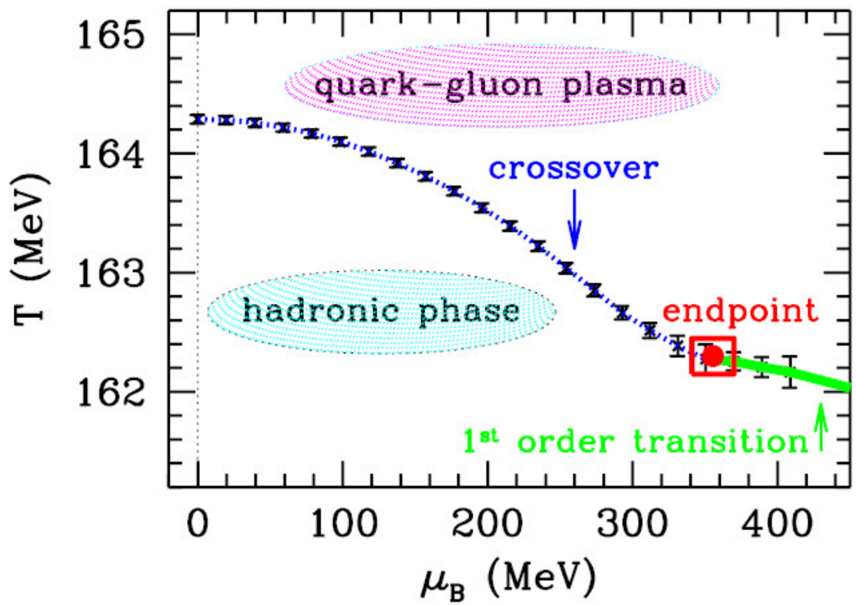
- Why Taylor series expansion? — i) Ease of taking continuum and thermodynamic limit & ii) Better control of systematic errors.

First Glimpse of QCD Critical Point





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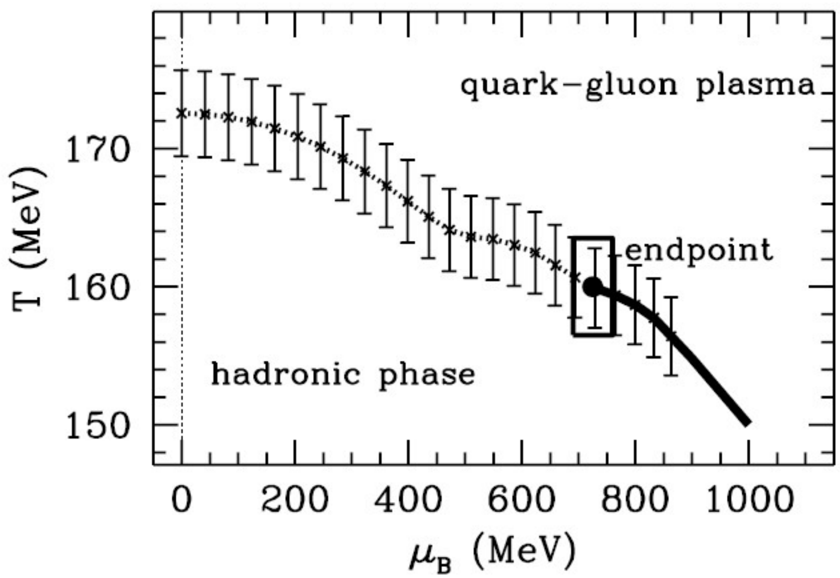

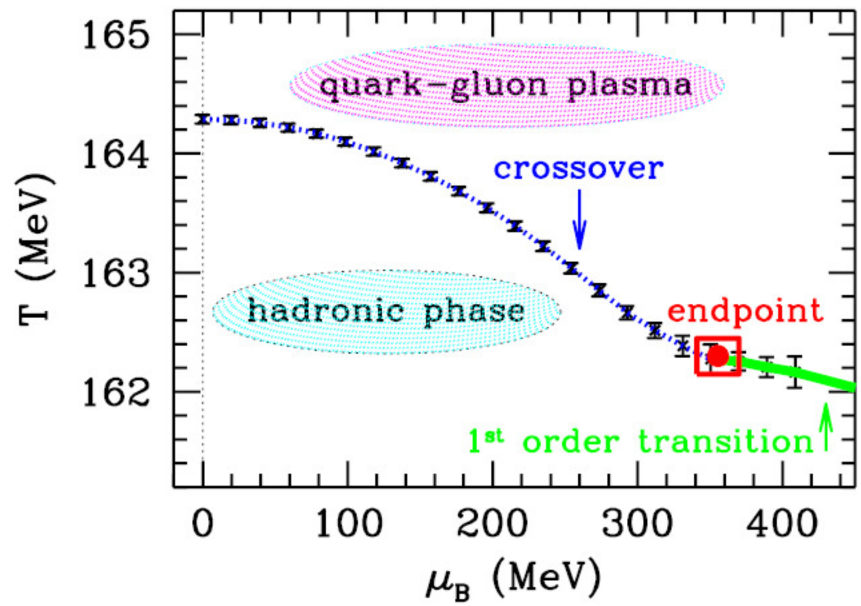

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Larger N_t or Continuum limit ?

QCD Critical Point : Taylor Expansion

- Note that 1) Specific Heat/Susceptibility diverges as one approaches critical point and 2) a series $1 + x + x^2 + x^3.... = 1/(1 - x)$, only if $x < 1$, it diverges otherwise.

- Employ Taylor expansion of baryonic susceptibility $\chi_B(\mu, T)$ in $z = \mu/T$, and look for its radius of convergence to obtain the nearest critical point.

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- Successive estimates for the radius of convergence can be obtained from these using $\sqrt{\frac{n(n+1)\chi_B^{(n+1)}}{\chi_B^{(n+3)}}}$ or $\left(n!\frac{\chi_B^{(2)}}{\chi_B^{(n+2)}}\right)^{1/n}$. We used both definitions and terms up to 8th order in μ.

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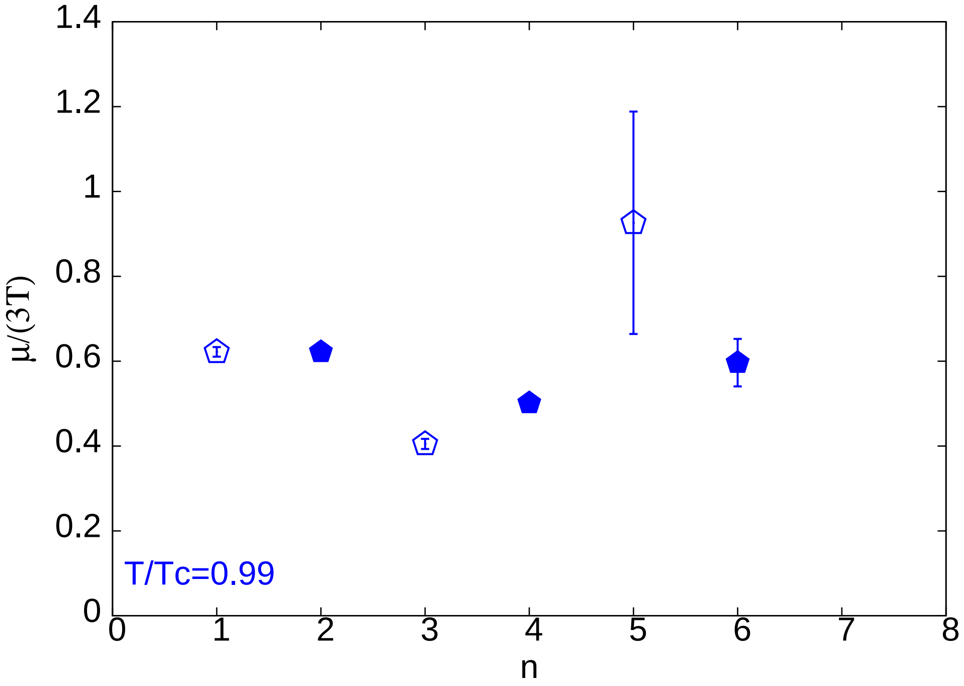
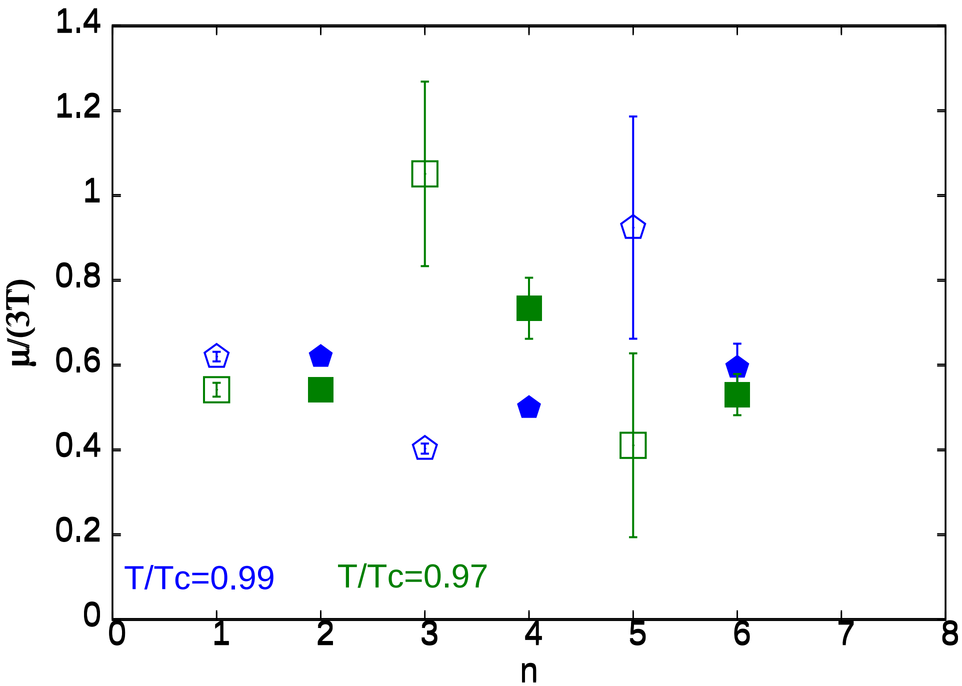
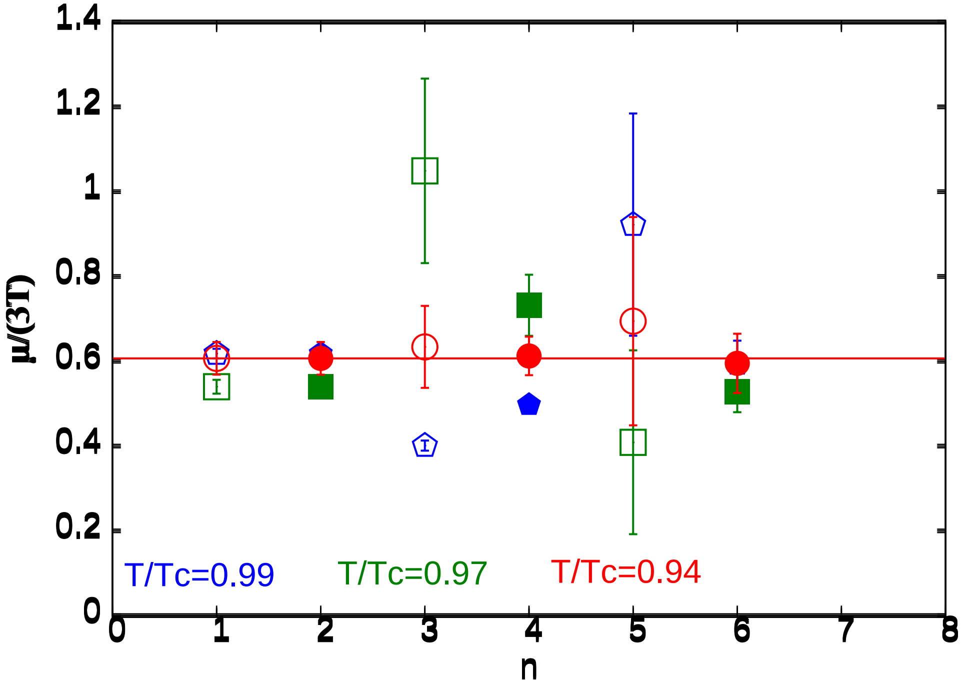
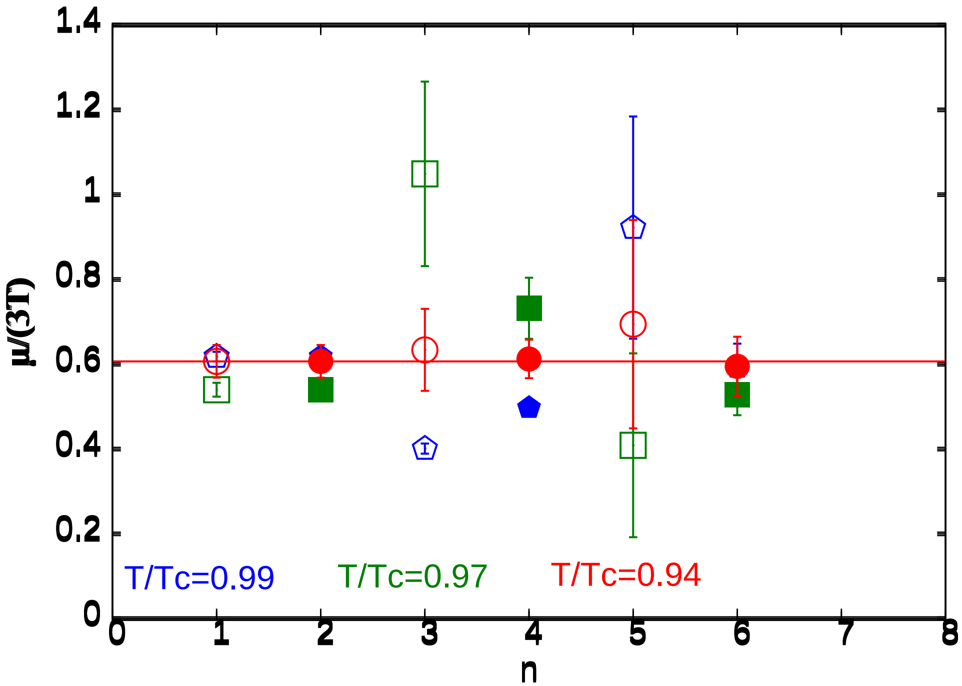
- All coefficients of the series must be POSITIVE for the critical point to be at real μ, and thus physical.

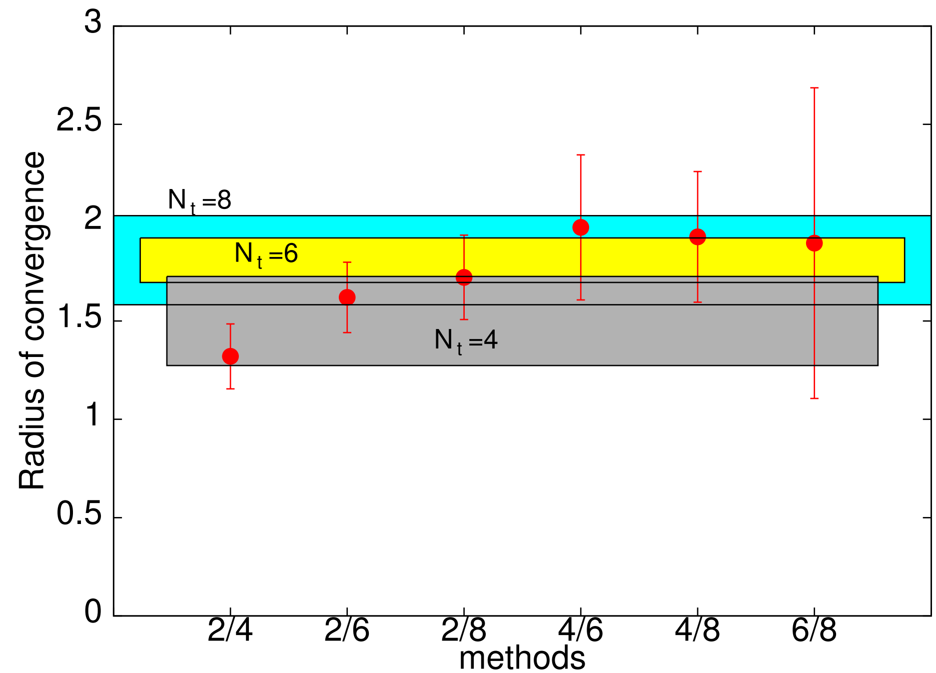


μ/(3T)
n
T/Tc=0.99


1.4
1.2
1
0.8
0.6
0.4
0.2
0
μ/(3T)
0
1
2
3
4
5
6
7
8
n
T/Tc=0.99
T/Tc=0.97


μ/(3T)
n
T/Tc=0.99
T/Tc=0.97
T/Tc=0.94
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
1
2
3
4
5
6
7
8





- $\frac{T^E}{T_c} = 0.94 \pm 0.01$, and $\frac{\mu_B^E}{T^E} = 1.8 \pm 0.2 (1.8 \pm 0.1)$ for the $N_t = 8(6)$ lattice (Datta-RVG-Gupta, '08, '13, '17). Recent high statistics coarser $(N_t = 4)$ lattice result was $\mu_B^E / T^E = 1.5 \pm 0.2$ (Gupta-Karthik-Majumdar PRD '14).

- Critical point at $\mu_B/T \sim 2$, based on results from TIFR('05, '08, '13, '17) & Budapest-Wuppertal ('04) groups.

- Note that for any fermion linear μ leads to $M' = \sum_{x,y} N(x,y)$, and $M'' = M''' = M''''... = 0$, in contrast to the exp($\pm a\mu$)-prescription where *all* derivatives are nonzero: $M', M'''... \neq 0$ and $M'', M'''', M''''''... \neq 0$.

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- Consequently, one has fewer terms in the Taylor coefficients, especially as the order increases. E.g., in the 4th order susceptibility, $\mathcal{O}_4 = -6\ \mathrm{Tr}\ (M^{-1}M')^4$ in the linear case, compared to
$\mathcal{O}_4 = -6\ \mathrm{Tr}\ (M^{-1}M')^4 + 12\ \mathrm{Tr}\ (M^{-1}M')^2 M^{-1}M'' - 3\ \mathrm{Tr}\ (M^{-1}M'')^2 - 3\ \mathrm{Tr}\ M^{-1}M'M^{-1}M''' + \mathrm{Tr}\ M^{-1}M''''$.

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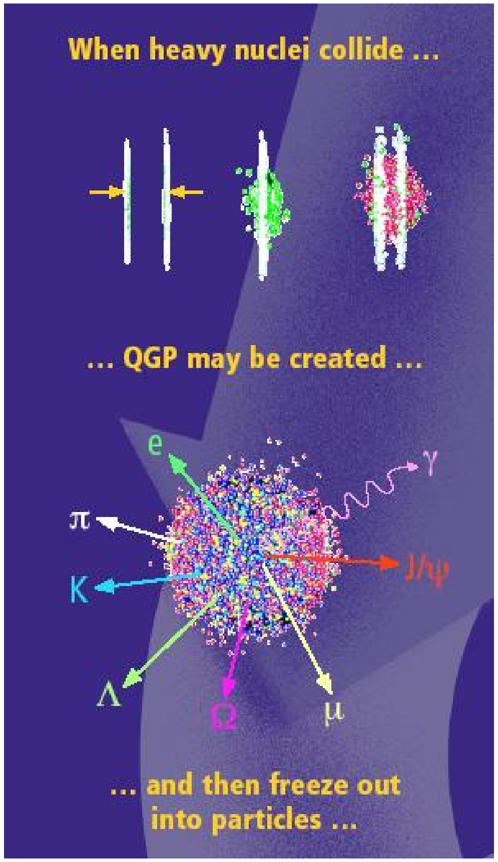
- The resultant computer time savings can be up to a factor of two, with still better error control (due to less cancellations). Moreover, higher orders crucially needed to establish the reliability can perhaps be more easily obtained.us

- Makes Lattice QCD at finite density a bit simpler [Bi-BNL-CCNU PRD 2017].

Searching Experimentally: Heavy Ion Collisions

$\Longrightarrow$ Heavy Ion Collisions at 99.5-99.995 % Velocity of Light.



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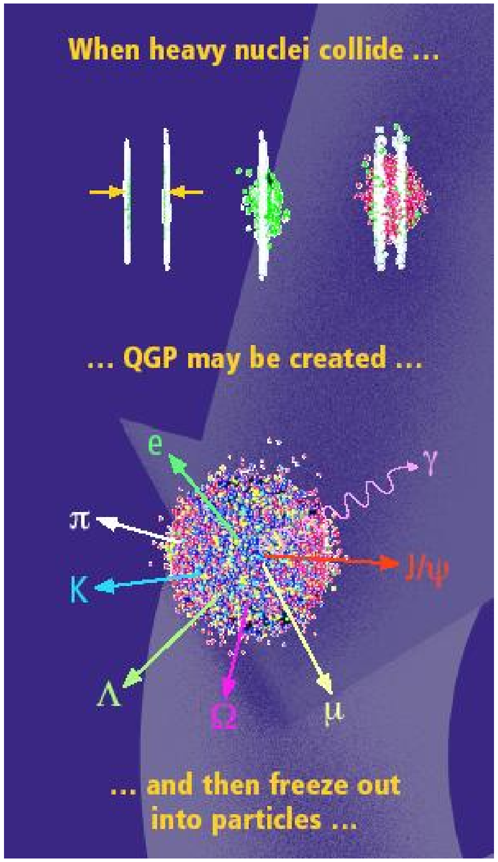

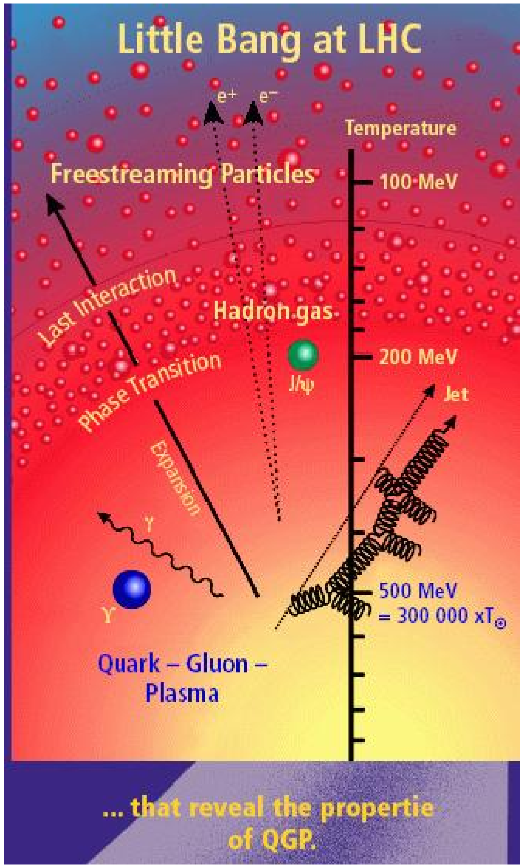

Fireball of QGP condenses into hadrons in $\approx 10^{-23}$ seconds.

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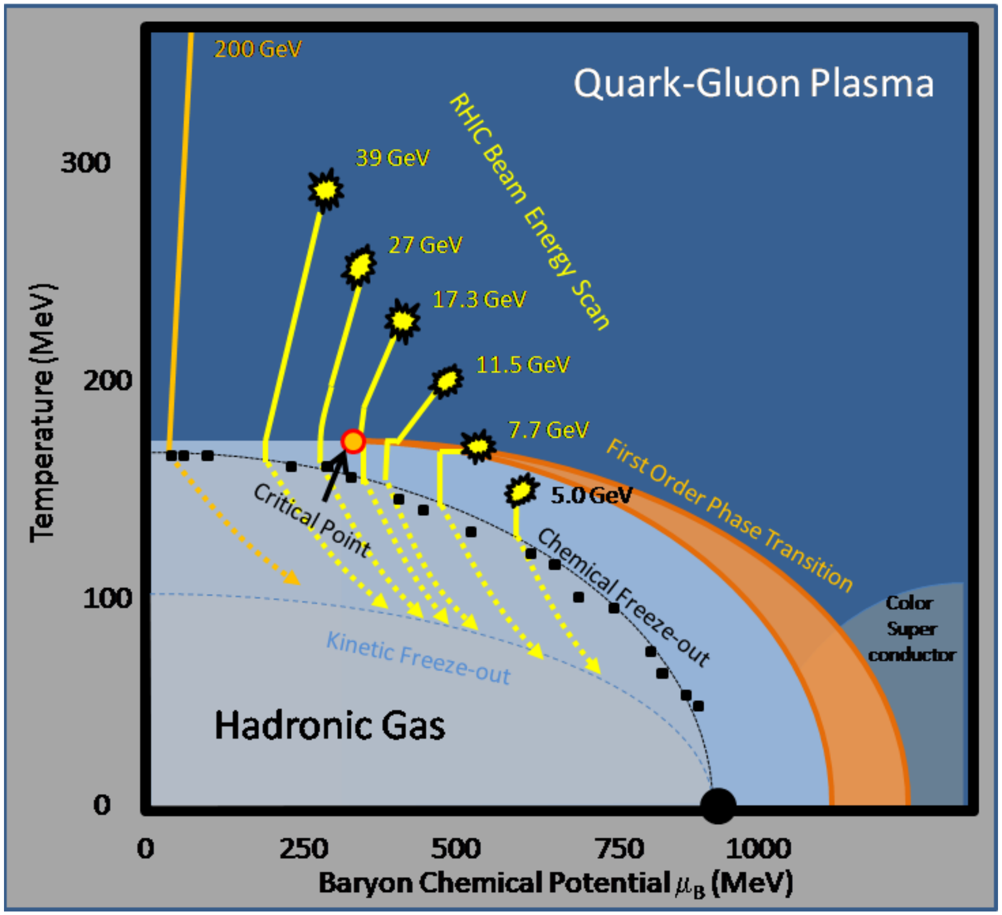

STAR Collaboration, Aggarwal et al.
arXiv : 1007.2637

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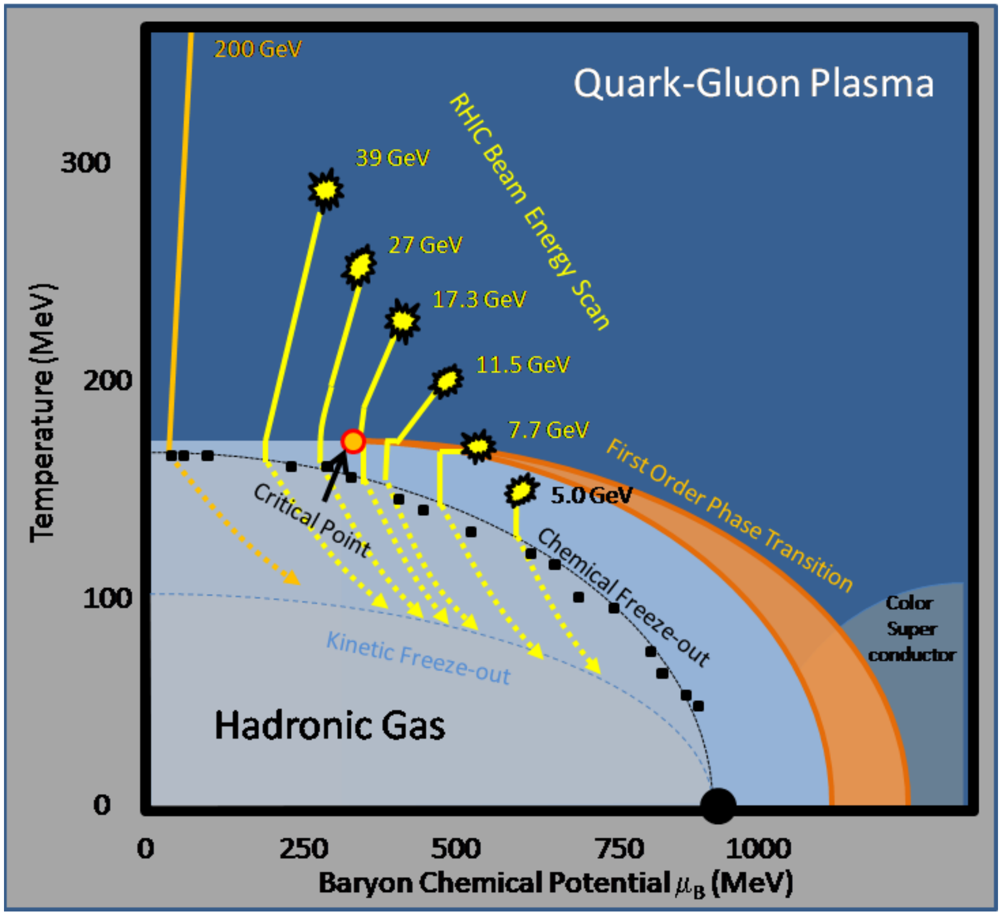

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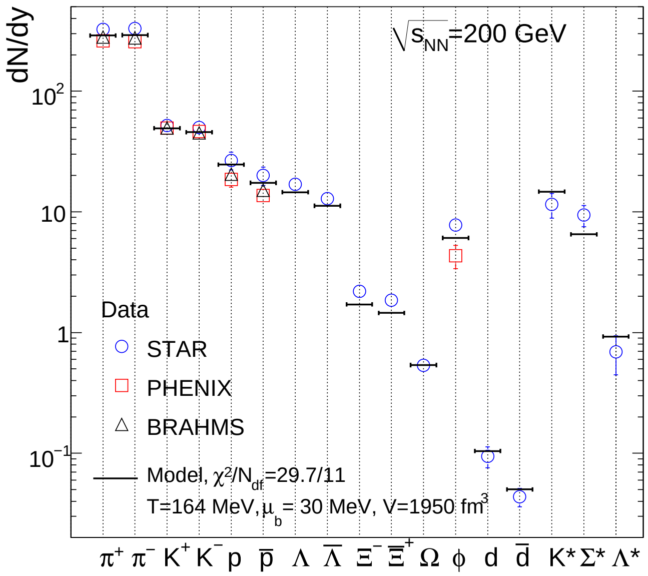
- Look for nonmonotonic dependence of the event-by-event fluctuations with colliding energy. No indications in early such results for π, K-mesons. E.g., CERN NA49 results (C. Roland NA49, J.Phys. G30 (2004) S1381-S1384).

The Freezeout Curve

- Hadron yields well described using Statistical Hadronization Models, leading to the freezeout curve in the T-μ_B plane. (Andronic, Braun-Munzinger & Stachel, PLB 2009 ; Oeschler, Cleymans, Redlich & Wheaton, 2009)



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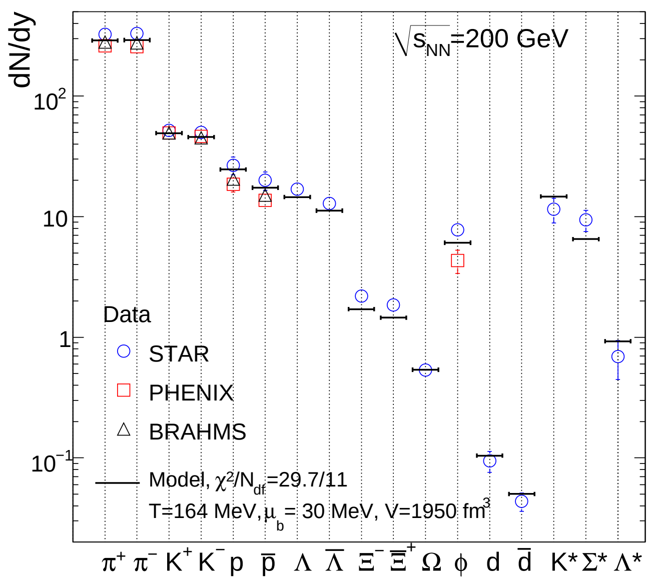
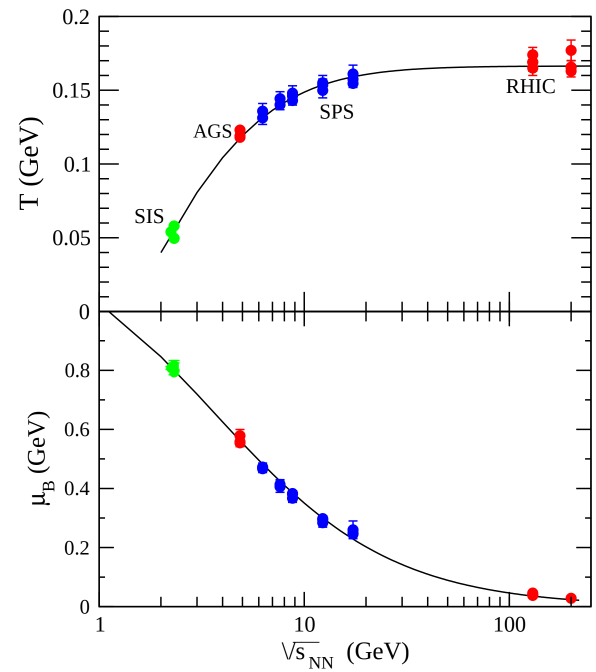
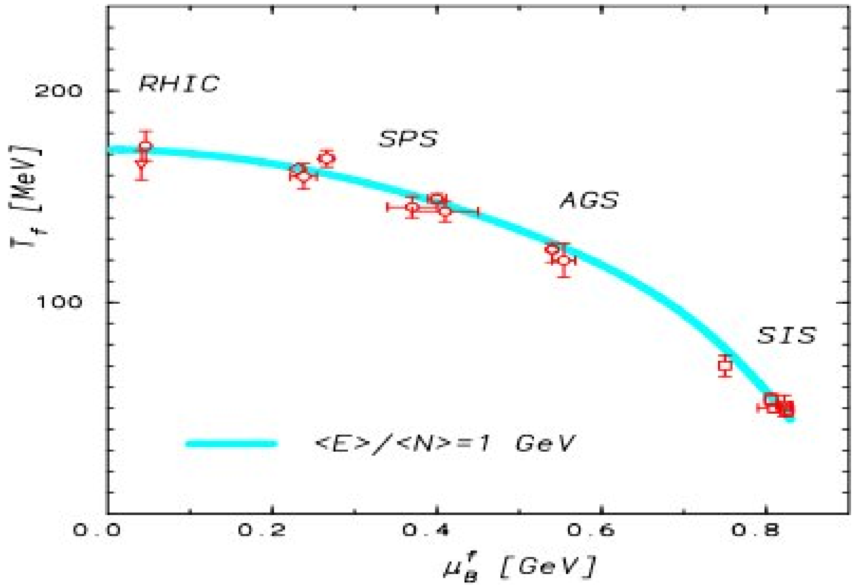




- Plotting these results in the T-μ_B plane, one has the freezeout curve, which was shown to correspond the $\langle E \rangle / \langle N \rangle \simeq 1$. (Cleymans and Redlich, PRL 1998)

Lattice predictions along the Freezeout Curve



(Braun-Munzinger, Redlich and Stachel nucl-th/0304013)

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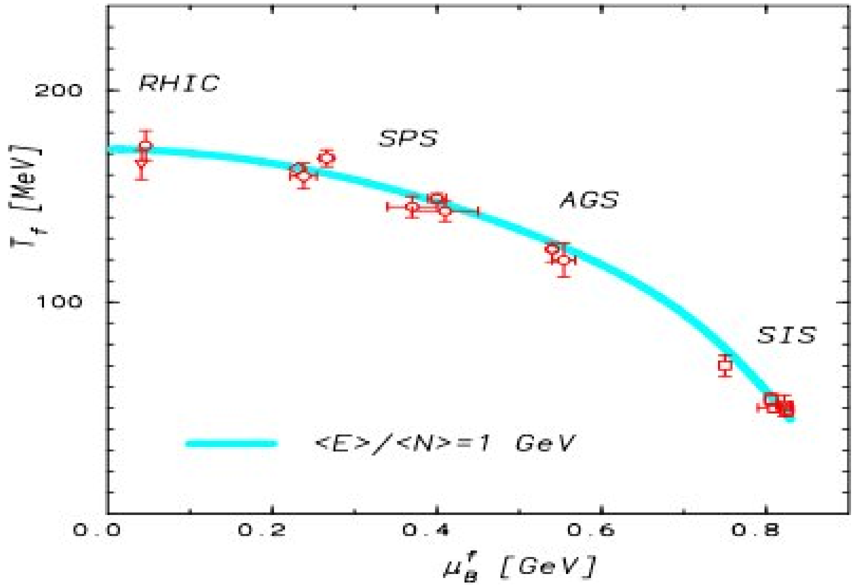
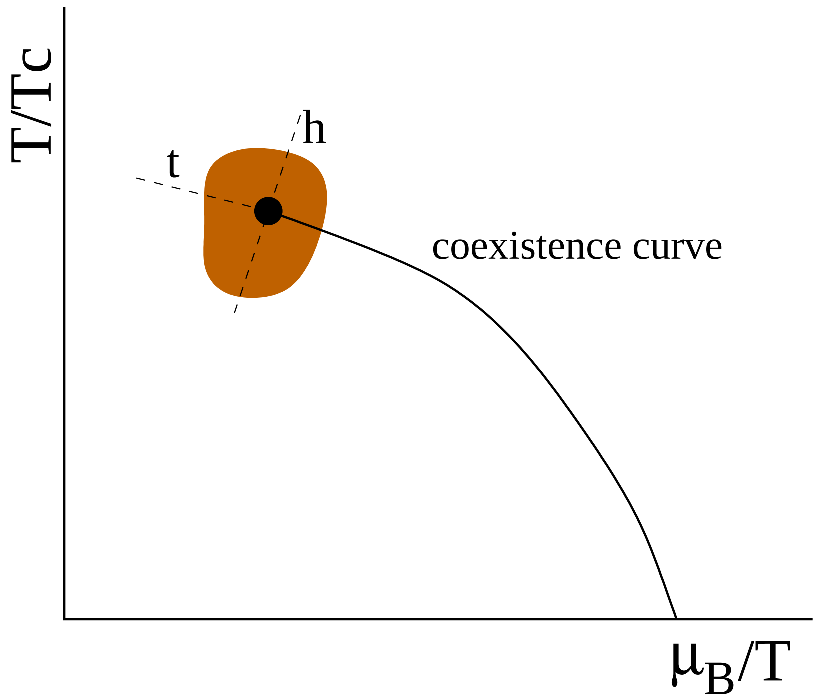
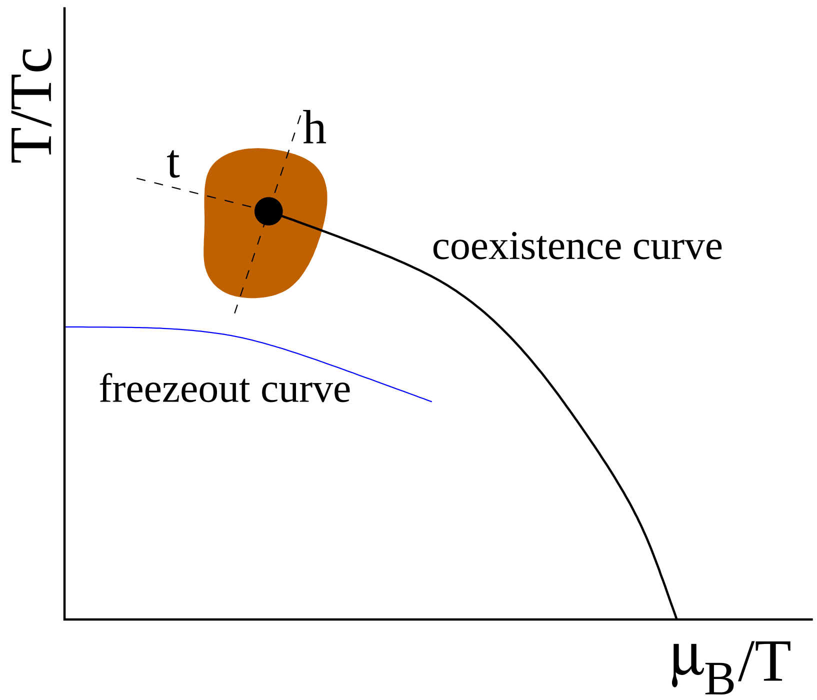


(Braun-Munzinger, Redlich and Stachel nucl-th/0304013)

- Note : Freeze-out curve is based solely on data on hadron yields, & gives the (T, μ) accessible in heavy-ion experiments.
- Our Key Proposal : Use the freezeout curve from hadron abundances to *predict baryon* fluctuations using lattice QCD along it. (Gavai-Gupta, TIFR/TH/10-01, arXiv 1001.3796)



T/Tc
h
t
coexistence curve
μ_B/T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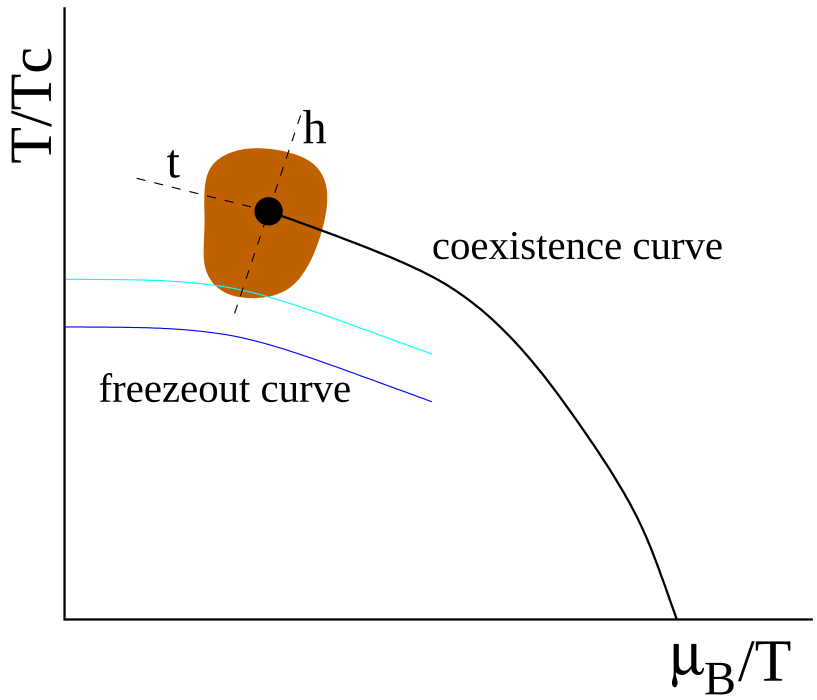
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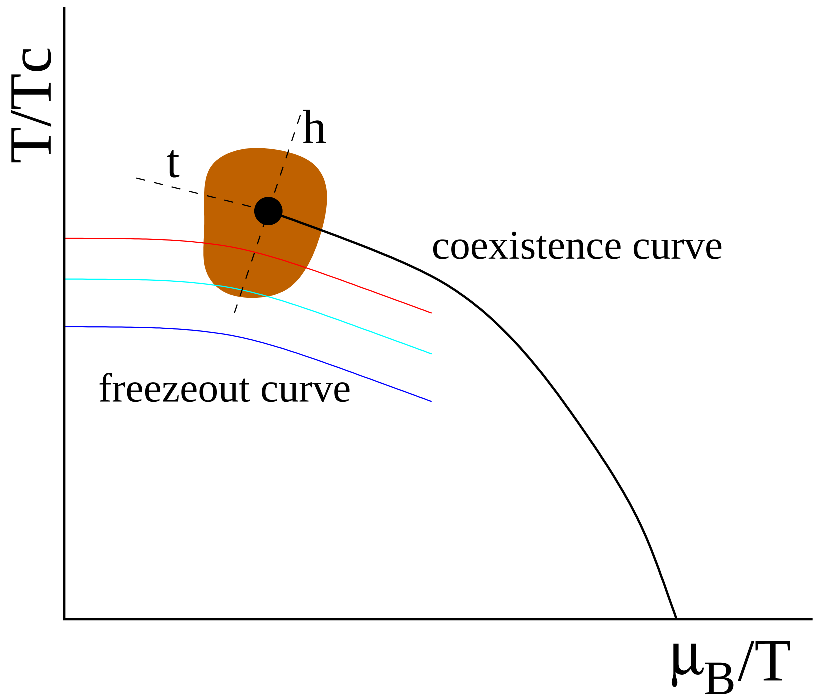
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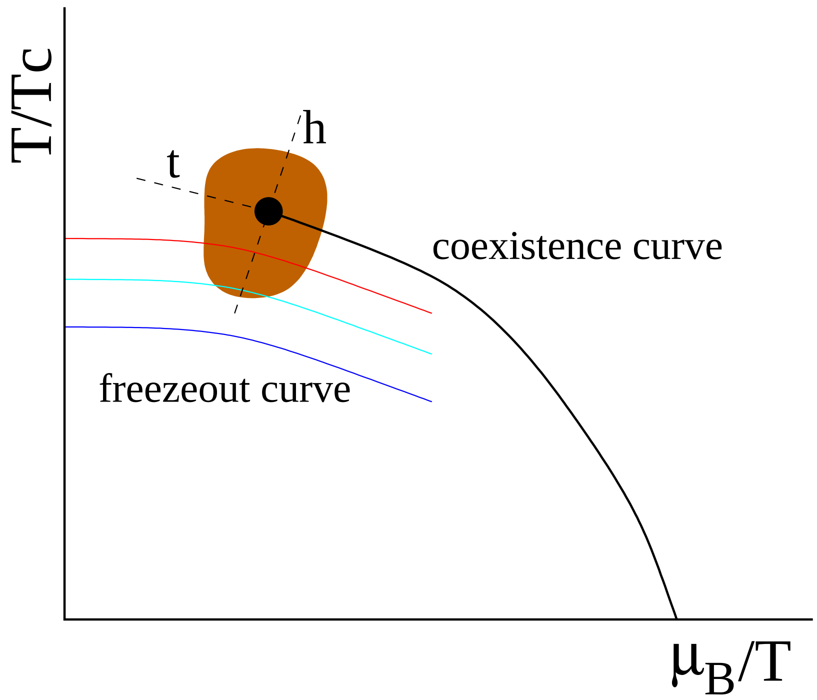
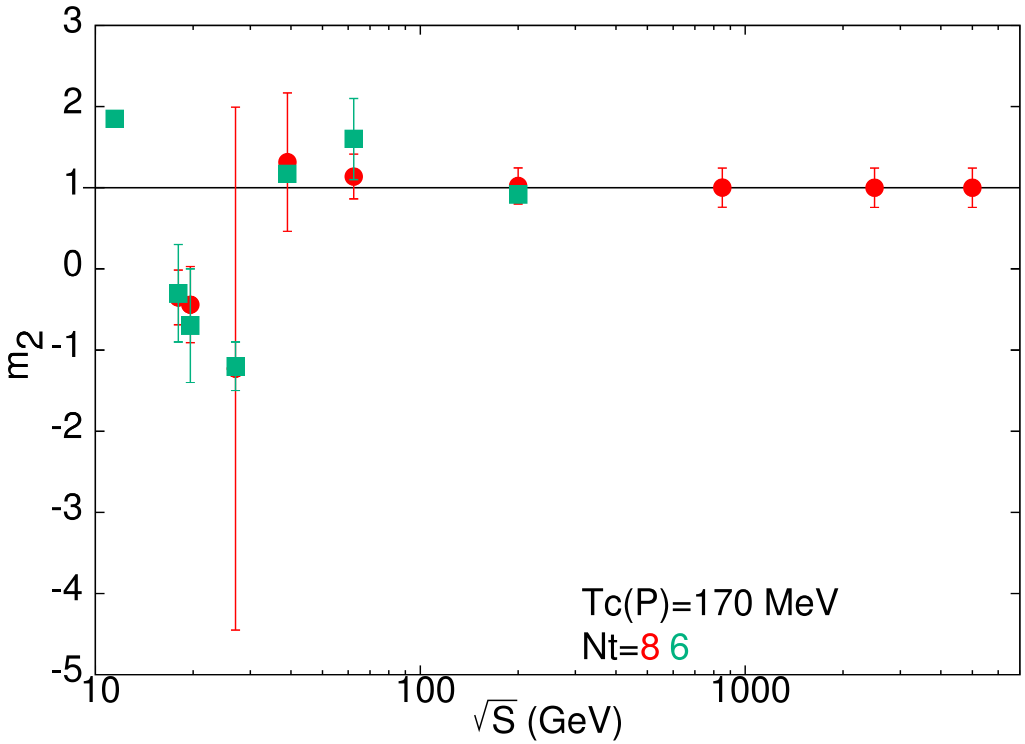


- Use the freezeout curve to relate $(T, \mu_B)$to $\sqrt{s}$ and employ lattice QCD predictions along it. (Gavai-Gupta, TIFR/TH/10-01, arXiv 1001.3796)

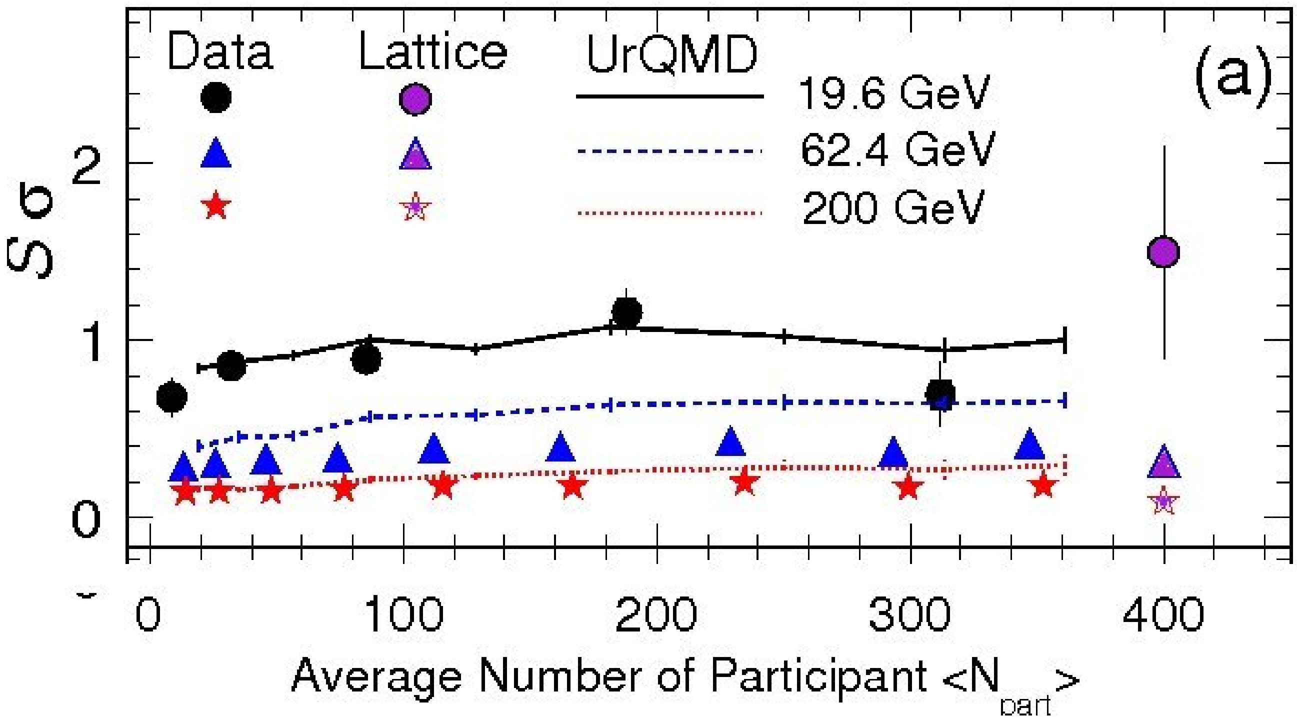
- Define $m_1 = \frac{T\chi^{(3)}(T,\mu_B)}{\chi^{(2)}(T,\mu_B)}$, $m_3 = \frac{T\chi^{(4)}(T,\mu_B)}{\chi^{(3)}(T,\mu_B)}$, and $m_2 = m_1 m_3$ and use the Padè method to construct them.



Gavai-Gupta, '10 & Datta-Gavai-Gupta, Lattice 2013

- Smooth & monotonic behaviour for large $\sqrt{s}$: $m_1 \downarrow$, $m_3 \uparrow$, and $m_2 \sim$ constant.
- Note that even in this smooth region, an experimental comparison is exciting : Direct Non-Perturbative test of QCD in hot and dense environment.

$$S\sigma \equiv m_1$$



Aggarwal et al., STAR Collaboration, arXiv : 1004.4959

- Reasonable agreement with our lattice results. Where is the critical point ?

- Our estimated critical point suggests non-monotonic behaviour in all m_i, which should be accessible to the low energy scan of RHIC BNL !

- Caution : Experiments measure *only* proton number fluctuations.

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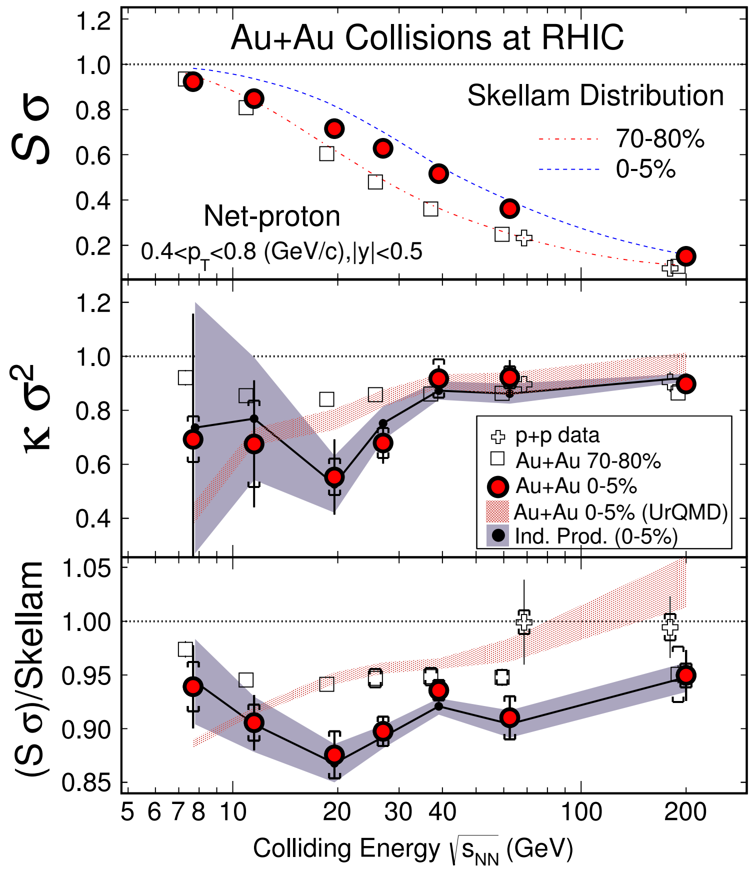
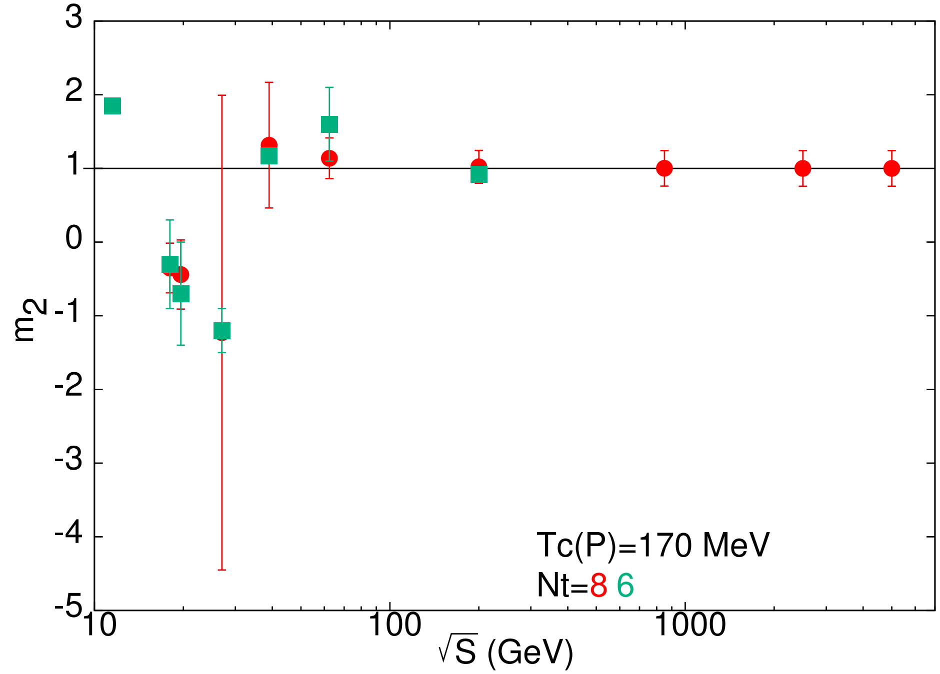
- Leads to a ratio χ_Q:χ_I:χ_B = 1:0:4

- Assuming protons, neutrons, pions to dominate, both χ_Q and χ_B can be shown to be fully reflected in proton number fluctuations.





L. Adamczyk *et al.*
STAR Collaboration PRL (2014)

Gavai-Gupta, '10
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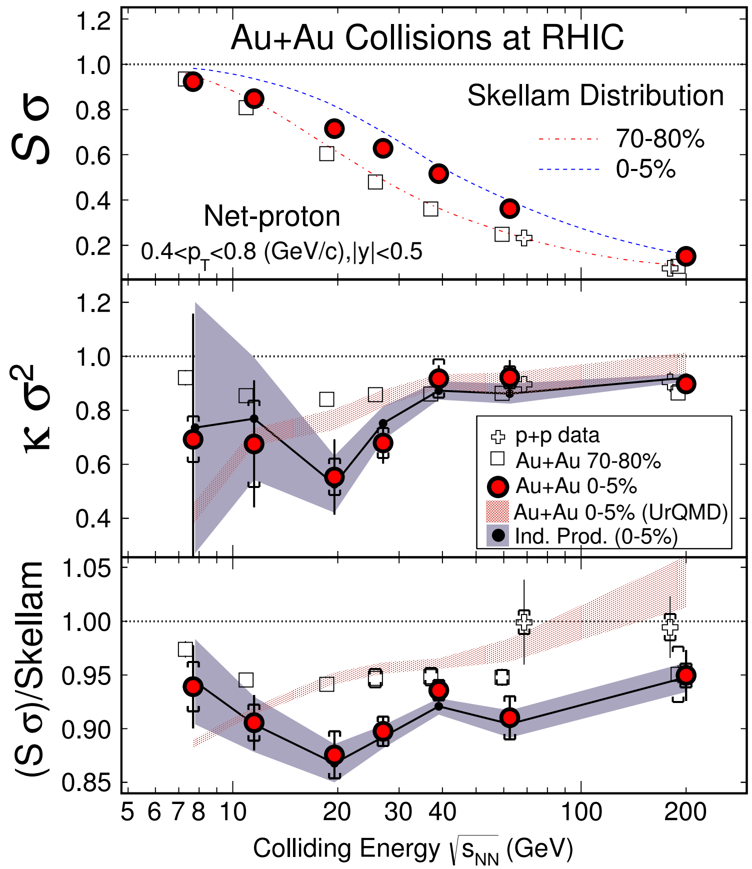

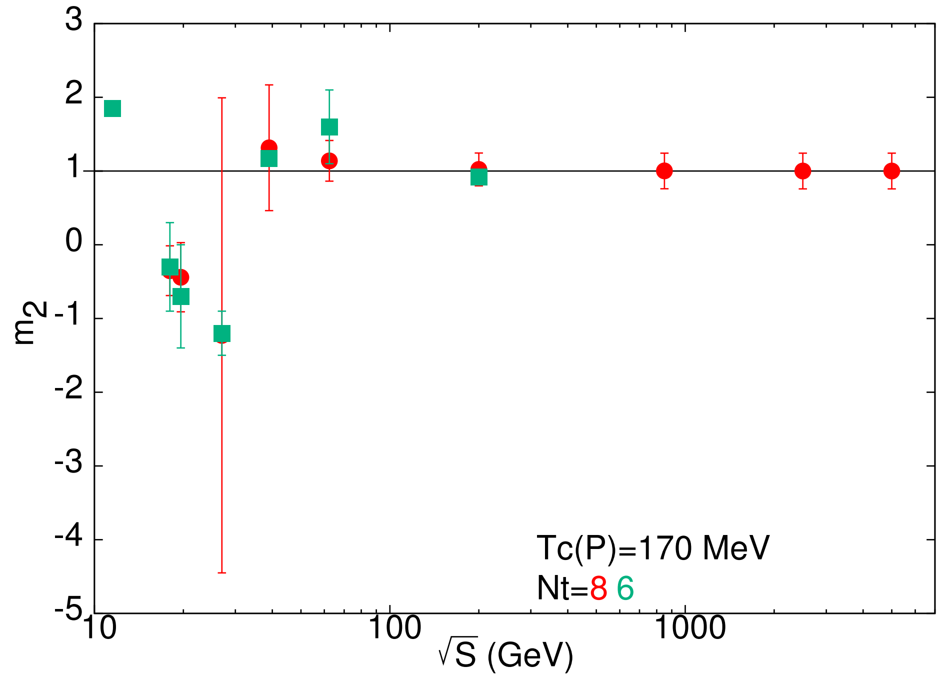

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"These observables show a centrality and energy dependence, which are neither reproduced by non-CP transport model calculations, nor by a hadron resonance gas model. " — STAR Collaboration PRL (2014).

Summary

- μ-dependent divergence is not unique to Lattice. Indeed, Lattice only reproduces faithfully what exists in the continuum field theory.

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- Subtraction of free theory divergences suffices even nonperturbatively. Proof limited to numerical simulations only, but so it is for the exponential prescription where analytic proof exists only for free theory.
- Chiral invariance crucial for critical point investigations but insisting on it for overlap quarks at finite density seems to always lead to a μ-dependent divergence.
- Lots of methods in the market for dealing with the phase/sign problem. Some can be used for QCD with light quarks. Possible hints of QCD critical point have been found, both theoretically, and even more interestingly experimentally.

Summary II

- Phase diagram in $T - \mu$ has begun to emerge: Different methods, $\rightsquigarrow$ similar qualitative picture. Critical Point at $\mu_B/T \sim 1.5 - 2$.

- Our results for $N_t = 8$ first to begin the inching towards continuum limit.

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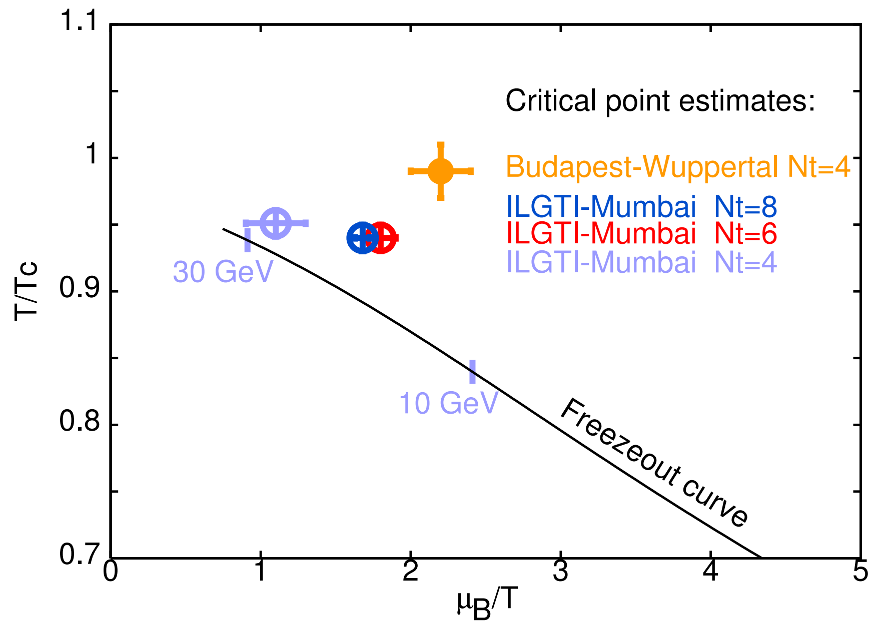
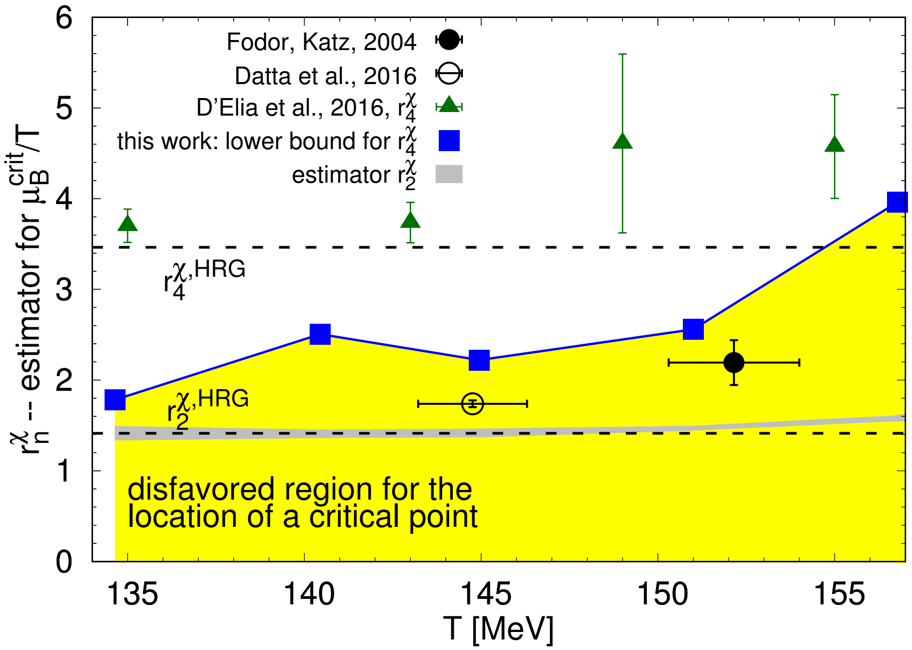
- Our results for $N_t = 8$ first to begin the inching towards continuum limit.
- We showed that Critical Point leads to structures in m_i on the Freeze-Out Curve. Possible Signature ?



♡ STAR, BNL results appear to agree with our Lattice QCD predictions. ☺

♠ Comparison with other group (Bazavov et al. PRD '17): 1-σ bound disfavours Mumbai & Budapest results.



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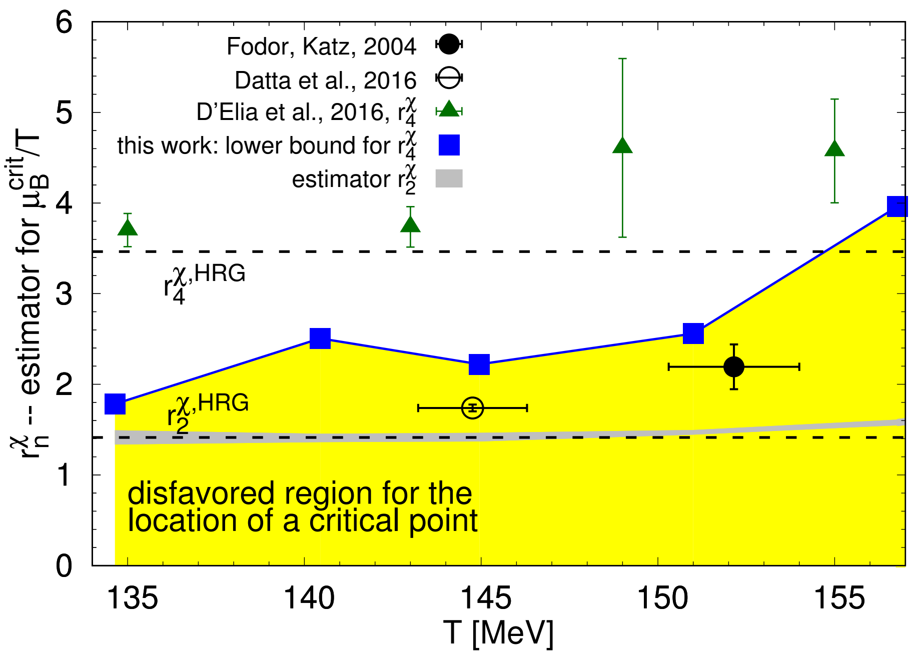
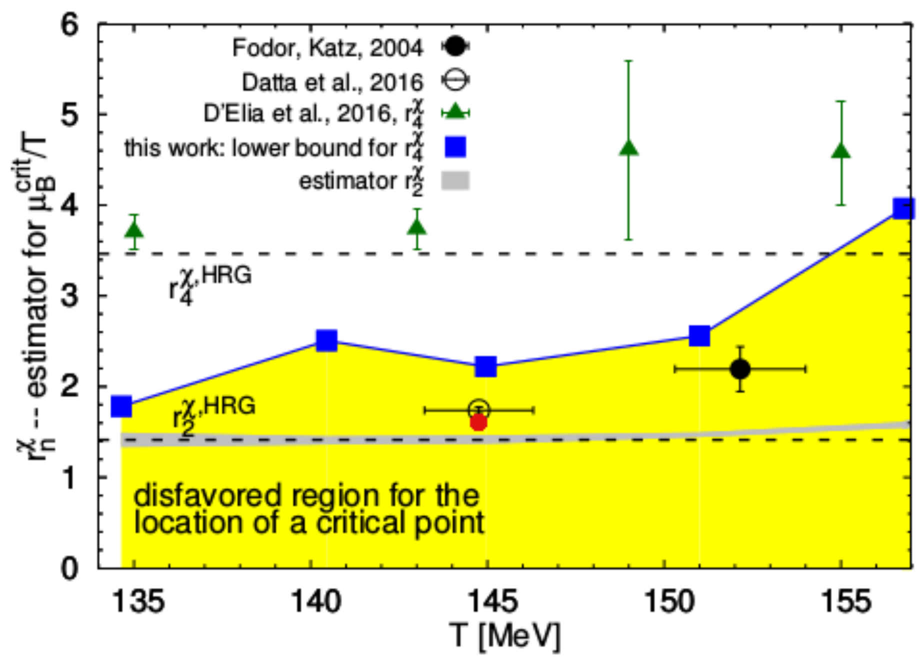
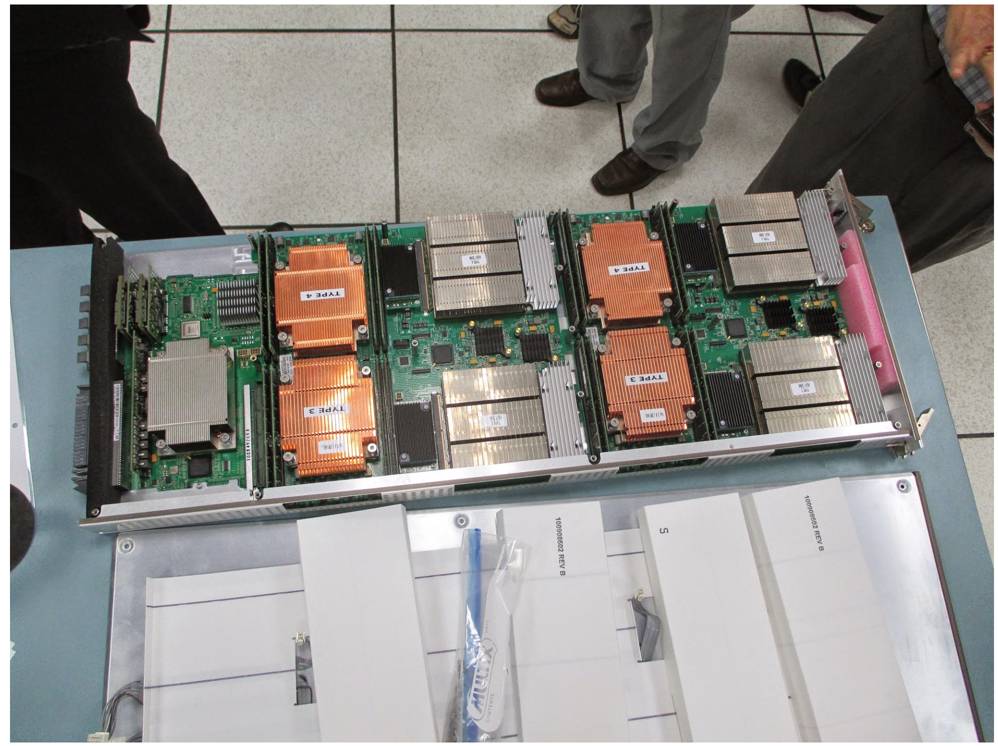




♡ Noting 2+1 flavours, smaller m_π, different discretization & μ-actions employed, $\Longrightarrow$ Good to see that a 2σ-level consistency is plausible.

Our Newest One: CRAY-XC30



CRAY-XC30 of I L G T I , T I F R, Mumbai

Our Workhorse: IBM Blue Gene/P