

Heavy quark free and internal energies in 2-flavor QCD

Olaf Kaczmarek



Felix Zantow



August 4, 2005

Motivation - Heavy quark bound states above deconfinement

Quarkonium suppression as a probe for thermal properties of hot and dense matter [Matsui and Satz]

- heavy quark potential gets screened
- screening radius related to parton density

$$r_D \sim \frac{1}{g\sqrt{n/T}}$$

- at high T screening radius smaller than size of a quarkonium state

Typical length scales of heavy quark bound states: $1/\Lambda_{QCD} \sim 1$ fm

- screening has to be strong enough to modify short distance behaviour
- detailed analysis of "heavy quark potentials"
 - temperature and r dependence
 - screening properties above deconfinement
 - What is the correct effective potential at finite temperature ?

$$F_1(r, T) = U_1(r, T) - T S_1(r, T)$$

Heavy quark bound states above deconfinement

Strong interactions in the deconfined phase $T \gtrsim T_c$

Possibility of heavy quark bound states?

Charmonium ($\chi_c, J/\psi$) as thermometer above T_c

Suppression patterns of charmonium/bottomonium

⇒ **Potential models**

→ heavy quark potential ($T=0$)

$$V_1(r) = -\frac{4}{3} \frac{\alpha(r)}{r} + \sigma r$$

→ heavy quark free energies ($T > T_c$)

$$F_1(r, T) \simeq -\frac{4}{3} \frac{\alpha(r, T)}{r} e^{-m(T)r}$$

→ heavy quark internal energies ($T \neq 0$)

$$F_1(r, T) = U_1(r, T) - T S_1(r, T)$$

⇒ **Charmonium correlation functions/spectral functions**

Polyakov loop correlation function and free energy:

L. McLerran, B. Svetitsky (1981)

$$\frac{Z_{Q\bar{Q}}}{Z(\mathbf{T})} \simeq \frac{1}{Z(\mathbf{T})} \int \mathcal{D}\mathbf{A} \dots \mathbf{L}(\mathbf{x}) \mathbf{L}^\dagger(\mathbf{y}) \exp\left(-\int_0^{1/T} dt \int d^3\mathbf{x} \mathcal{L}[\mathbf{A}, \dots]\right)$$

$$= -\frac{F_{Q\bar{Q}}(\mathbf{r}, \mathbf{T})}{T}$$

$Q\bar{Q} = 1, 8, \text{av}$

O. Philipsen (2002)

O. Jahn, O. Philipsen (2004)

Lattice data used in our analysis:

$N_f = 0:$

$32^3 \times 4, 8, 16$ -lattices

(*Symanzik*)

O. Kaczmarek,

F. Karsch,

P. Petreczky,

F.Z. (2002, 2004)

$N_f = 2:$

$16^3 \times 4$ -lattices

(*Symanzik, p4-stagg.*)

$m_\pi/m_\rho \simeq 0.7$ ($m/T = 0.4$)

O. Kaczmarek, F.Z. (2005),

O. Kaczmarek et al. (2003)

$N_f = 3:$

$16^3 \times 4$ -lattices

$m_\pi/m_\rho \simeq 0.4$

P. Petreczky,

K. Petrov (2004)

Details of the calculation

$N_f = 2$ with $m/T = 0.4$ ($m_\pi/m_\rho \approx 0.7$ at T_c)

Lattice size: $16^3 \times 4$, $T_c \approx 170\text{MeV}$

(generated by the Bielefeld-Swansea collaboration)

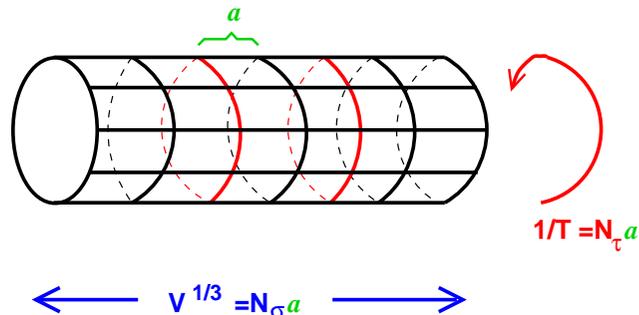
Symanzik improved gauge action and
p4-improved staggered fermion action

Physical scale is determined by string tension

$T=0$ potential obtained from Wilson loops

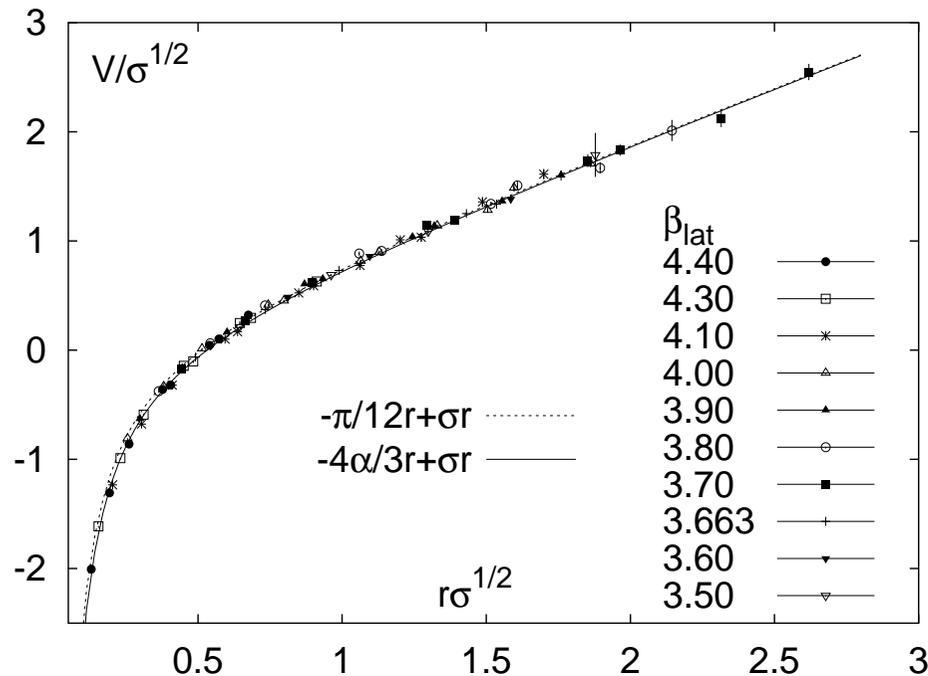
[F. Karsch, E. Laermann and A. Peikert, Nucl. Phys . B 605 (2001) 579]

Coulomb gauge fixing [O. Philipsen, Phys. Lett. B535 (2002) 138]



$$\begin{aligned}
 -\ln \left(\langle \tilde{\text{Tr}} L(\mathbf{x}) \tilde{\text{Tr}} L^\dagger(\mathbf{y}) \rangle \right) &= \frac{F_{\bar{q}q}(r, T)}{T} \\
 -\ln \left(\langle \tilde{\text{Tr}} L(\mathbf{x}) L^\dagger(\mathbf{y}) \rangle \right) \Big|_{GF} &= \frac{F_1(r, T)}{T} \\
 -\ln \left(\frac{9}{8} \langle \tilde{\text{Tr}} L(\mathbf{x}) \tilde{\text{Tr}} L^\dagger(\mathbf{y}) \rangle - \frac{1}{8} \langle \tilde{\text{Tr}} L(\mathbf{x}) L^\dagger(\mathbf{y}) \rangle \right) \Big|_{GF} &= \frac{F_8(r, T)}{T}
 \end{aligned}$$

Zero temperature potential



Large distance behaviour

consistent with string model prediction:

$$V(r) = -\frac{\pi}{12r} + \sigma r, \text{ for large } r$$

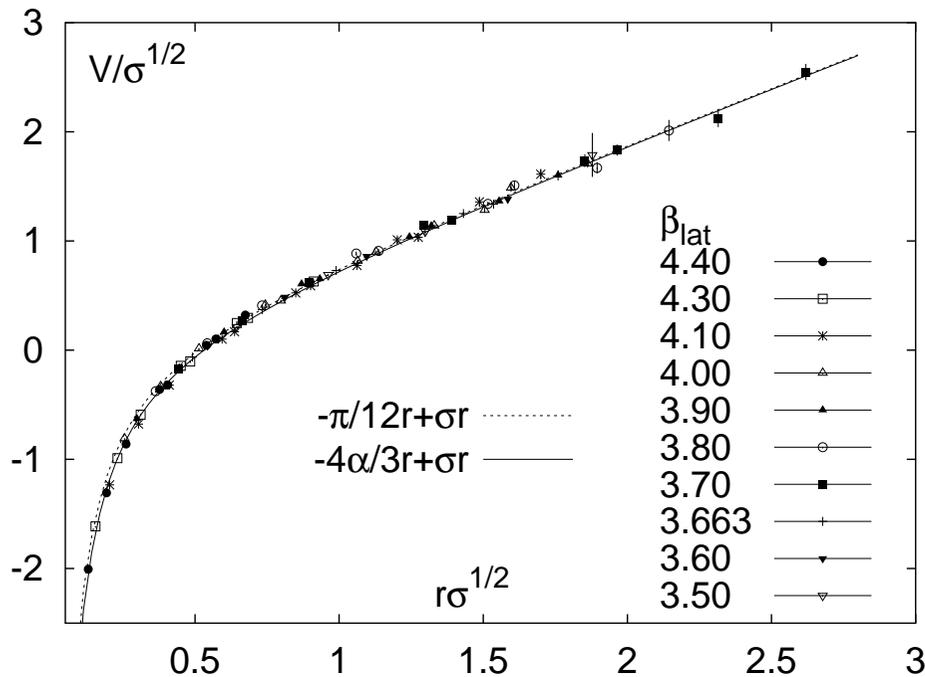
consistent with quenched potential for $r \gtrsim 0.4 \text{ fm}$

no string breaking observed

due to the used operator

$$r_{\text{str}} \approx 1.3 \text{ fm}$$

Zero temperature potential



Short distance behaviour

deviations at small r

enhancement of the running coupling

$$\text{fit: } V(r) = -0.2822(28)/r + \sigma r$$

r -dependent running coupling $\alpha(r)$

Large distance behaviour

consistent with string model prediction:

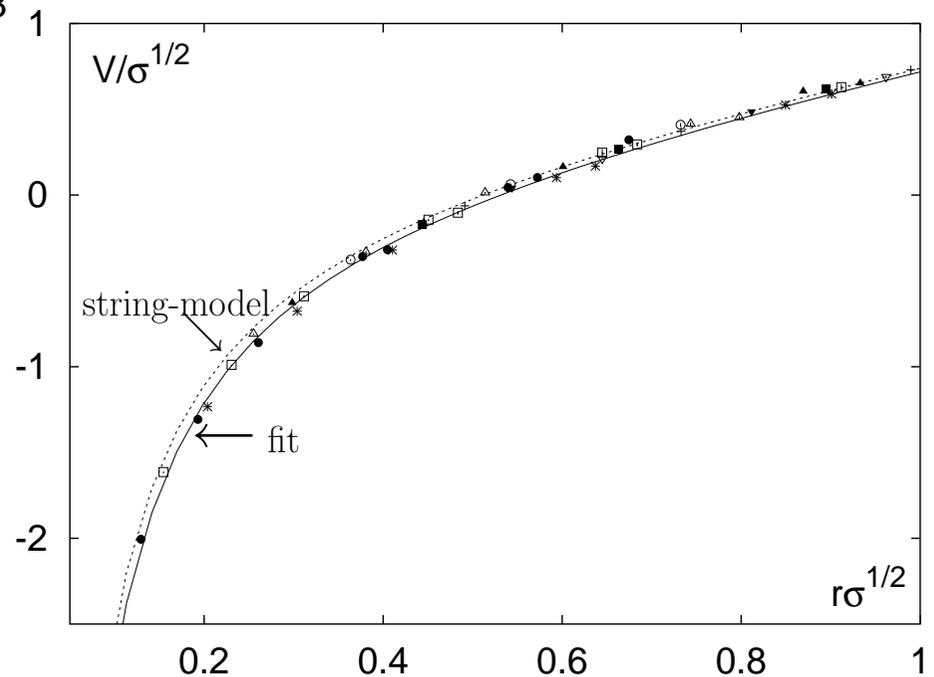
$$V(r) = -\frac{\pi}{12r} + \sigma r, \text{ for large } r$$

consistent with quenched potential for $r \gtrsim 0.4 \text{ fm}$

no string breaking observed

due to the used operator

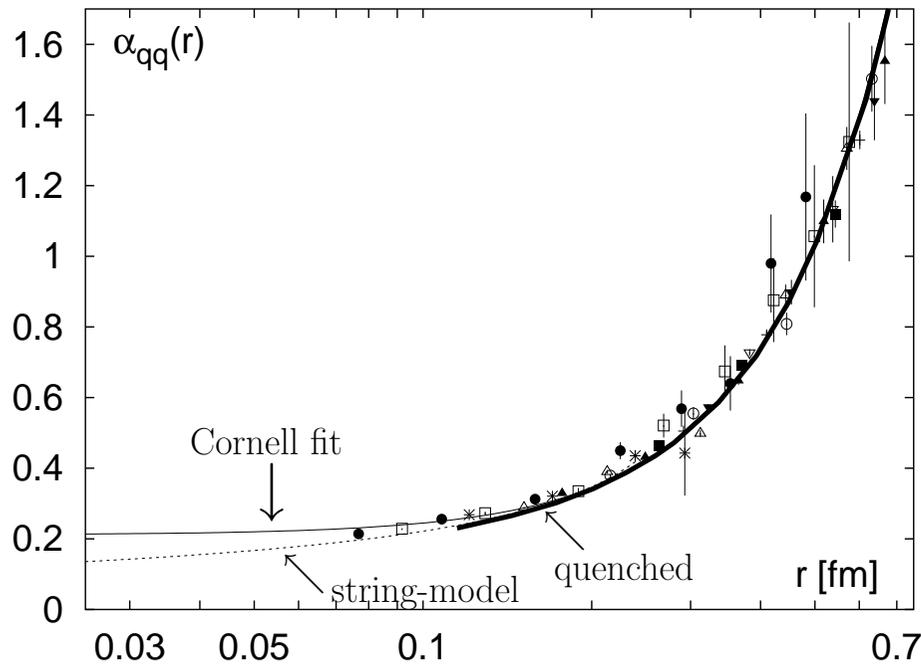
$$r_{str} \approx 1.3 \text{ fm}$$



Zero temperature running coupling

QCD running coupling in the qq -scheme

$$\alpha_{qq}(r) = \frac{3}{4} r^2 \frac{dV(r)}{dr}$$



Large distance behavior

non-perturbative confining part for $r \gtrsim 0.4$ fm

$$\alpha_{qq}(r) \simeq 3/4 r^2 \sigma$$

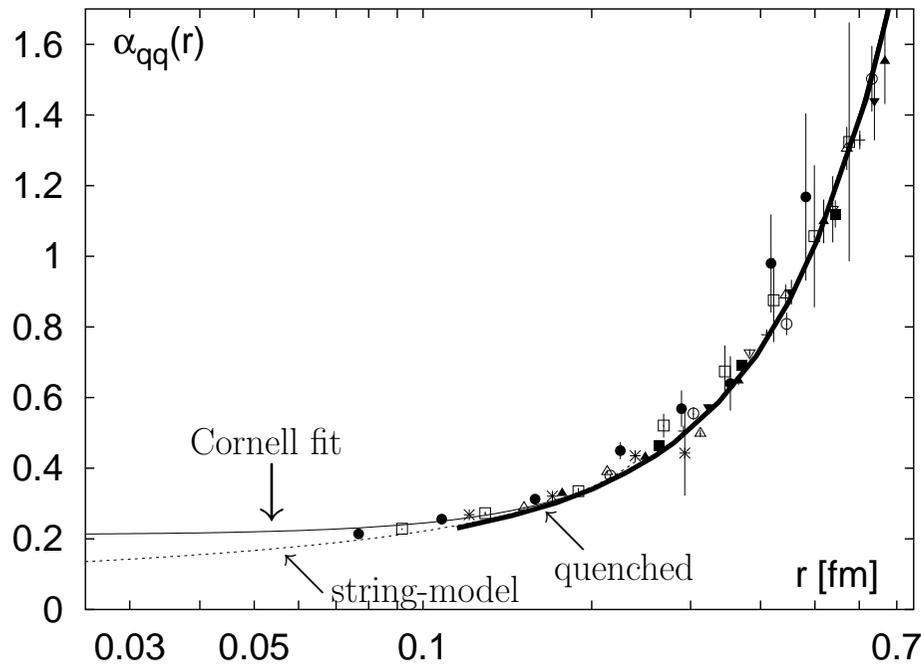
consistent with quenched potential

consistent with string model prediction

Zero temperature running coupling

QCD running coupling in the qq -scheme

$$\alpha_{qq}(r) = \frac{3}{4} r^2 \frac{dV(r)}{dr}$$



leading order perturbation theory:

$$\alpha(r) \simeq \frac{1}{8\pi} \frac{1}{\beta_0 \log(1/(r\Lambda_{\text{QCD}}))}$$

Large distance behavior

non-perturbative confining part for $r \gtrsim 0.4$ fm

$$\alpha_{qq}(r) \simeq 3/4 r^2 \sigma$$

consistent with quenched potential

consistent with string model prediction

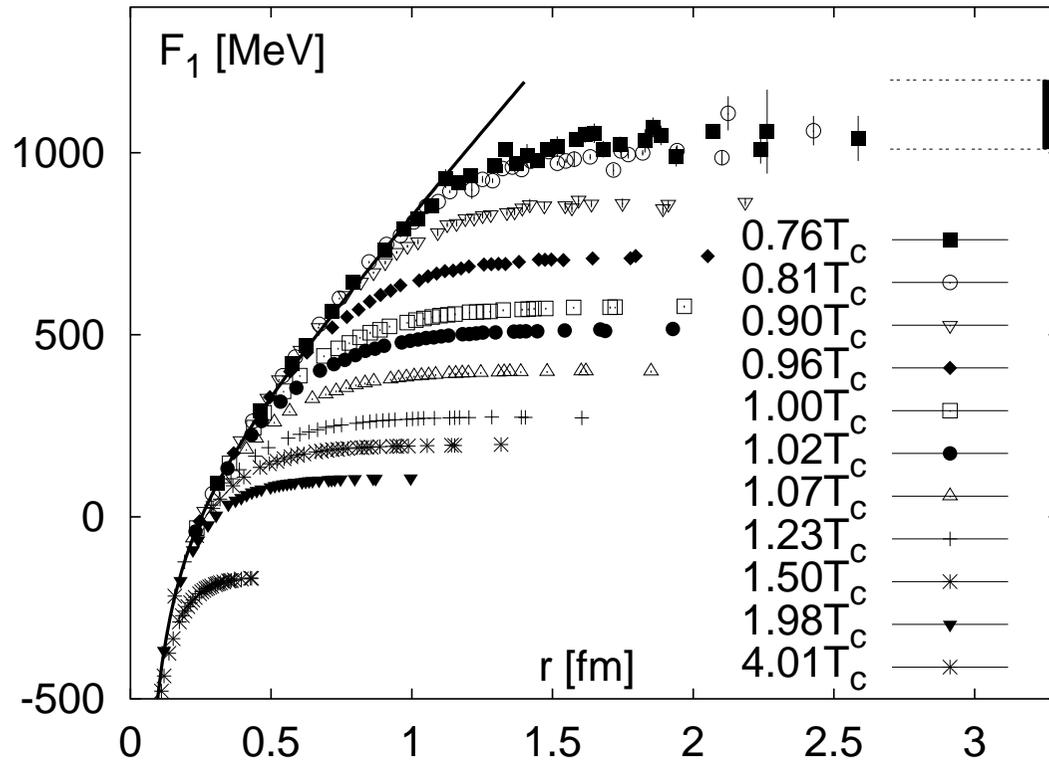
Short distance behavior

logarithmic weakening, i.e. $\alpha_{\text{qcd}} = \alpha_{\text{qcd}}(r)$

flavor and quark mass dependence

$$\beta_0 = \frac{33 - 2N_f}{48\pi^2}$$

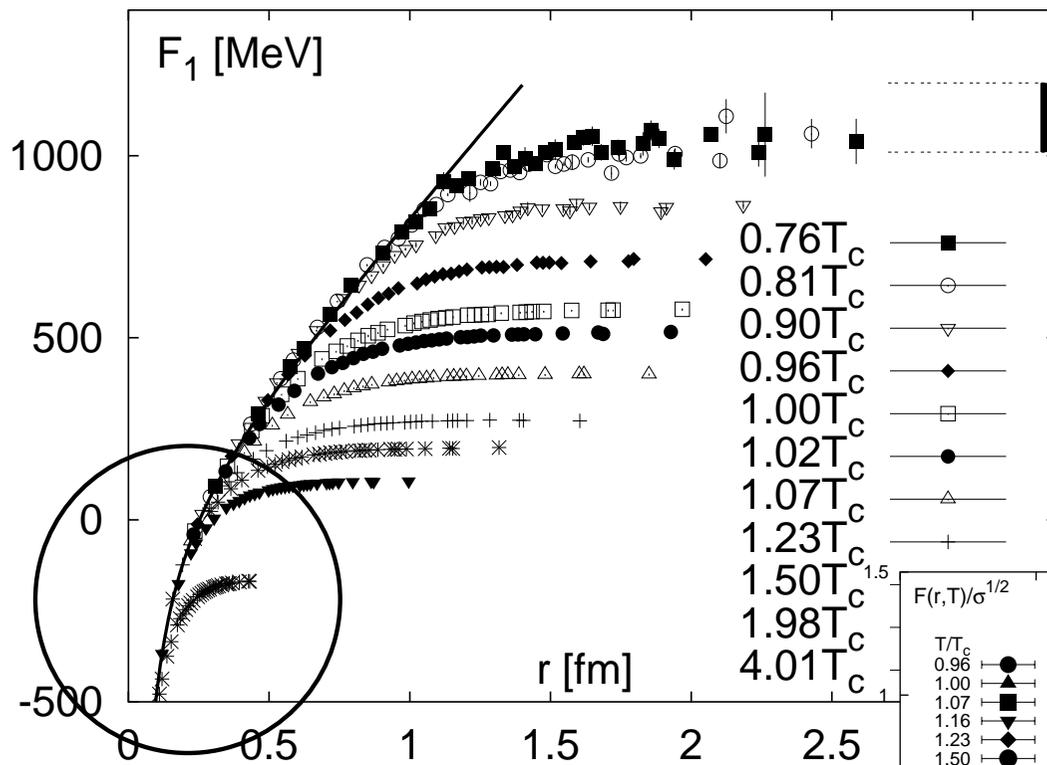
Heavy quark free energy



Renormalization of $F(r, T)$
 by
 matching with $T=0$ potential

$$e^{-F_1(r, T)/T} = (Z_r(g^2))^{2N_\tau} \langle \text{Tr} (L_x L_y^\dagger) \rangle$$

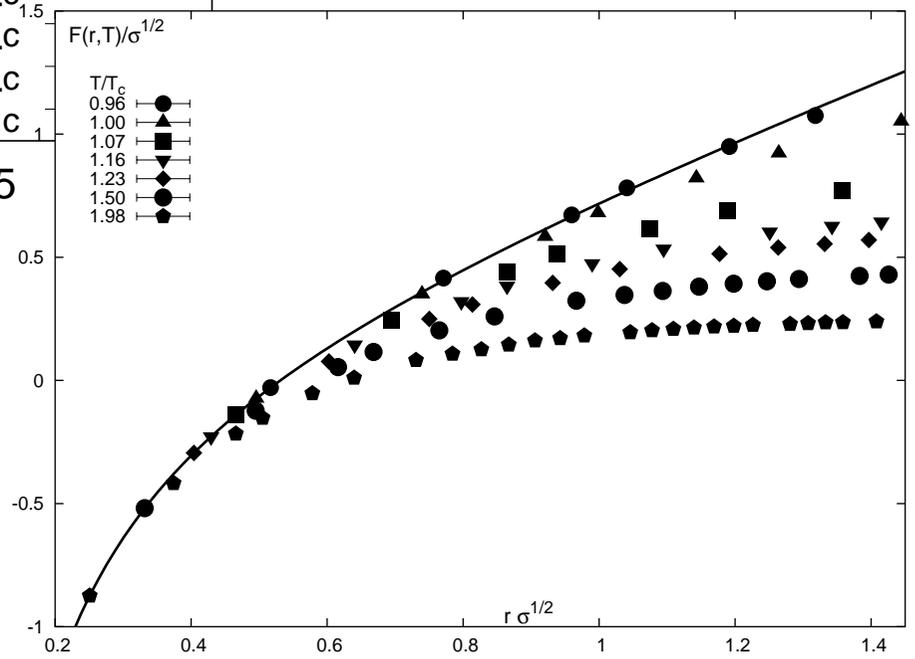
Heavy quark free energy



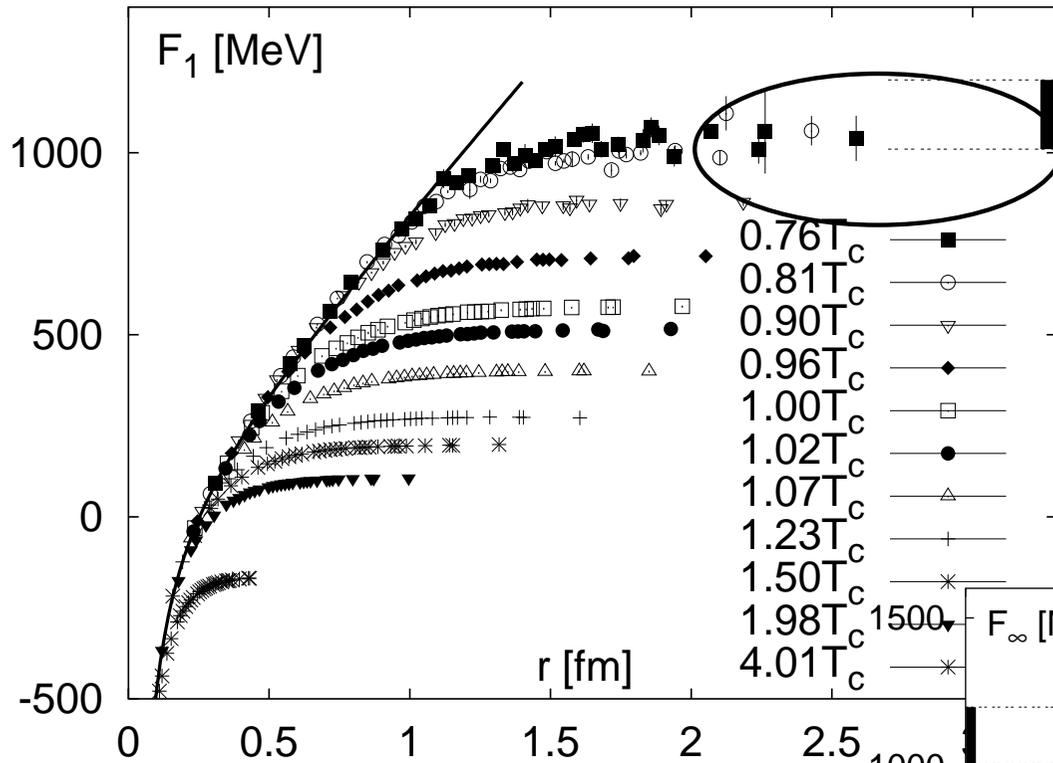
Renormalization of $F(r, T)$
by
matching with $T=0$ potential

$$e^{-F_1(r, T)/T} = (Z_r(g^2))^{2N_\tau} \langle \text{Tr} (L_x L_y^\dagger) \rangle$$

T -independent
 $r \ll 1/\sqrt{\sigma}$
 $F(r, T) \sim g^2(r)/r$

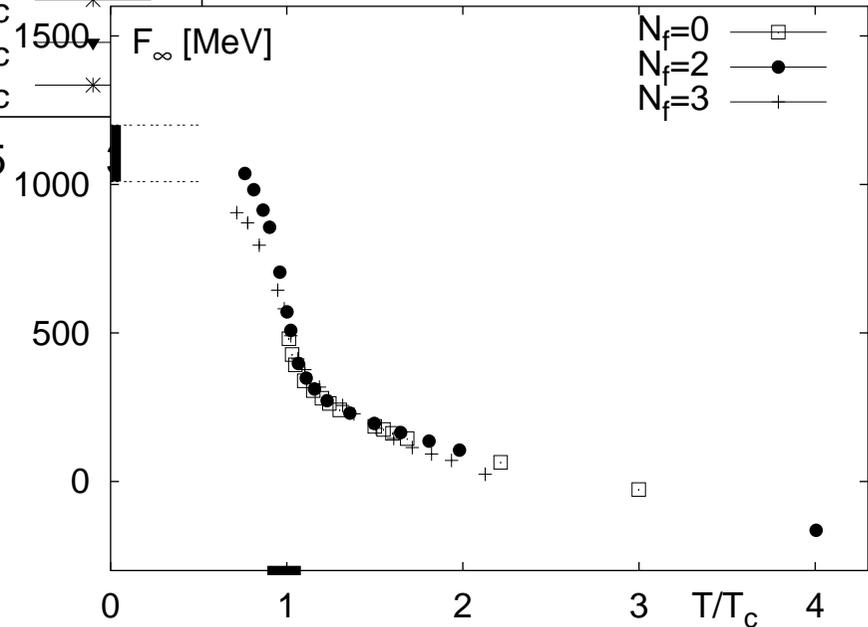


Heavy quark free energy

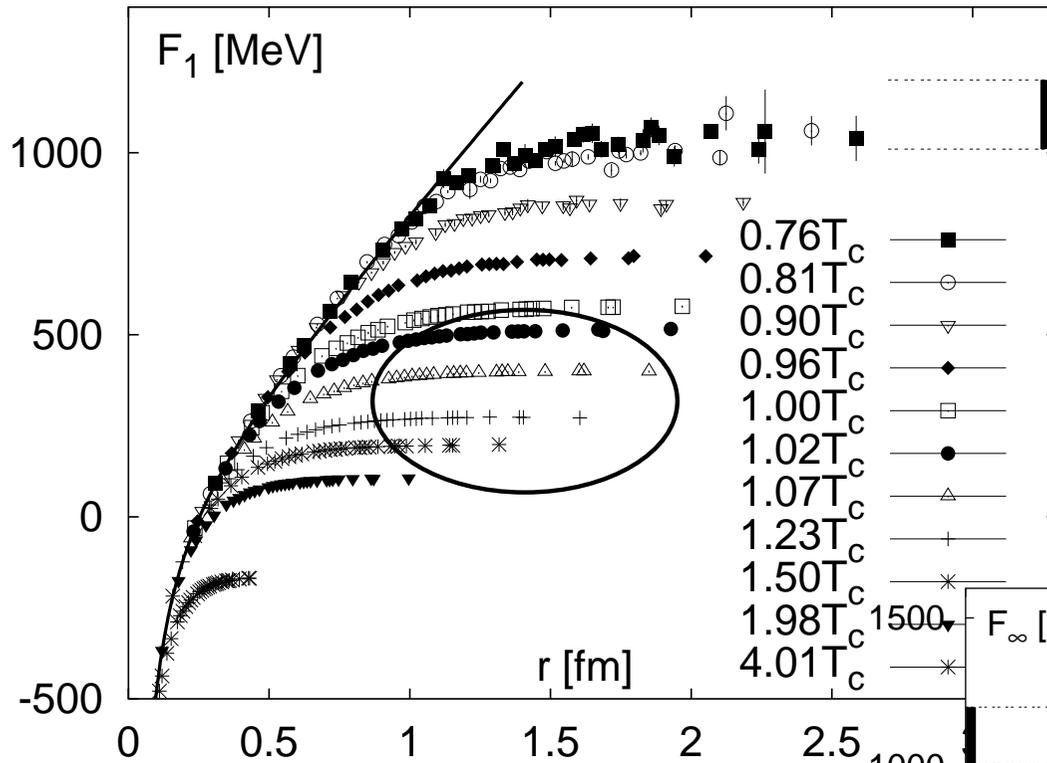


String breaking
 $T < T_c$
 $F(r\sqrt{\sigma} \gg 1, T) < \infty$

T-independent
 $r \ll 1/\sqrt{\sigma}$
 $F(r, T) \sim g^2(r)/r$



Heavy quark free energy



String breaking

$$T < T_c$$

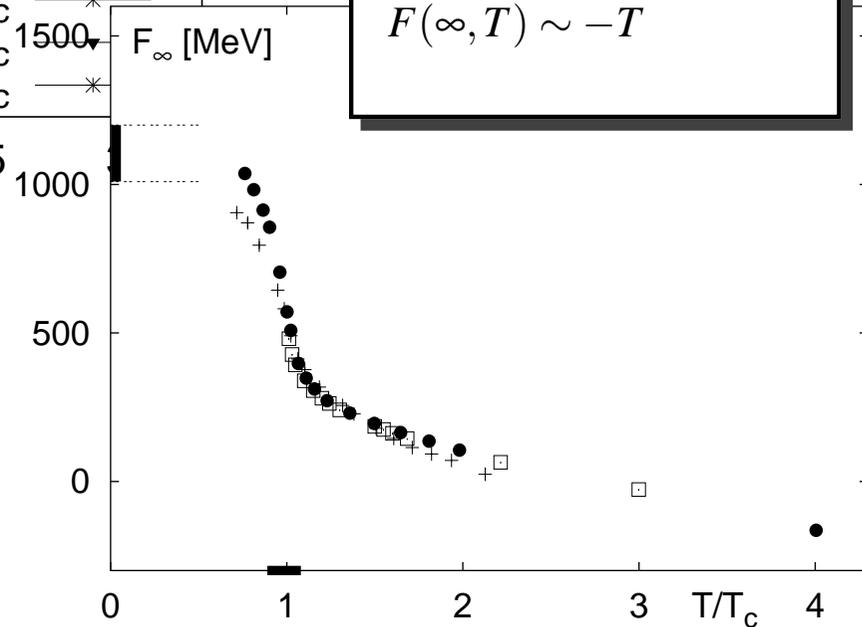
$$F(r\sqrt{\sigma} \gg 1, T) < \infty$$

high-T physics

$$rT \gg 1 ; \text{screening}$$

$$\mu(T) \sim g(T)T$$

$$F(\infty, T) \sim -T$$

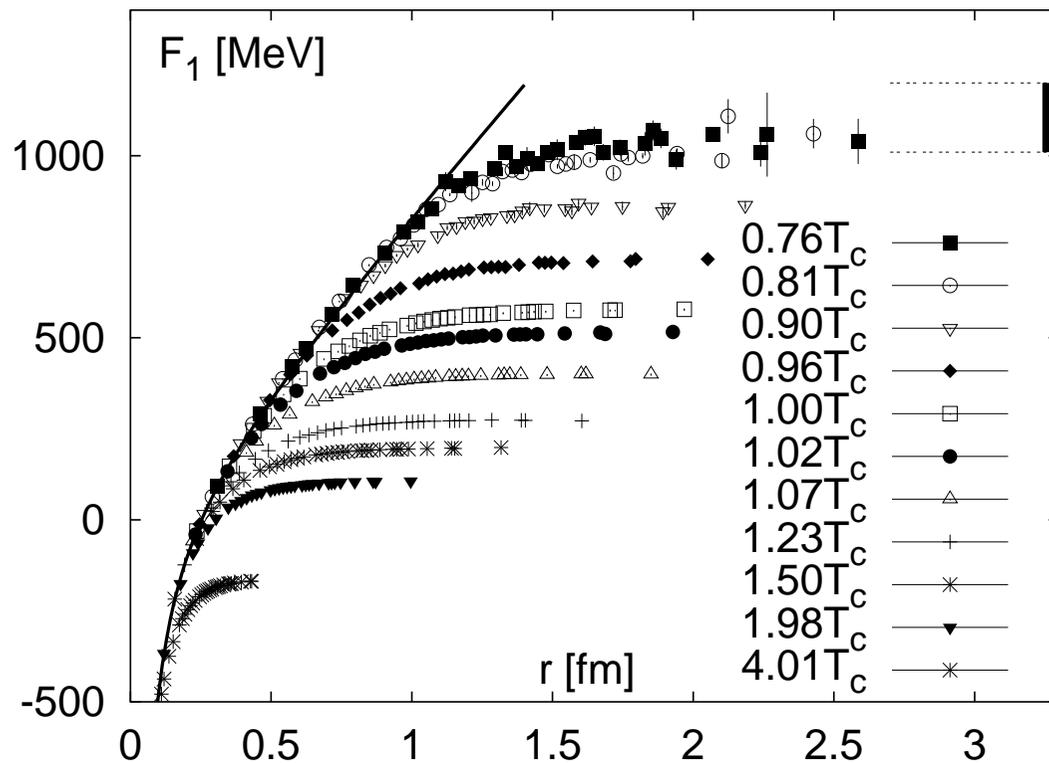


T -independent

$$r \ll 1/\sqrt{\sigma}$$

$$F(r, T) \sim g^2(r)/r$$

Heavy quark free energy



String breaking

$$T < T_c$$

$$F(r\sqrt{\sigma} \gg 1, T) < \infty$$

high-T physics

$$rT \gg 1 ; \text{screening}$$

$$\mu(T) \sim g(T)T$$

$$F(\infty, T) \sim -T$$

T -independent

$$r \ll 1/\sqrt{\sigma}$$

$$F(r, T) \sim g^2(r)/r$$

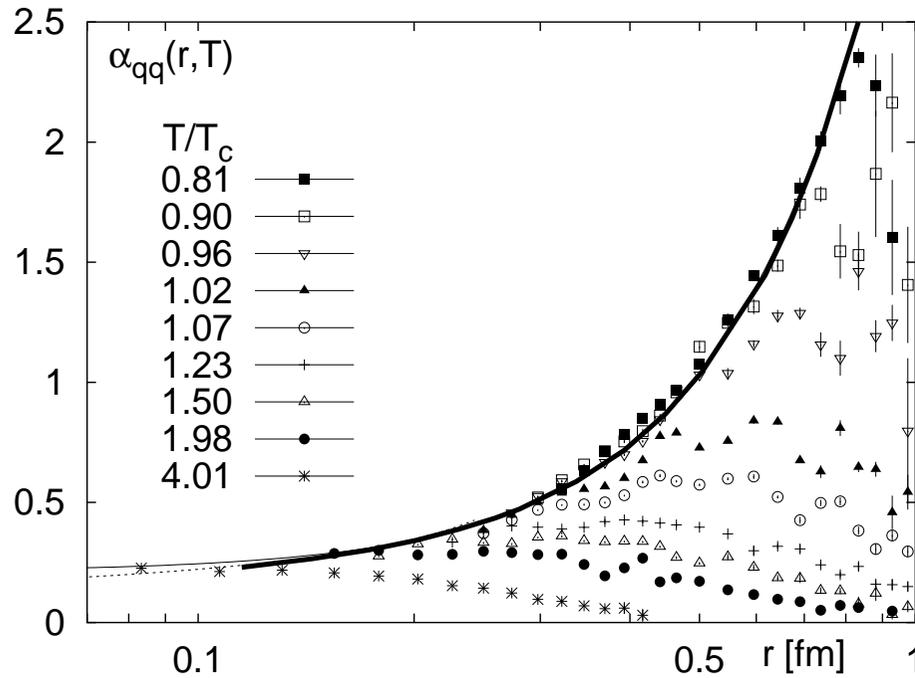
Complex r and T dependence

Small vs. large distance behavior

Running coupling vs. screening

Where do temperature effects set in?

Temperature depending running coupling



Free energy in perturbation theory:

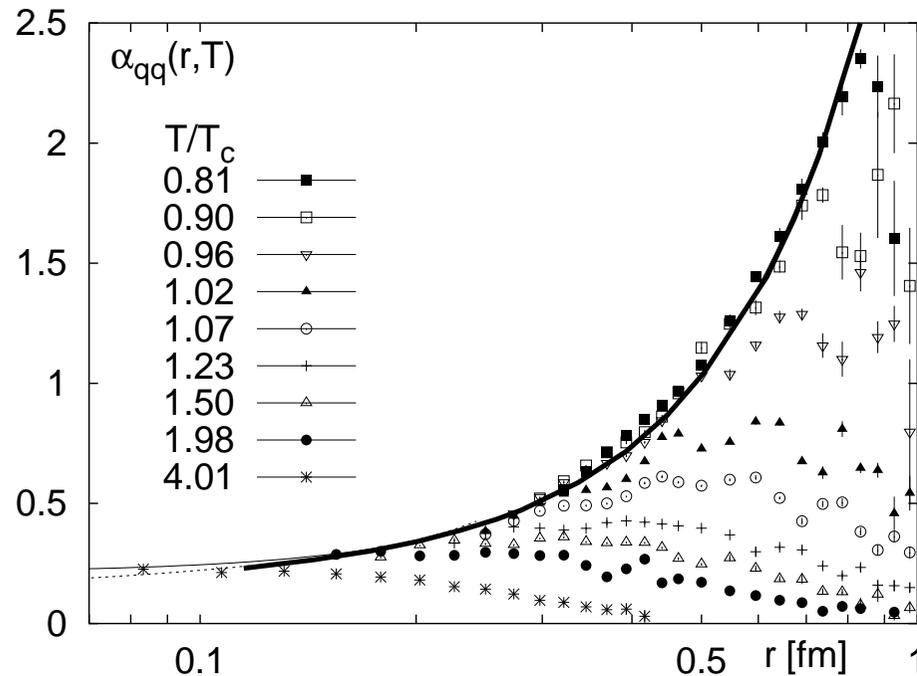
$$F_1(r, T) \equiv V(r) \simeq -\frac{4}{3} \frac{\alpha(r)}{r} \quad \text{for} \quad r\Lambda_{\text{QCD}} \ll 1$$

$$F_1(r, T) \simeq -\frac{4}{3} \frac{\alpha(T)}{r} e^{-m_D(T)r} \quad \text{for} \quad rT \gg 1$$

QCD running coupling in the qq -scheme

$$\alpha_{qq}(r, T) = \frac{3}{4} r^2 \frac{dF_1(r, T)}{dr}$$

Temperature depending running coupling



Free energy in perturbation theory:

$$F_1(r, T) \equiv V(r) \simeq -\frac{4}{3} \frac{\alpha(r)}{r} \quad \text{for} \quad r\Lambda_{\text{QCD}} \ll 1$$

$$F_1(r, T) \simeq -\frac{4}{3} \frac{\alpha(T)}{r} e^{-m_D(T)r} \quad \text{for} \quad rT \gg 1$$

QCD running coupling in the qq -scheme

$$\alpha_{qq}(r, T) = \frac{3}{4} r^2 \frac{dF_1(r, T)}{dr}$$

non-perturbative confining part for $r \gtrsim 0.4$ fm

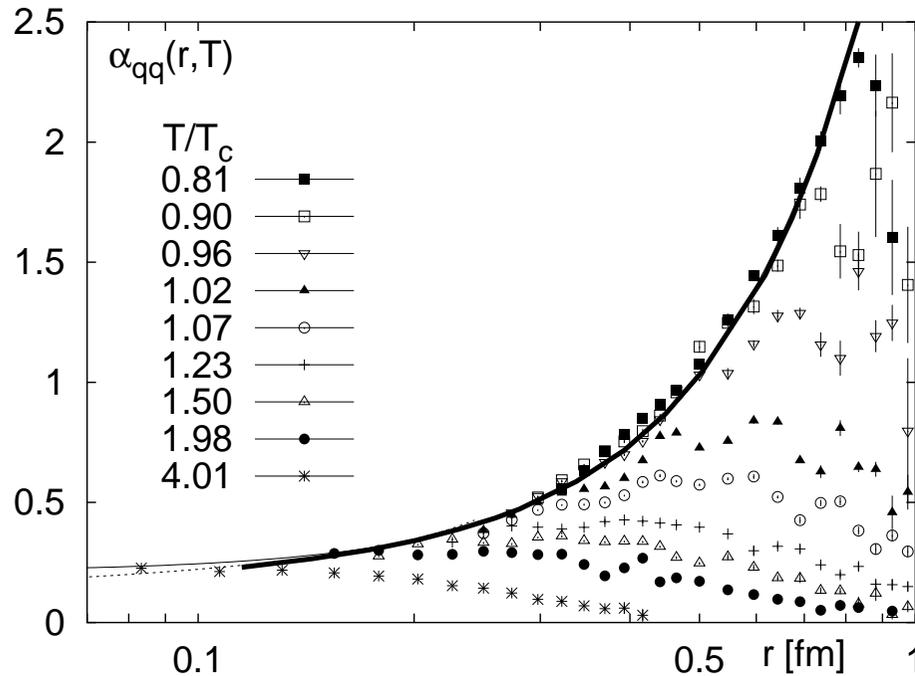
$$\alpha_{qq}(r) \simeq 3/4r^2\sigma$$

present below and just above T_c

temperature effects set in at smaller r with increasing T

maximum due to screening

Temperature depending running coupling



Free energy in perturbation theory:

$$F_1(r, T) \equiv V(r) \simeq -\frac{4}{3} \frac{\alpha(r)}{r} \quad \text{for} \quad r\Lambda_{\text{QCD}} \ll 1$$

$$F_1(r, T) \simeq -\frac{4}{3} \frac{\alpha(T)}{r} e^{-m_D(T)r} \quad \text{for} \quad rT \gg 1$$

QCD running coupling in the qq -scheme

$$\alpha_{qq}(r, T) = \frac{3}{4} r^2 \frac{dF_1(r, T)}{dr}$$

non-perturbative confining part for $r \gtrsim 0.4$ fm

$$\alpha_{qq}(r) \simeq 3/4 r^2 \sigma$$

present below and just above T_c

temperature effects set in at smaller r with increasing T

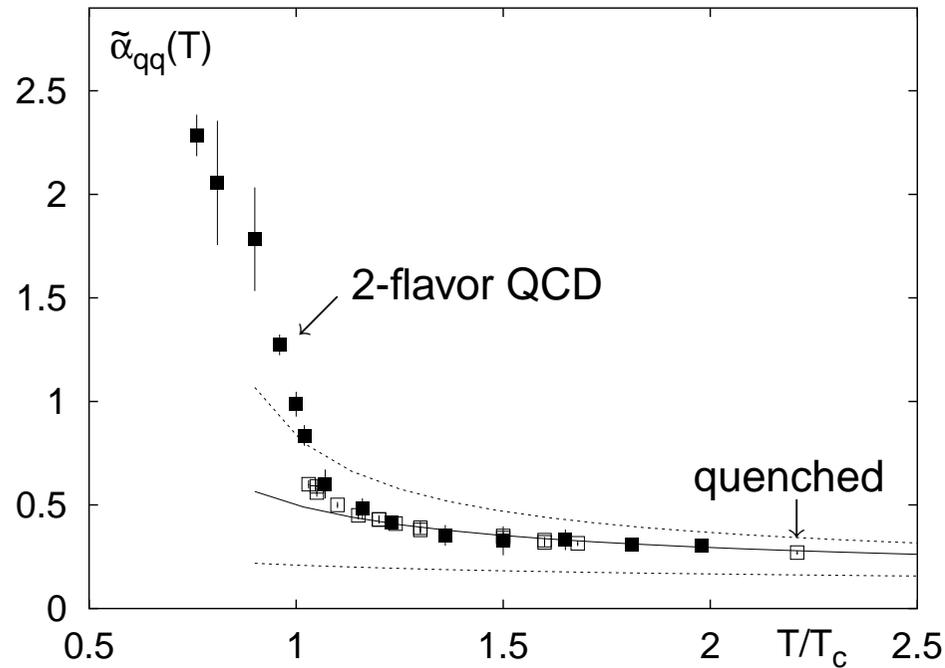
maximum due to screening

⇒ At which distance do T -effects set in ?

⇒ definition of the screening radius/mass

⇒ definition of the T -dependent coupling

Temperature depending running coupling



define $\tilde{\alpha}_{qq}(T)$ by maximum of $\alpha_{qq}(r, T)$:

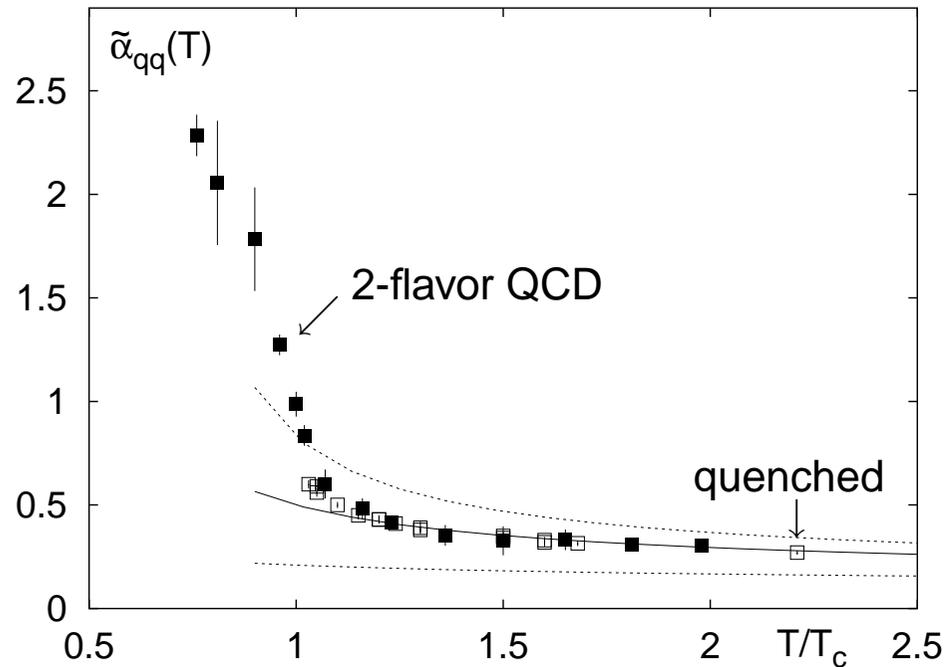
$$\tilde{\alpha}_{qq}(T) \equiv \alpha_{qq}(r_{max}, T)$$

perturbative behaviour at high T :

$$g_{2\text{-loop}}^{-2}(T) = 2\beta_0 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right) + \frac{\beta_1}{\beta_0} \ln\left(2 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right)\right),$$

Using $T_c/\Lambda_{\overline{MS}} = 0.77(21)$ we find $\mu = 1.14(2)\pi$

Temperature depending running coupling



define $\tilde{\alpha}_{qq}(T)$ by maximum of $\alpha_{qq}(r, T)$:

$$\tilde{\alpha}_{qq}(T) \equiv \alpha_{qq}(r_{max}, T)$$

perturbative behaviour at high T :

$$g_{2\text{-loop}}^{-2}(T) = 2\beta_0 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right) + \frac{\beta_1}{\beta_0} \ln\left(2 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right)\right),$$

Using $T_c/\Lambda_{\overline{MS}} = 0.77(21)$ we find $\mu = 1.14(2)\pi$

non-perturbative large values near T_c

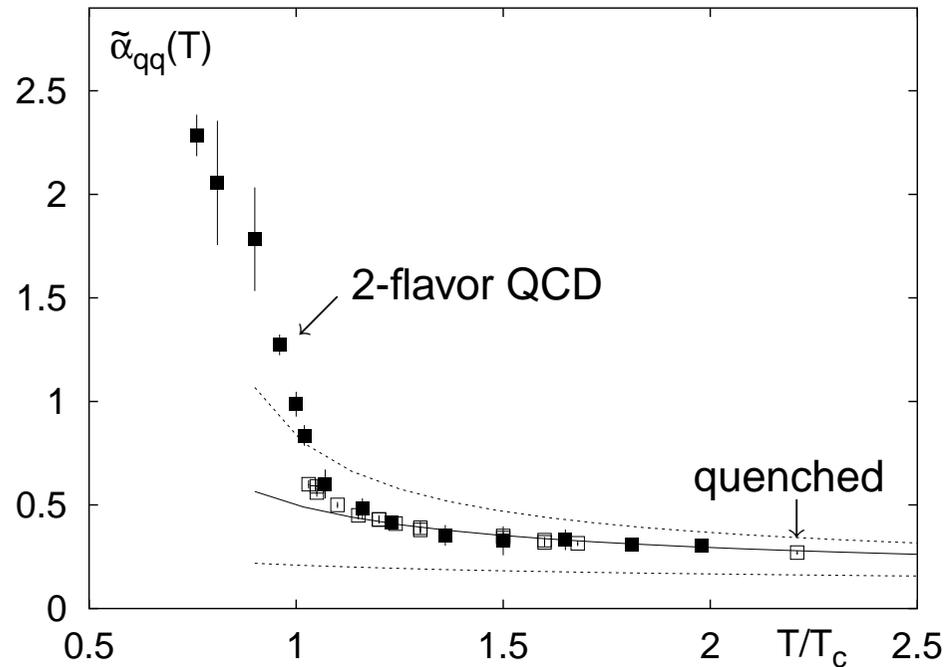
not a large Coulombic coupling

remnants of confinement at $T \gtrsim T_c$

string breaking and screening difficult to separate

slope at high T well described by perturbation theory

Temperature depending running coupling



define $\tilde{\alpha}_{qq}(T)$ by maximum of $\alpha_{qq}(r, T)$:

$$\tilde{\alpha}_{qq}(T) \equiv \alpha_{qq}(r_{max}, T)$$

perturbative behaviour at high T :

$$g_{2\text{-loop}}^{-2}(T) = 2\beta_0 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right) + \frac{\beta_1}{\beta_0} \ln\left(2 \ln\left(\frac{\mu T}{\Lambda_{\overline{MS}}}\right)\right),$$

Using $T_c/\Lambda_{\overline{MS}} = 0.77(21)$ we find $\mu = 1.14(2)\pi$

non-perturbative large values near T_c

not a large Coulombic coupling

remnants of confinement at $T \gtrsim T_c$

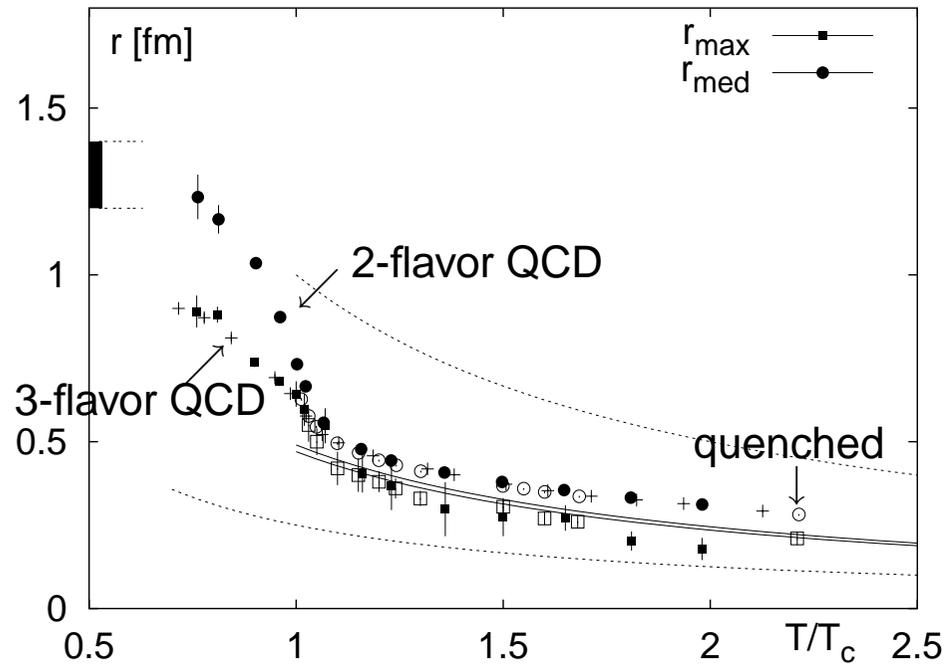
string breaking and screening difficult to separate

slope at high T well described by perturbation theory

⇒ At which distance do T -effects set in ?

⇒ definition of the screening radius/mass

Screening/String breaking radius



At which distances do medium effects set in?

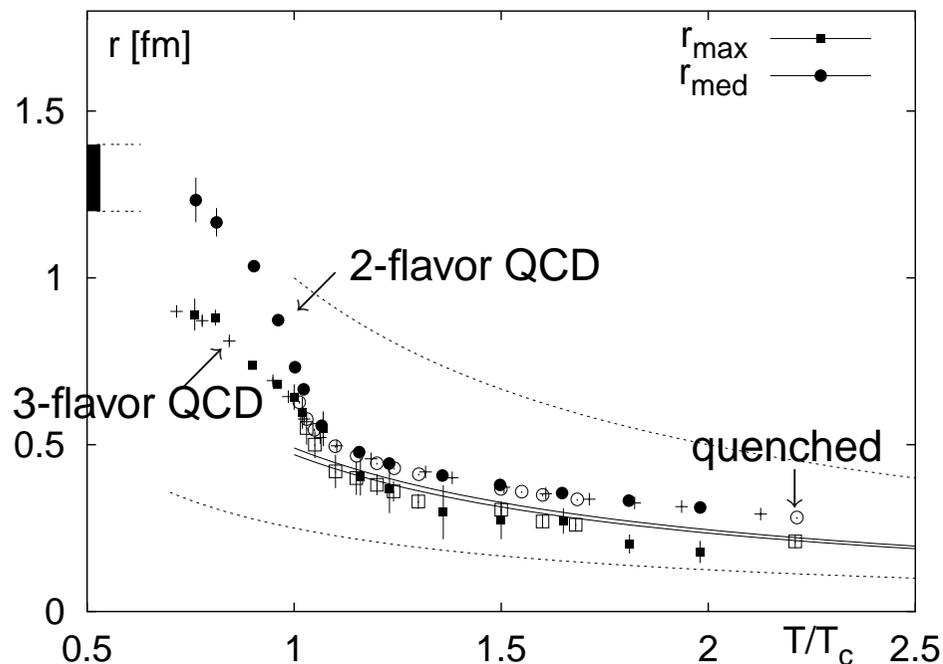
Definitions of the screening radius:

$$\tilde{\alpha}(T) \equiv \alpha_{qq}(r_{max}, T)$$

$$V(r_{med}) \equiv F_{\infty}(T)$$

Both define similar scales, but $r_{max} \lesssim r_{med}$

Screening/String breaking radius



At which distances do medium effects set in?

Definitions of the screening radius:

$$\tilde{\alpha}(T) \equiv \alpha_{qq}(r_{max}, T)$$

$$V(r_{med}) \equiv F_{\infty}(T)$$

Both define similar scales, but $r_{max} \lesssim r_{med}$

Above T_c :

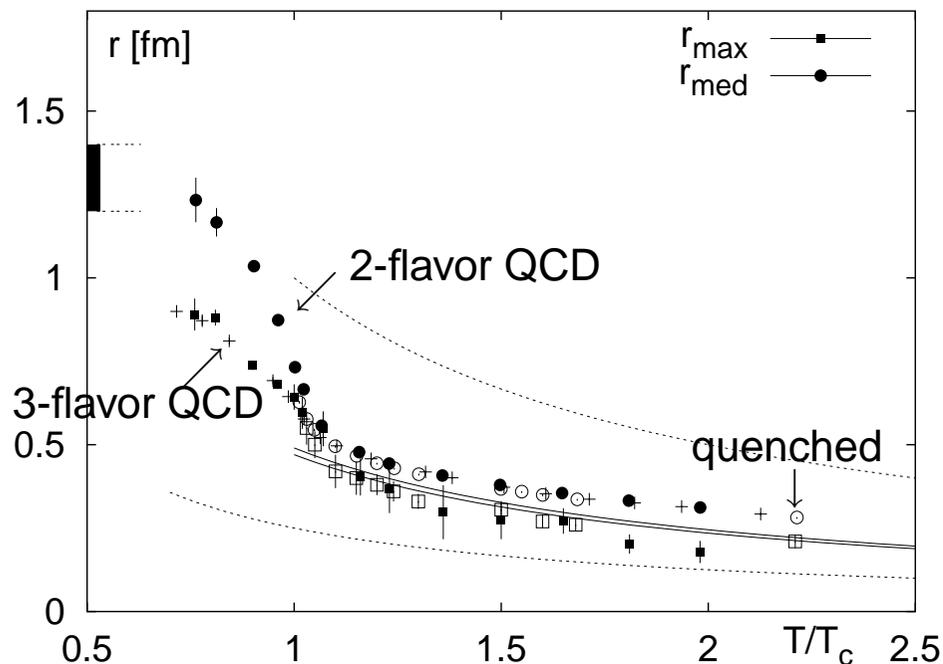
Only small flavor/quark mass effects

Both scales almost coincide

Change in r_{max} from 0.6 fm (T_c) to 0.25 fm ($2 T_c$)

$$r_{max} = 0.48(1) \text{ fm} \cdot T_c / T$$

Screening/String breaking radius



At which distances do medium effects set in?

Definitions of the screening radius:

$$\tilde{\alpha}(T) \equiv \alpha_{qq}(r_{max}, T)$$

$$V(r_{med}) \equiv F_{\infty}(T)$$

Both define similar scales, but $r_{max} \lesssim r_{med}$

Above T_c :

Only small flavor/quark mass effects

Both scales almost coincide

Change in r_{max} from 0.6 fm (T_c) to 0.25 fm ($2 T_c$)

$$r_{max} = 0.48(1) \text{ fm} \cdot T_c / T$$

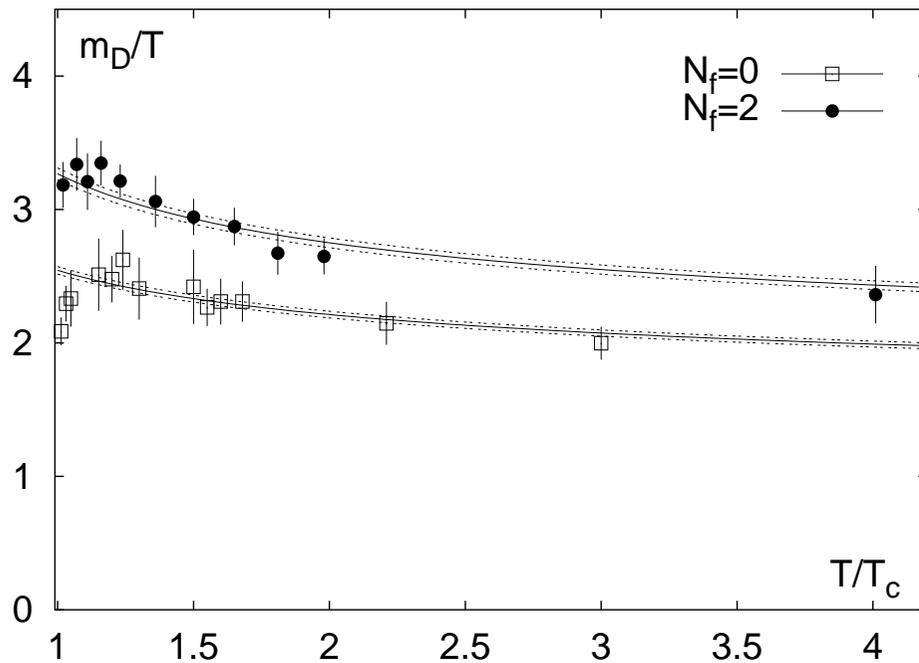
Below T_c :

Large flavor/quark mass effects

Both scales fall apart

Rapid increase to values expected at $T=0$

Screening mass



Screening masses obtained from fits to:

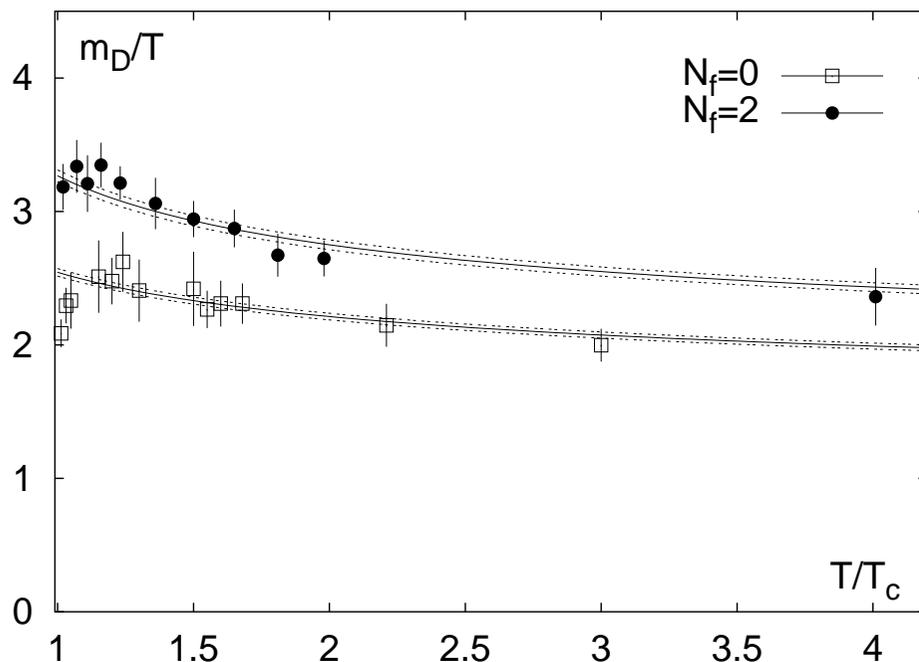
$$F_1(r, T) - F_1(r = \infty, T) = -\frac{4\alpha(T)}{3r} e^{-m_D(T)r}$$

at large distances $rT \gtrsim 1$

leading order perturbation theory:

$$\frac{m_D(T)}{T} = A \left(1 + \frac{N_f}{6}\right)^{1/2} g(T)$$

Screening mass



Screening masses obtained from fits to:

$$F_1(r, T) - F_1(r = \infty, T) = -\frac{4\alpha(T)}{3r} e^{-m_D(T)r}$$

at large distances $rT \gtrsim 1$

leading order perturbation theory:

$$\frac{m_D(T)}{T} = A \left(1 + \frac{N_f}{6}\right)^{1/2} g(T)$$

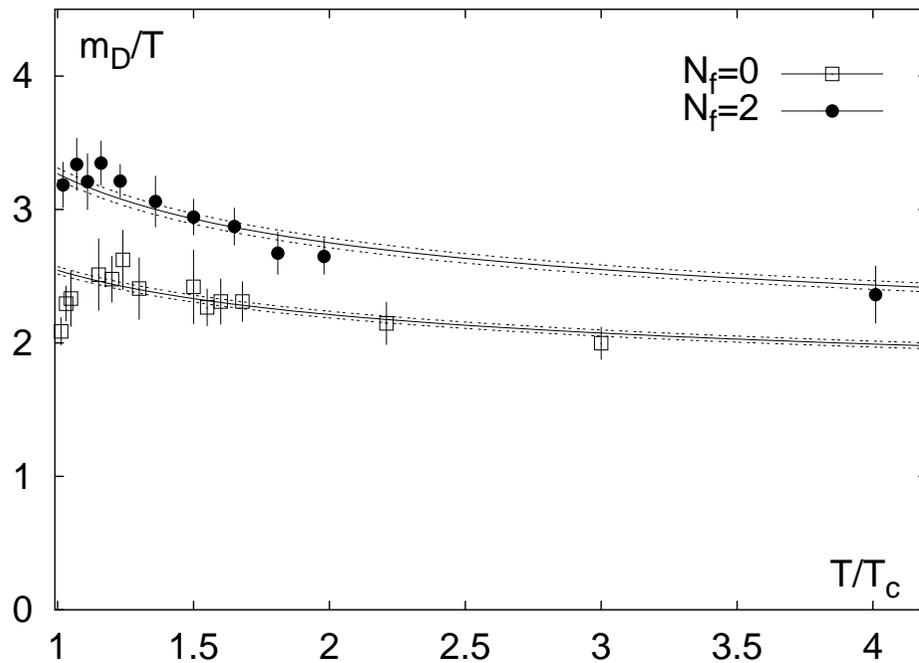
T dependence qualitatively described by perturbation theory

But $A \approx 1.4 - 1.5 \implies$ non-perturbative effects

$A \rightarrow 1$ in the (very) high temperature limit

Difference between $N_f = 0, 2$ disappears when converting to physical units

Screening mass



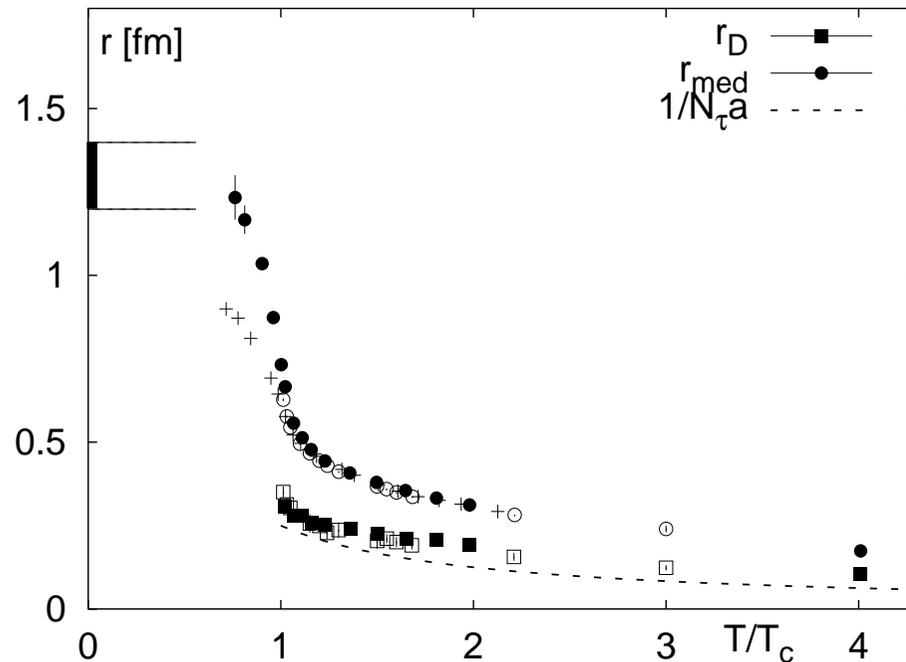
Screening masses obtained from fits to:

$$F_1(r, T) - F_1(r = \infty, T) = -\frac{4\alpha(T)}{3r} e^{-m_D(T)r}$$

at large distances $rT \gtrsim 1$

leading order perturbation theory:

$$\frac{m_D(T)}{T} = A \left(1 + \frac{N_f}{6}\right)^{1/2} g(T)$$



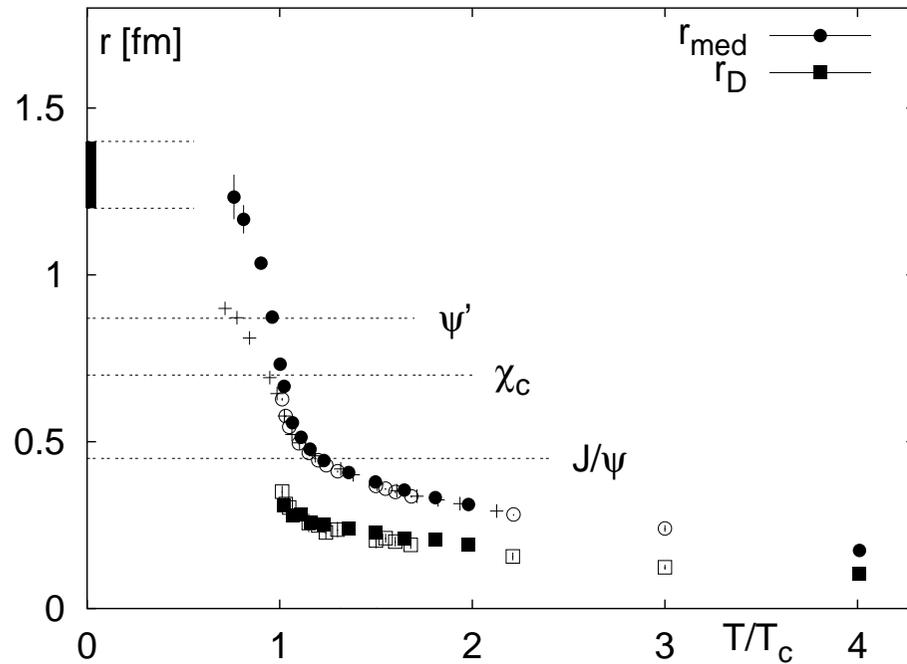
Debye screening radius $r_D = 1/m_D$

of the order of smallest attainable distance

r_{med} about twice as large

r_{med} indicates where medium effects become relevant

Heavy quark bound states above T_c ?



bound states above deconfinement?

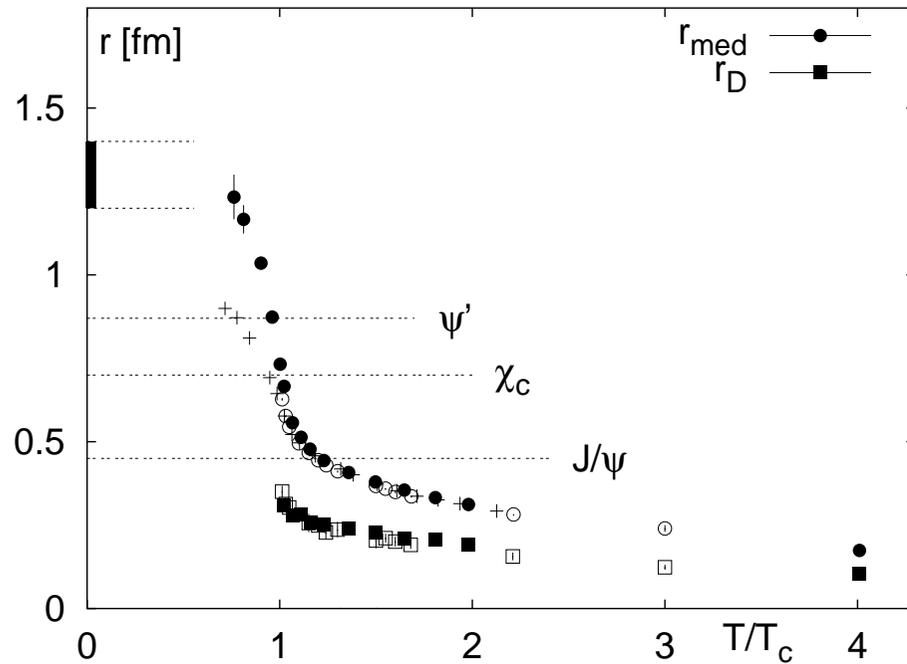
first estimate:

mean charge radii of charmonium states compared to r_{med}

thermal modifications on ψ' and χ_c already at T_c

J/ψ may survive above deconfinement

Heavy quark bound states above T_c ?



bound states above deconfinement?

first estimate:

mean charge radii of charmonium states compared to r_{med}

thermal modifications on ψ' and χ_c already at T_c

J/ψ may survive above deconfinement

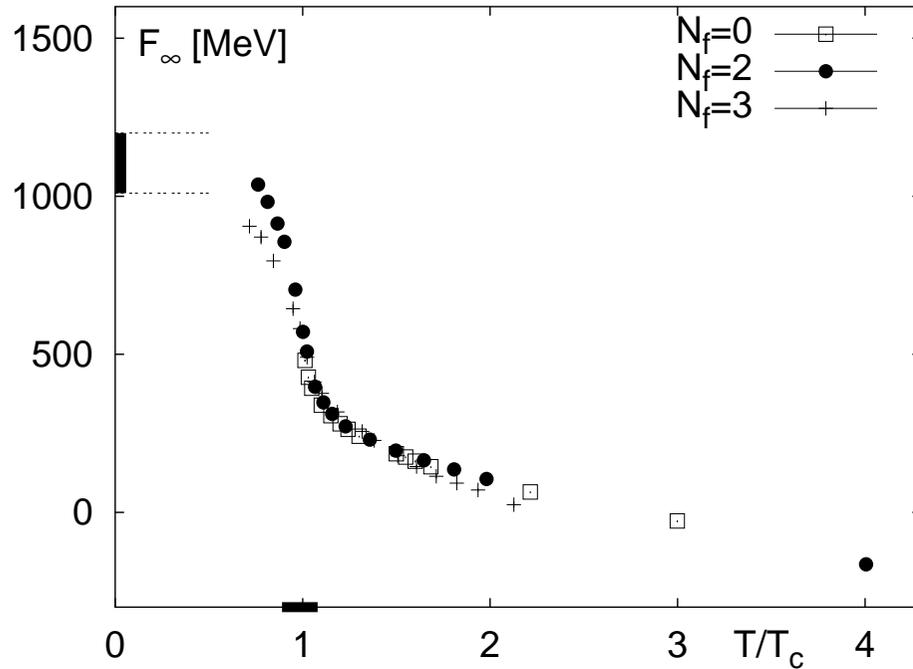
Better estimate:

effective potentials in Schrödinger Equation

Potential models, effective potential $V_{eff}(r, T)$

But: Free energies vs. internal energies $F(r, T) = U(r, T) - TS(r, T)$

Free energy vs. Entropy for $r \rightarrow \infty$



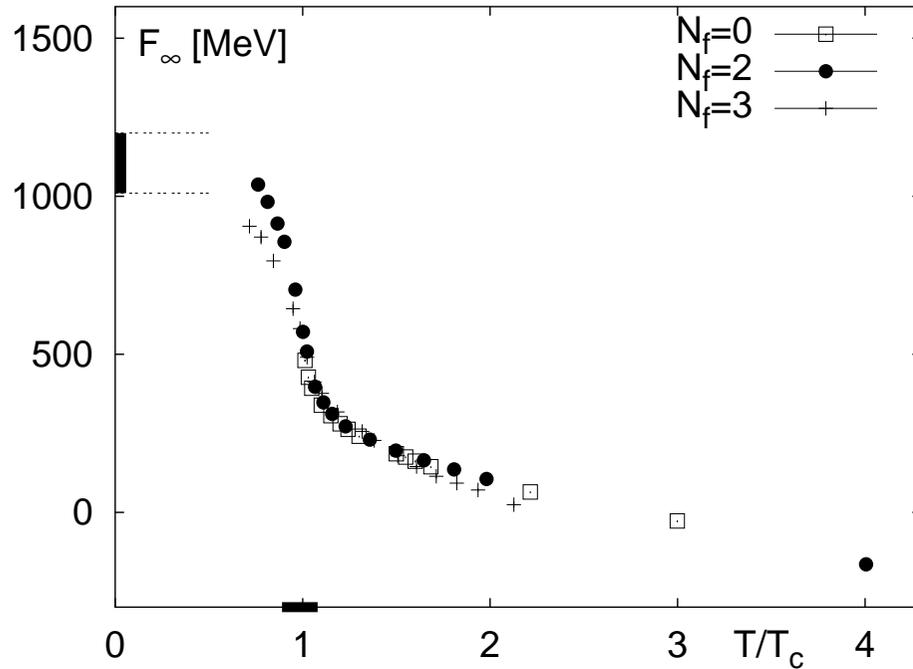
Free energies not only determined by potential energy

$$F_\infty = U_\infty - TS_\infty$$

Entropy contributions play a role at finite T

$$S_\infty = -\frac{\partial F_\infty}{\partial T}$$

Free energy vs. Entropy for $r \rightarrow \infty$

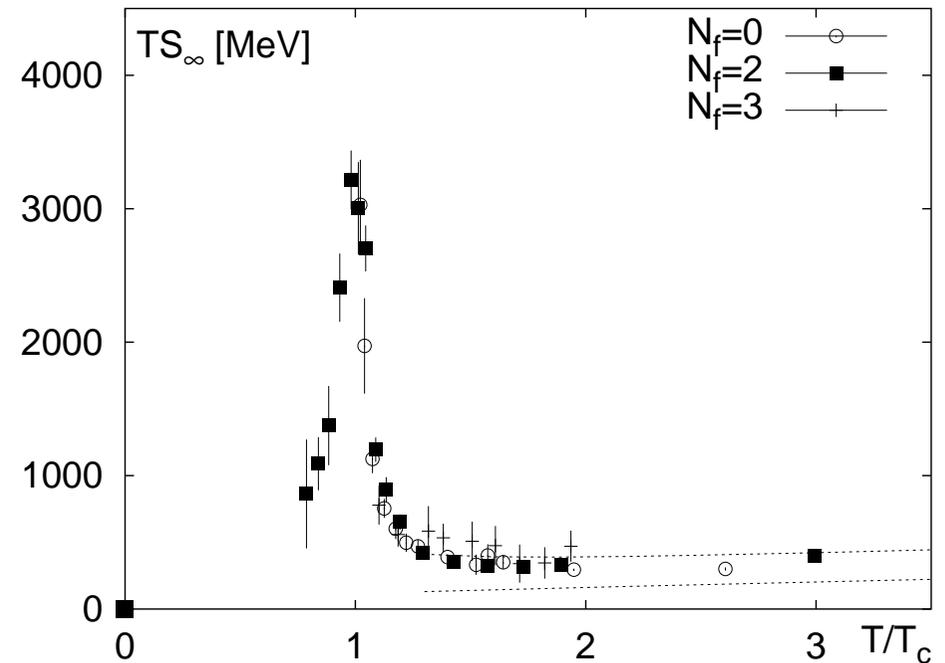


Free energies not only determined by potential energy

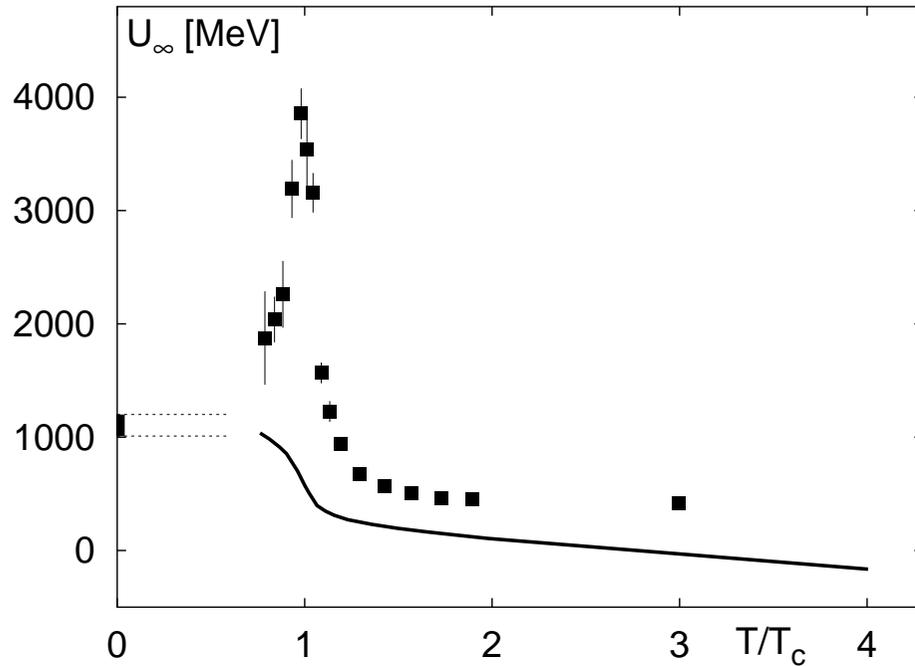
$$F_\infty = U_\infty - TS_\infty$$

Entropy contributions play a role at finite T

$$S_\infty = -\frac{\partial F_\infty}{\partial T}$$



Free energy vs. Entropy for $r \rightarrow \infty$



Internal energy:

$$U_\infty = -T^2 \frac{\partial F_\infty / T}{\partial T}$$

enhancement compared to free energies

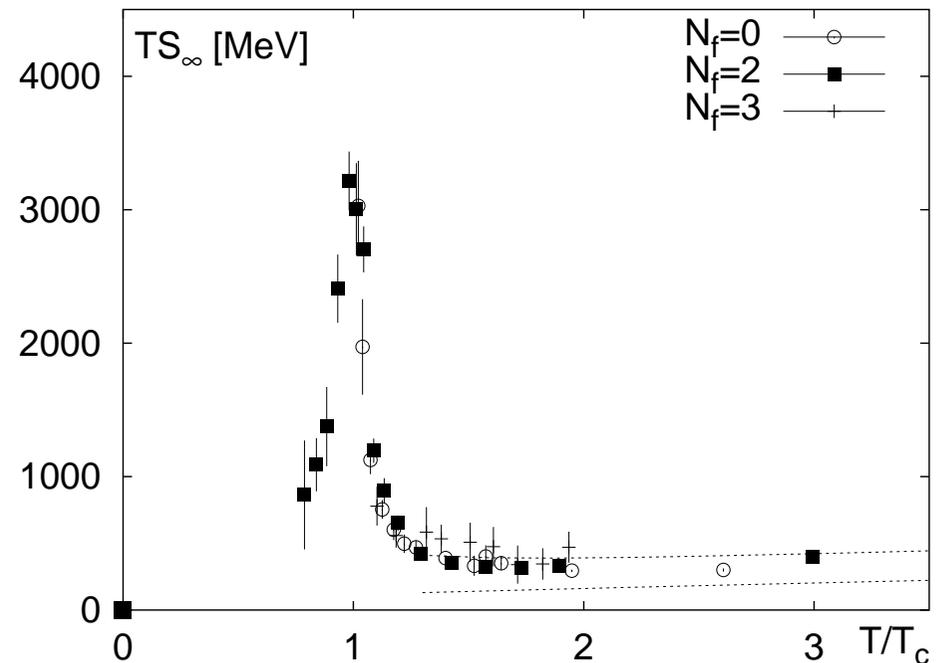
strongest enhancement around T_c

Free energies not only determined by potential energy

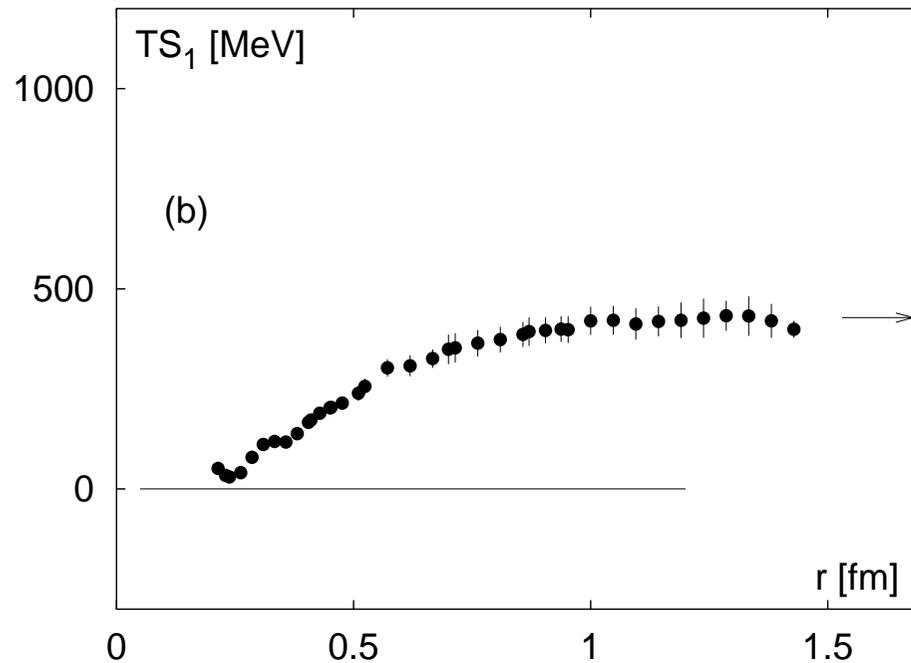
$$F_\infty = U_\infty - TS_\infty$$

Entropy contributions play a role at finite T

$$S_\infty = -\frac{\partial F_\infty}{\partial T}$$



r -dependence of internal energies



$$F_1(r, T) = U_1(r, T) - TS_1(r, T)$$

$$S_1(r, T) = \frac{\partial F_1(r, T)}{\partial T}$$

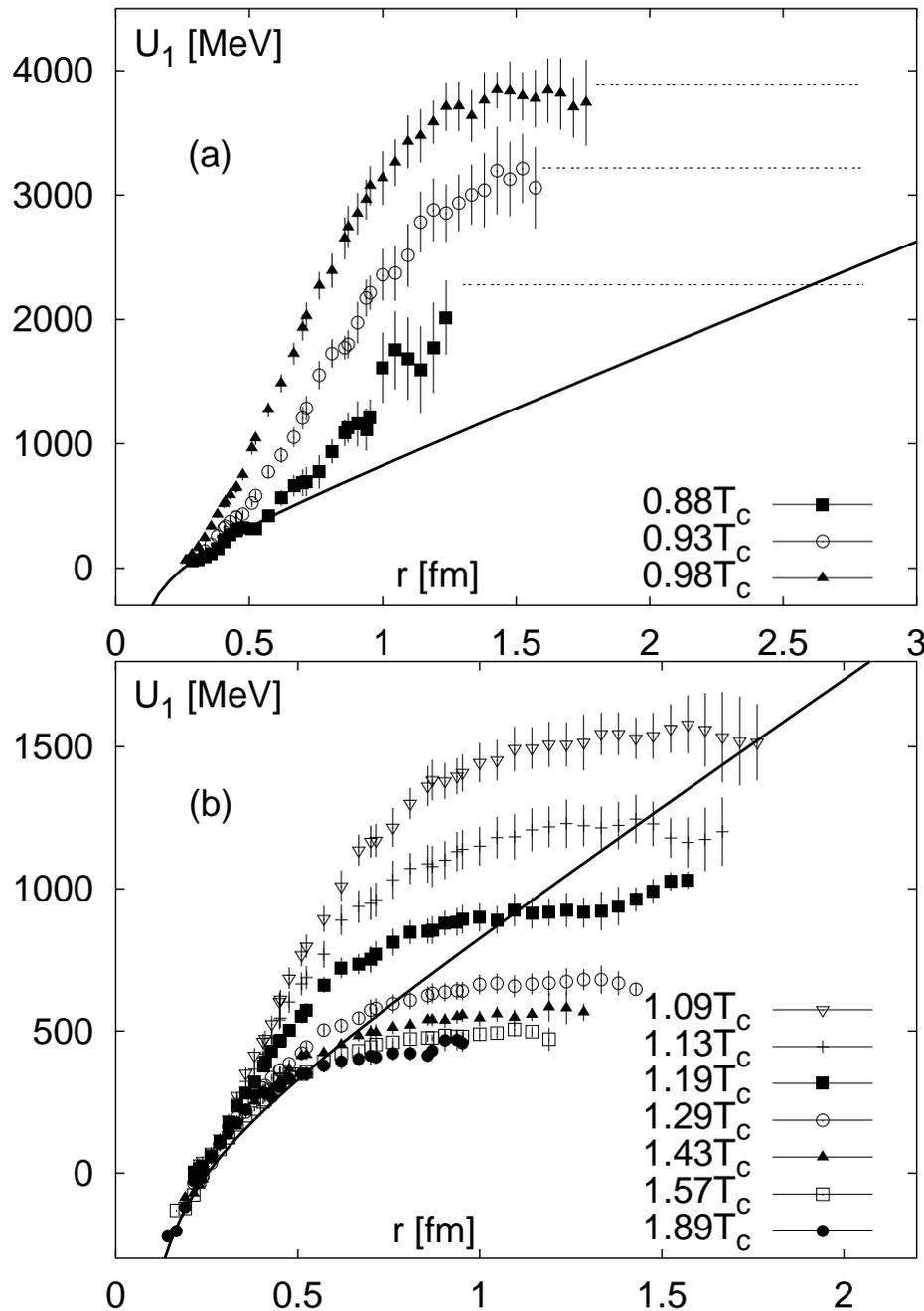
$$U_1(r, T) = -T^2 \frac{\partial F_1(r, T)/T}{\partial T}$$

Entropy contributions vanish in the limit $r \rightarrow 0$

$$F_1(r \ll 1, T) = U_1(r \ll 1, T) \equiv V_1(r)$$

important at intermediate/large distances

r -dependence of internal energies



$$F_1(r, T) = U_1(r, T) - T S_1(r, T)$$

$$S_1(r, T) = \frac{\partial F_1(r, T)}{\partial T}$$

$$U_1(r, T) = -T^2 \frac{\partial F_1(r, T)/T}{\partial T}$$

Entropy contributions vanish in the limit $r \rightarrow 0$

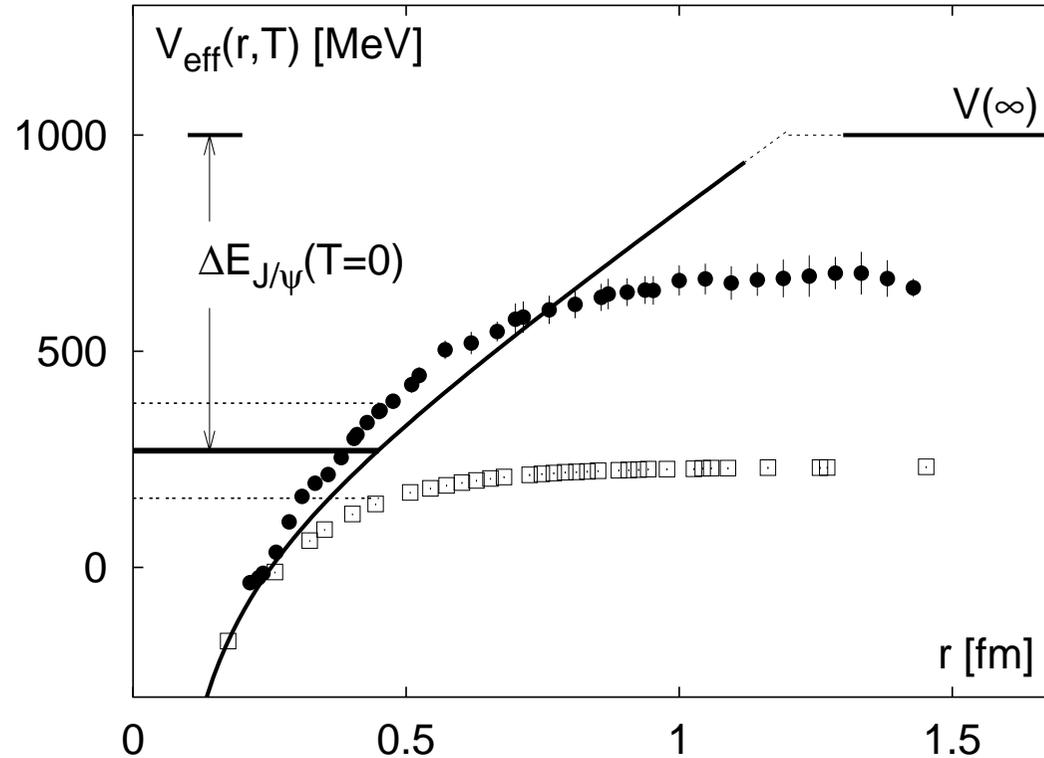
$$F_1(r \ll 1, T) = U_1(r \ll 1, T) \equiv V_1(r)$$

important at intermediate/large distances

⇒ Implications on heavy quark bound states?

⇒ What is the correct $V_{eff}(r, T)$?

Heavy quark bound states



steeper slope of $V_{eff}(r, T) = U_1(r, T)$

$\Rightarrow J/\psi$ stronger bound using $V_{eff} = U_1(r, T)$

\Rightarrow dissociation at higher temperatures compared to $V_{eff}(r, T) = F_1(r, T)$

Estimates on bound states from Schrödinger equation

Schrödinger equation for heavy quarks:

$$\left[2m_f + \frac{1}{m_f} \Delta^2 + V_{eff}(r, T) \right] \Phi_i^f = E_i^f(T) \Phi_i^f, \quad f = \text{charm, bottom}$$

T -dependent color singlet heavy quark potential mimics in-medium modifications of $q\bar{q}$ interaction

reduction to 2-particle interaction clearly too simple, in particular close to T_c

recent analysis:

using $V_{eff} = F_1$: S.Digal, P.Petreczky, H.Satz, Phys. Lett. B514 (2001)57

using $V_{eff} = V_1$: C.-Y. Wong, hep-ph/0408020

using $V_{eff} = V_1$: W.M. Alberico, A. Beraudo, A. De Pace, A. Molinari, hep-ph/0507084

state	J/ψ	χ_c	ψ'	Υ	χ_b	Υ'	χ'_b	Υ''
$E_s^i [GeV]$	0.64	0.20	0.005	1.10	0.67	0.54	0.31	0.20
T_d/T_c	1.1	0.74	0.1-0.2	2.31	1.13	1.1	0.83	0.74
T_d/T_c	~ 2.1	~ 1.2	~ 1.2	~ 5.0	~ 1.95	~ 1.65	-	-
T_d/T_c	1.75-1.95	1.13-1.15	1.10-1.11	4.4-4.7	1.5-1.6	1.4-1.5	~ 1.2	~ 1.2

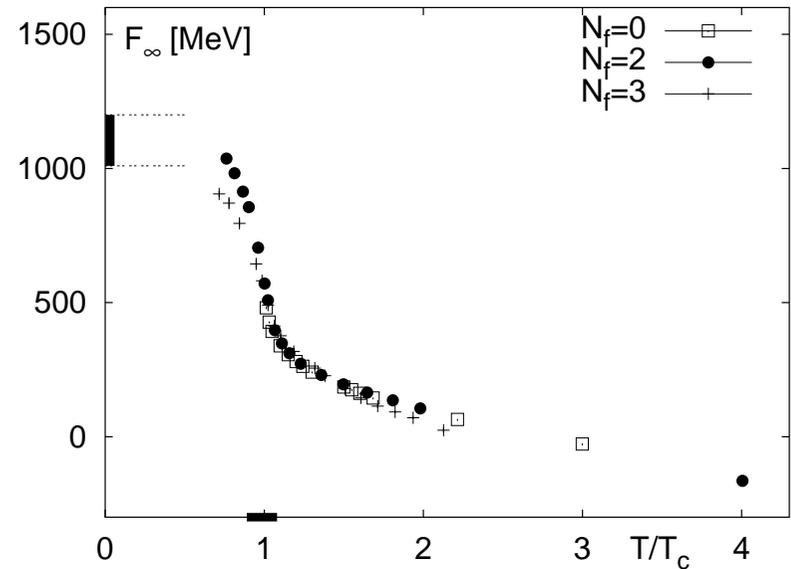
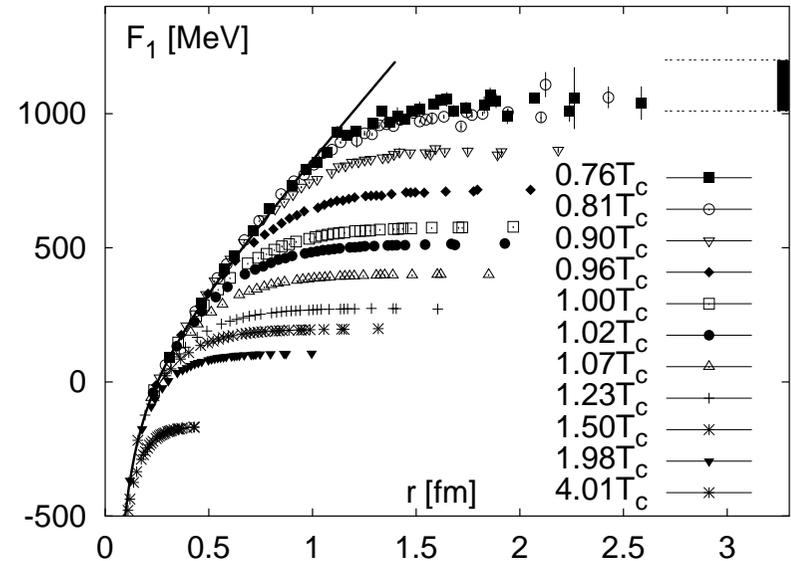
Renormalized Polyakov loop

$$L_{ren} = \exp\left(-\frac{F(r = \infty, T)}{2T}\right)$$

Defined by long distance behaviour of $F(r, T)$.

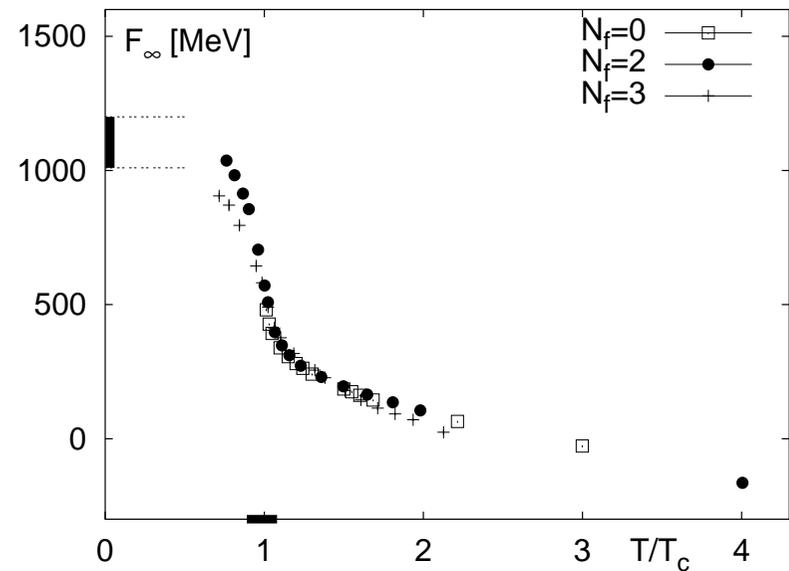
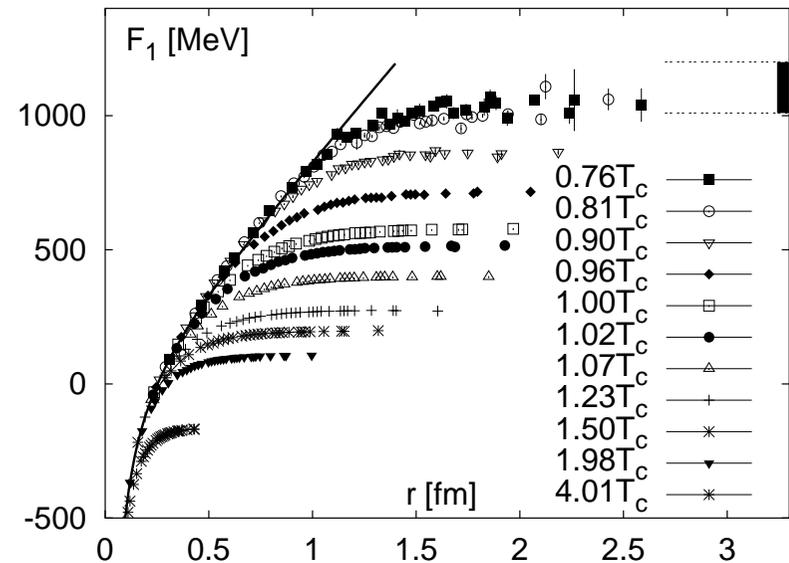
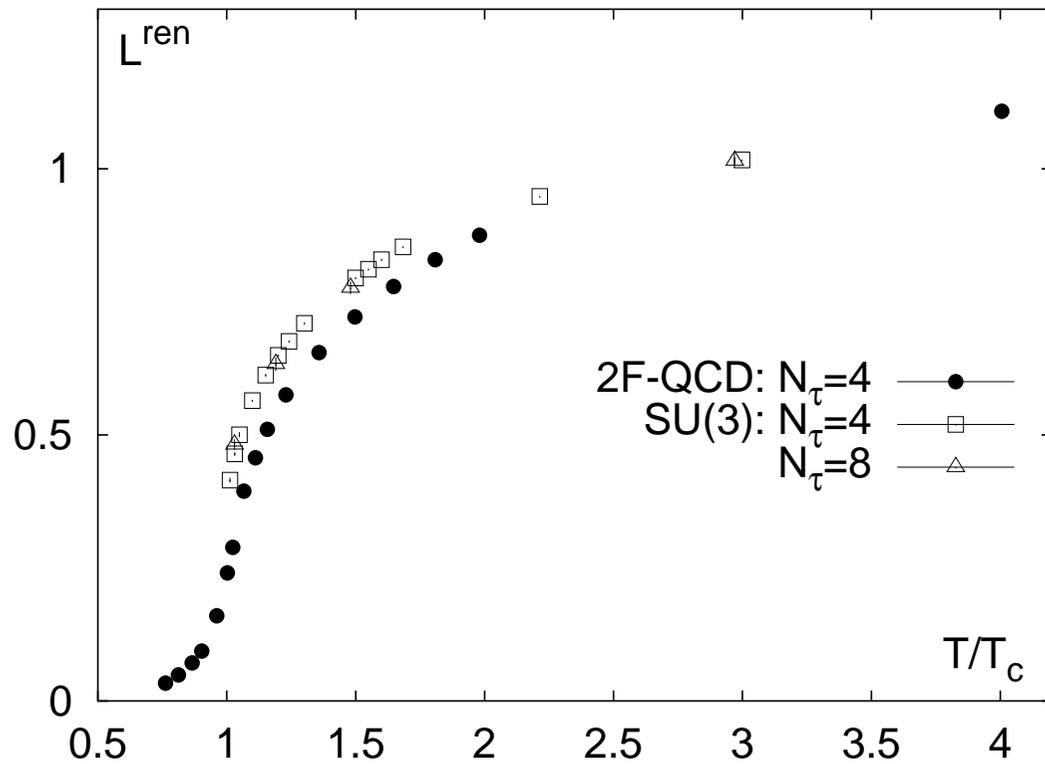
Renormalized by renormalization of $F(r, T)$ at small distances.

$$L_{ren} = (Z_R(g^2))^{N_t} L_{lattice}$$



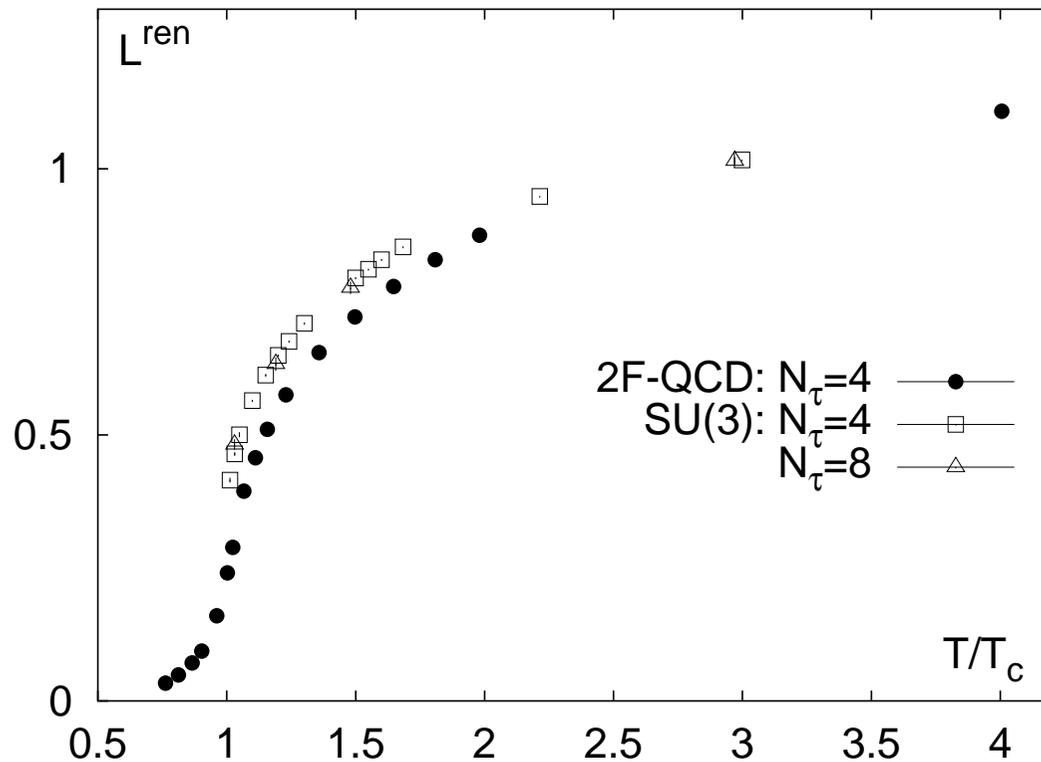
Renormalized Polyakov loop

$$L_{ren} = \exp\left(-\frac{F(r = \infty, T)}{2T}\right)$$



Renormalized Polyakov loop

$$L_{ren} = \exp\left(-\frac{F(r = \infty, T)}{2T}\right)$$



Quenched QCD:

$L_{ren} = 0$ for $T < T_c$.

Finite gap at T_c

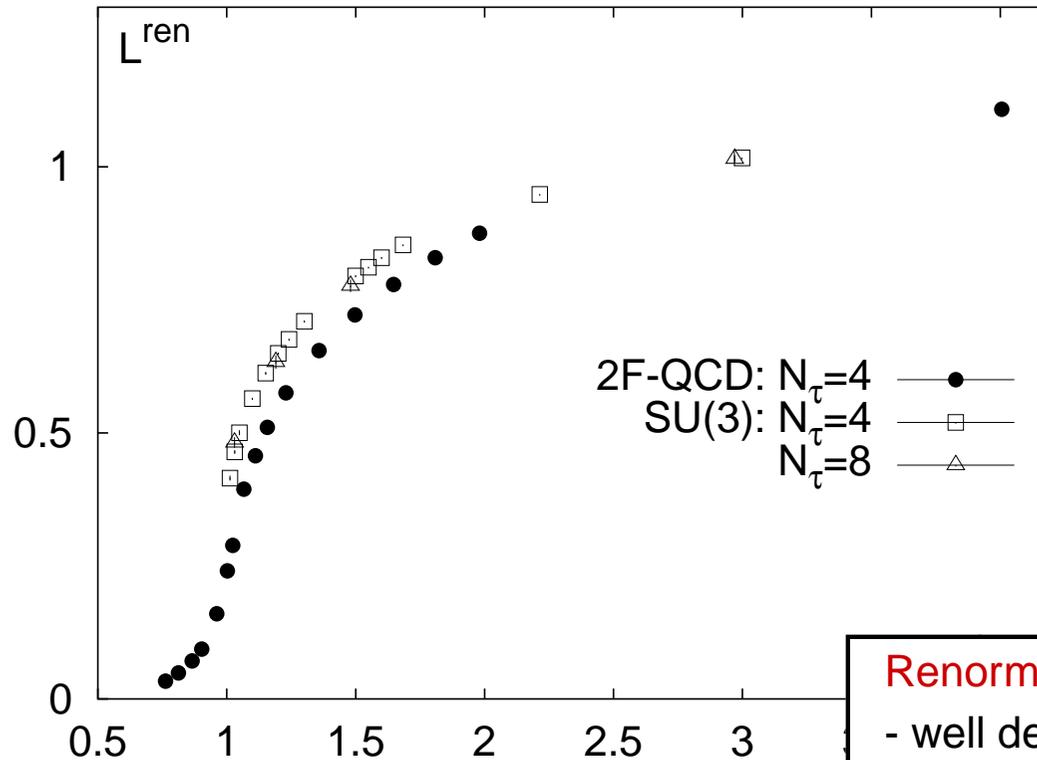
Full QCD:

L_{ren} finite for all T .

Strong increase near T_c .

Renormalized Polyakov loop

$$L_{ren} = \exp\left(-\frac{F(r = \infty, T)}{2T}\right)$$



Quenched QCD:

$L_{ren} = 0$ for $T < T_c$.

Finite gap at T_c

Full QCD:

L_{ren} finite for all T .

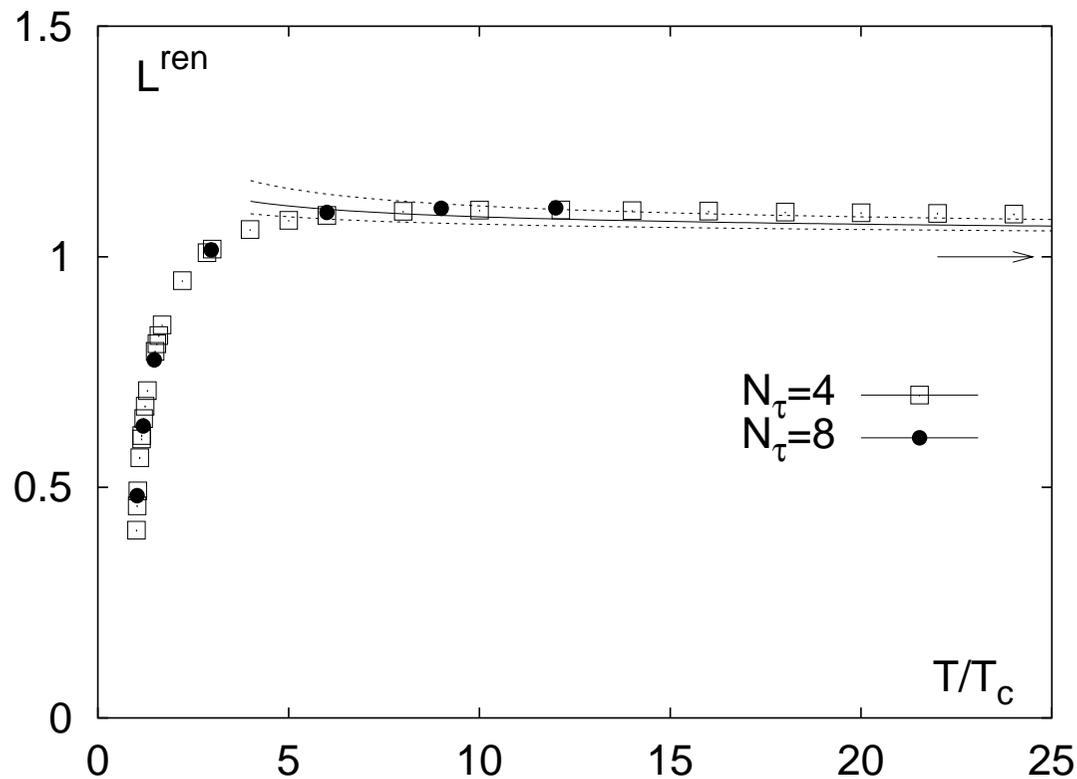
Strong increase near T_c .

Renormalized Polyakov loop

- well defined in quenched and full QCD
- non-zero for finite quark mass
- strong increase near T_c

Renormalized Polyakov loop

$$L_{ren} = \exp\left(-\frac{F(r = \infty, T)}{2T}\right)$$



Quenched QCD:

$L_{ren} = 0$ for $T < T_c$.

Finite gap at T_c

Full QCD:

L_{ren} finite for all T .

Strong increase near T_c .

Heavy quark free and internal energies

Complex r and T dependence

Running coupling shows remnants of confinement above T_c

Entropy contributions play a role at finite T

Separation of entropy and internal energy contributions possible

Potential energy larger than free energy

Charmonium in the quark gluon plasma

First estimates from potential models

Higher dissociation temperature using V_1

(directly produced) J/ψ exist well above T_c

Heavy quark free and internal energies

Smaller quark masses

Smaller lattice spacing to analyze small r dependence

Better understanding of the different contributions

Charmonium in the quark gluon plasma

What is the correct V_{eff} in potential models

Full QCD calculations of correlation/spectral functions

Relevant processes for charmonium production/dissociation ?

Density dependence of heavy quark free energies

→ poster by M. Döring

Extension to qq and qqq free energies