Progress in lattice QCD at non-zero temperature and density (part I)

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- Deconfinement and color screening
- Chiral transition at non-zero temperature and density
- Equation of state at zero density
- Taylor expansion: fluctuations and correlations of conserved charges
- Taylor expansion: chiral transition and equation of state
- Heavy quark diffusion coefficient from lattice QCD
- Complex heavy quark potential at $T>0$

comparison with weak coupling calculations (HTL, EQCD, pNRQCD)

Comparison with Hadron Resonance Gas (HRG) model

63. Cracow School of Theoretical Physics, Nuclear Matter at Extremes Densities and High Temperatures, September 17-23, 2023, Zakopane, Poland

Finite Temperature QCD and its Lattice Formulation

$$\langle O \rangle = \mathrm{Tr} O e^{-\beta H - \mu N}$$

$$\beta = 1/T$$

evolution operator in imaginary time

$$\langle O \rangle = \int \mathcal{D}A_\mu \mathcal{D}\psi \mathcal{D}\bar{\psi} O e^{-\int_0^\beta d\tau d^3x \mathcal{L}_{QCD}}$$

$$A_\mu(0,\mathbf{x}) = A_\mu(\beta,\mathbf{x}) \quad \psi(0,\mathbf{x}) = -\psi(\beta,\mathbf{x})$$

Integral over functions → Lattice → integral with very large (but finite) dimension (> 1000)

$$\langle O \rangle = \int \prod_x dU_\mu(x) O(det D_q[U,m,\mu]) e^{-\sum_x S_G[U(x)]}, U_\mu(x) = e^{igaA_\mu(x)}$$

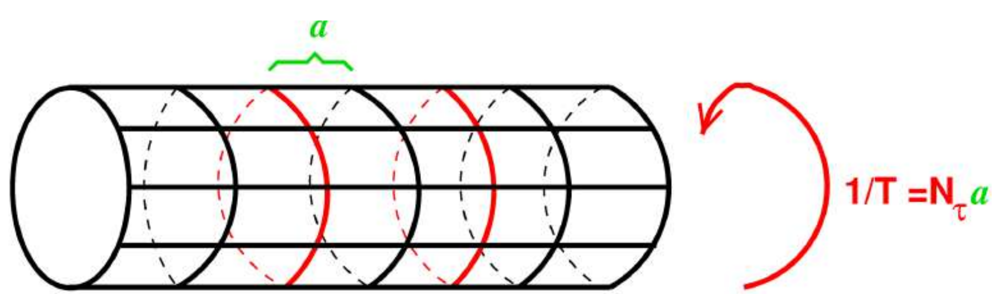
$\mu \neq 0$: $det D_q(U,m,\mu)$ complex → Monte-Carlo Methods / sign-problem

continuum limit

$N_\tau \to \infty$, N_σ / N_τ fixed

Costs : ?

$$\sim a^{-7} \sim N_\tau^7$$



Quenched QCD: $det D_q(U,m,\mu) = 1$

improved discretization schemes are needed : p4, asqtad, stout, HISQ

Symmetries of QCD in the vacuum and for T>0

- Chiral symmetry : For light quarks $m_{u,d} << \Lambda_{QCD}$ QCD Lagrangian has

Nobel Prize 2008

$SU_A(2)$ symmetry $\psi \rightarrow e^{i\phi^a T^a \gamma_5}\psi$ $\qquad \psi_{L,R} \rightarrow e^{i\phi^a_{L,R} T^a} \psi_{L,R}$

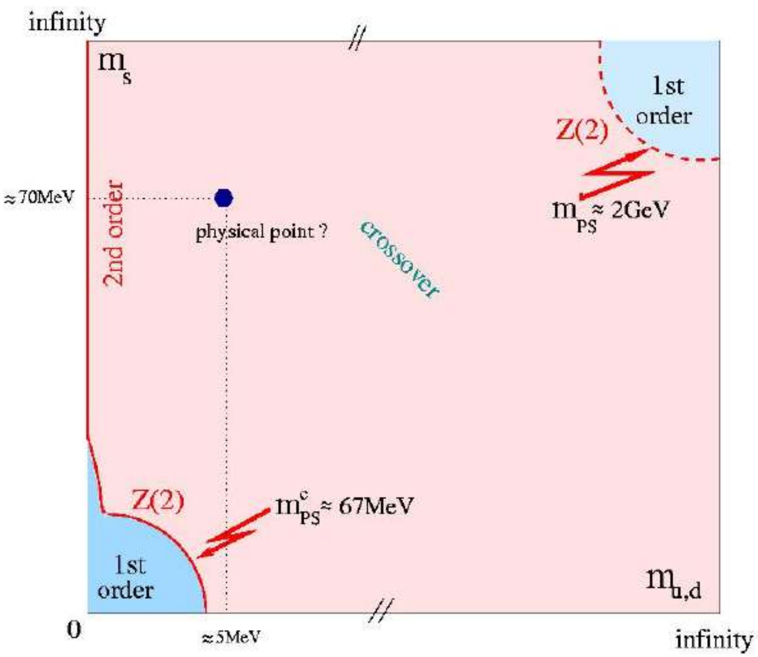
The vacuum breaks the symmetry $\langle \bar\psi \psi \rangle = \langle \bar\psi_L \psi_R \rangle + \langle \bar\psi_R \psi_L \rangle \neq 0$

spontaneous symmetry breaking or Nambu-Goldstone realization of the symmetry

hadrons with opposite parity have very different masses, interactions between hadrons are weak at low *E*

$U_A(1)$ symmetry $\psi \rightarrow e^{i\phi\gamma_5}\psi$ is broken by anomaly (ABJ) : $\langle \partial^\mu j^a_\mu \rangle = -\frac{\alpha_s}{4\pi} \langle \epsilon^{\alpha\beta\gamma\delta} F^a_{\alpha\beta} F^a_{\gamma\delta} \rangle$

⇒ *η'* meson mass, *π*-a_0 mass difference



Pisarski, Wilczek, PD29 (1984) 338

$T \gg \Lambda_{QCD}$: $\langle \bar\psi \psi \rangle \simeq 0$, $U_A(1)$ symmetry ?

For large quark masses center symmetry there is an approximate center Z(N) symmetry that is broken at high temperature and its breaking is associated with deconfinement

Evidence for 2nd order transition in the chiral limit => universal properties of QCD transition:

$SU_A(2) \sim O(4)$ relation to spin models	transition is a crossover for physical quark masses

Center symmetry and deconfinement transition

Above the phase transition temperature Z(N) (center) symmetry of SU(N) gauge theory is broken
Quarks transform non-trivially under Z(N) symmetry group
=> static charges in fundamental representations can be screened by gluons !

Lattice set-up:

$U_\mu(\tau,x) = e^{igA_\mu(\tau,x)},\ N_\sigma^3 \times N_\tau,\ T = 1/(N_\tau a)$

Thermodynamic limit: $N_\sigma/N_\tau \to \infty$; Continuum limit : $N_\tau \to \infty$, T-fixed Temperature is set by $a \leftrightarrow \beta = 2N_c/g^2$; allowable gauge transformations: $U_\mu(x) \to \Omega(x+\mu)U_\mu(x)\Omega^\dagger(x)$

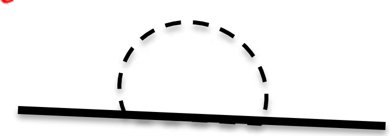
$$\Omega(0,\vec{x}) = \Omega(\beta,\vec{x})C, \quad C = e^{2\pi i n/N_c} I \quad \to Z(N) - \text{symmetry}$$

$$L(\vec{x}) = \frac{1}{N_c} \mathrm{tr} \prod_{\tau=1}^{N_\tau} U_0(\tau,\vec{x})$$

Polyakov loop is changed $L(\vec{x}) \to e^{2\pi n i/N_c} L(\vec{x})$

$< L > \neq 0 \ \to Z(N)$ spontaneously broken; $< L >= e^{-F_Q/T}$ -free energy of an isolated static quark is finite $\Rightarrow$ deconfinement

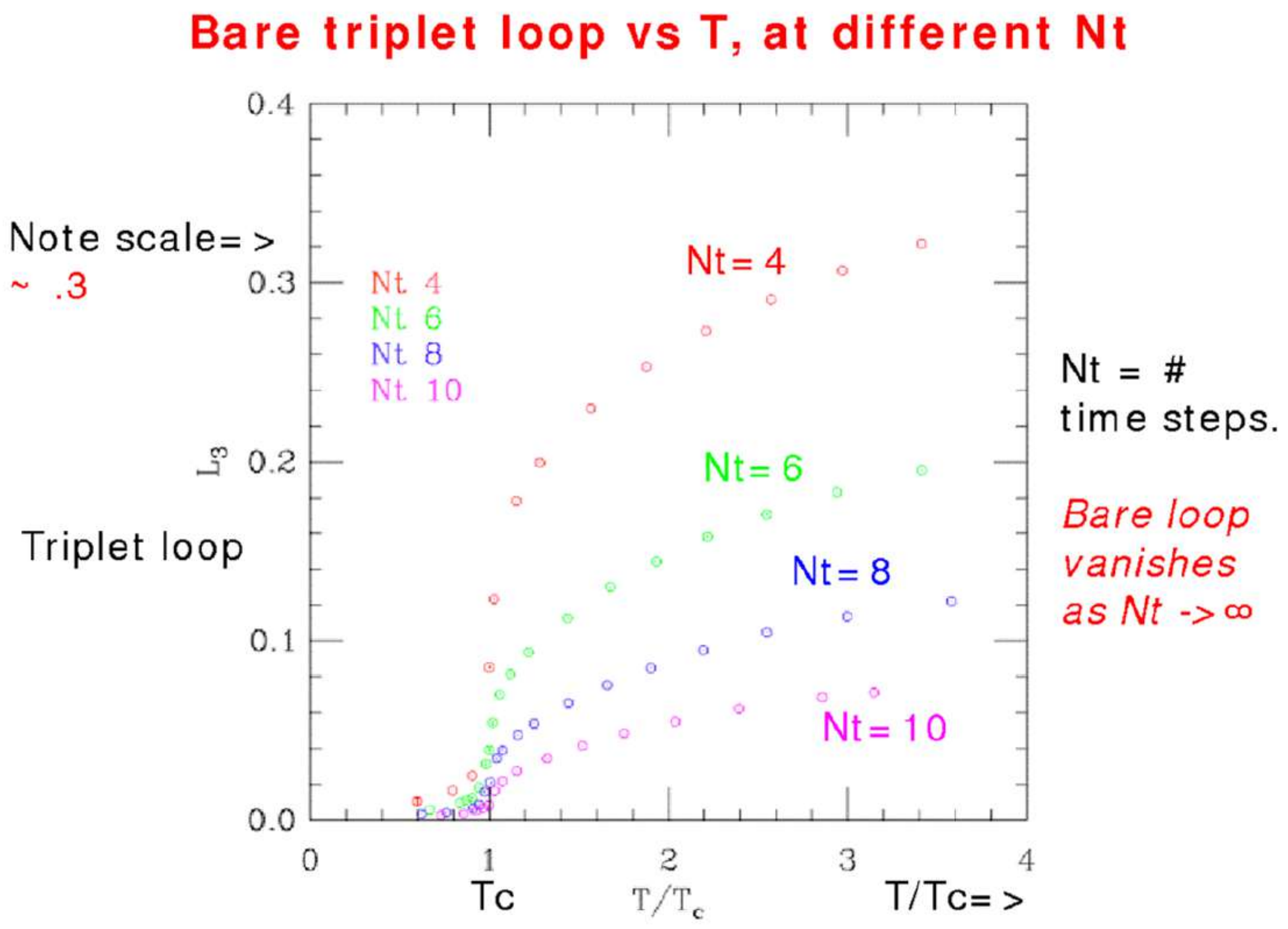
L is order parameter



The free energy of static quark is infinite in the Continuum limit due to linear *1/a* divergence => needs renormalization

Continuum limit for *L* ?

Dumitru et al, hep-th/0311223

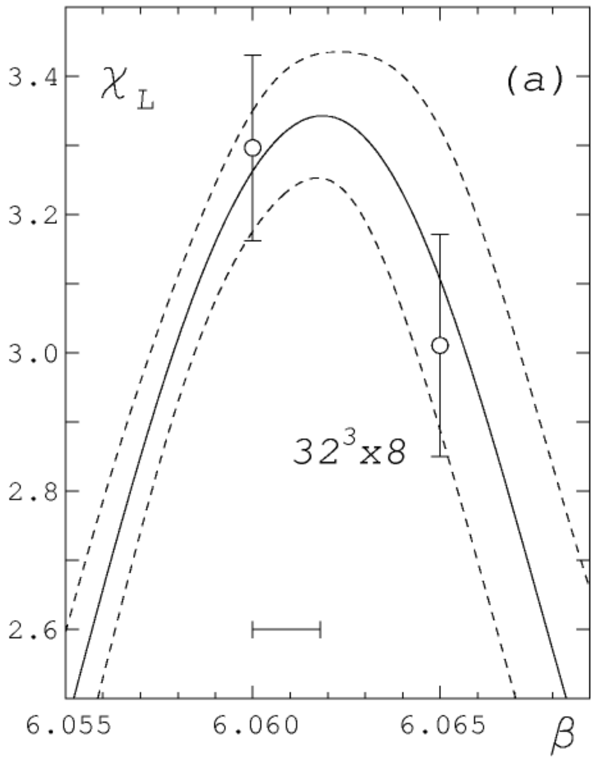


needs renormalization !

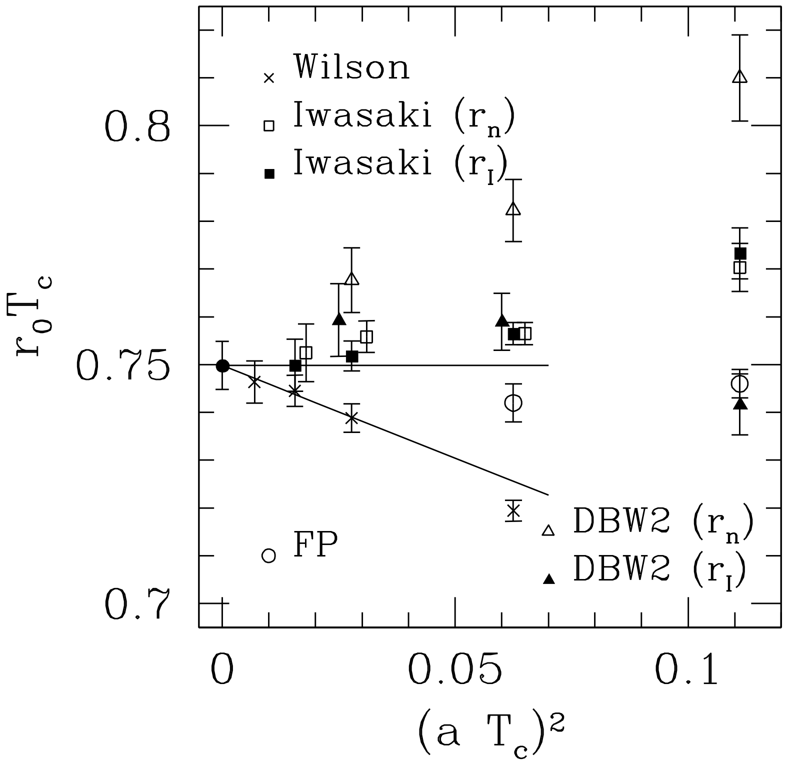
How to determine the deconfinement transition temperature ?

$$\frac{\chi_L}{T^2} = N_\sigma^3 \left(\langle L^2 \rangle - \langle L \rangle^2 \right) = \langle (\delta L)^2 \rangle \text{ has a peak at } \beta_c$$

Boyd et al., Nucl. Phys. B496 (1996) 167



Necco, Nucl. Phys. B683 (2004) 167



- Use different volumes and Ferrenberg-Swedsen re-weighting to combine information collected at different gauge couplings

Finite volume behavior can tell the order of the phase transition, e.g. for 1st order transition the peak height scales as spatial volume !

Correlator of Polyakov loops and deconfinement

The correlation function of Polyakov loops defines the free energy of static quark anti-quark pair (also an order parameter)

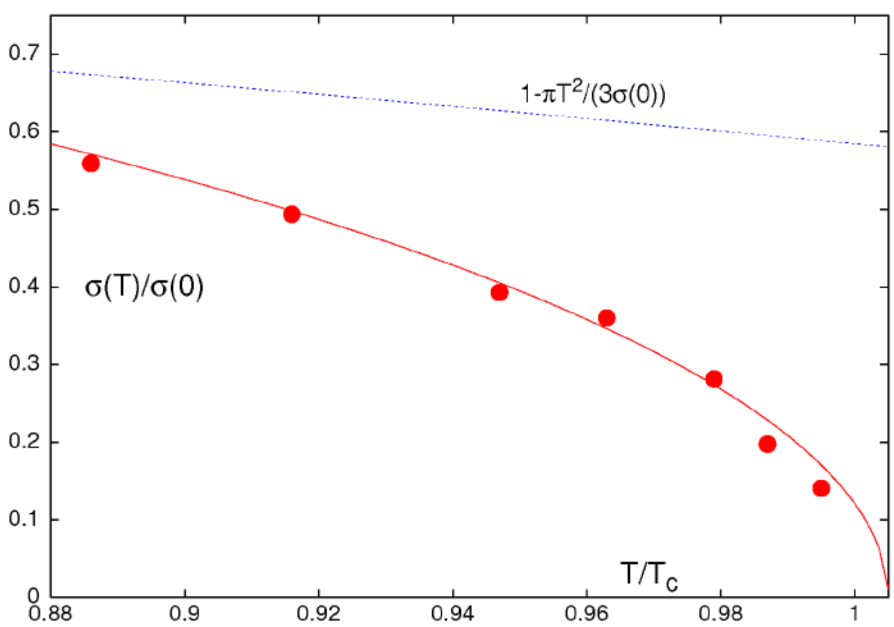
$T < T_c :$

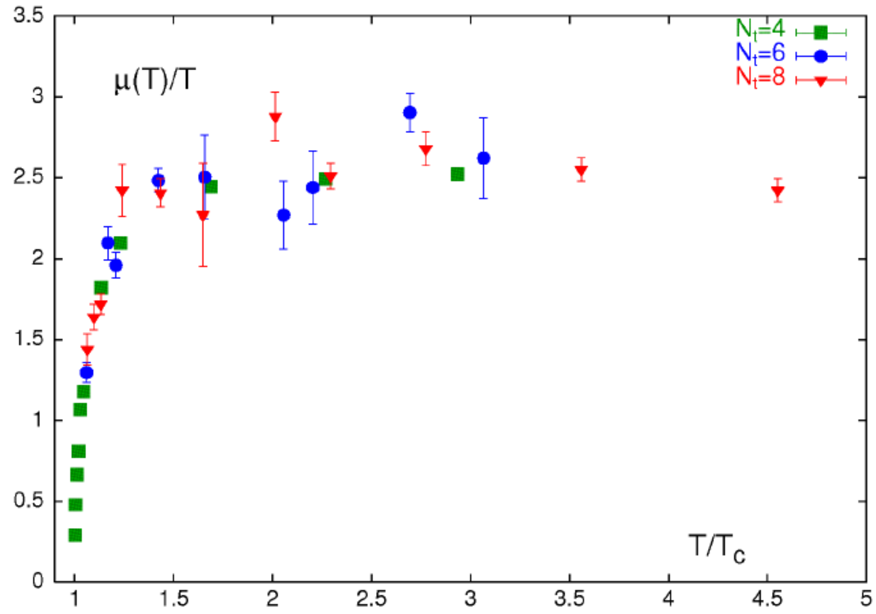
$$< L(r)L^\dagger(0) > \sim e^{-\sigma(T)r/T}$$

$T > T_c :$

$$\ln\left(\frac{< L(r)L^\dagger(0) >}{|< L >|^2}\right) \sim e^{-\mu(T)r}$$

Kaczmarek, Phys. Rev. D62 (2000) 034021



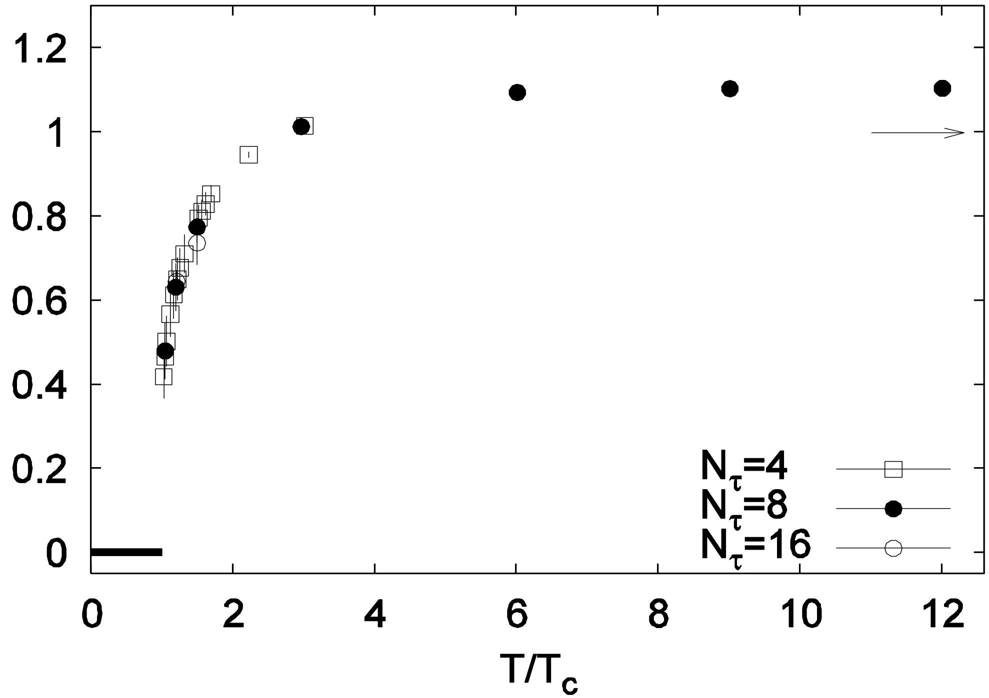


small inverse correlation length => weak 1st order phase transition SU(3) gauge theory is far from the large *N*-limit !

The renormalized Polyakov loop in pure glue theory

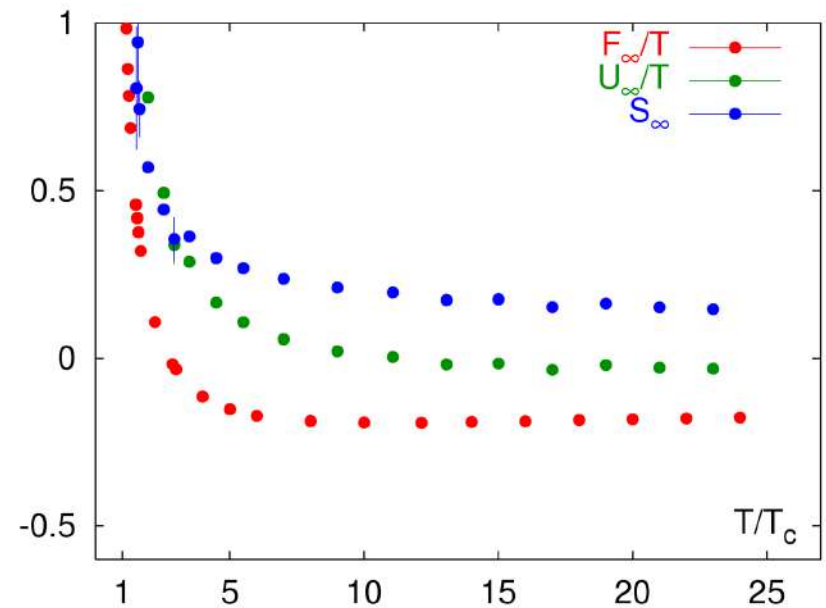
$$r \ll 1/T: \; F_{Q\bar{Q}}(r,T) = V(r, T=0) + T \ln 9$$
$\Rightarrow$ normalize the $Q\bar{Q}$ free energy to the $T=0$ potential

$$\lim_{r\to\infty} \langle L(r) L^\dagger(0)\rangle = \exp(-F_{Q\bar{Q}}(r\to\infty, T)/T) = \exp(-F_\infty/T) = |\langle L\rangle|^2, F_Q = F_\infty/2$$



$$L_{ren} = \exp(-F_\infty(T)/(2T))$$

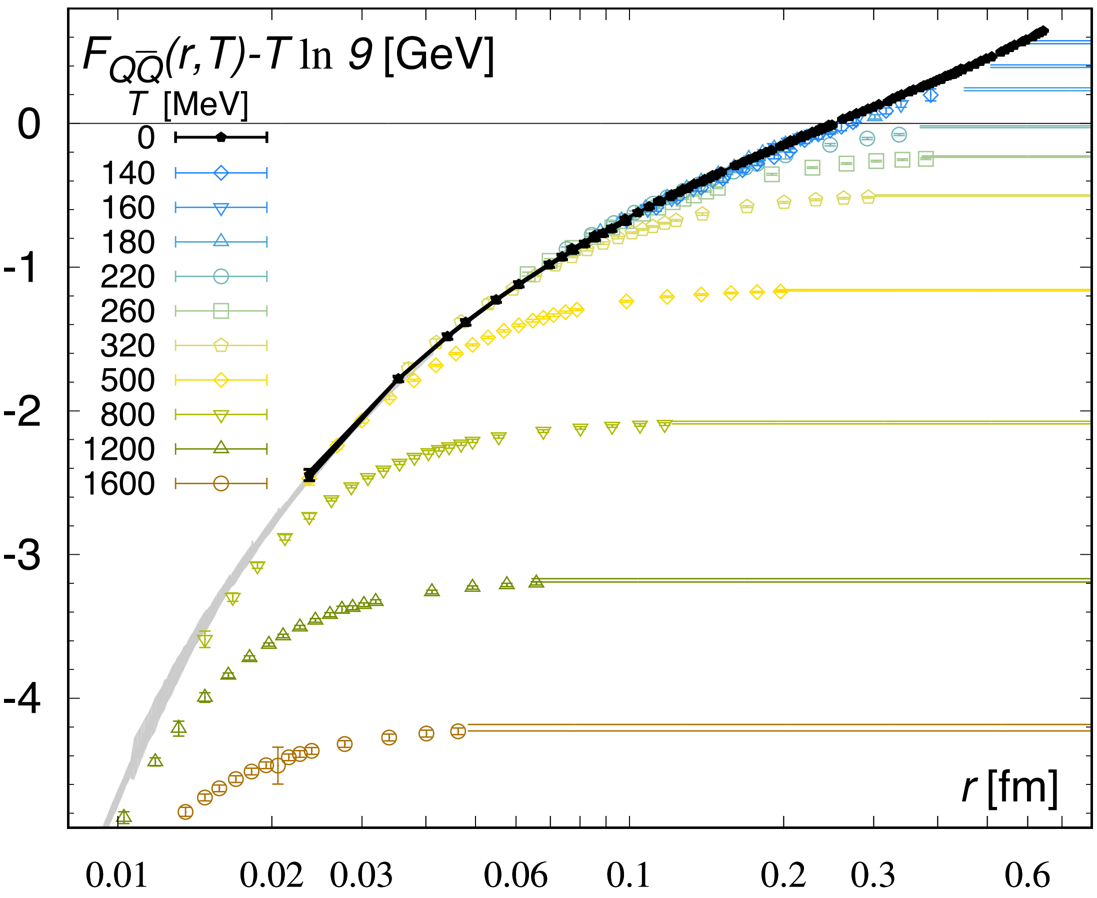
Kaczmarek et al, PLB 543 (2002) 41,
PRD 70 (2004) 074505, hep-lat/0309121



$$\text{LO}: F_Q = -TS_Q = -\frac{4}{3}\alpha_s m_D$$

Deconfinement and color screening in QCD

2+1 flavor QCD, continuum extrapolated, TUMQCD, PRD 98 (2018) 054511

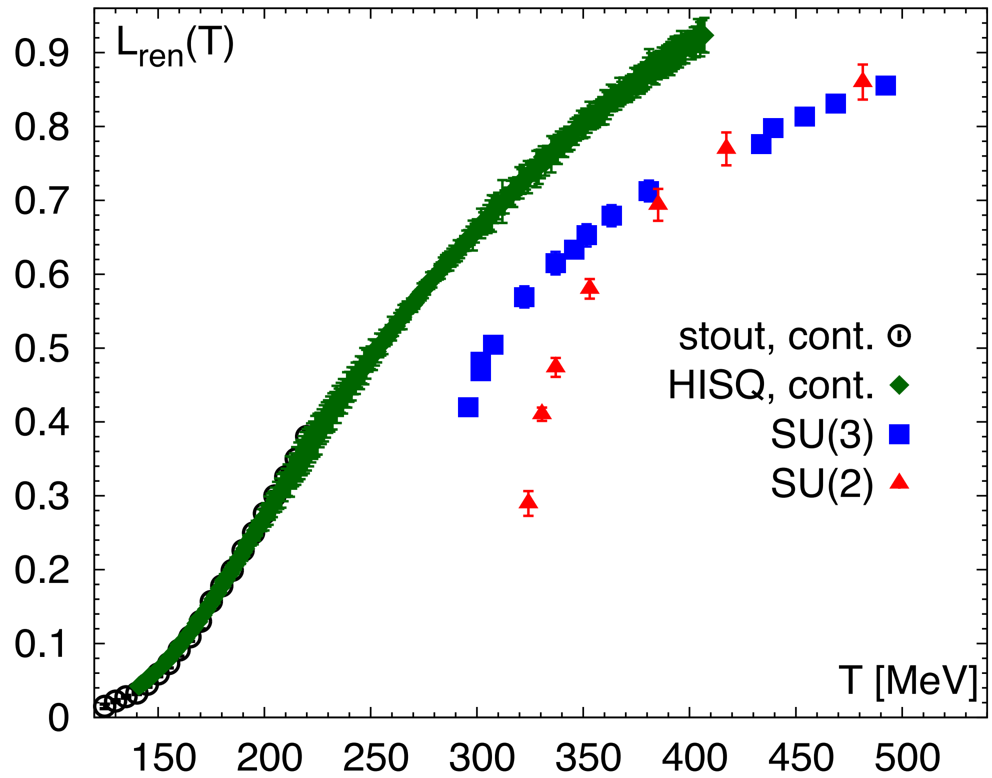


The free energy of static quark anti-quark pair agrees with the *T=0* potential for $r \ll 1/T$

The free energy of static quark anti-quark pair is screened for $r>r_{scr}$ at any temperature

$r_{scr} \sim 1/T$ => Debye screening

Deconfinement and color screening in QCD (cont'd)



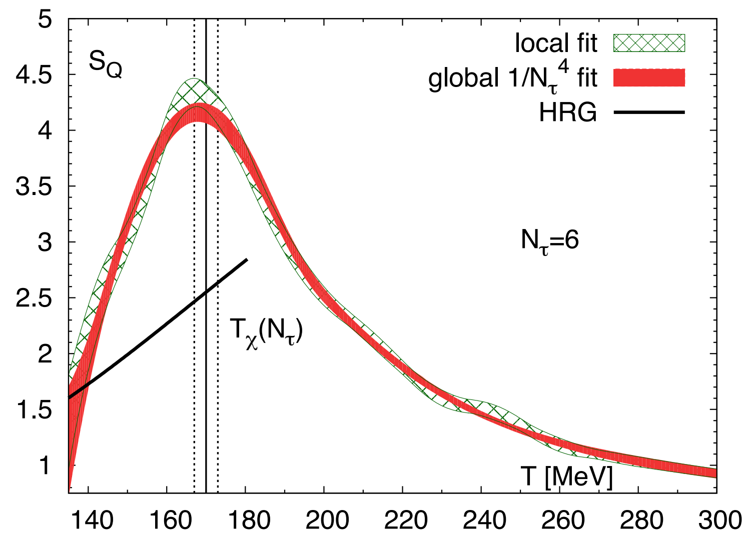
Pure glue ≠ QCD !

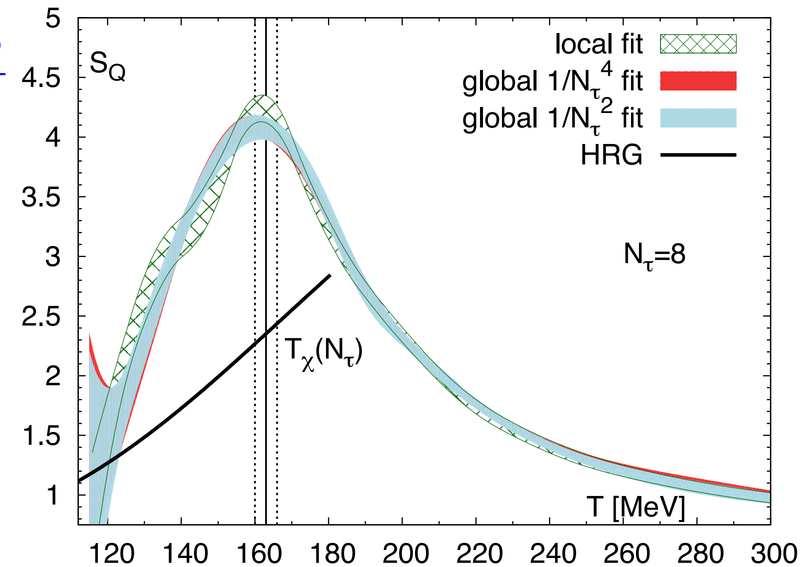
Deconfinement transition happens at lower temperature but the Polyakov loop behaves smoothlyaround T_c , *Z(3) symmetry plays no apparent role*

How to define deconfinement transition in QCD ?

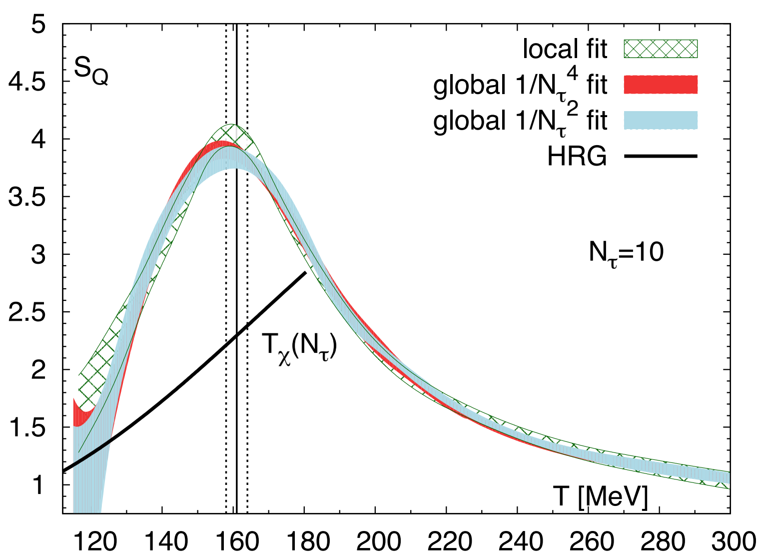
The entropy of static quark

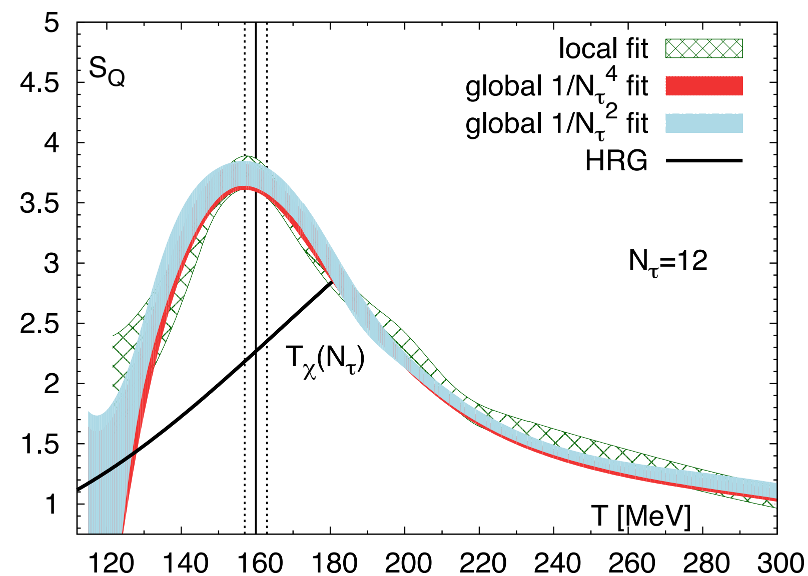
$$S_Q = -\frac{\partial F_Q}{\partial T}$$





TUMQCD, PRDD93 (2016) 114502



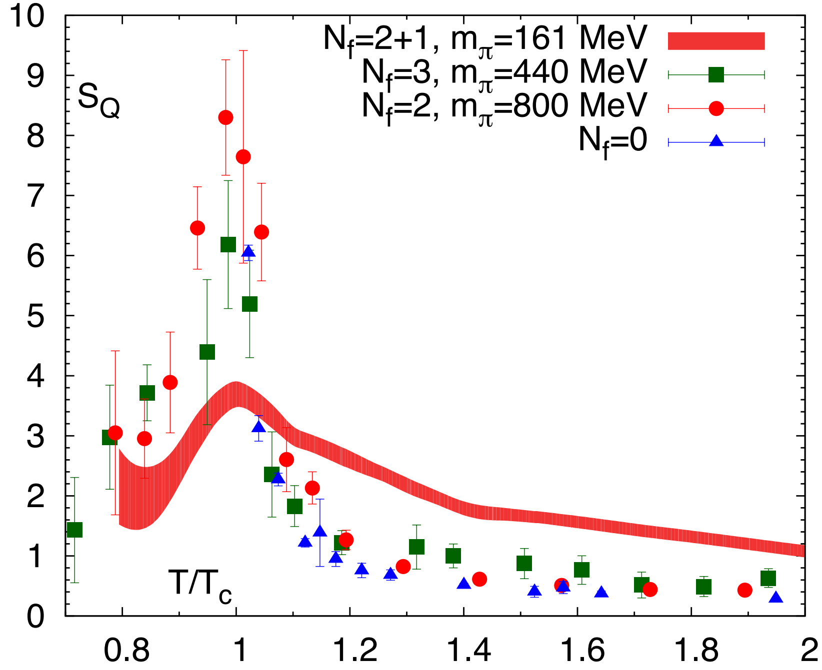


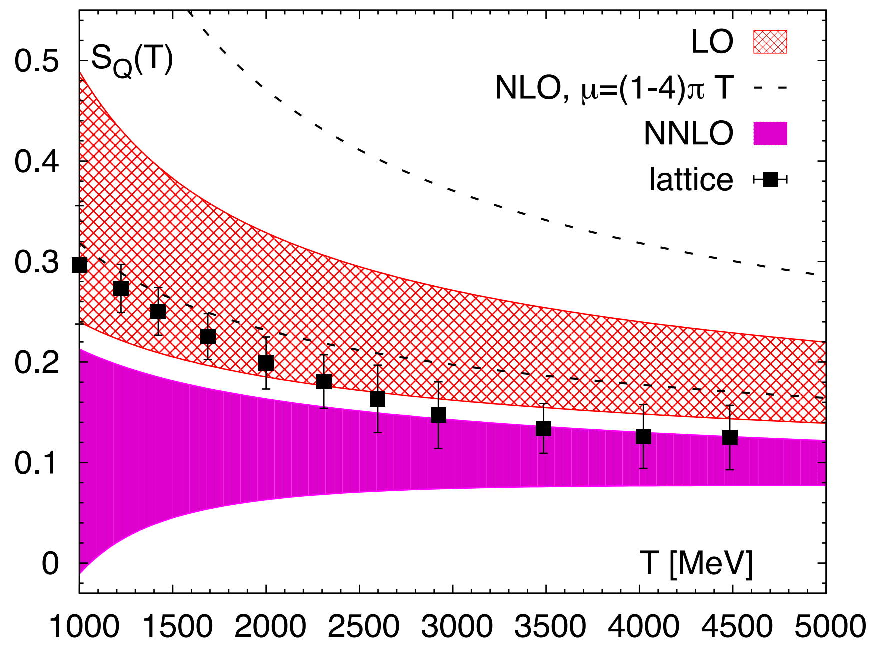
The onset of screening corresponds to peak is S_Q and its position coincides with T_c

The entropy of static quark

TUMQCD, PRDD93 (2016) 114502

$$S_Q = -\frac{\partial F_Q}{\partial T}$$





At low *T* the entropy S_Q increases reflecting the increase of states the heavy quark can be coupled to; at high temperature the static quark only "sees" the medium within a Debye radius, as *T* increases the Debye radius decreases and S_Q also decreases

The peak in the entropy is broader and smaller for smaller quark mass

Weak coupling (EQCD) calculations work for *T> 2000* MeV
Berwein et al, PRD 93 (2016) 034010

Free energy of a static quark anti-quark pair at high T

The work to separate the $Q\bar{Q}$ pair from distance r_1 to r_2 : $F_{Q\bar{Q}}(r_2) - F_{Q\bar{Q}}(r_1)$

Leading order in perturbation theory:

$$F_{Q\bar{Q}}(r,T) = -\frac{1}{9}\frac{\alpha_s^2}{r^2 T}\exp(-2m_D r) + F_\infty$$

In QED at leading order:

$$F_{Q\bar{Q}}(r,T) = -\frac{\alpha}{r}\exp(-m_D r) + F_\infty$$

Conjecture: in QCD the work is reduced due to cancelation of color singlet and octet contribution

Fierz idenity: $\delta_{ij}\delta_{lk} = \frac{1}{N_c}\delta_{ik}\delta_{lj} + 2T^a_{ik}T^a_{lj}$

$$e^{-F_{Q\bar{Q}}(r,T)/T} = \frac{1}{9}e^{-F_S(r,T)/T} + \frac{8}{9}e^{-F_O(r,T)/T}$$

$$e^{-F_S(r,T)/T} = \frac{1}{N_c}\langle \mathrm{tr} W(r) W^\dagger(0)\rangle, \quad W(r) = \prod_{\tau=0}^{N_\tau - 1} U_0(\mathbf{r},\tau)$$

LO:

$$F_S = -\frac{4}{3}\frac{\alpha_s}{r}e^{-m_D r} + F_\infty, \quad F_O = +\frac{1}{6}\frac{\alpha_s}{r}e^{-m_D r} + F_\infty$$

➡ The LO result for $F_{Q\bar{Q}}$ is recovered

Free energy of a static quark anti-quark pair at high T (cont'd)

The definition of F_S requires gauge fixing. Is it possible to have a gauge invariant decomposition of $F_{Q\bar{Q}}$ into singlet and octet contributions ?

Yes, for $r \ll 1/T$ using pNRQCD

$$e^{-F_{Q\bar{Q}}(r,T)/T} = \langle S(r,1/T)S(r,0)\rangle + L_A \langle O^a(r,1/T)O^a(r,0)\rangle$$

L_A is Polyakov loop in the adjoint representation

$$e^{-F_{Q\bar{Q}}(r,T)/T} = \frac{1}{9} e^{-f_s(r,T)/T} + \frac{8}{9} e^{-f_o(r,T)/T},$$

$$f_s = V_s(r) + \mathcal{O}(\alpha_s^2 r T^2),\ f_o = V_o(r) - \frac{N_c \alpha_s m_D}{2} + \mathcal{O}(\alpha_s^2 r T^2)$$

Brambilla et al, PRD 82 (2010) 074019

$$F_s = f_s + \mathcal{O}(\alpha_s^3 T) + \mathcal{O}(\alpha_s^2 r T^2),\ F_O = f_o + \mathcal{O}(\alpha_s^3 T) + \mathcal{O}(\alpha_s^2 r T^2)$$

Berwein et al, PRD 96 (2017) 014025

The naïve and the pNRQCD decomposition into singlet and octet agree

To calculate $F_{Q\bar{Q}}(r,T)$ and $F_S(r,T)$ for $r \sim 1/m_D$ another EFT, namely EQCD, should be used

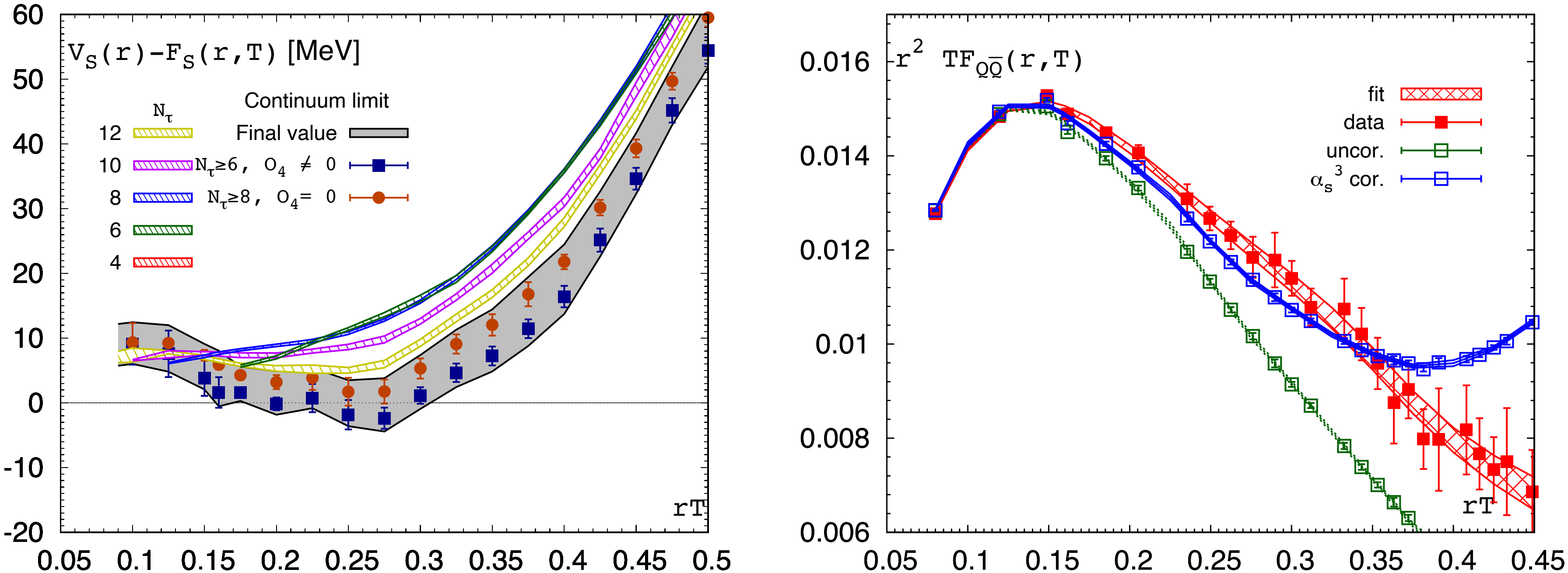
Free energy at short distances: lattice results vs. pNRQCD

The difference between V_s and F_S is small as expected for $rT < 0.3$

Construct pNRQCD prediction for $F_{Q\bar{Q}}$ using the lattice data for F_S and V_s as proxy for f_s together with the relation:

$$f_o = -\frac{1}{8} f_s + \frac{3\alpha_s^3}{8r}\left(\frac{\pi^2}{4} - 3\right)$$

works !



T=407 MeV

TUMQCD, PRD 98 (2018) 054511

The interaction of static Q and $\bar{Q}$ is vacuum like for $rT < 0.3$

Free energy in the screening regime: lattice vs. weak coupling

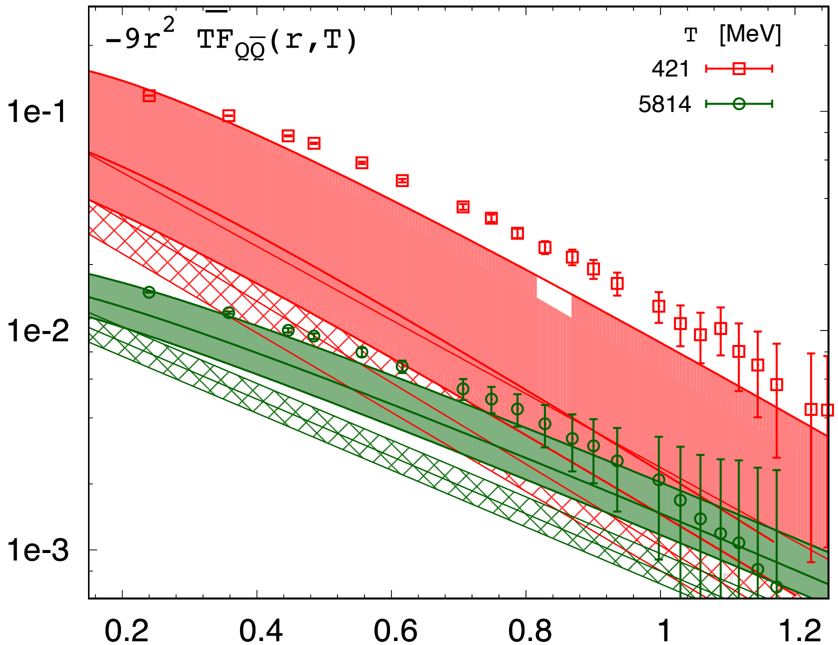
NLO in EQCD results are available for $\bar{F}_i(r,T) = F_i(r,T) - F_\infty(T)$

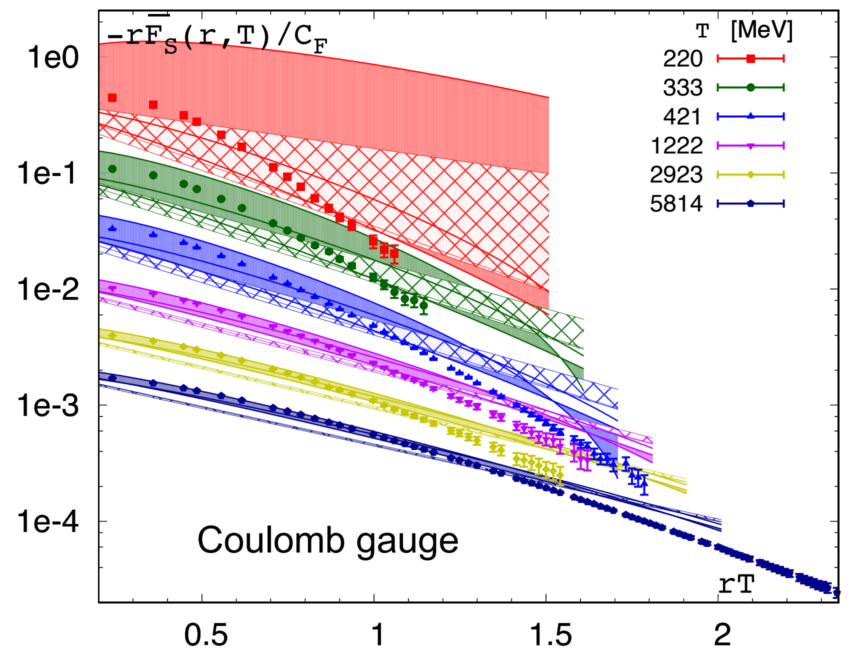
Nadkarni, PRD 33 (1986) 3738

$$F_{Q\bar{Q}}(r,T) = -\frac{\alpha_s^2 e^{-2m_D r}}{9r^2 T}(1+\alpha_s(\delta Z_1(\mu) + rTf(rm_D)))$$

Burnier et al, JHEP 01 (2010) 054

$$F_S(r,T) = -\frac{4\alpha_s e^{-m_D r}}{3r}(1+\alpha_s(\delta Z_1(\mu) + rTf_1(rm_D)))$$





TUMQCD, PRD 98 (2018) 054511

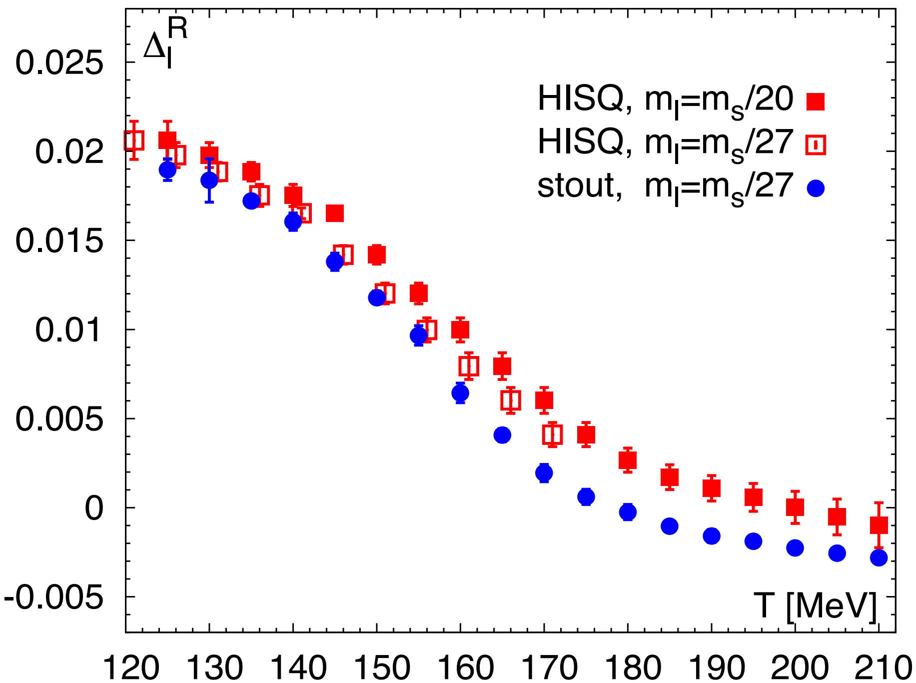
Lattice results are in reasonable agreement with NLO weak coupling result for *rT<0.6*, at larger distances, non-pertubtative effects (due to chromo-magnetic sector) become important

The chiral transition at non-zero temperature

Renormalized chiral condensate

$$\langle\bar\psi\psi\rangle \Rightarrow \Delta_l^R(T) = \\ = m_s r_1^4(\langle\bar\psi\psi\rangle_T - \langle\bar\psi\psi\rangle_{T=0}) + d, \\ d = m_s r_1^4 \langle\bar\psi\psi\rangle_{T=0}^{m_q=0}, \quad r_1 = 0.3106\text{fm}$$

HotQCD, PRD85 (2012) 054503;
Bazavov, PP, PRD 87(2013)094505,
Borsányi et al, JHEP 1009 (2010) 073

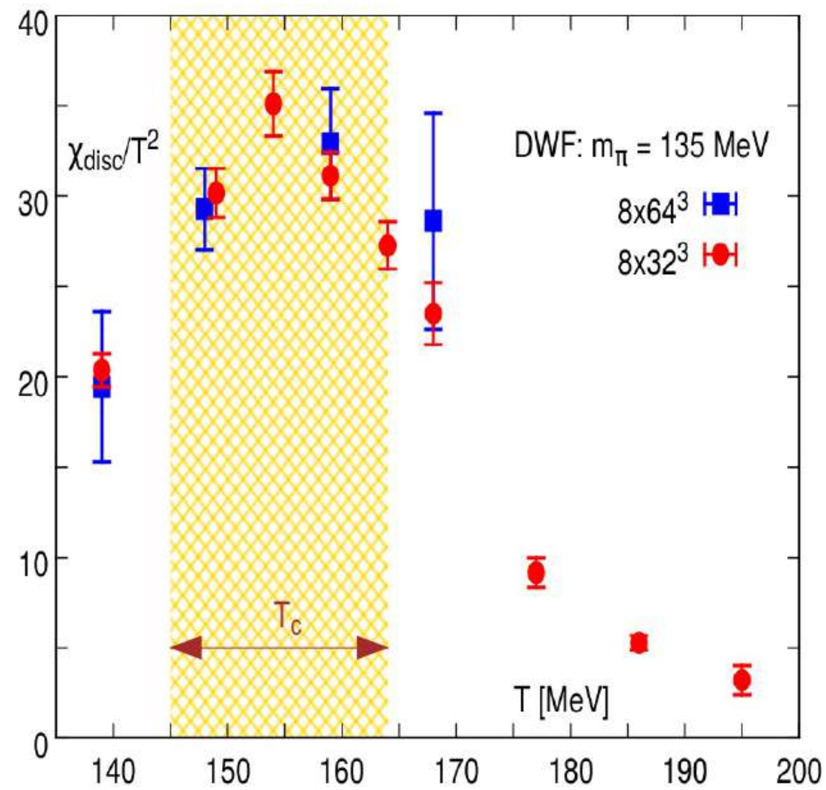


$$T_c = (154 \pm 8 \pm 1(scale))\text{MeV}$$

Fluctuations of the order parameter:

$$\chi_{disc} = VT^{-1}\left(\langle(\bar\psi\psi)^2\rangle - \langle\bar\psi\psi\rangle^2\right)$$

HotQCD, PRL 113 (2014)082001



$$T_c = (155 \pm 8 \pm 1)\text{MeV}$$

No increase with the volume
$\Rightarrow$ Crossover transition

O(4) scaling and the chiral transition temperature

$$SU_A(2) \times SU_V(2) \sim O(4)$$

For sufficiently small m_l and in the vicinity of the transition temperature:

$$f(T, m_l) = -\frac{T}{V} \ln Z = f_{reg}(T, m_l) + f_s(t, h), \; t = \frac{1}{t_0}\left(\frac{T - T_c^0}{T_c^0} + \kappa \frac{\mu_q^2}{T^2}\right), \; H = \frac{m_l}{m_s}, h = \frac{H}{h_0}$$

governed by universal *O(4)* scaling $\quad M = -\frac{\partial f_s(t,h)}{\partial H} = h^{1/\delta} f_G(z), \;\; z = t/h^{1/\beta\delta}$

$$\langle q\bar{q} \rangle = T(\partial \ln Z)/\partial m_f$$

T_c^0 is critical temperature in the mass-less limit, h_0 and t_0 are scale parameters

Pseudo-critical temperatures for non-zero quark mass are defined as peaks in the response functions (susceptibilities) :

$$\chi_{m,l} = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial m_l^2} \sim m_l^{1/\delta - 1} \quad \chi_{t,l} = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial m_l \partial t} \sim m_l^{\frac{\beta-1}{\beta\delta}} \quad \chi_{t,t} = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial t^2} \sim |t|^{-\alpha}$$

$$T_{m,l} \quad = \quad T_{t,l} \quad = \quad T_{t,t} \quad = \quad T_c^0$$

in the zero quark mass limit

$$\frac{\chi_{l,m}}{T^2} = \frac{T^2}{m_s^2}\left(\frac{1}{h_0} h^{1/\delta - 1} f_\chi(z) + reg.\right)$$

universal scaling function has a peak at $z = z_p$

$$T_c(H) = T_{m,l} = T_c^0 + T_c^0 \frac{z_p}{z_0} H^{1/(\beta\delta)} + \ldots$$

Caveat : staggered fermions *O(2)*

$m_l \rightarrow 0$, $a > 0$,

proper limit $a \rightarrow 0$, before $m_l \rightarrow 0$

The chiral cross-over temperature for physical masses

Chiral order parameter:

$$\Sigma = \frac{1}{f_K^4}\left[m_s\langle \bar{u}u + \bar{d}d\rangle - (m_u + m_d)\langle \bar{s}s\rangle\right] \qquad \langle q\bar{q}\rangle = T(\partial \ln Z)/\partial m_f$$

and the corresponding susceptibilities:

$$\chi^\Sigma = m_s\left(\frac{\partial}{\partial m_u} + \frac{\partial}{\partial m_d}\right)\Sigma \qquad \chi = \frac{m_s^2}{f_K^4}\left[\langle(\bar{u}u + \bar{d}d)^2\rangle - \left(\langle \bar{u}u\rangle + \langle \bar{d}d\rangle\right)^2\right]$$

For non-zero chemical potential we use Taylor expansion

$$\Sigma(T,\mu_X) = \sum_{n=0}^{\infty}\frac{C_{2n}^{\Sigma}(T)}{(2n)!}\left(\frac{\mu_X}{T}\right)^{2n} \quad \chi(T,\mu_X) = \sum_{n=0}^{\infty}\frac{C_{2n}^{\chi}(T)}{(2n)!}\left(\frac{\mu_X}{T}\right)^{2n} \qquad C_0^\Sigma = \Sigma \quad C_0^\chi = \chi$$

Derivatives in μ_X^2 are similar to derivatives in T $\quad$ $e.g.\ \partial_T C_0^\chi \sim C_2^\chi$

$\Rightarrow$ the following quantities will peak at T_c

$\chi^\Sigma,\ C_0^\chi(T) \sim \chi_{l,m} \qquad \partial_T C_0^\Sigma,\ C_2^\Sigma(T) \sim \chi_{t,m}$

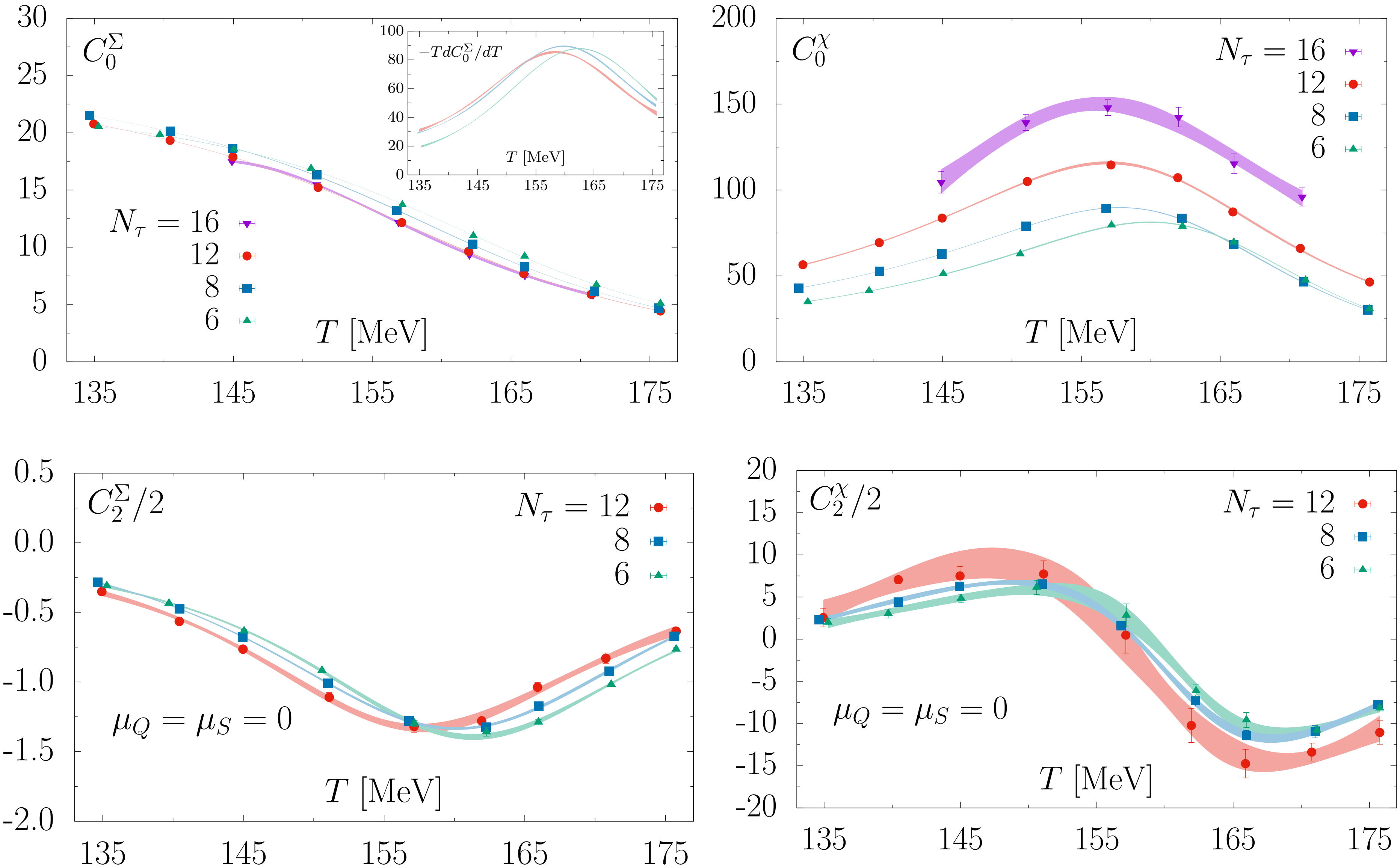
HotQCD, PLB795 (2019) 15

5 different definitions of T^{pc}:

$$\partial_T C_0^\chi = 0,\ \partial_T \chi^\Sigma = 0\ , C_2^\chi = 0 \qquad \partial_T^2 C_0^\Sigma = 0,\ \partial_T C_2^\Sigma = 0$$

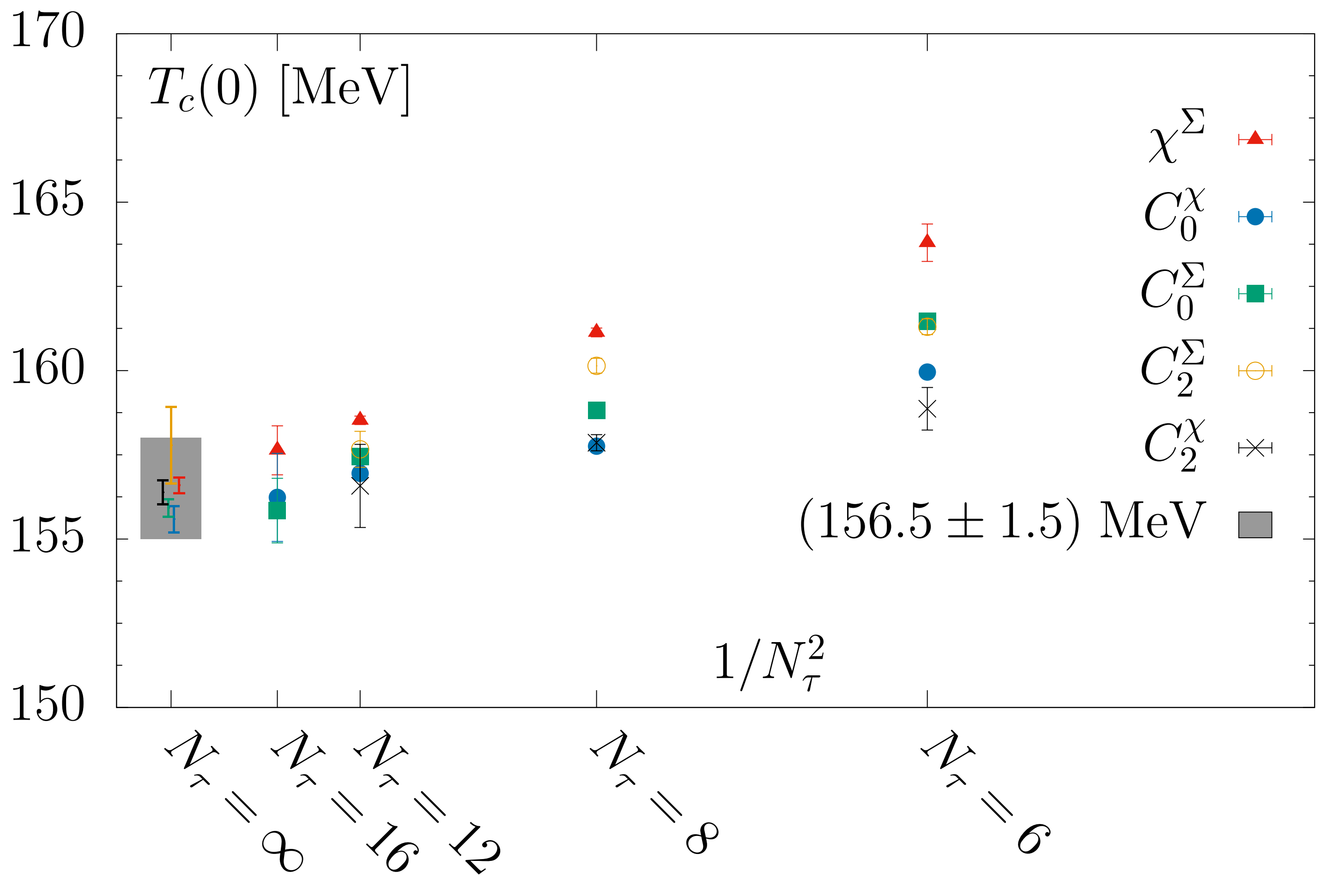
The 5 different T_c values reduce to $T_{l,m}$ and $T_{l,t}$ if regular part is zero

Lattice calculations based on 100K - 500 K configurations, $N_\tau = 6 - 12$, and 4K configurations for $N_\tau = 16$



HotQCD, PLB795 (2019) 15

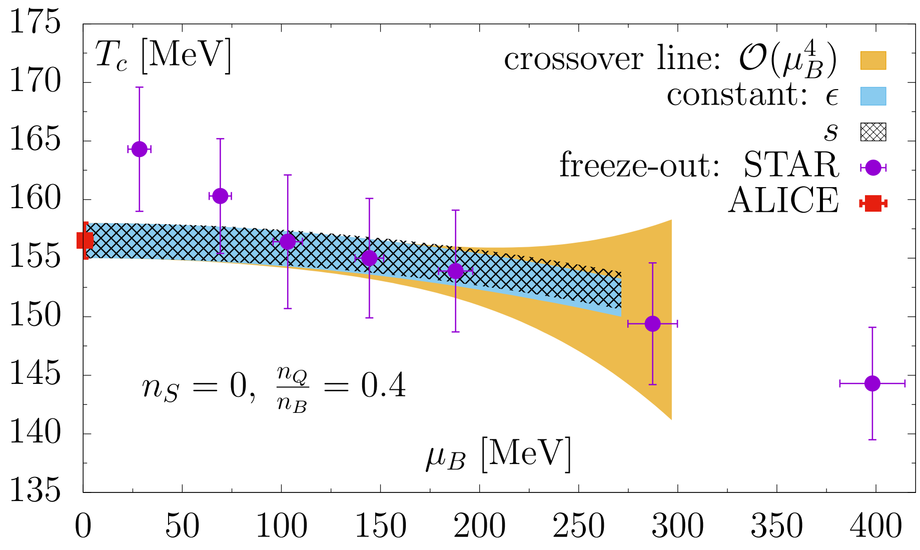
Different definitions of T_c surprisingly agree in the continuum limit and we for zero chemical potential we get $T_c = 156 \pm 1.5$ MeV



HotQCD, PLB795 (2019) 15

The chiral cross-over temperature at non-zero density

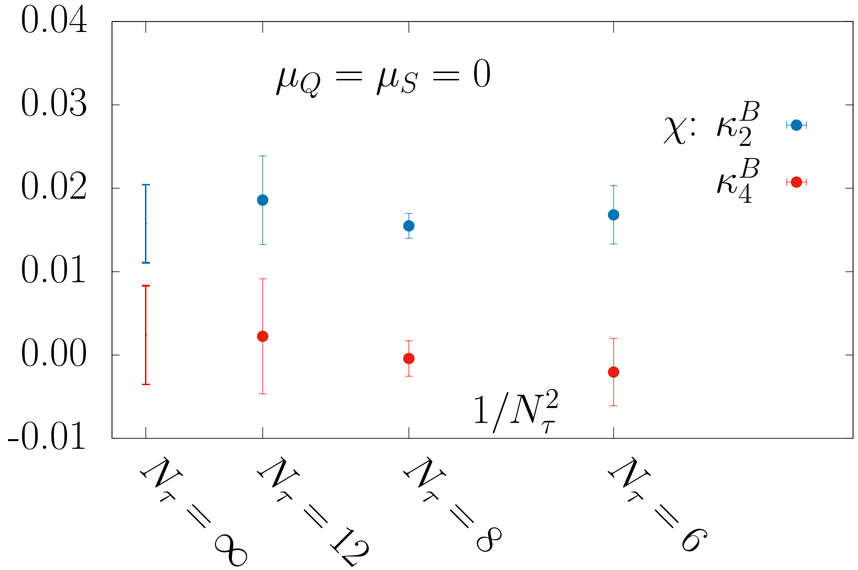
$$T_c(\mu_B) = T_c(0)\left[1 - \kappa_2^B\left(\frac{\mu_B}{T_c(0)}\right)^2 - \kappa_4^B\left(\frac{\mu_B}{T_c(0)}\right)^4\right]$$



The freeze-out condition corresponding to constant energy density or constant entropy density agrees with the crossover line within errors

The μ_B dependence of T_c is small

$$\kappa_2^{B,\chi} \simeq \kappa_2^{B,\Sigma}$$



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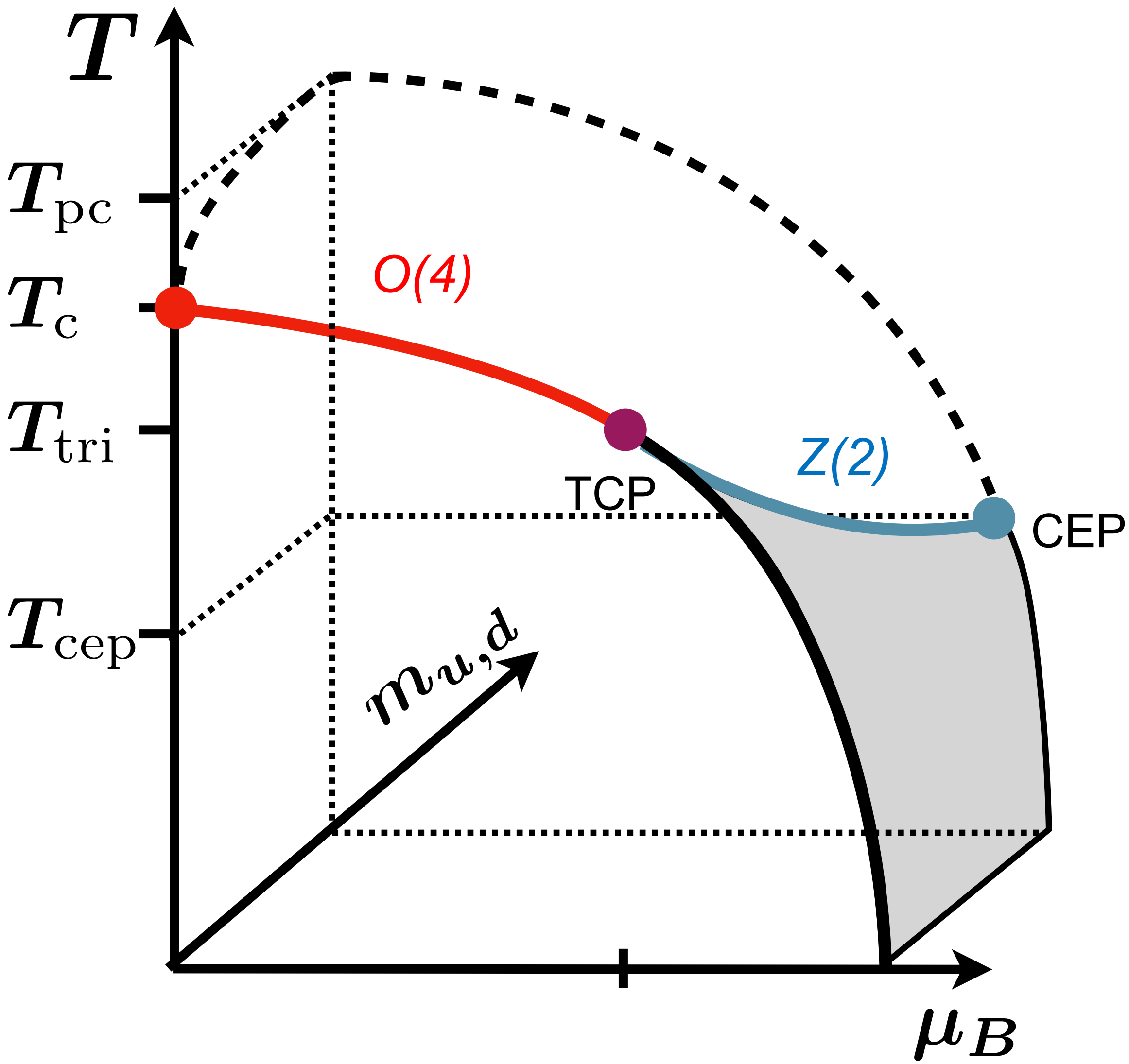
QCD phase diagram in extended parameter space

The QCD phase diagram in $T - \mu_B$ plane is related to the nature of the QCD phase transition at zero light quark masses



Chiral phase transition in 2+1 flavor QCD

What is the nature of the chiral transition in 2+1 flavor QCD for fixed m_s and $m_l \to 0$?

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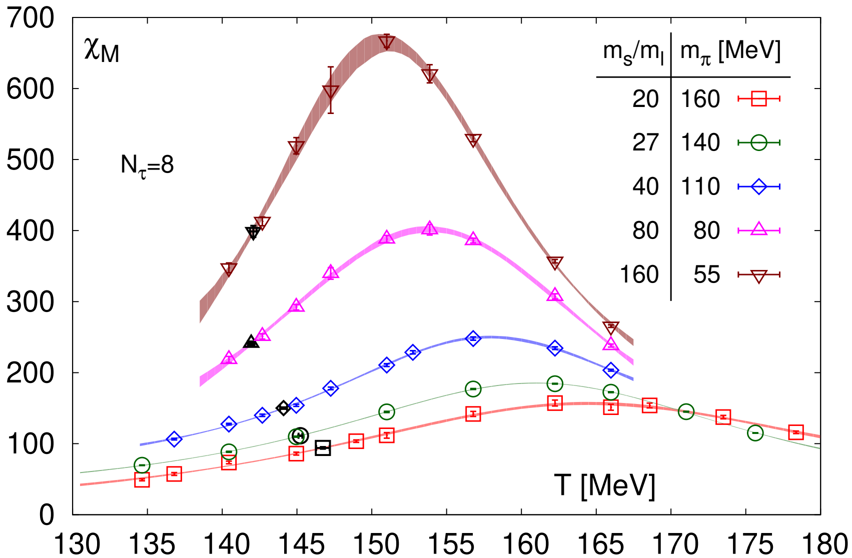
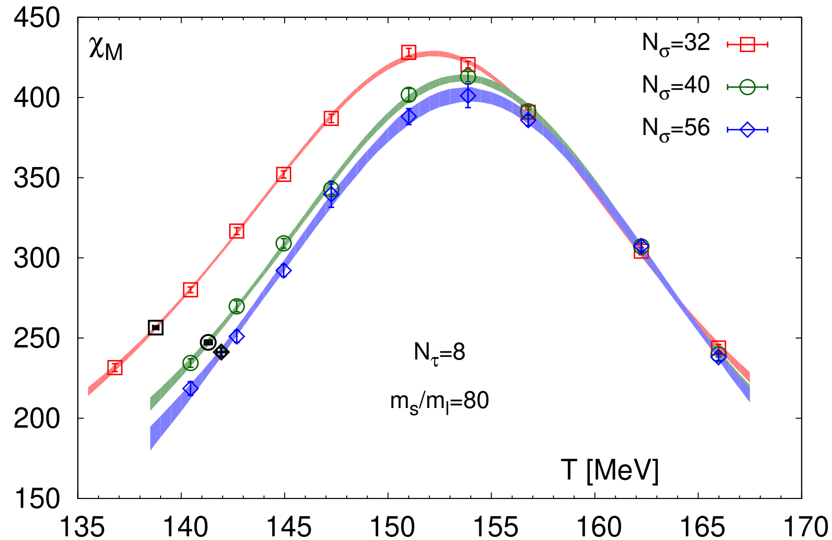


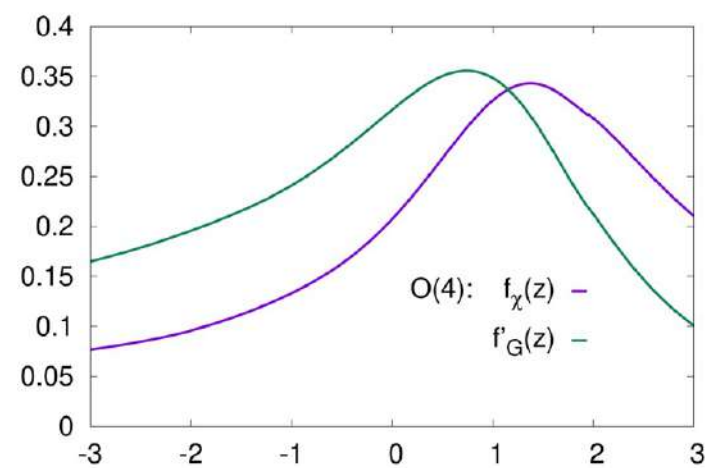


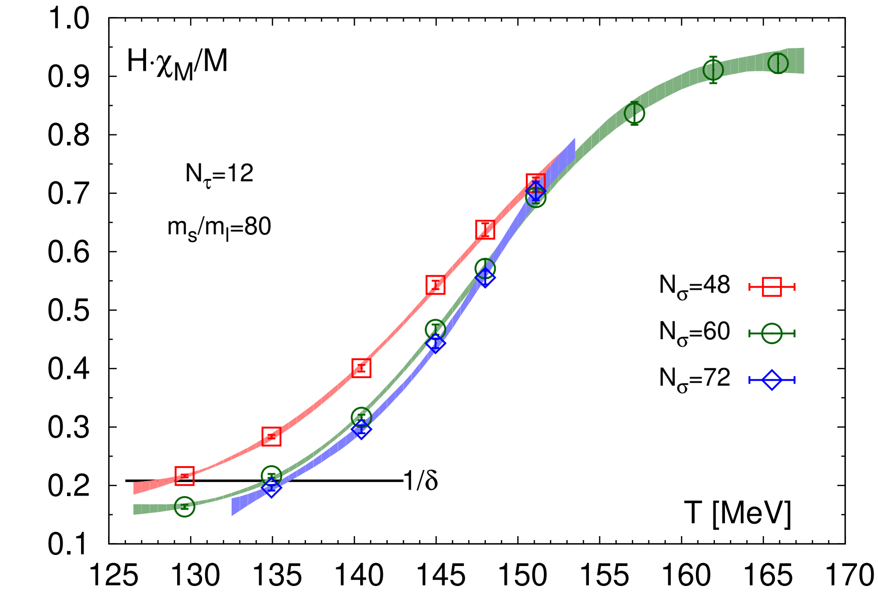
$$M = h^{1/\delta} f_G(z, z_L) + f_{sub}(T, H, L) \ ,$$

$$\chi_M = h_0^{-1} h^{1/\delta-1} f_\chi(z, z_L) + \tilde{f}_{sub}(T, H, L) \ .$$

$$T_p(H, L) = T_c^0 \left(1 + \frac{z_p(z_L)}{z_0} H^{1/\beta\delta}\right) \ + \ \text{sub leading}$$

$$T_X(H, L) = T_c^0 \left(1 + \left(\frac{z_X(z_L)}{z_0}\right) H^{1/\beta\delta}\right)$$



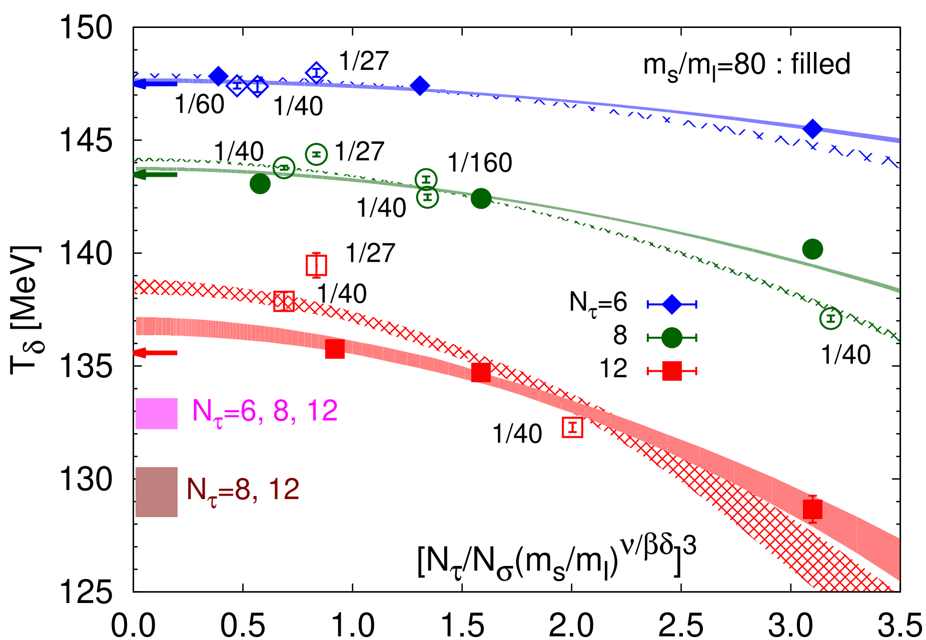


$$\frac{H\chi_M(T_\delta, H, L)}{M(T_\delta, H, L)} = \frac{1}{\delta} \, ,$$

$$\chi_M(T_{60}, H) = 0.6\chi_M^{max} \, .$$

$$T_X(H, L) = T_c^0 \left(1 + \left(\frac{z_X(z_L)}{z_0}\right) H^{1/\beta\delta}\right)$$
$$+ c_X H^{1-1/\delta+1/\beta\delta} \quad , \quad X = \delta, \; 60$$

$$z_{60} \simeq z_\delta \simeq 0$$



Use $O(4)$ fits for m_l and volume dependence

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Continuum extrapolations:

$$T_c^0 = 132^{+3}_{-6} \text{ MeV}$$

$$T^{CEP} < 132 \text{ MeV}$$