

The transition temperature in QCD

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Introduction (a little bit of history)

Previous results on the transition temperature in QCD

Lattice QCD

- HISQ action

- Force filter

- Staggered fermions and taste symmetry

- Pion splittings

- Lattice scale setting

Finite-temperature transition in QCD

- Chiral condensate and susceptibility

- $O(N)$ scaling analysis

- Deconfinement

Conclusion

“Statistical Thermodynamics of Strong Interactions”

- ▶ Hagedorn (1965) applied a thermodynamical description to high-energy collisions:

The essential idea is now the following one: the thermodynamical system consisting of more or less excited hadrons is itself nothing else than a highly excited hadron (because in the sense of our above statement we have no way to distinguish between a resonance, a fire-ball and our thermodynamical system—except that they differ in the degree of excitation).

- ▶ Limiting temperature $T_0 = 158 \pm 3$ MeV

- ▶ Hagedorn (1968)

A fireball is

(T) → a statistical equilibrium (hadronic black body radiation) of an undetermined number of all kinds of fireballs; each of which, in turn, is considered to be

- ▶ Limiting temperature $T_0 = 160$ MeV

“Statistical Thermodynamics of Strong Interactions”

- ▶ Hagedorn (1970)

A fireball is:

→ *a statistical equilibrium (hadronic black-body radiation) of an undetermined number of all kinds of fireballs, each of which, in turn, is considered to be* (P)

- ▶ The number of hadronic states between m and $m + dm$ is given asymptotically by

$$\lim_{m \rightarrow \infty} \rho(m) dm = \frac{a}{m^{5/2}} \exp \left[\frac{m}{T_0} \right] dm$$

- ▶ T_0 is “the highest possible temperature”

Reinterpretation of T_0

- ▶ After the discovery of asymptotically-free theories existence of the limiting temperature was reinterpreted as a transition to a new phase of matter, quark-gluon plasma
- ▶ Collins, Perry (1975), Cabbibo, Parisi (1975), conjectured phase structure is shown

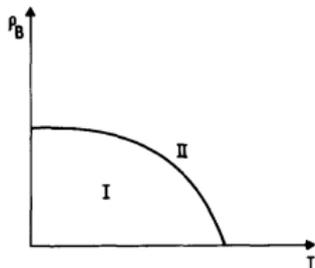


Fig. 1. Schematic phase diagram of hadronic matter. ρ_B is the density of baryonic number. Quarks are confined in phase I and unconfined in phase II.

Reinterpretation of T_0

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- ▶ Collins, Perry (1975), Cabbibo, Parisi (1975), conjectured phase structure is shown (left), current expectations (right)

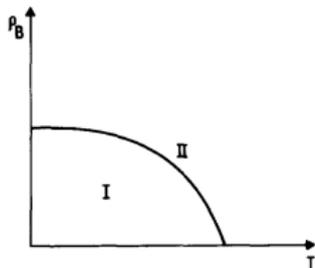
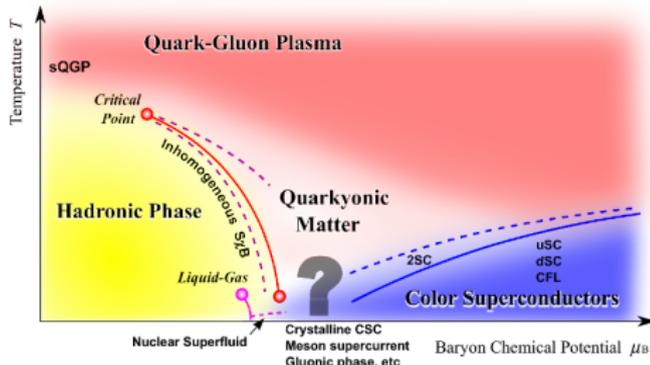


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Hadron Resonance Gas model

- ▶ Following Hagedorn's picture, the Hadron Resonance Gas model¹ approximates the spectrum with currently known states from PDG

$$p^{HRG}/T^4 = \frac{1}{VT^3} \sum_{i \in \text{mesons}} \ln Z_{m_i}^M(T, V, \mu_{X^a}) \\ + \frac{1}{VT^3} \sum_{i \in \text{baryons}} \ln Z_{m_i}^B(T, V, \mu_{X^a}),$$

where

$$\ln Z_{m_i}^{M/B} = \mp \frac{Vd_i}{2\pi^2} \int_0^\infty dk k^2 \ln(1 \mp z_i e^{-\varepsilon_i/T}) \quad ,$$

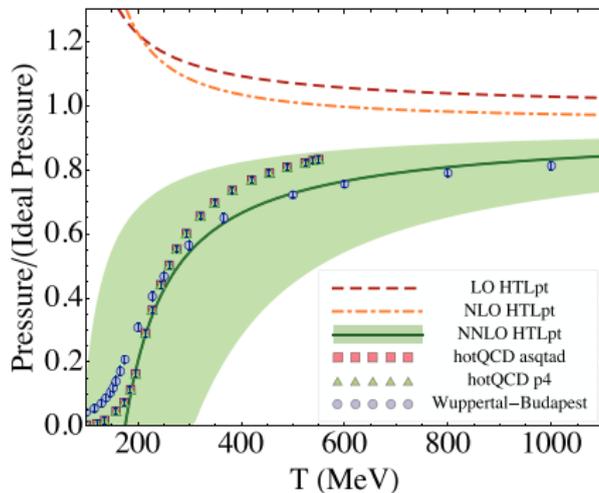
with energies $\varepsilon_i = \sqrt{k^2 + m_i^2}$, degeneracy factors d_i and fugacities

$$\ln z_i = \sum_a X_i^a \mu_{X^a}/T \quad .$$

¹Hagedorn (1965), Dashen, Ma, Bernstein (1969), Venugopalan, Prakash (1992)

High-temperature phase and perturbation theory

- ▶ Deconfinement is signaled by liberation of degrees of freedom with quark and gluon quantum numbers
- ▶ The high-temperature phase (due to asymptotic freedom) is accessible² to perturbation theory
- ▶ Recent results by Strickland et al. (2011) in 3-loop hard-thermal-loop³ perturbation theory are shown

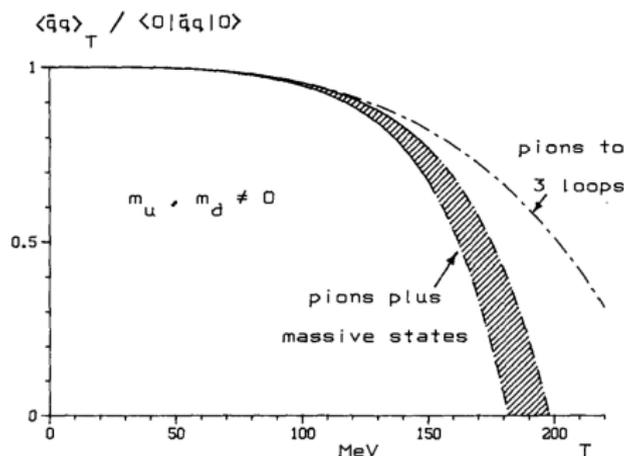


²Kapusta (1979)

³Braaten, Pisarski (1990)

Chiral symmetry restoration

- ▶ The high-temperature phase is chirally symmetric, a chiral symmetry restoration transition is expected
- ▶ The quark condensate should disappear at some temperature, early estimates, for instance, Gerber, Leutwyler (1989) give $T_c = 190$ MeV (170 MeV in the chiral limit)



Early lattice results

First study of the deconfinement transition in $SU(2)$ pure gauge theory:

- ▶ McLerran, Svetitsky (1981) $T_{cr} = 200$ MeV, Polyakov loop (left)
- ▶ Kuti et al. (1981) $T_c = 160 \pm 30$ MeV,
- ▶ Engels et al. (1981) $T_c = 210 \pm 10$ MeV, energy density (right)

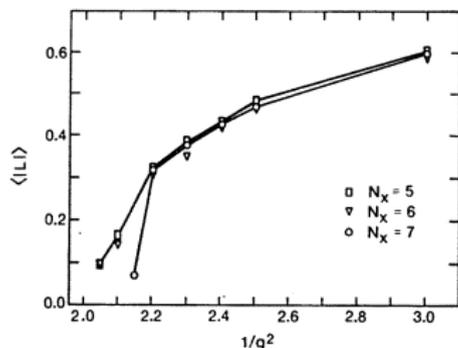


Fig. 2. Magnetization curves for $N_f = 3$. We display $\langle |L| \rangle$ rather than $\langle L \rangle$ to remove effects of domain nucleation as shown in fig. 1. Points for $N_x = 5$ and for $N_x = 7$ are joined to guide the eye.

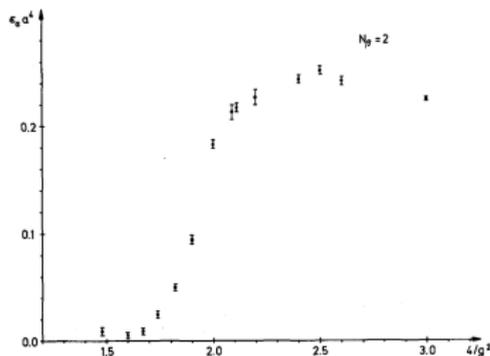


Fig. 3. Energy density of gluon matter versus $4/g^2$, at fixed lattice size $N_\beta = 2$, after about 500 iterations.

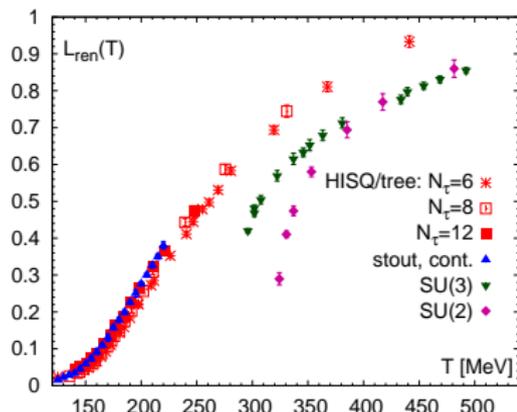
Pure gauge vs QCD

The Polyakov loop:

$$L_{ren}(T) = z(\beta)^{N_\tau} L_{bare}(\beta), \quad L_{bare}(\beta) = \left\langle \frac{1}{3} \text{Tr} \prod_{x_0=0}^{N_\tau-1} U_0(x_0, \vec{x}) \right\rangle$$

- ▶ Related to the free energy of a static quark anti-quark pair

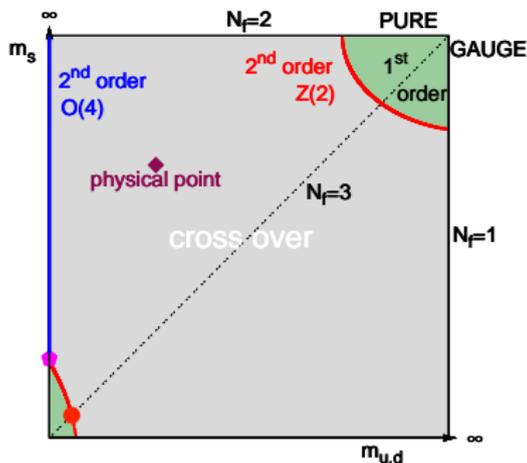
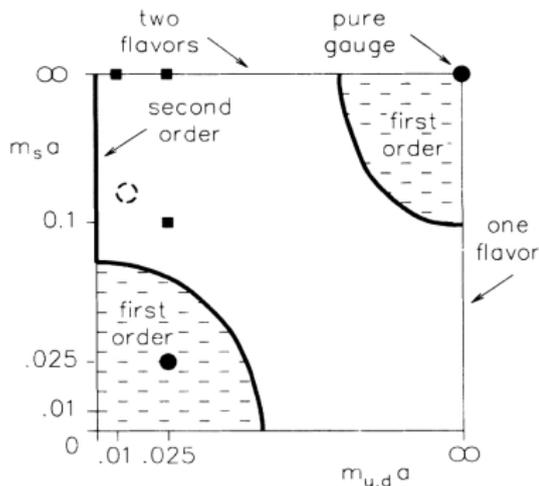
$$L_{ren}(T) = \exp(-F_\infty(T)/(2T))$$



- ▶ The increase of $L_{ren}(T)$ (and decrease of $F_\infty(T)$) is related to the onset of screening at higher temperatures.
- ▶ The order parameter in pure gauge theory but not in full QCD, the behavior in $SU(2)$, $SU(3)$ and 2+1 flavor QCD is quite different!

Pure gauge vs QCD

- ▶ Pure gauge = infinitely heavy quarks
- ▶ Real world = almost massless quarks ($m_u, m_d \ll \Lambda_{QCD}$)
- ▶ Pisarski, Wilczek (1984) discussed possible behavior in the chiral limit, Brown et al. (1990) later attempted to address this problem on the lattice, conjectured phase diagram (left),
- ▶ a more recent study by Ding et al (2011) puts an upper bound $m_\pi = 75$ MeV (right)



- ▶ Where is the real world in this phase diagram?

2+1 flavor QCD

- ▶ Lattice QCD calculations of mid-2000's: Bernard et al. (2005), Cheng et al (2006), Aoki et al (2006) indicate that at the physical quark masses the transition is indeed an analytic crossover (at $\mu = 0$)
- ▶ If there is no genuine phase transition, is it possible to identify some transition temperature? Is there one? Are there many?

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Transition temperature(s)

- ▶ Bernard et al. [MILC] (2005) $T_c = 169(12)(4)$ MeV (chiral and deconfinement)
- ▶ Cheng et al. [RBC-Bielefeld] (2006) $T_c = 192(7)(4)$ MeV (chiral and deconfinement)
- ▶ Aoki et al. [BW] (2006)-(2010) $T_c = 151(3)(3)$ MeV (chiral),
 $T_c = 175(4)(3)$ MeV (deconfinement)
- ▶ Bazavov et al. [HotQCD], PRD85 (2012) 054503
 $T_c = 154(9)$ MeV (chiral), no T_c associated with deconfinement

HotQCD collaboration

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M. Cheng (Boston)

N. Christ (Columbia)

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Lattice QCD

- ▶ An observable \mathcal{O} in the path integral representation of QCD in the imaginary time (Euclidian) formalism:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\bar{\psi} D\psi DA \mathcal{O} \exp(-S),$$
$$Z = \int D\bar{\psi} D\psi DA \exp(-S), \quad S = \int d^4x \mathcal{L}_E,$$

where S is the action of the theory.

- ▶ Integrals may not be expanded (no small parameter), but may still be evaluated by other means.
- ▶ Lattice⁴ – discrete Euclidian space-time, serves as a regulator (momenta are bound) and allows for stochastic evaluation of path integrals,
 - ▶ quarks live on sites and gluons on links as SU(3) matrices

$$U_{x,\mu} = \mathcal{P} \exp \left\{ ig \int_x^{x+a\hat{\mu}} dy_\nu A_\nu(y) \right\}.$$

⁴Wilson, Phys. Rev. D 10, 2445 (1974)

Lattice QCD

- ▶ Lattice action

$$S = S_G + S_F, \quad S_F = \sum_{x,y} \bar{\psi}_x M_{x,y} \psi_y$$

($M_{x,y}$ is the fermion matrix) preserves the gauge symmetry, but there is the infamous fermion doubling problem – 16 species of fermions in 4D.

- ▶ Staggered fermions⁵ remove the 4-fold degeneracy, reduce 16 to 4 (call them tastes to distinguish from physical flavors), preserve a part of the chiral symmetry at non-zero lattice spacing.
- ▶ Rooting procedure⁶ is used to further reduce the number of species.
- ▶ Irrelevant operators (that vanish in the continuum limit) can be added to the lattice action to remove leading discretization effects – the idea of improved actions⁷.
- ▶ The p4⁸, asqtad⁹ and HISQ¹⁰ actions have similar improvement at high temperatures and differ by the degree of improvement at low temperatures.

⁵Kogut and Susskind, Phys. Rev. D 11, 395 (1975)

⁶Sharpe, PoS LAT2006, 022 (2006), Creutz, PoS LAT2007, 007 (2007)

⁷Symanzik, Nucl. Phys. B 226, 187 (1983)

⁸Heller, Karsch and Sturm, Phys. Rev. D 60, 114502 (1999)

⁹Orginos and Toussaint, Phys. Rev. D 59, 014501 (1999)

¹⁰E. Follana et al., Phys. Rev. D 75, 054502 (2007)

Lattice QCD

- ▶ Integrate fermionic degrees of freedom explicitly, then introduce bosonic fields to exponentiate the fermionic determinant:

$$\begin{aligned} Z &= \int \prod_{x,\mu} dU_{x,\mu} (\det M(U))^{1/4} \exp\{-S_G\} \\ &= \int \prod_{x,\mu} dU_{x,\mu} \prod_x [d\Phi_x^\dagger d\Phi_x] \exp\{-S_G - \Phi^\dagger (M^\dagger M)^{-1/4} \Phi\}. \end{aligned}$$

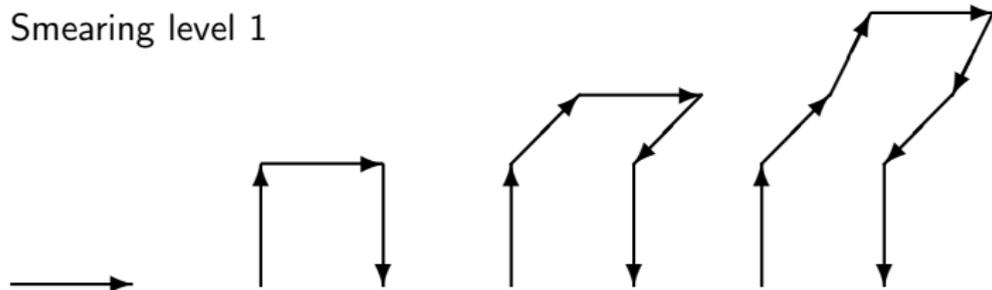
- ▶ If the weight is real this resembles canonical ensemble and we can use importance sampling techniques to estimate the integrals stochastically.
- ▶ Develop a Markov Chain Monte Carlo procedure to sample the phase space.
- ▶ Temperature is set by compactifying the temporal dimension, $T = 1/(N_\tau a)$, hold N_τ fixed and vary a .
- ▶ Lower temperatures – coarser lattices.
- ▶ Establish lines of constant physics (LCP), i.e. change bare quark masses with lattice spacing such that m_π , m_K are fixed.

HISQ action

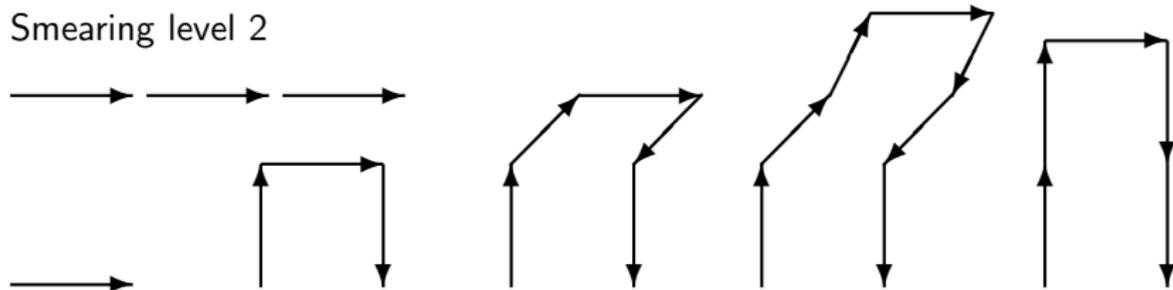
- ▶ **H**ighly – More improvement compared to previously used staggered actions (e.g., asqtad).
- ▶ **I**mproved – Adding higher-order (irrelevant) operators to the action allows for suppression of the discretization effects at $O(a^2)$.
- ▶ **S**taggered – A particular fermion discretization scheme which partially deals with the fermion doubling problem, conserves a part of the chiral symmetry on the lattice and is relatively cheap to simulate numerically.
- ▶ **Q**uarks.

HISQ action

Smearing level 1



Smearing level 2



HISQ force

- ▶ Calculate as the derivative of the action using the chain rule:

$$\frac{\partial S_F}{\partial U} = \frac{\partial S_F}{\partial X} \frac{\partial X}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U},$$

- ▶ where

- ▶ U – fundamental gauge links
- ▶ V – fat links level 1
- ▶ W – reunitarized links
- ▶ X – fat links level 2

- ▶ For projecting to $U(3)$ we have chosen

$$W = VQ^{-1/2}, \quad Q = V^\dagger V.$$

- ▶ To calculate the inverse square root one can apply the Cayley-Hamilton theorem¹¹

$$Q^{-1/2} = f_0 + f_1 Q + f_2 Q^2.$$

(All derivatives can be evaluated analytically!)

- ▶ For singular matrices V we use the singular value decomposition (SVD) algorithm:

$$V = A \Sigma B^\dagger, \quad A, B \in U(3) \quad \rightarrow \quad W = AB^\dagger.$$

¹¹Morningstar and Peardon, Phys. Rev. D 69, 054501 (2004),

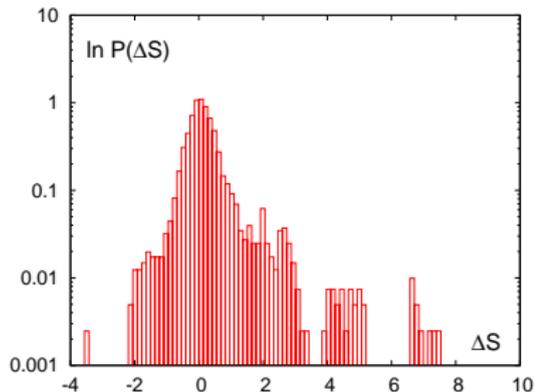
Example of reunitarization for $U(1)$

- ▶ Let $V = r e^{i\theta}$, then $W = e^{i\theta}$.
- ▶ The derivative

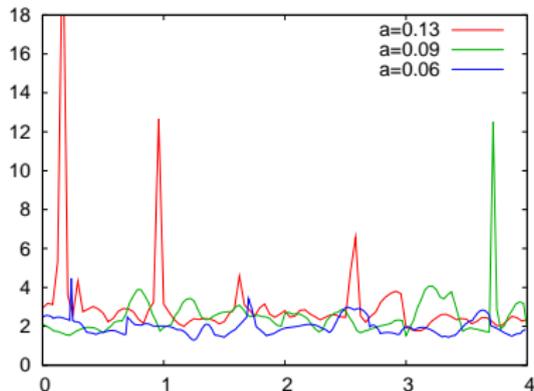
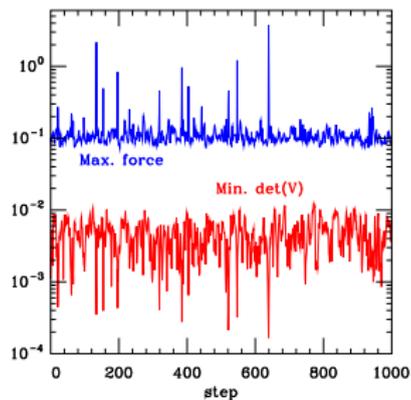
$$\begin{aligned}\frac{\partial W}{\partial V} &= \left(\frac{\partial W}{\partial V} \right)_{V^\dagger} = \frac{\partial(W, V^\dagger)}{\partial(V, V^\dagger)} \\ &= \frac{\partial(W, V^\dagger)}{\partial(r, \theta)} \cdot \frac{\partial(r, \theta)}{\partial(V, V^\dagger)} = \frac{1}{2r}.\end{aligned}$$

- ▶ For the matrix case the derivative is dominated by the smallest singular value of smeared link V .

Change in the action and fermion force



- ▶ Outliers in the histogram are caused by exceptionally large forces (coming from a small number of links).
- ▶ Less pronounced on finer lattices.



Filtered fermion force

- ▶ To deal with exceptionally large forces we introduce an “eigenvalue filter”.
- ▶ In the fermion force, if the lowest eigenvalue of a smeared link V is smaller than a certain cutoff, we replace

$$Q^{-1/2} \rightarrow (Q + \delta I)^{-1/2},$$

where δ is typically set to $5 \cdot 10^{-5}$.

- ▶ This effectively makes the guiding Hamiltonian slightly different from the original Hamiltonian, however, the integration algorithm by construction is reversible and area preserving
- ▶ With the HISQ action we use the RHMC algorithm, so the accept/reject step at the end of MD trajectory ensures correct equilibrium distribution.

Taste symmetry

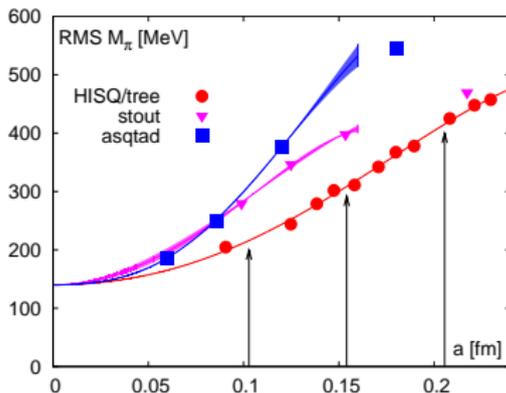
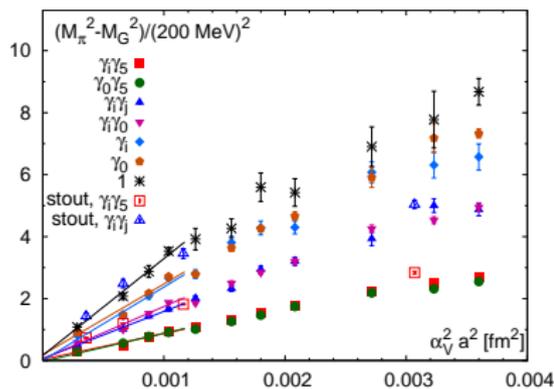
- ▶ Staggered fermion discretization describes a theory with four tastes. The rooting procedure (reducing four flavors to one by taking the fourth root of the fermion determinant) amounts to averaging between staggered tastes.
- ▶ Four tastes are not equivalent at non-zero lattice spacing because the taste symmetry is broken.
- ▶ As a result, only one of the pseudo-scalar mesons is massless in the chiral limit and the other 15 pseudo-scalar mesons have masses of order a^2 .
- ▶ Violations of the taste symmetry have been identified as the dominant source of the cutoff effects at $O(a^2)$ in the asqtad and p4 actions. They lead to distortion of the hadron spectrum at non-zero lattice spacing.
- ▶ In thermodynamics calculations deviations from the physical hadron spectrum show up at low temperatures, where agreement with the Hadron Resonance Gas (HRG) model is expected.
- ▶ The cutoff effects can be reduced either by going to finer lattices (e.g., asqtad $N_t = 8$ to $N_t = 12$) or by using an action with higher degree of improvement (e.g. HISQ).

Taste symmetry

- ▶ Taste violations affect the pseudo-scalar meson sector most
- ▶ The quadratic mass splitting of non-Goldstone mesons and the Goldstone meson is of order $\alpha^2 a^2$ (left panel).
- ▶ These splittings are to a good approximation mass independent
- ▶ The root-mean-squared (RMS) pion mass for asqtad, stout and HISQ (right panel)¹²:

$$m_{\pi}^{RMS} = \sqrt{\frac{1}{16} \left(m_{\gamma_5}^2 + m_{\gamma_0 \gamma_5}^2 + 3m_{\gamma_i \gamma_5}^2 + 3m_{\gamma_i \gamma_j}^2 + 3m_{\gamma_i \gamma_0}^2 + 3m_{\gamma_i}^2 + m_{\gamma_0}^2 + m_1^2 \right)}.$$

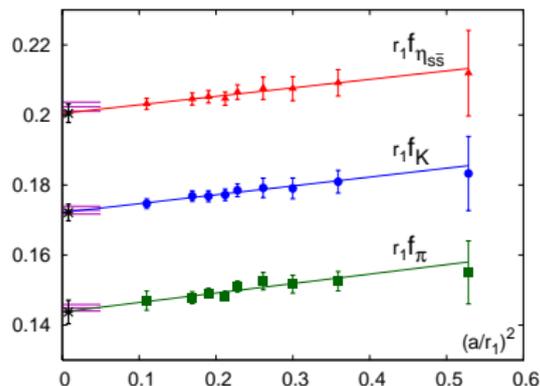
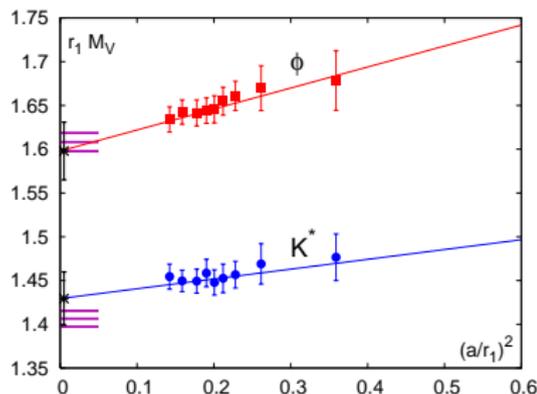
- ▶ Arrows on the right panel indicate $T = 160$ MeV on lattices with $N_{\tau} = 6, 8$ and 12 (from right to left)



¹²Bazavov, Petreczky (2010)

Hadron masses and decay constants

- ▶ ρ , K^* (left) and pseudoscalar decay constants (right) are shown
- ▶ Hadron spectrum on the lattice is heavier than physical, thus, at non-zero lattice spacing one expects the transition region to be at higher temperatures (and even more so for lattice actions with stronger cut-off effects)

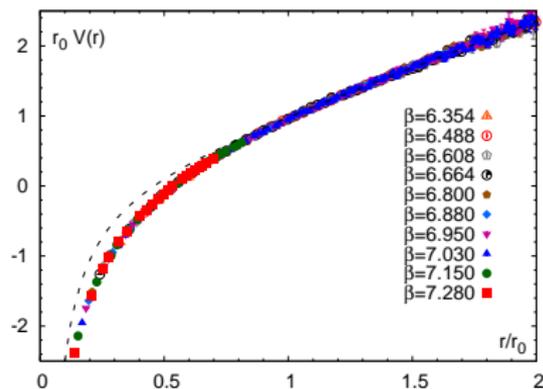
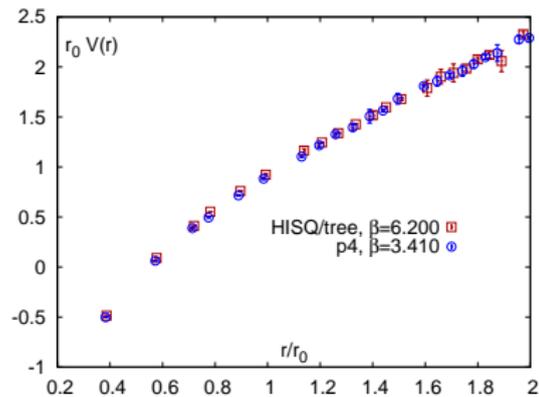


Scale setting, r_1

- ▶ The lattice spacing is determined from the static quark anti-quark potential, which does not show any noticeable cutoff dependence.
- ▶ Sommer scale¹³

$$\left(r^2 \frac{dV_{q\bar{q}}(r)}{dr} \right)_{r=r_n} = \begin{cases} 1.65, & n=0 \\ 1.0, & n=1 \end{cases}$$

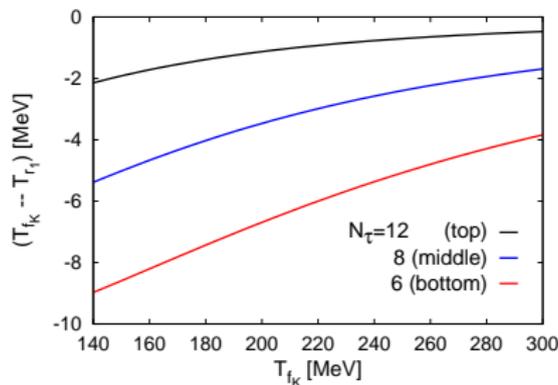
$r_0 = 0.468$ fm or $r_1 = 0.3106$ fm is used to convert to physical units.



¹³Sommer (1994)

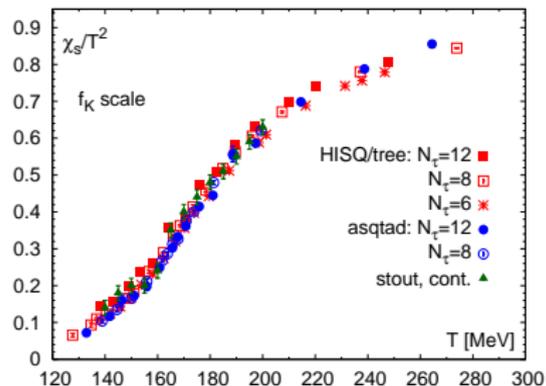
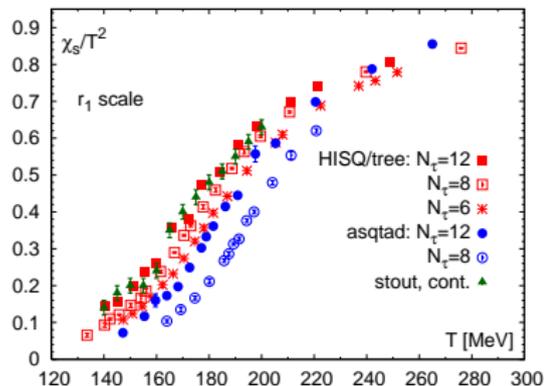
Scale setting with f_K

- ▶ Setting the scale with a hadronic quantity, f_K , may help to reduce the cut-off effects
- ▶ An uncertainty in temperature set with r_1 and f_K scale is shown



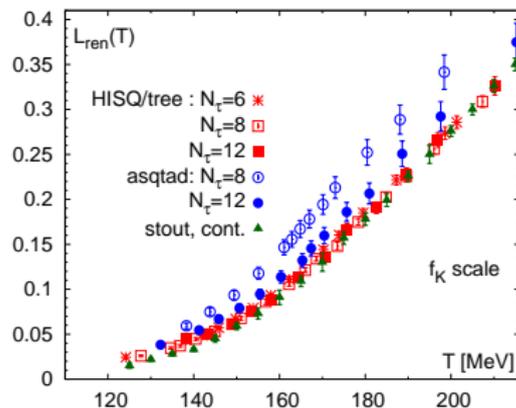
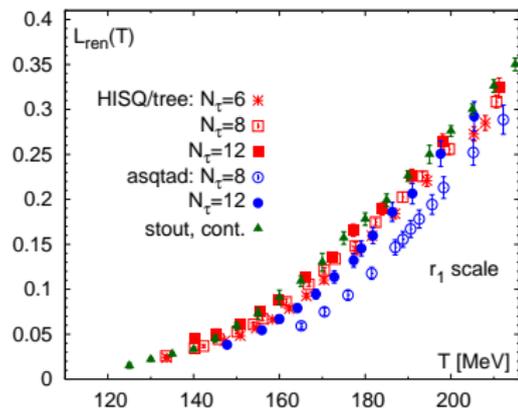
Scale setting with f_K

- ▶ The strangeness fluctuations with the asqtad and HISQ action with r_1 (left) and f_K (right) scale



Scale setting with f_K

- ▶ The renormalized Polyakov loop with r_1 (left) and f_K (right) scale
- ▶ Notice that the cut-off effects are very different in the Polyakov loop and f_K , thus, using f_K does not help



Chiral symmetry restoration

Chiral condensate:

$$\langle \bar{\psi}\psi \rangle_{q,x} = \frac{1}{4} \frac{1}{N_\sigma^3 N_\tau} \text{Tr} \langle D_q^{-1} \rangle, \quad q = l, s, \quad x = 0, \tau.$$

The susceptibility:

$$\chi_{m,q}(T) = \frac{\partial \langle \bar{\psi}\psi \rangle_l}{\partial m_q} = 2\chi_{q,disc} + \chi_{q,con},$$

$$\chi_{q,disc} = \frac{1}{16N_\sigma^3 N_\tau} \left\{ \langle (\text{Tr} D_q^{-1})^2 \rangle - \langle \text{Tr} D_q^{-1} \rangle^2 \right\},$$

and

$$\chi_{q,con} = \frac{1}{4} \text{Tr} \sum_x \langle D_q^{-1}(x,0) D_q^{-1}(0,x) \rangle, \quad q = l, s.$$

The renormalized condensate:

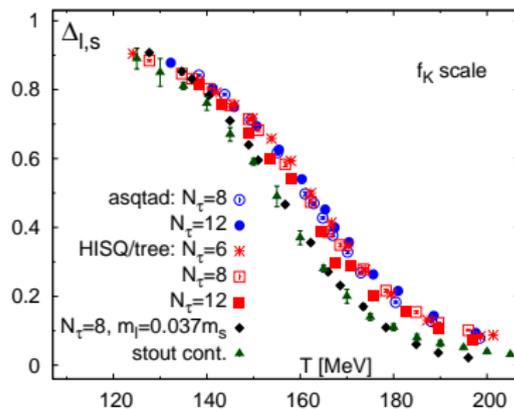
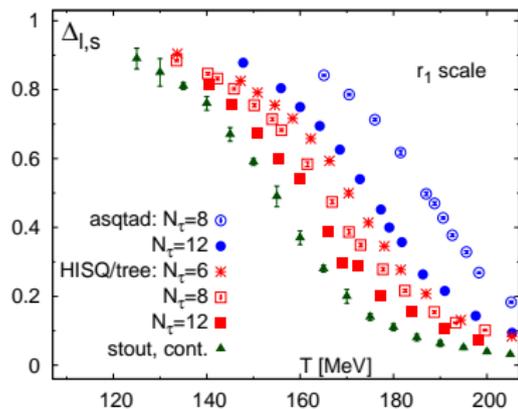
$$\Delta_{l,s}(T) = \frac{\langle \bar{\psi}\psi \rangle_{l,\tau} - \frac{m_l}{m_s} \langle \bar{\psi}\psi \rangle_{s,\tau}}{\langle \bar{\psi}\psi \rangle_{l,0} - \frac{m_l}{m_s} \langle \bar{\psi}\psi \rangle_{s,0}}$$

or

$$\Delta_l^R = d + m_s r_0^4 (\langle \bar{\psi}\psi \rangle_{l,\tau} - \langle \bar{\psi}\psi \rangle_{l,0}).$$

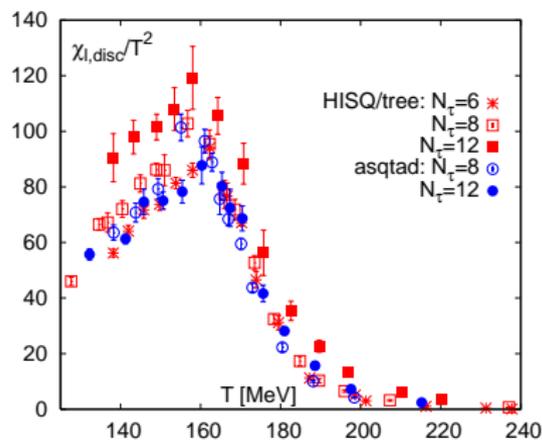
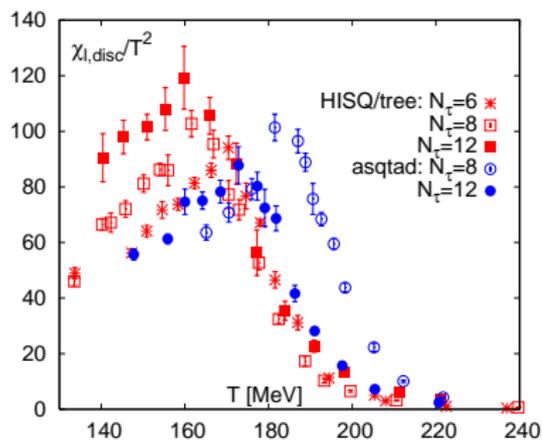
Chiral condensate

- ▶ Renormalized chiral condensate with r_1 (left) and f_K (right) scale



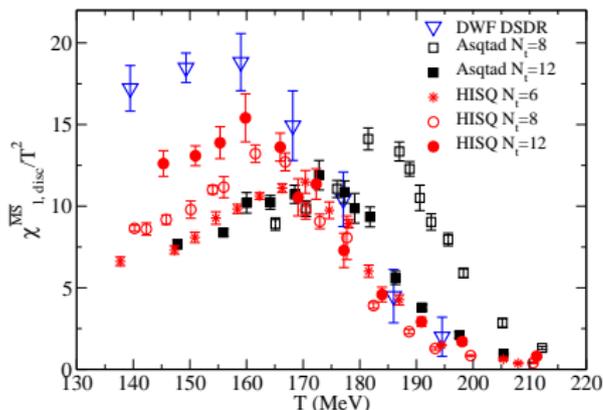
Chiral susceptibility

- ▶ Disconnected chiral susceptibility with r_1 (left) and f_K (right) scale



Chiral susceptibility

- ▶ Comparison of the disconnected chiral susceptibility with staggered and domain-wall fermions (DWF), r_1 scale, HotQCD (2012)



- ▶ Good agreement in the location of the peak, extra support for the validity of staggered studies
- ▶ DWF simulations are done at $m_\pi = 200$ MeV, note that for HISQ at $N_\tau = 12$ RMS pion mass is around 200 MeV

Chiral condensate (scaling)

- ▶ In the limit of vanishing light quark masses and for sufficiently large strange quark mass QCD is expected to have a second order phase transition in $O(4)$ universality class.
- ▶ Staggered fermions preserve only a part of the chiral symmetry, thus, the relevant universality class in the chiral limit at non-zero lattice spacing is $O(2)$.
- ▶ In the numerical analysis the difference between $O(2)$ and $O(4)$ is rather small, so we refer to scaling properties as $O(N)$ scaling.
- ▶ Previous studies with the p4 action demonstrated that even for non-vanishing light quark masses, provided they are small enough, universal scaling properties can be used to define pseudo-critical temperature.
- ▶ $O(N)$ scaling analysis has been extended to asqtad and HISQ/tree.
- ▶ The multiplicatively renormalized chiral condensate (the order parameter in the chiral limit):

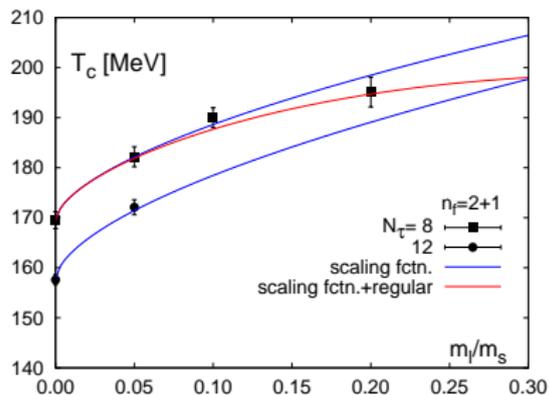
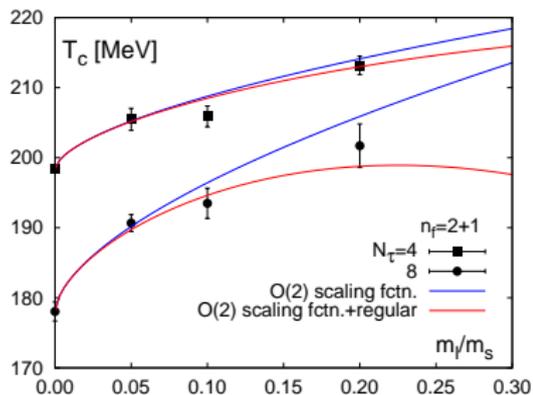
$$M_b = \frac{m_s}{T^4} \langle \bar{\psi}\psi \rangle_l.$$

- ▶ At sufficiently low mass the chiral condensate is described by a universal scaling function f_G plus additional scaling violating terms:

$$M_b(T, m_l, m_s) = h^{1/\delta} f_G(t/h^{1/\beta\delta}) + a_t \Delta TH + b_1 H,$$

$$H = \frac{m_l}{m_s}, \quad \Delta T = \frac{T - T_c^0}{T_c^0}, \quad h = H/h_0, \quad t = \Delta T/t_0.$$

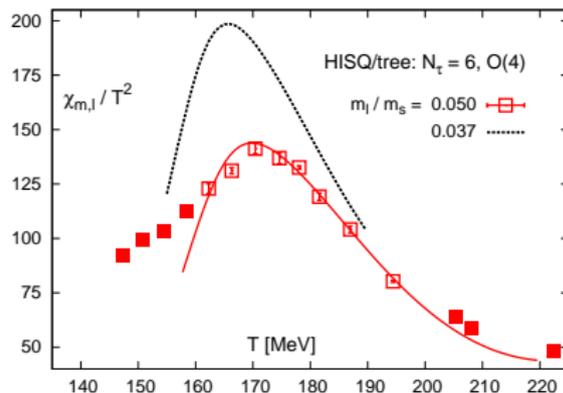
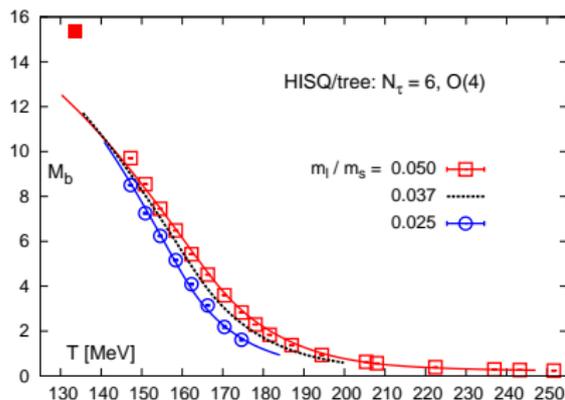
$O(N)$ scaling analysis



- ▶ The pseudo-critical temperature as function of light quark mass at $N_\tau = 4$ and 8 for the p4 action (left) and $N_\tau = 8$ and 12 for the asqtad action (right).
- ▶ Points represent the pseudo-transition temperature T_C determined from the peak of the disconnected chiral susceptibility.
- ▶ Lines are predictions from the fits to the chiral condensate.

Chiral condensate and susceptibility, HISQ

- ▶ Simultaneously fit the chiral condensate and susceptibility
- ▶ This gives dependence on the quark mass, determine the transition temperature for each $N_\tau = 6, 8, 12$
- ▶ For $N_\tau = 6$ and 8 lower than physical, $m_l = m_s/40$ quark masses are also available, $N_\tau = 6$ is shown

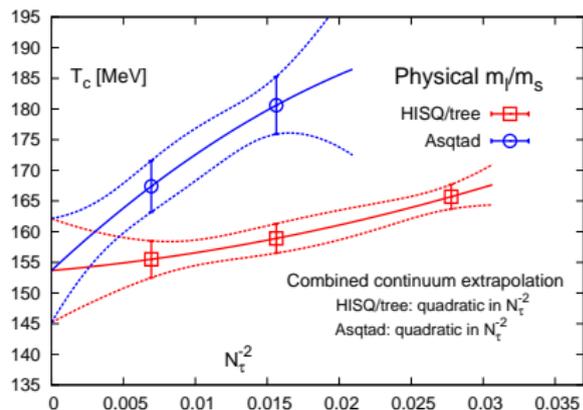
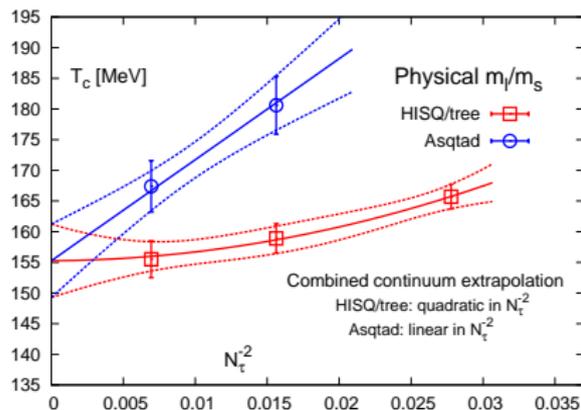


Combined extrapolation to the continuum

- ▶ Combined extrapolation using asqtad and HISQ data sets, quadratic for HISQ and linear (left) and quadratic (right) for asqtad
- ▶ Notice, HISQ has substantially smaller cut-off effects
- ▶ The final result for the chiral transition temperature **at the physical quark masses in the continuum limit**

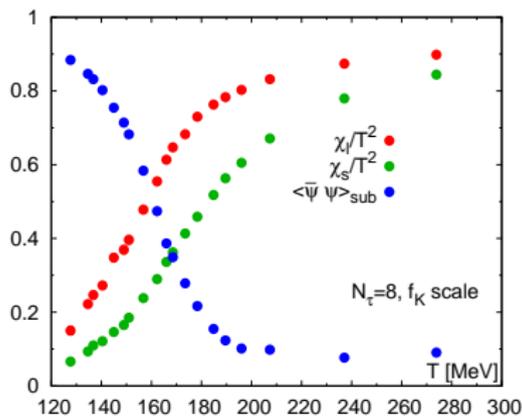
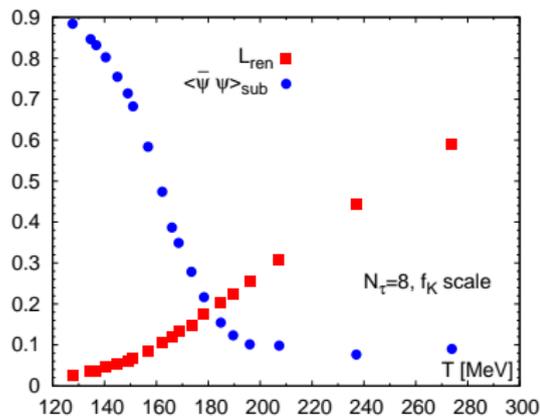
$$T_c = 154 \pm 9 \text{ MeV}$$

(derived from the chiral susceptibility which diverges in the chiral limit)



Back to deconfinement

- ▶ Probes of the deconfinement, i.e. the Polyakov loop or quark number susceptibilities, show gradual rise in a wide temperature range
- ▶ Compare the behavior of the chiral condensate and the Polyakov loop (left) and the chiral condensate and light and strange quark number susceptibility (right)
- ▶ The deconfinement phenomenon happens gradually and is indicated by full temperature dependence of various observables (inflection points are not helpful here), therefore no unique temperature can be associated with deconfinement



Conclusion

- ▶ QCD at zero chemical potential at the physical light and strange quark masses exhibits an analytic crossover between the confined and deconfined phase
- ▶ Lattice QCD calculations with staggered fermions allow for calculations at (almost) physical light quark masses
- ▶ Taste symmetry breaking in staggered formulation is by far the largest source of cut-off effects
- ▶ Highly Improved Staggered Quarks action substantially reduces the cut-off effects, allows for better control in the low-temperature phase
- ▶ Calculation with the HISQ action on lattices with the temporal extent $N_\tau = 6, 8$ and 12 at $m_l = m_s/20$ and $N_\tau = 6$ and 8 at $m_l = m_s/40$, relying on universal $O(N)$ scaling in the chiral limit, gives **at the physical quark masses in the continuum limit** the chiral symmetry restoration temperature $T_c = 154(9)$ MeV
- ▶ **Deconfinement** happens gradually, as manifested in the behavior of various thermodynamic quantities in the wide temperature range, so **no unique temperature is associated with it**