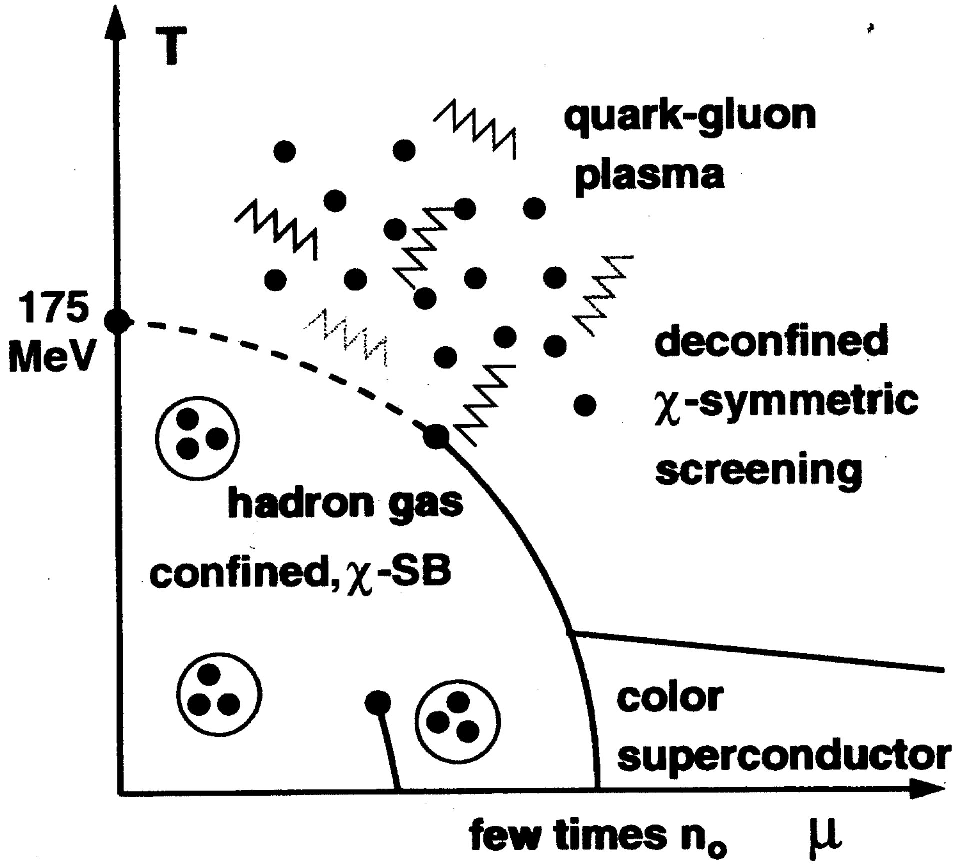
Thermodynamics of two and three flavour QCD

Martina Franca, June 16-20, 2001

- Introduction
  - basic concepts, lattice formulation
  - short vs. long distance physics, improved actions
- The QCD phase diagram
  - chiral symmetry restoration and/or deconfinement
  - flavour and quark mass dependence
  - heavy quark free energy, critical temperature
- Bulk thermodynamics
  - flavour dependence of the high temperature limit
  - QCD equation of state, critical energy density
- Hadrons in a thermal medium
  - Deconfinement ⇒heavy quark bound states
  - χ-symmetry restoration ⇒light meson spectrum
- Conclusions

QCD Thermodynamics

Generic phase diagram of strongly interacting matter



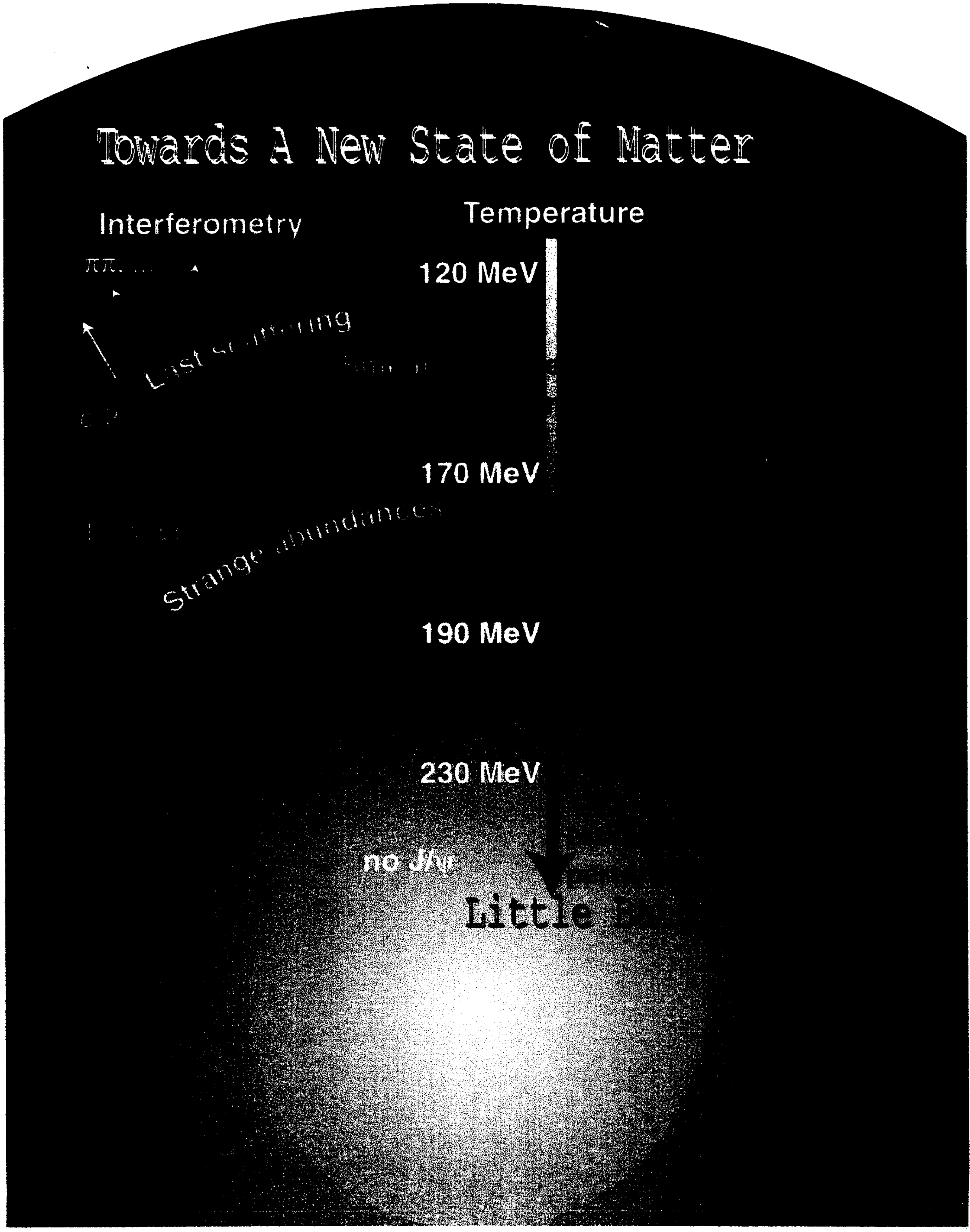
- **phase transition from a hadron gas to a quark-gluon plasma**

- qualitative features can be understood in terms of models (bags, percolation, strings, ...) and approximations (resonance gas, perturbation theory, instanton liquid, ...)

- quantitative can come from numerical simulations of

lattice regularized QCD

– Lattice Thermodynamics



Towards A New State of Matter

Interferometry

Temperature

$\pi\pi$. ...

120 MeV

Last scattering

170 MeV

Strange abundances

190 MeV

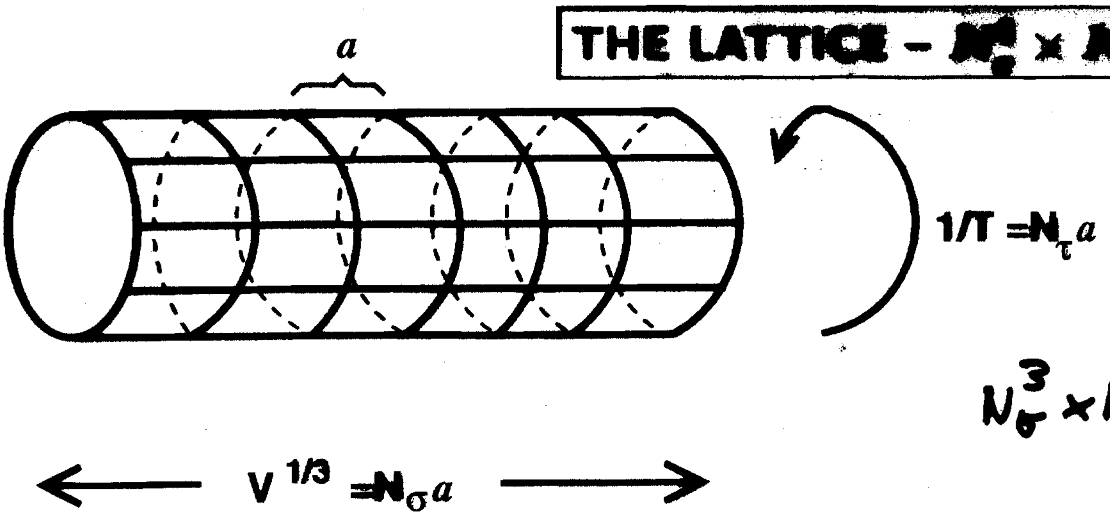
230 MeV

no J/ψ

Little

Lattice regularized QCD thermodynamics

THE LATTICE – $N_\sigma^3 \times N_\tau$



$N_\sigma^3 \times N_\tau$

partition function: $Z(V,T) = \int \mathcal{D}\mathcal{A}\mathcal{D}\psi\mathcal{D}\bar{\psi}e^{-S_E}$ $\mu=0$

$$\boxed{S_E = \int_0^{1/T} dx_0 \int_V d^3x \mathcal{L}_E(\mathcal{A},\psi,\bar{\psi})}$$

discrete space-time: $Z(V,T) \rightarrow Z(N_\sigma, N_\tau, a) \leftarrow a(g^2, m_q)$

The lattice problems ⇔	solutions
• **finite cut-off effects:** $a > 0 \Leftrightarrow N_\tau < \infty$ **continuum limit at fixed** $T = 1/N_\tau a$ ⇒**requires** $a \rightarrow 0$, $N_\tau \rightarrow \infty$	**improved** **actions**
• **finite volume effects:** **thermodynamic limit** ⇒**requires** $N_\sigma \rightarrow \infty$	**large** **computers**
• **broken symmetries:** **rotational-, flavor-, chiral-sym.** ⇒**requires appropriate actions** **and/or**	**SF, WF, DWF** **impr. actions** **+cont. limit**

Bielefelder Parallelrechnerkomplex

zur Untersuchung von wechselwirkender Elementarteilchenmaterie

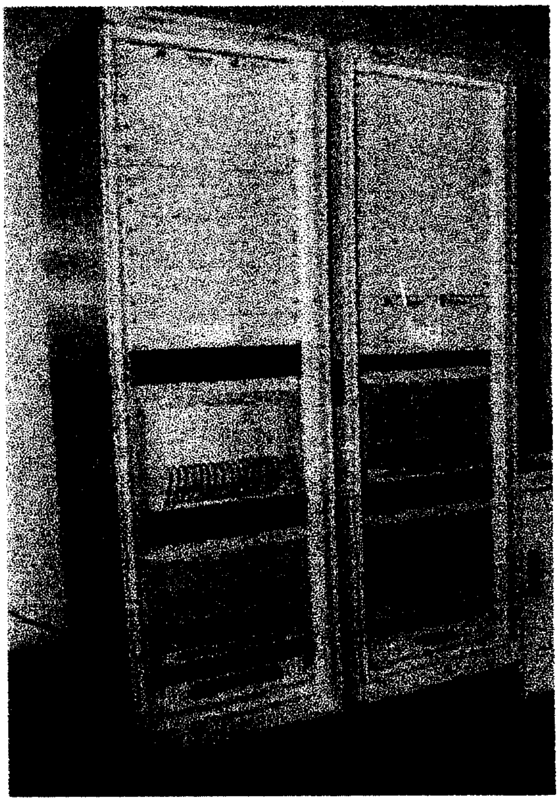
- **APE100 → APEmille:**
  Parallelrechner, entwickelt an der Universität Rom
- **in Bielefeld eingesetzt seit 1993**

integrierte Rechenleistung: 110 GFlops

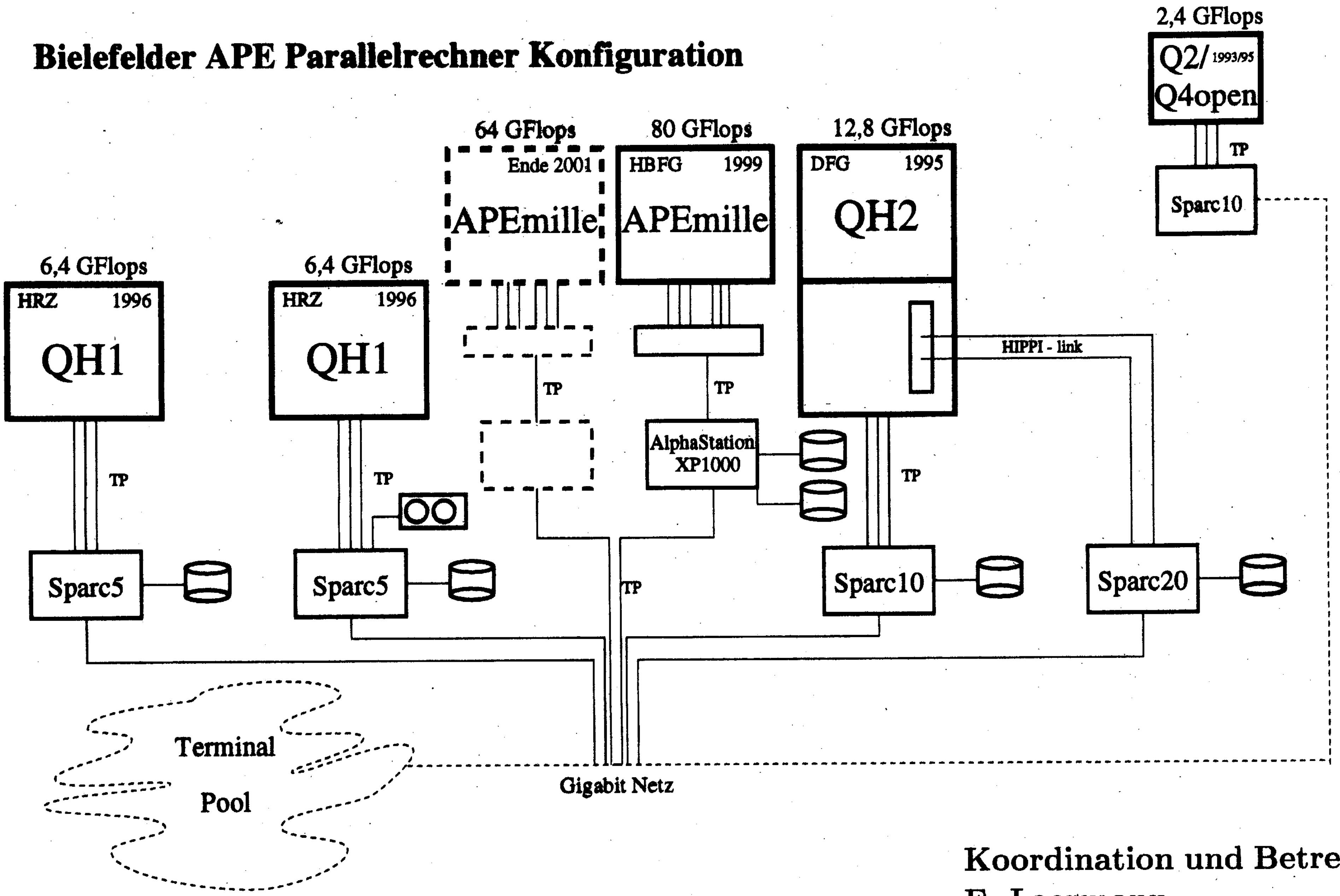
256-Knoten APE100
(Fak. f. Phys. seit 1/1995)

2×128-Knoten APE100
(HRZ, 12/1996)

60-Knoten APEmille
(Fak. f. Phys. seit 12/1999)



Bielefelder APE Parallelrechner Konfiguration



Koordination und Betreuung:
E. Laermann
O. Kaczmarek

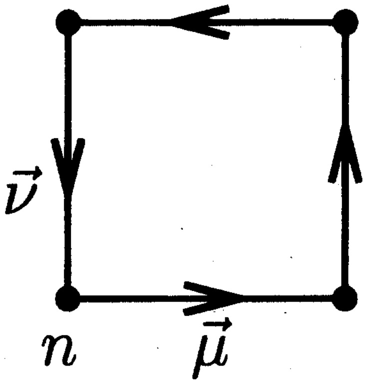
Improved actions for Thermodynamics

Lattice discretization ⇔ultraviolet cut-off effects

- **standard Wilson action**

$$S_E = \frac{2N_c}{g^2} \sum_{n,\mu<\nu} P_{n,\mu,\nu} \qquad \beta \equiv \frac{2N_c}{g^2} \leftarrow g^2(a)$$

$$P_{n,\mu,\nu} = 1 - \frac{1}{N_c} \mathrm{Re}\ \mathrm{Tr}\ U_{n,\mu} U_{n+\mu,\nu} U^\dagger_{n+\nu,\mu} U^\dagger_{n,\nu}$$



$$n \equiv (n_0,\ n_1,\ n_2,\ n_3)$$

$$x = n \cdot a$$

$$U_{n,\mu} = \exp(iagA_\mu(x)) \ , A_\mu \equiv A_\mu^\alpha \lambda^\alpha$$

$$\Longrightarrow \quad \frac{1}{4} a^4 F^c_{\mu\nu} F^c_{\mu\nu} + \mathcal{O}(a^6)$$

$$\Downarrow$$

$\mathcal{O}(a^2)$ **correction to** S_E

leads to $\mathcal{O}((aT)^2 \equiv 1/N_\tau^2)$ **systematic errors in** $\epsilon/T^4,\ P/T^4$**...**

CPU-time increases like N_τ^z , $z \simeq 10$

Cut-off dependence in the $T \to \infty$ limit

cut-off dependence ⇔ N_τ-dependence

Wilson action

perturbative calculation of the energy density ⇒ weak coupling expansion for spacelike (P_σ) and timelike (P_τ) plaquette expectation values on lattices of size $N_\sigma^3 \times N_\tau$

$$\boxed{\frac{\epsilon}{T^4} = \frac{6N_c}{g^2}(P_\sigma - P_\tau)N_\tau^4 + \mathcal{O}(g^2)}$$

$$\Uparrow \quad P_{\sigma,\tau} = g^2 \frac{N_c^2 - 1}{N_c} P_{\sigma,\tau}^{(2)} + \mathcal{O}(g^4)$$

$$\boxed{\frac{\epsilon}{T^4} = \frac{3}{2} N_\tau^4 (N_c^2 - 1) \int \frac{\mathrm{d}^3 p}{(2\pi)^3} (\frac{4}{3} \frac{\coth(N_\tau \Omega/2)}{\coth(\Omega/2)} - 1)}$$

with $\sinh^2(\Omega/2) = \sum_{\mu=1}^{3} \sin^2(p_\mu/2)$

- expand in $1/N_\tau$

$$\boxed{\frac{\epsilon}{T^4} = (N_c^2 - 1)\frac{\pi^2}{15}[1 + \frac{30}{63}(\frac{\pi}{N_\tau})^2 + \frac{1}{3}(\frac{\pi}{N_\tau})^4 + ...]}$$

$$\Uparrow \quad \sim (aT)^2$$

cut-off dependence $\sim 50\%$ for $N_\tau = 4$

Improved Actions

Some tree level improved actions

- $\mathcal{O}(a^2)$ improved

$$S^{(1,2)} = \sum_{x,\nu>\mu} \frac{5}{3}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\square_{\mu\nu}(x)\right)-\frac{1}{6}\left(1-\frac{1}{2N}\mathrm{Re}\ \mathrm{Tr}\left(\boxed{}_{\mu\nu}(x)+\boxed{\begin{matrix}\\\end{matrix}}_{\mu\nu}(x)\right)\right)$$

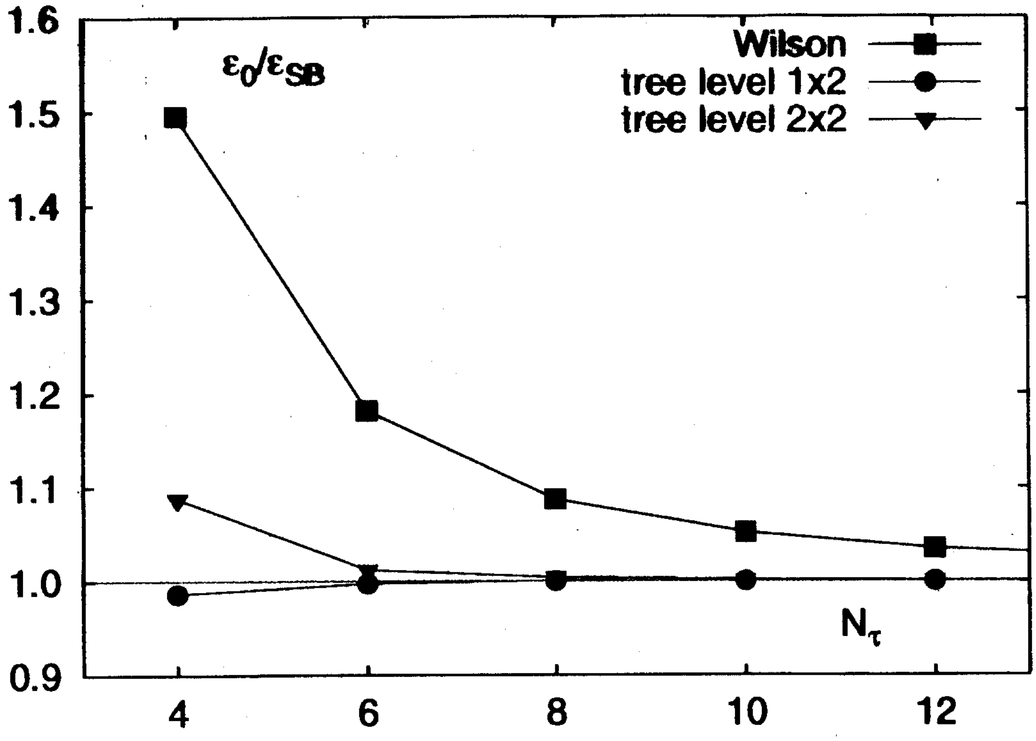
$$S^{(2,2)} = \sum_{x,\nu>\mu} \frac{4}{3}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\square_{\mu\nu}(x)\right)-\frac{1}{48}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\boxed{\begin{matrix}&\\&\end{matrix}}_{\mu\nu}(x)\right)$$

- $\mathcal{O}(a^4)$ improved

$$S^{(3,3)} = \sum_{x,\nu>\mu} \frac{3}{2}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\square_{\mu\nu}(x)\right)-\frac{3}{80}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\boxed{\begin{matrix}&\\&\end{matrix}}_{\mu\nu}(x)\right)$$
$$+\frac{1}{810}\left(1-\frac{1}{N}\mathrm{Re}\ \mathrm{Tr}\,\boxed{\begin{matrix}&&\\&&\\&&\end{matrix}}_{\mu\nu}(x)\right)$$

Improved High-T Limit

reduced cut-off dependence of the
energy density in the high temperature limit: $\mathcal{O}(a^2) \rightarrow \mathcal{O}(a^4)$



$$(1 \times 1)\text{-action:}\ \frac{\epsilon}{\epsilon_{SB}} = 1 + 0.476 \left(\frac{\pi}{N_\tau}\right)^2 + \dots.$$

$$(1 \times 2)\text{-action:}\ \frac{\epsilon}{\epsilon_{SB}} = 1 + 0.044 \left(\frac{\pi}{N_\tau}\right)^4 + \dots.$$

$$(2 \times 2)\text{-action:}\ \frac{\epsilon}{\epsilon_{SB}} = 1 + 0.178 \left(\frac{\pi}{N_\tau}\right)^4 + \dots.$$

computational effort $\sim N_\tau^{10}$

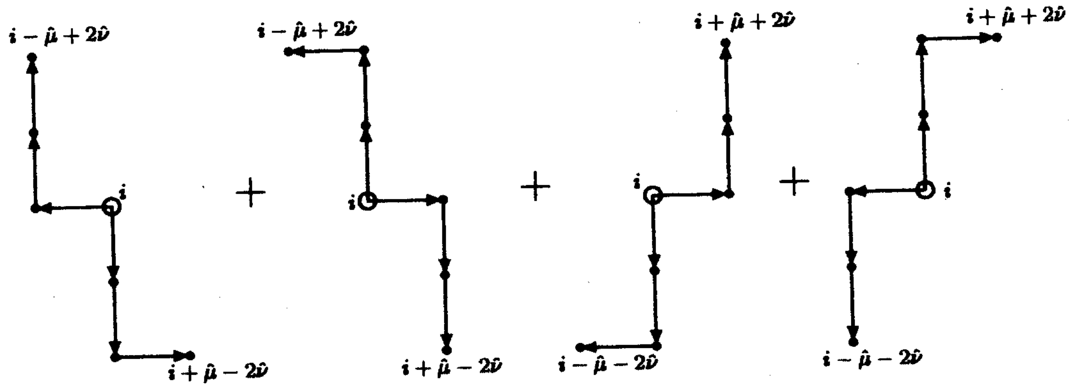
Staggered fermion action with improved rotational invariance (p4-action)

- 1-link and L-shaped **3-link paths**
- Coefficients fixed by demanding rotational invariance of the fermion propagator up to order p^4
- **Fat links**† to improve flavour symmetry

$$M[U]_{ij} = m\,\delta_{ij} + \eta_i \left\{ \frac{3}{8}\, A[U]_{ij} + \frac{1}{48}\,\frac{1}{2}\, B[U]_{ij} \right\}$$

$A[U]_{ij} =$

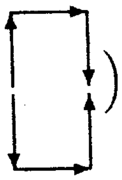
$B[U]_{ij} =$



⇒ Improved rotational symmetry - rapid approach to continuum ideal gas limit.

Fat-Links in the one-link derivative $A[U]$:

$$U_{\text{fat}} = \boldsymbol{\longrightarrow} = \frac{1}{1+6\omega}\Big(\longrightarrow + \omega$$



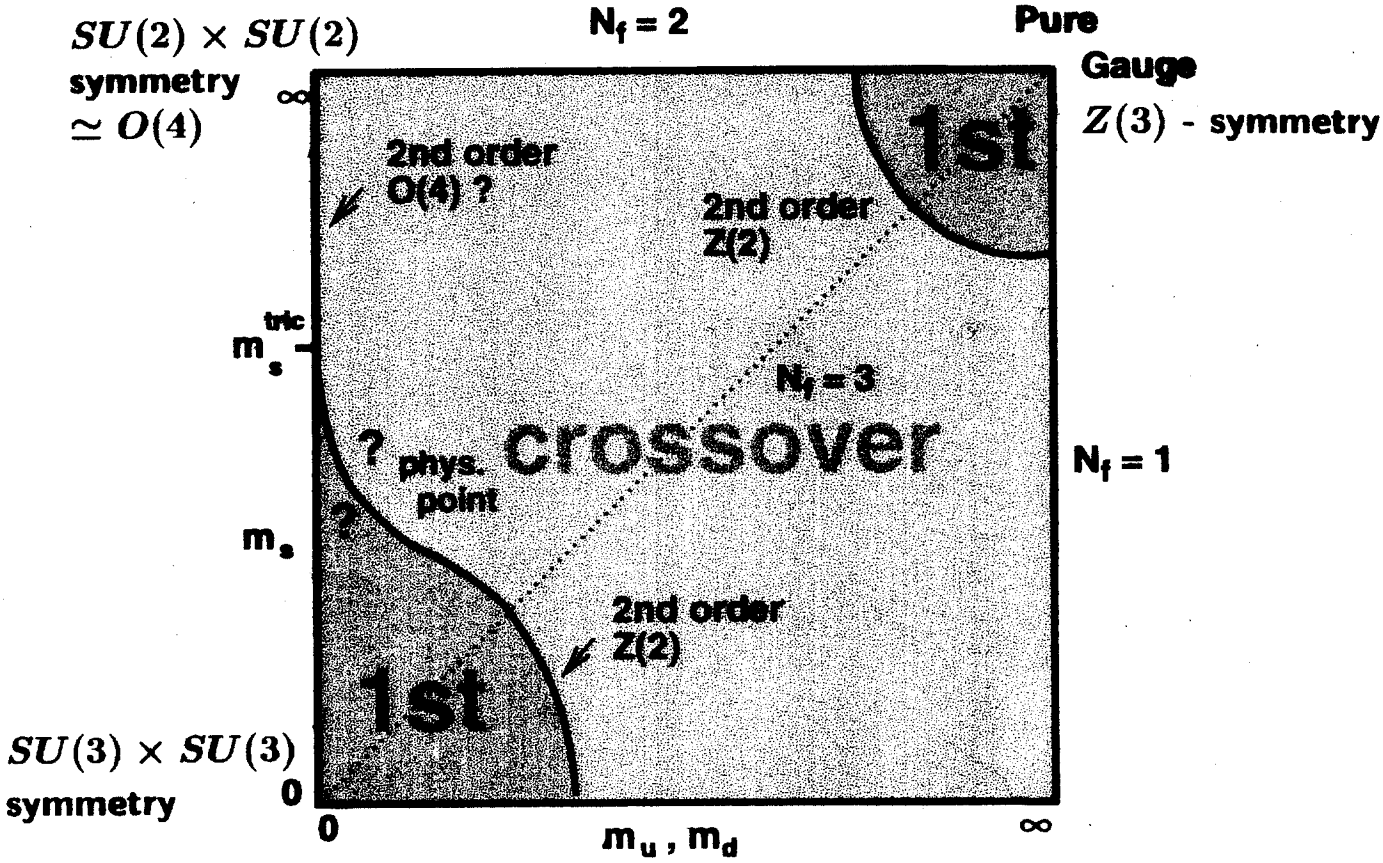
⇒ Improved flavour symmetry - reduced pion splitting

† **T. Blum et al., Phys. Rev. D55 (1997) 1133**

The QCD phase diagram

order of the transition; its flavour and quark mass dependence

universal critical behaviour?



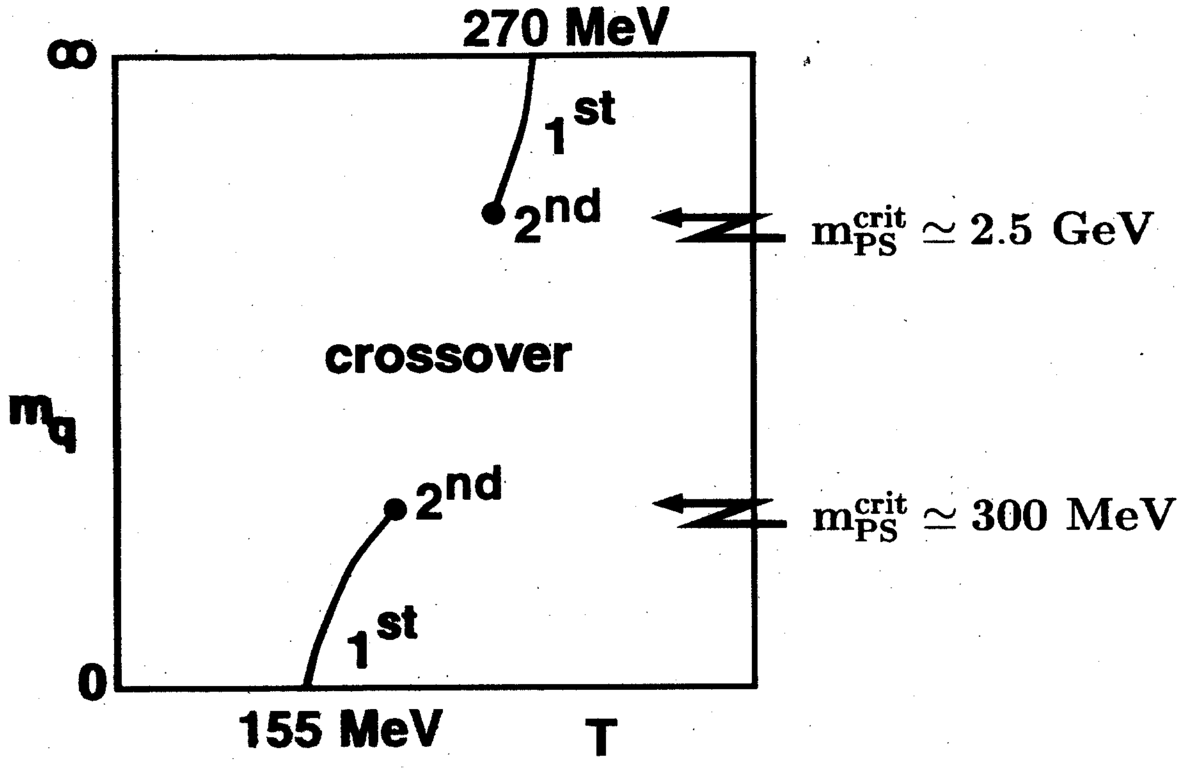
global symmetries

- suggest order of the transition
- control universal properties at 2^{nd} order phase transitions

quantitative results for $T_c(m_q)$ (or $T_c(m_\pi)$??)

- How does the transition temperature depend on m_q, m_π,...?

Deconfinement and chiral symmetry in 3-flavour QCD

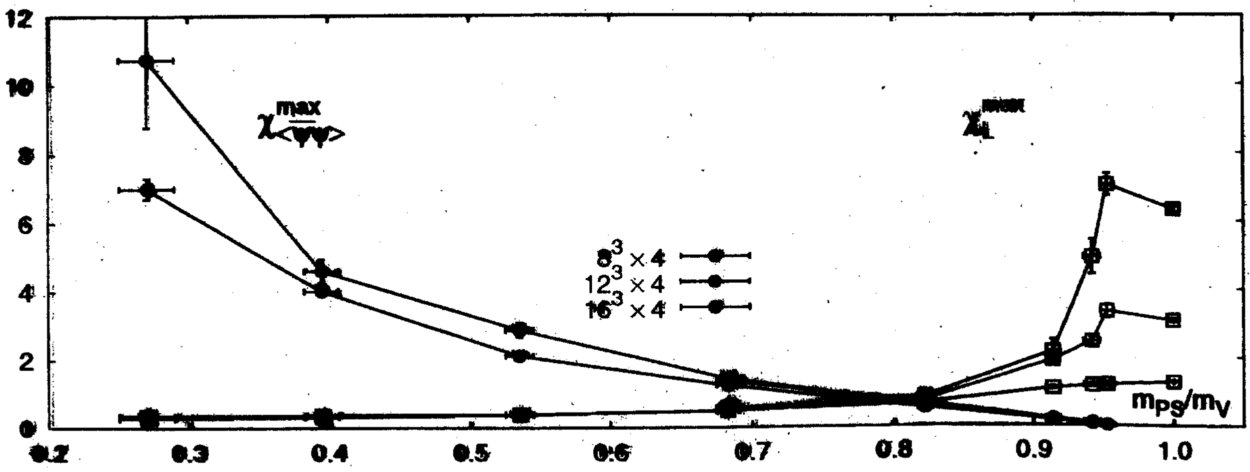


peak heights of susceptibilities

crossover : ⇔ $\chi \sim$ **const.**

$\mathbf{1^{st}}$**order :** ⇔ $\chi \sim \mathbf{V}$

$n_f = 3$, p4-action, $0.27 \leq m_{PS}/m_V \leq 1$



Deconfinement

$m_q \to \infty$: Polyakov Loop order parameter

$$e^{-\frac{1}{T}V_{q\bar{q}}(R,T)} \equiv \langle \mathrm{Tr}\, L_{\vec{0}}\ \mathrm{Tr}\, L^{+}_{\vec{R}} \rangle$$

$$L_{\vec{x}} \equiv \prod_{i=1}^{N_\tau} U_{(\vec{x},i),\hat{4}}$$

⇔ Location of "critical point" for $m_q \leq \infty$

⇒ peak in Polyakov loop susceptibility

$$\boxed{\chi_L = V\left(\langle L^2\rangle - \langle L\rangle^2\right)}$$

$$L \equiv \frac{1}{V}\sum_{\vec{x}} \mathrm{Tr}\, L_{\vec{x}}$$

Chiral Symmetry Restoration

$m_q \to 0$: chiral condensate is order parameter

$$\langle \bar{\psi}\psi \rangle = \frac{T}{V}\frac{\partial}{\partial m} \ln Z_{QCD}$$

⇔ Location of "critical point" for $m_q \geq 0$

⇒ peak in chiral susceptibility

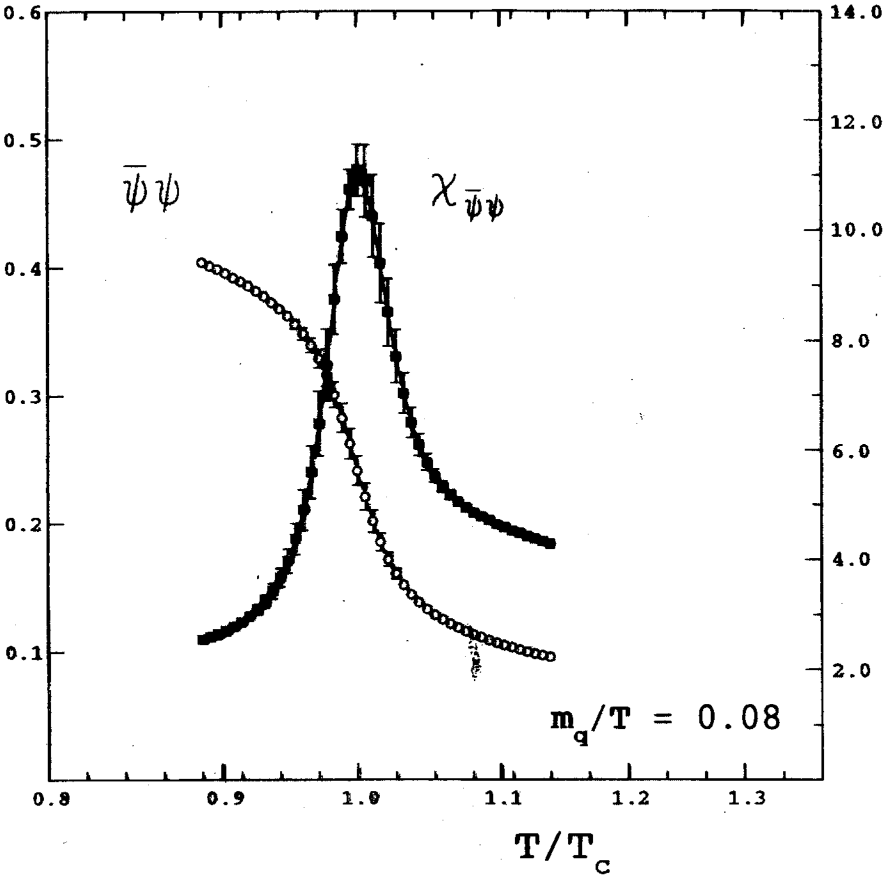
$$\boxed{\chi_m = \frac{\partial}{\partial m}\langle \bar{\psi}\psi \rangle}$$

⇒

⇒ $\chi_L^{peak} = \chi_m^{peak}$

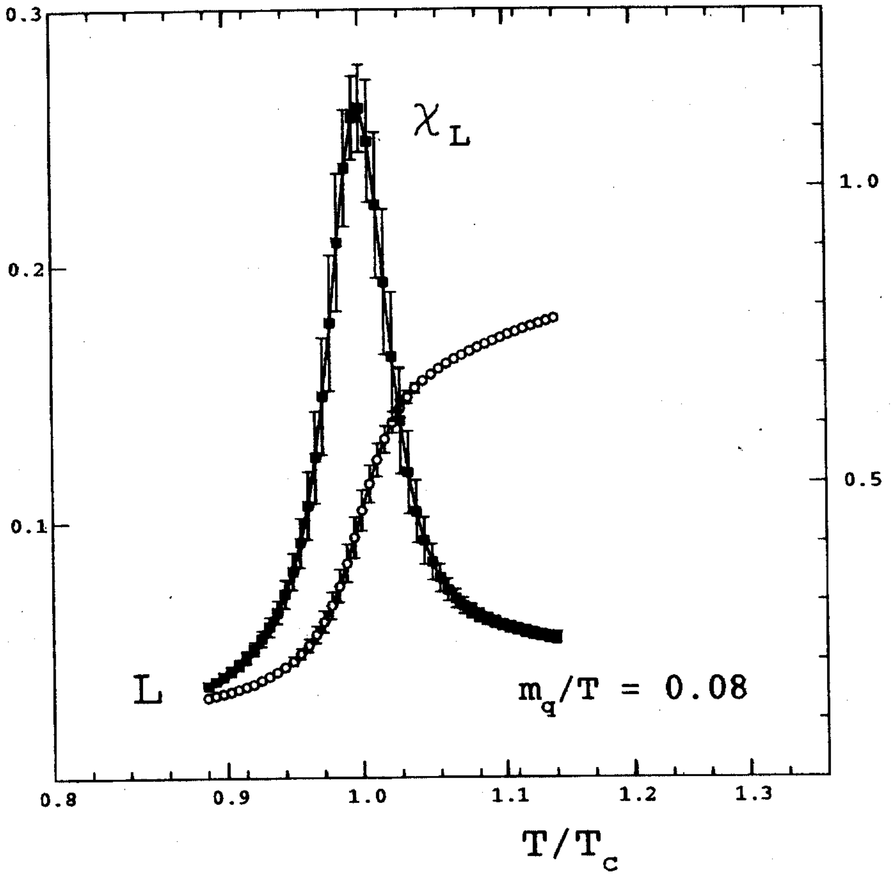
Chiral Symmetry Restoration

vanishing of the chiral condensate

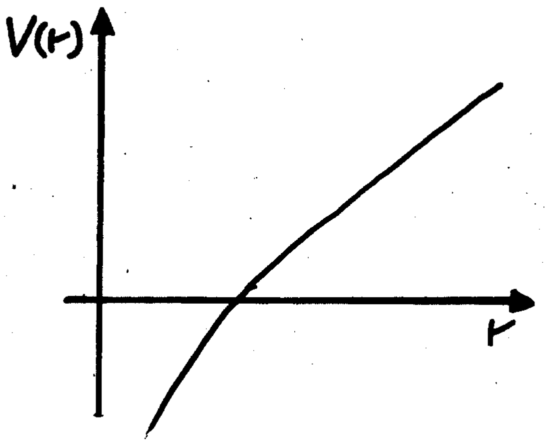


Deconfinement

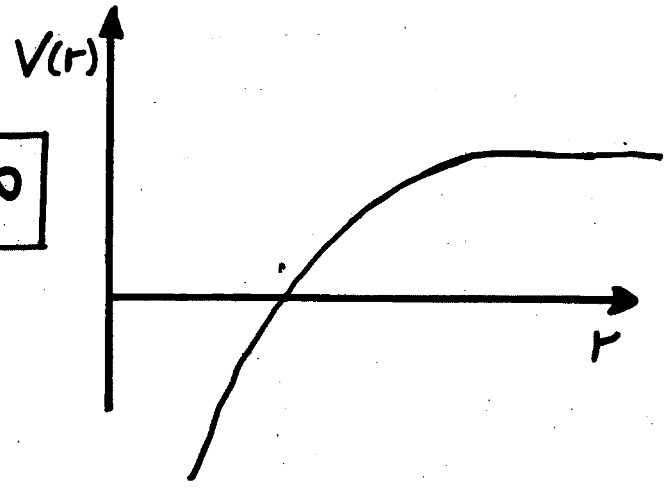
screening of the heavy quark potential



T_c and the heavy quark potential



$$\boxed{m_q \equiv \infty}$$



Confinement Phase

$$V(r,T) \simeq \frac{-\alpha(T)}{r} + \sigma(T)\, r$$

string tension

$$T \lesssim T_c : \sigma(T) \sim \left(1 - \frac{T}{T_c}\right)^{\nu}$$

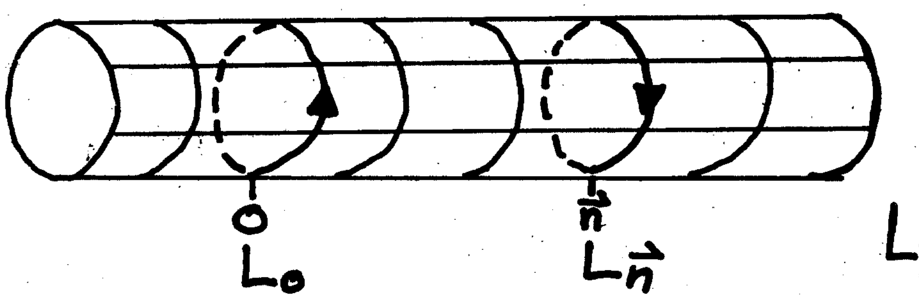
Quark-Gluon Plasma

$$V(r,T) \simeq -\frac{\alpha(T)}{r^d}\, e^{-\mu(T) r}$$

screening mass

$$T \gg T_c : \mu(T) = 2 m_D(T$$
$$= 2\sqrt{\frac{N}{3}}\, g(T)\, T$$

Lattice Potential



$$L_{\vec{n}} \equiv \prod_{n_0=1}^{N_\tau} U_{(n_0,\vec{n}),0}$$

Polyakov Loop

$$\boxed{e^{-V(r,T)/T} = \langle \mathrm{Tr}\, L_0\, \mathrm{Tr}\, L^{+}_{\vec{n}} \rangle}$$

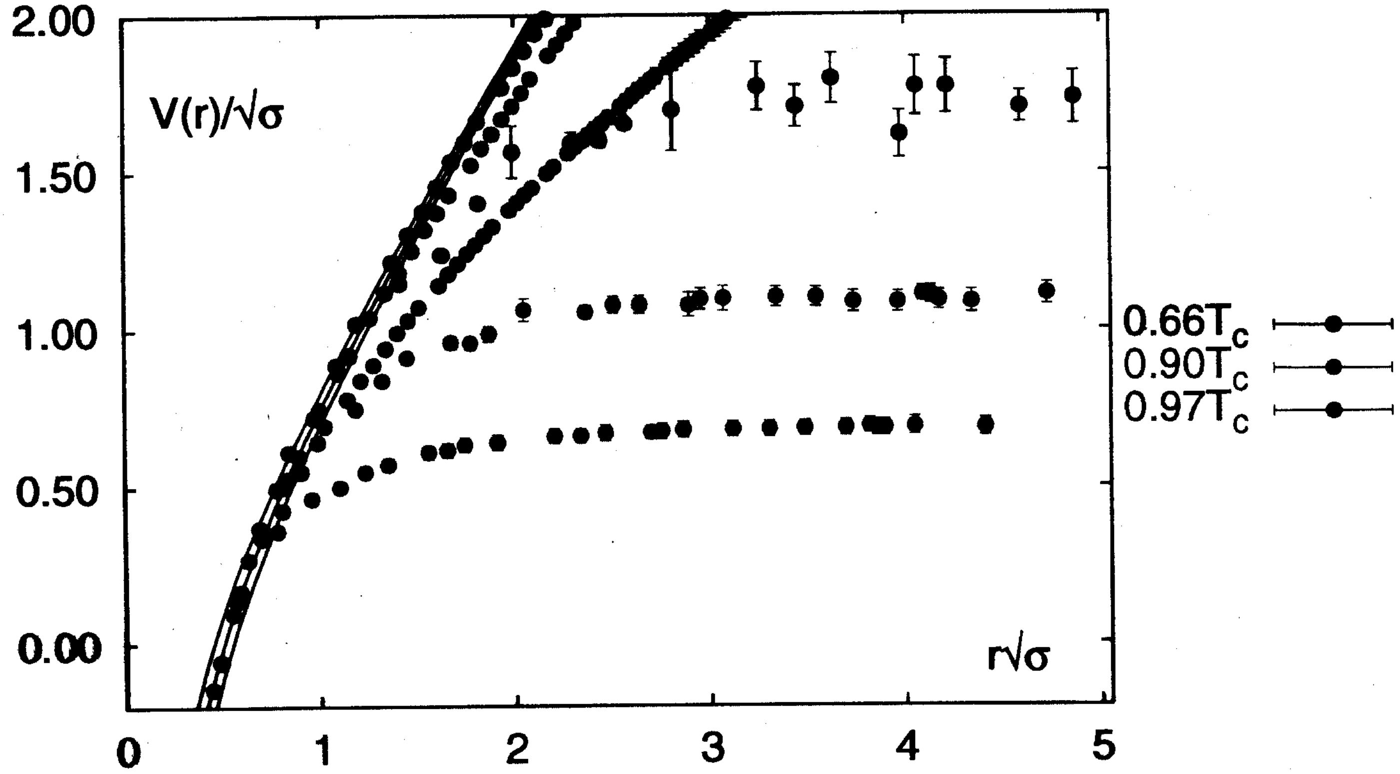
heavy quark free energy

$$\xrightarrow[|\vec{n}| \to \infty]{} |\langle \mathrm{Tr} L \rangle|^2$$

Heavy quark free energy

SU(3) vs. 3-flavour QCD

- drastic changes of large distance behaviour already below T_c

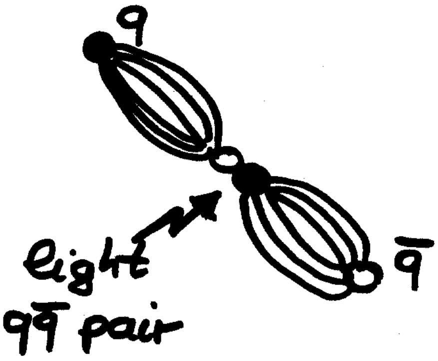


dynamical, light quarks screen the heavy quark free energy already below T_c

string breaking

$$\Downarrow$$

$$V_{q\bar{q}}(r \to \infty) < \infty \quad \forall T$$

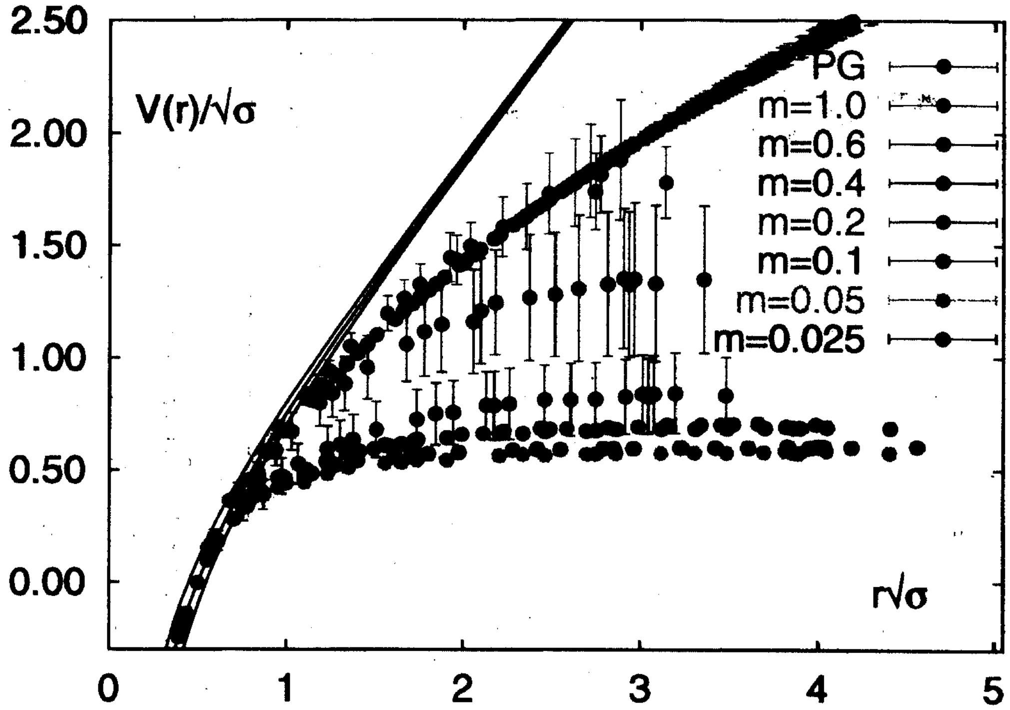


- quark mass and T-dependence in 3-flavour QCD

Heavy Quark "Potential" close to T_c

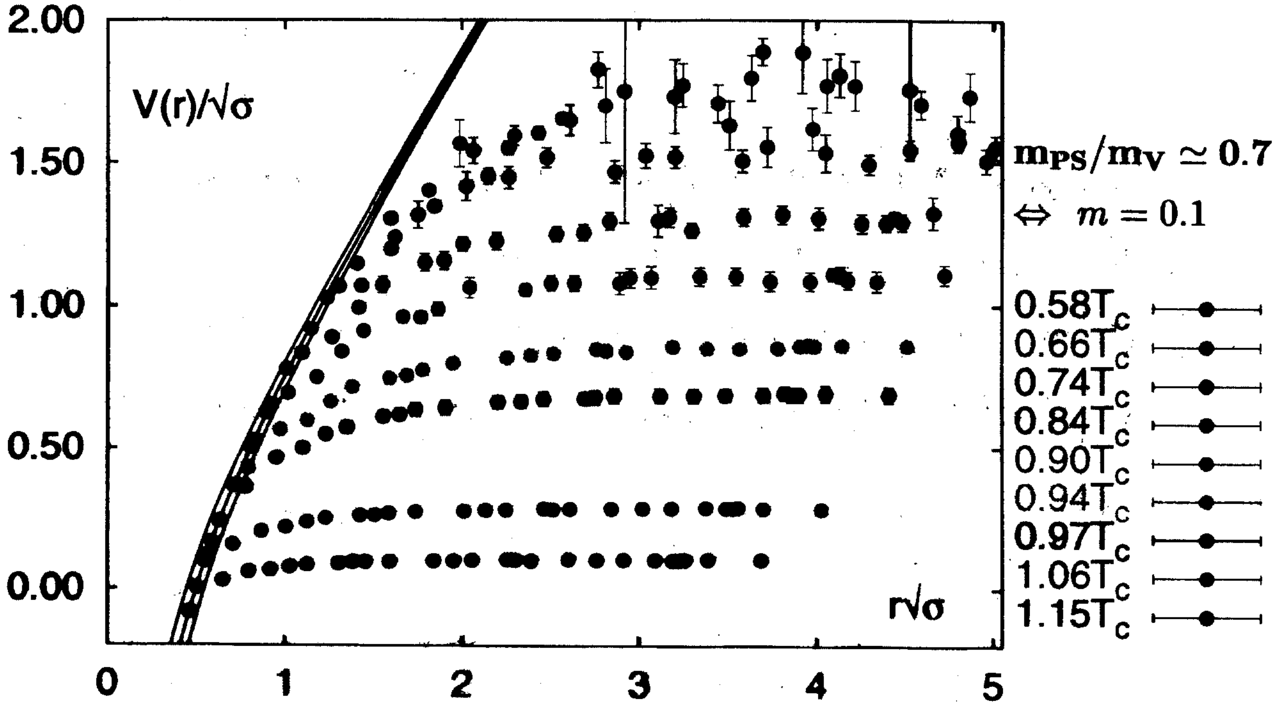
FK, E. Laermann, A. Peikert, hep-lat/0012023

$n_f = 3$, p4-action, $16^3 \times 4$ lattices



$T \simeq 0.97T_c$

⇕ $r \simeq 0.5$ fm **onset of screening shifts from $r \simeq 1$ fm at $T = 0$ to $r \simeq 0.5$ fm at $T \simeq T_c$**



$m_{PS}/m_V \simeq 0.7$

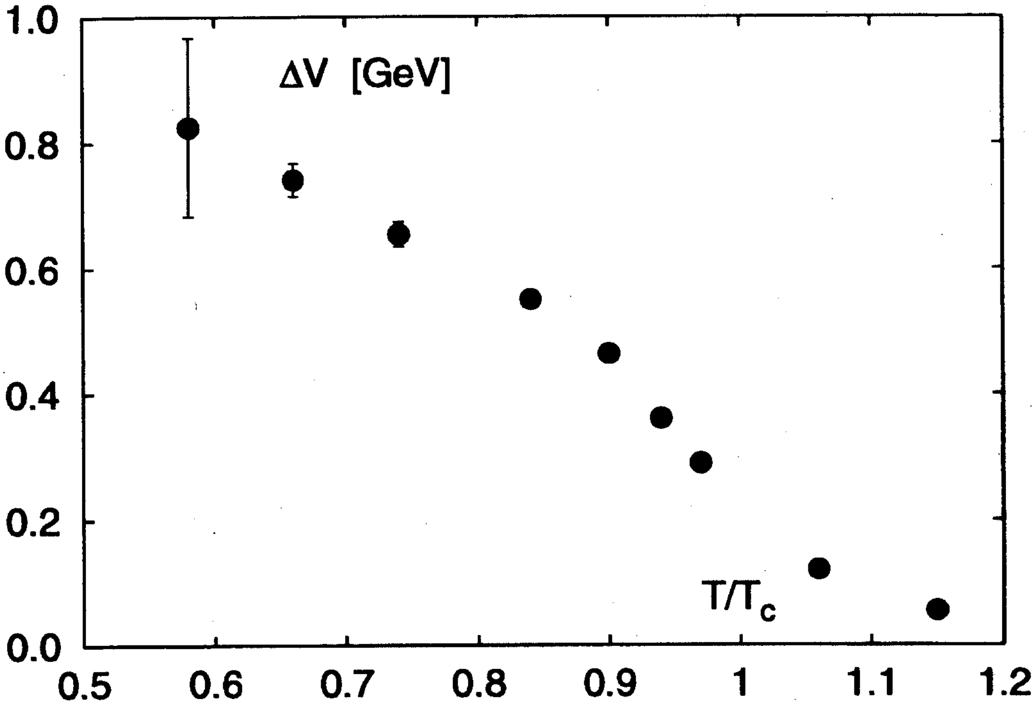
⇔ $m = 0.1$

⇑ $r \simeq 0.3$ fm

Temperature dependence of the depth of the heavy quark free energy (potential)

3-flavor QCD, $m_{PS}/m_V \simeq 0.7$

$$\Delta V \equiv \lim_{r\to\infty} V(r) - V(0.23\ \mathrm{fm})$$



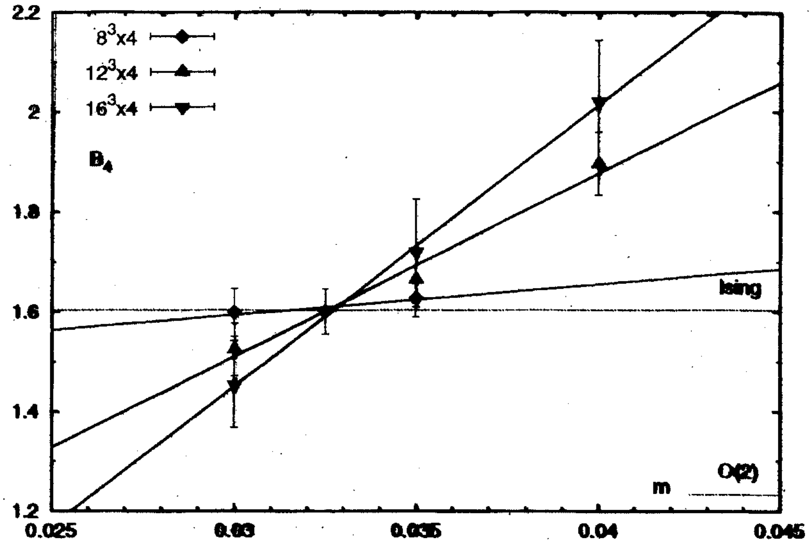
a more detailed analysis of the consequences for heavy quark spectroscopy does require a detailed, quantitative analysis of the short distance part of the heavy quark potential/free energy

some heavy quark bound states
may get destroyed already
below T_c

Chiral critical point in 3-flavour QCD

F.K, E. Laermann and Ch. Schmidt, in preparation

- **standard staggered fermion action; $16^3 \times 4$ lattices**
- **3-4 β-values for ma =0.03, 0.035 and 0.04**



critical point

$\beta_c = 5.147(4)$

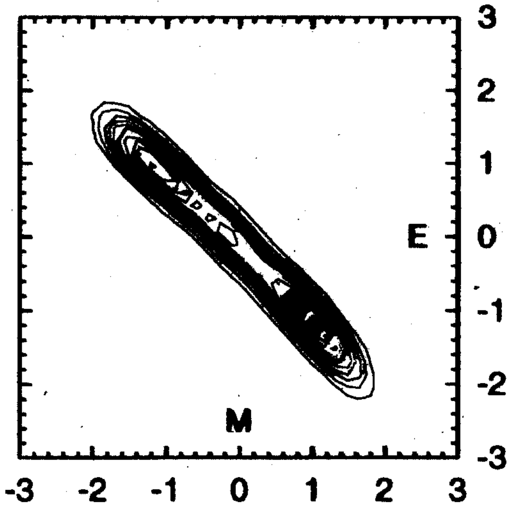
$m_c = 0.034(4)$

$dm_c(\beta)/d\beta = 0.552(1)$

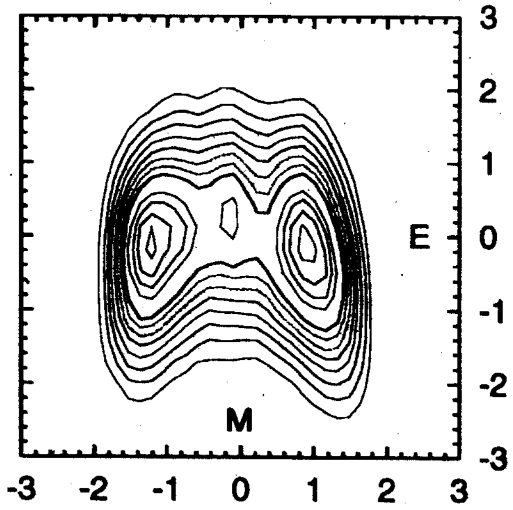
$$B_4 \equiv \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$$

$\Rightarrow$ **after rotation:** $\boxed{\textbf{universal 3-d Ising } E - M \textbf{ distribution}}$

original fields



rotated fields



$$M = \bar{\psi}\psi + 0.3\, S_G$$

$$E = S_G + 0.552\, \bar{\psi}\psi$$

consistent with:

S. Aoki et al. (JLQCD), Nucl. Phys. B (Proc. Suppl.) 73 (1999) 459.

Quark Mass Dependence of $\mathbf{T_c}$

need a m_q (and n_f) independent observable to set a scale

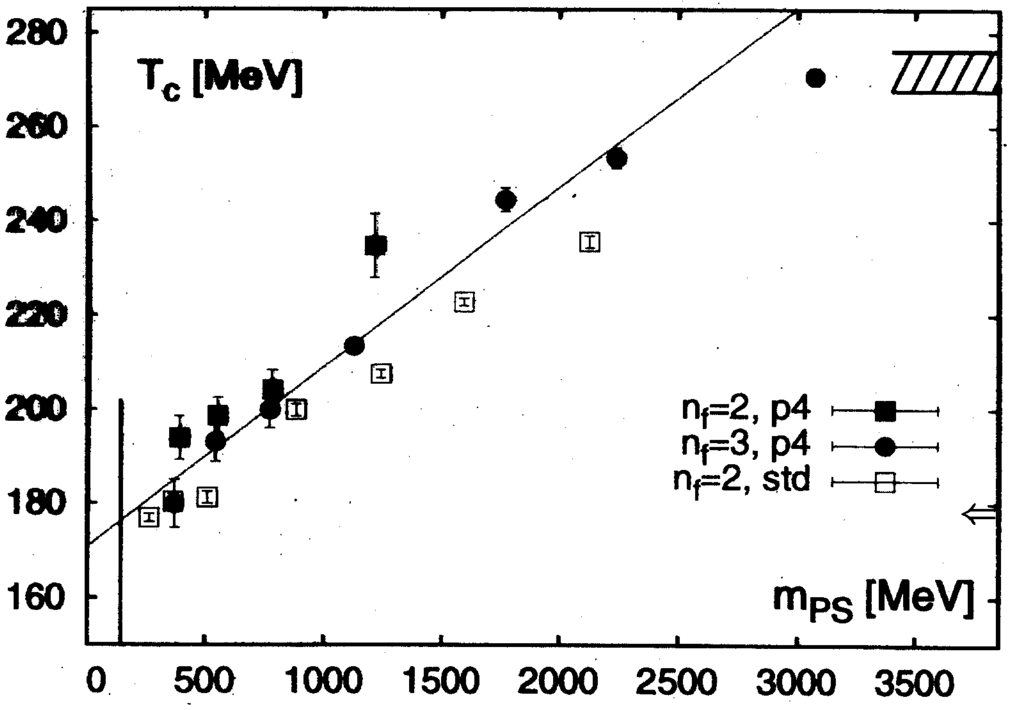
$$\frac{\sqrt{\sigma}}{m_\rho} = \begin{cases} 0.552(13) & \text{, quenched } (m_q \to \infty) \\ 0.532(18) & \text{, partially quenched, } m_q = 0.1,\ n_f = 3 \\ 0.53(3) & \text{, chiral limit, } n_f = 3 \end{cases}$$

$\Rightarrow$ $\sqrt{\sigma}$, quenched hadron masses are good scale parameters

$$\boxed{\mathbf{T_c(m_{PS}) \simeq T_c(0) + 0.04(1) m_{PS}}}$$

⇐ **favours percolation picture**

⇓ $\mathbf{m_{PS} \sim 2}$ **GeV**



SU(3) limit

⇐ **indicator for cut-off effects**

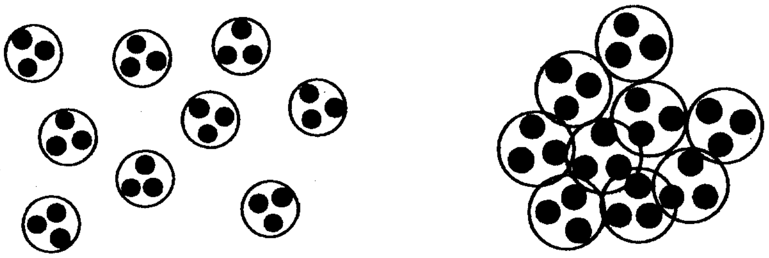
- **weak quark mass dependence of $\mathbf{T_c/\sqrt{\sigma}}$**

$\Rightarrow$**gross features of the transition not controled by "light" mesons**

Percolation and the Bag Model

qualitative understanding of the QCD Phase Transition

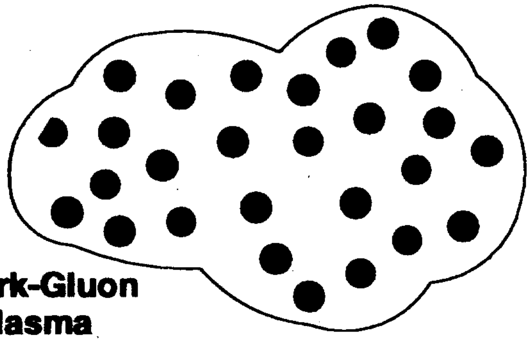
percolation model:



bags percolate

⇕

phase transition



need $\mathcal{O}(1)$ hadrons per hadronic volume: $V_H = 4\pi r_H^3/3$

particle density: $\frac{n_H}{T^3} = \sum_H \frac{g_H}{2\pi^2}\left(\frac{m_H}{T}\right)^2 \sum_{k=1}^{\infty} \frac{1}{k} K_2(km_H/T)$

glueballs: $m_G/T_c \simeq 5 \quad \Rightarrow \quad n_G/T^3 \simeq 0.0067\, g_G$

pions: $m_\pi/T_c \simeq 1 \quad \Rightarrow \quad n_\pi/T^3 \simeq (n_f^2 - 1)\pi^2/90$

$$\Downarrow$$

$$T_c \quad \simeq \quad \left(0.4\,(n_f^2 - 1)\, r_\pi^3 \; + \; 0.03\, g_G\, r_G^3\right)^{-1/3}$$

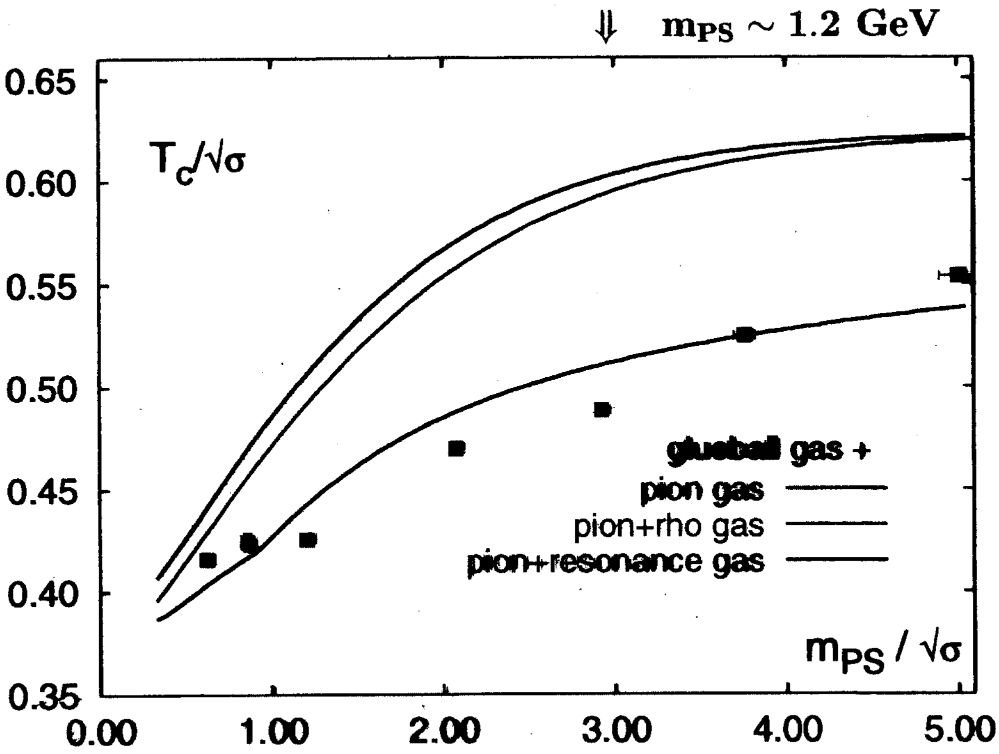
drops with increasing n_f;
increases with increasing m_π
approaches pure gauge value for $m_\pi \simeq m_G$

- **weak quark mass dependence of $T_c/\sqrt{\sigma}$**

  for $m_{PS}/m_V \lesssim 0.5$ or ($m_{PS} \lesssim m_G$)!

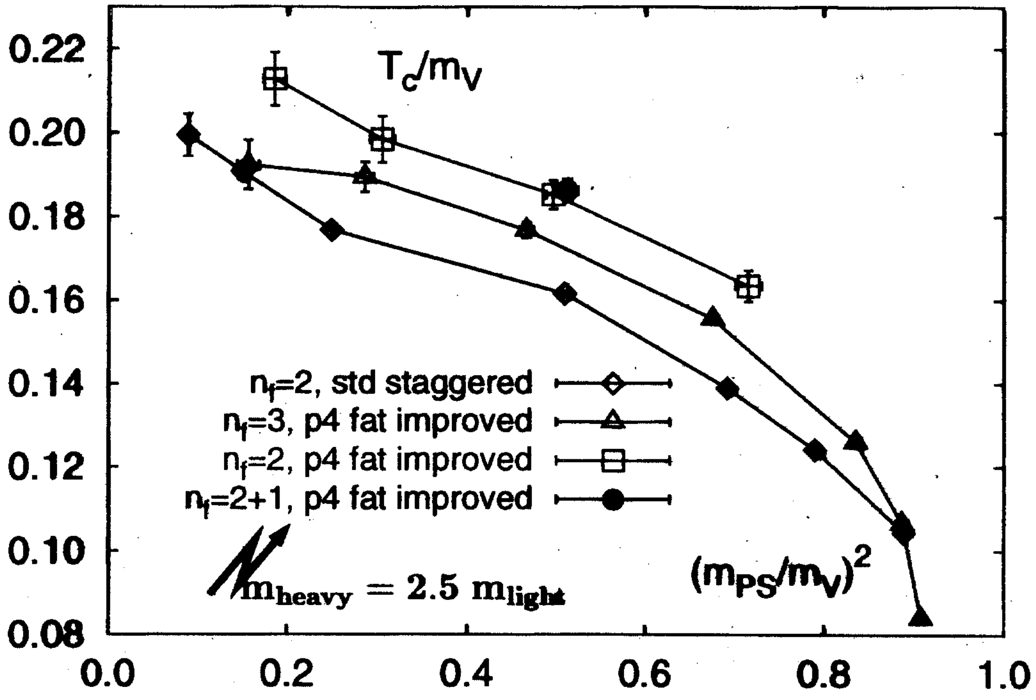
$\Rightarrow$ **in accordance with resonance gas models**

$$\frac{n_H}{T^3} = \frac{1}{2\pi^2}\int_0^\infty \mathrm{d}m\ \rho(m) \int_0^\infty \mathrm{d}p\ p^2 \exp(-\beta\sqrt{p^2+m^2})$$
$$\rho(m) = \delta(m-m_\pi) + c\,\Theta(m-\bar{m})\ m^a \exp(bm)$$



curves show lines of constant density;
percolation transition: $\boxed{n_H V_H = 0.35 \quad \text{with} \quad r_H \simeq 0.8\ \text{fm}}$

Flavor Dependence of T_c



$$\boxed{T_{c,nf=2} - T_{c,nf=3} \simeq 20\ \text{MeV}}$$

- **weak flavor dependence**
- **similar m_q-dependence**
- **T_c for (2+1)-flavor QCD $\simeq$ T_c for 2-flavor QCD**

$$n_f = 2 : \quad T_c = (173 \pm 8 \pm (\text{sim.sys.err.}))\ \text{MeV}$$

$$n_f = 3 : \quad T_c = (154 \pm 8 \pm (\text{sim.sys.err.}))\ \text{MeV}$$

2-flavor QCD: T_c/m_V

O(4) scaling: $\boxed{T_c(m_\pi) - T_c(0) \sim m_\pi^{2/\beta\delta} \sim m_\pi^{1.1}}$

m_q-dependent m_v: $m_v \simeq m_\rho + \tilde{c}_\rho\, m_q$

⇒ **direct chiral extrapolation of T_c/m_v difficult**

expect: $\boxed{\frac{T_c}{m_v} = \frac{T_c(0) + c_t\, x^{1.1}}{m_\rho + c_\rho\, x^2}}$, $x = m_{PS}/m_v$

improved Wilson fermions (CP-PACS); first $\beta_c(m_q) \rightarrow \beta_c(0)$:

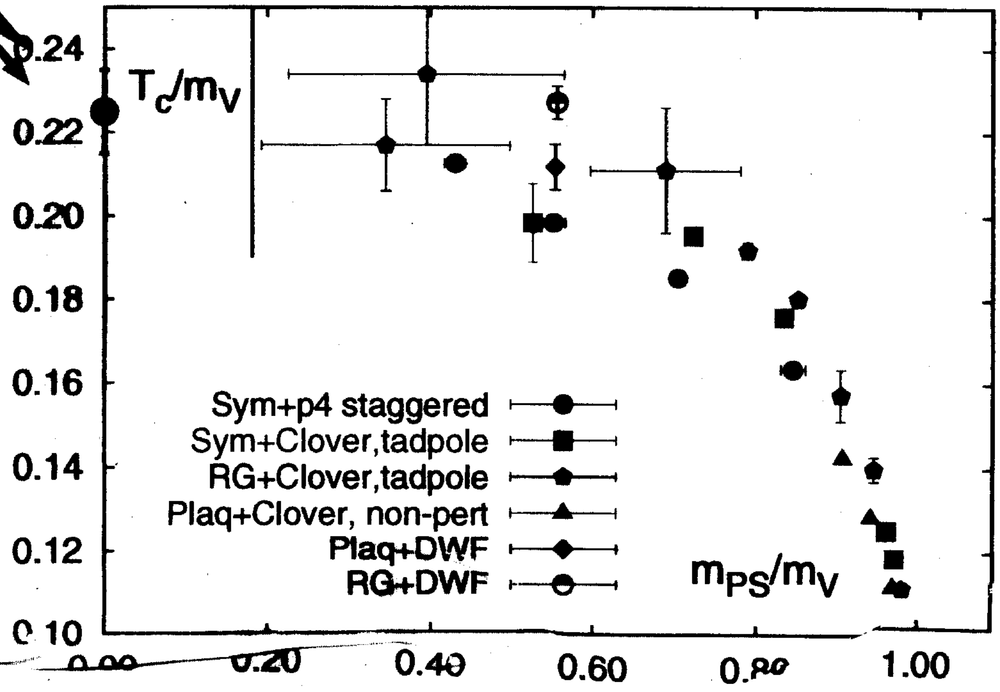
$$T_c/m_\rho = 0.2224\ (51)$$

improved staggered fermions (Bielefeld); extrapolation in x^2:

$$T_c/m_\rho = 0.225\ (10)$$

⇒ expect sys.err. of similar size

$\boxed{\sim 173(8)(..)\ \text{MeV}}$



improvement mandatory

(..)systematic/ discretisation errors not yet under control

$m_{PS} \sim 0.3$ GeV ⇑ ⇑ $m_{PS} \sim 1.2$ GeV

SF: Sym+ rot. improved SF; **Bielefeld**

WF: Plaq+Clover/Sym+Clover; **R.G. Edwards, U.M. Heller, PL B462 (1999) 132**
RG+Clover: **CP-PACS**

DWF: **Plaq+DWF/RG+DWF, Columbia-RIKEN-BNL group**

Bulk Thermodynamics

everything can be obtained from the partition function $\boxed{Z(T,V,m_q) \Rightarrow Z(N_\tau, N_\sigma, \beta, m)}$

- free energy density: $\boxed{f = -\frac{T}{V} \ln Z}$

  not directly accessible to MC-calculations $\Rightarrow$

  trick: integral method, e.g.

$$\frac{f}{T^4}\bigg|_{T_0}^{T} = - \int_{T_0}^{T} \mathrm{d}t \frac{\partial t^{-3} V^{-1} \ln Z(t, V, m_q)}{\partial t} \qquad (\star)$$

- pressure: $\boxed{P = -f}$

  requires large volumes for homogeneity to hold:

  $(\partial \ln Z / \partial V)_T = \ln Z / V$

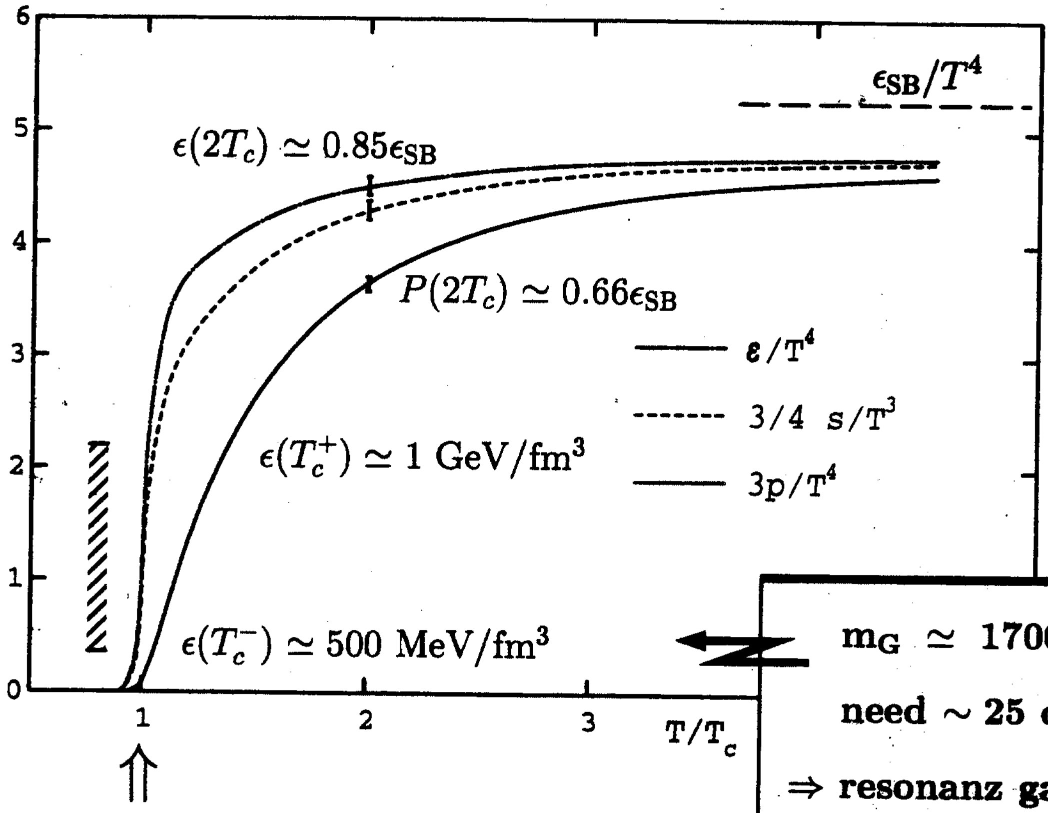
- energy density: $\boxed{\frac{(\epsilon - 3P)}{T^4} = T \frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{P}{T^4}\right)}$

  from $(\star)$

$$\frac{(\epsilon - 3P)}{T^4} = T \frac{\partial t^{-3} V^{-1} \ln Z(t, V, m_q)}{\partial t}$$

- entropy density: $\boxed{\frac{s}{T^3} = \frac{\epsilon + P}{T^4}}$

SU(3) Equation of State



$m_G \simeq$ 1700 MeV

need ~ 25 d.o.f.

⇒ resonanz gas

$T_c \simeq (0.63 - 0.65)\sqrt{\sigma} \simeq 270$ MeV

- **substantial deviations from ideal gas even for T$\gtrsim$2T$_c$**
- **continuum approaches (HTL-resummed perturbation theory) have difficulties in reproducing the EoS for $T \lesssim 2T_c$**

J.O. Andersen et al., PR D61 (2000) 014017;

J.-P. Blaizot, et al., PRL 83 (1999) 2906; PL B470 (1999) 181

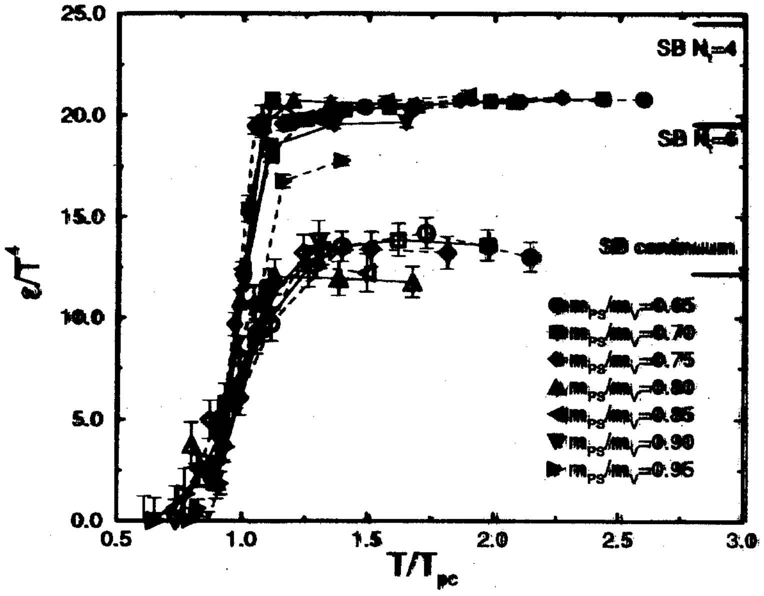
⇒ **large thermal gluon mass; strong T-dependence**

P. Lévai and U. Heinz, PR C57 (1998) 1879

Energy Density

new results:

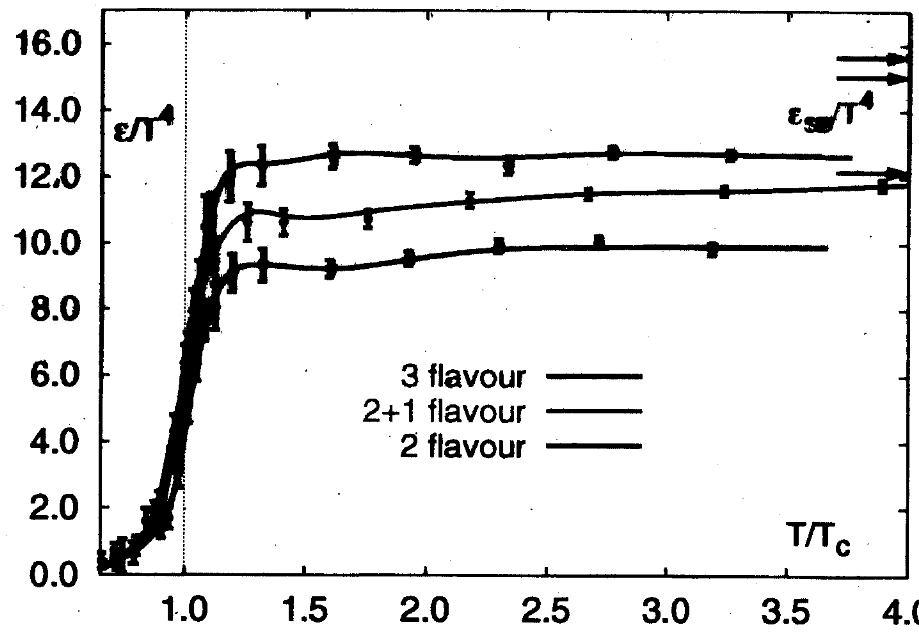
Clover improved WF (CP-PACS in prep.), S. Ejiri, hep-lat/0011006v2
rot. sym. improved SF (Bielefeld): + hep-lat/0103028
A. Peikert et al., Phys. Lett. B478 (2000) 447



$n_f = 2$ Clover fermions:

large cut-off dependence for T > T_c

small cut-off dependence at T_c



improved staggered fermions:

small cut-off dependence

critical energy density: $\boxed{\epsilon_c \simeq (6 \pm 2)\ T_c^4}$

even massless pions would contribute only 10% to this!

detailed analysis of volume and quark mass dependence still needed!

Some Quantitative Results

- The QCD (phase) transition is weakly dependent on n_f and m_{PS}.
  - L-calculations will provide T_c with less than 10% errors in the near future; current estimate:

    $n_f = 2 :\quad T_c = (173 \pm 8 \pm (\text{sim.sys.err.}))$ MeV

    $n_f = 3 :\quad T_c = (154 \pm 8 \pm (\text{sim.sys.err.}))$ MeV

- bulk thermodynamics, e.g. the pressure in units of the ideal gas pressure, is only weakly flavor dependent
  - critical energy density:

    $\epsilon_c = (6 \pm 2)\, T_c^4 \quad \Rightarrow \quad \epsilon_c \simeq (700 \pm 300)\ \text{MeV}/\text{fm}^3$

    + error on T_c

- screening of the heavy quark free energy sets in at rather short distances: $r \sim 0.3$ fm

- MEM provides a promissing approach towards the study of thermal masses in the vicinity of T_c

QCD with a realistic mass spectrum

$$m_u = m_d \simeq 0 \ , \ m_s \simeq T_c$$

– first order or crossover? –

quantitative results on this question

$$+$$

T_c, ϵ_c, **e.o.s, ...**

are within reach