Computational particle physics: lattice QCD

(approaching the continuum limit with physical quark masses)

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Nara, December 14, 2012

(talk for non-experts)

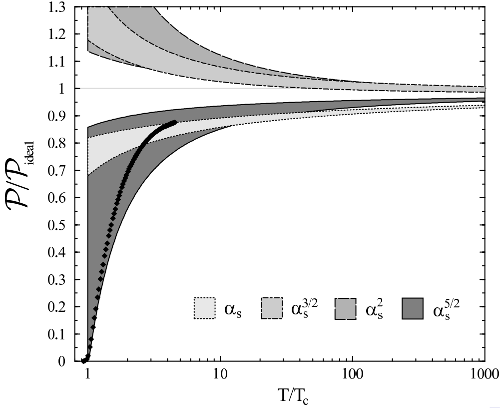
SFB TR55

Outline

QCD: need for a systematic non-perturbative method

in some cases (g-2): perturbative approach is good; in other cases: bad

pressure at high temperatures converges at T=10^{300} MeV



Lattice field theory

systematic non-perturbative approach (numerical solution):

quantum fields on the lattice

quantum theory: path integral formulation with $S = E_{kin} - E_{pot}$

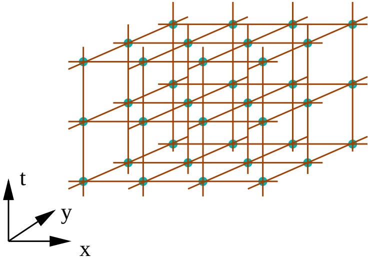
quantum mechanics: for all possible paths add exp(iS)
quantum fields: for all possible field configurations add exp(iS)

Euclidean space-time ($t = i\tau$): exp(-S) sum of Boltzmann factors

we do not have infinitely large computers ⇒ two restrictions

a. put it on a space-time grid (proper approach: asymptotic freedom)
formally: four-dimensional statistical system
b. finite size of the system (can be also controlled)

⇒ stochastic approach, with reasonable spacing/size: solvable

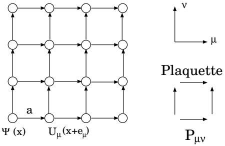


fine lattice to resolve the
structure of the proton ($\lesssim$0.1 fm)
few fm size is needed
50-100 points in 'xyz/t' directions
$a \Rightarrow a/2$ means 100-200$\times$CPU

mathematically
10^9 dimensional integrals

advanced techniques,
good balance and
order of Pflops are needed

Lattice Lagrangian: gauge fields



$$\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(D_\mu \gamma^\mu + m)\psi$$

anti-commuting $\psi(x)$ quark fields live on the sites
gluon fields, $A^a_\mu(x)$ are used as links and plaquettes

$$U(x,y) = \exp\left(ig_s \int_x^y dx'^\mu\, A^a_\mu(x')\lambda_a/2\right)$$

$$P_{\mu\nu}(n) = U_\mu(n) U_\nu(n+e_\mu) U^\dagger_\mu(n+e_\nu) U^\dagger_\nu(n)$$

$S = S_g + S_f$ consists of the pure gluonic and the fermionic parts

$$S_g = 6/g_s^2 \cdot \sum_{n,\mu,\nu} [1 - \mathrm{Re}(P_{\mu\nu}(n))]$$

Lattice Lagrangian: fermionic fields

quark differencing scheme:

$$\bar{\psi}(x)\gamma^\mu \partial_\mu \psi(x) \to \bar{\psi}_n \gamma^\mu (\psi_{n+e_\mu} - \psi_{n-e_\mu})$$

$$\bar{\psi}(x)\gamma^\mu D_\mu \psi(x) \to \bar{\psi}_n \gamma^\mu U_\mu(n) \psi_{n+e_\mu} + \ldots$$

fermionic part as a bilinear expression: $S_f = \bar{\psi}_n M_{nm} \psi_m$
we need 2 light quarks (u,d) and the strange quark: $n_f = 2 + 1$

(complication: doubling with 16 fermions $\Rightarrow$ staggered/Wilson)

Euclidean partition function is given by the Boltzmann weights

$$Z = \int \prod_{n,\mu} [dU_\mu(x)][d\bar{\psi}_n][d\psi_n] e^{-S_g - S_f} = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

using two fermionic fields instead of one: $\det^2(M[U])$

Importance sampling

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability $\propto$ its weight

importance sampling, Metropolis algorithm:
(all other algorithms are based on importance sampling)

$$P(U \to U') = \min \left[1, \exp(-\Delta S_g) \det(M[U'])/\det(M[U])\right]$$

gauge part: trace of 3$\times$3 matrices (easy, without M: quenched)
fermionic part: determinant of $10^6 \times 10^6$ sparse matrices (hard)

more efficient ways than direct evaluation (Mx=a), but still hard

Hadron spectroscopy in lattice QCD

Determine the transition amplitude between:
having a “particle” at time 0 and the same “particle” at time t
$\Rightarrow$ Euclidean correlation function of a composite operator $\mathcal{O}$:

$$C(t) = \langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle$$

insert a complete set of eigenvectors $|i\rangle$

$$= \sum_i \langle 0|e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}|i\rangle\langle i|\mathcal{O}^\dagger(0)|0\rangle = \sum_i |\langle 0|\mathcal{O}^\dagger(0)|i\rangle|^2\,e^{-(E_i-E_0)t},$$

where $|i\rangle$: eigenvectors of the Hamiltonian with eigenvalue E_i.

and $$\mathcal{O}(t) = e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}.$$

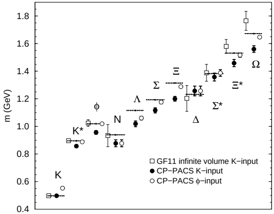
t large $\Rightarrow$ lightest states (created by $\mathcal{O}$) dominate: $C(t) \propto e^{-M\cdot t}$
$\Rightarrow$ exponential fits or mass plateaus M_t=log[C(t)/C(t+1)]

Quenched results

QCD is 40 years old $\Rightarrow$ properties of hadrons (Rosenfeld table)

non-perturbative lattice formulation (Wilson) immediately appeared
needed 20 years even for quenched result of the spectrum (cheap)
instead of det(M) of a $10^6 \times 10^6$ matrix trace of 3×3 matrices

always at the frontiers of computer technology:
GF11: IBM "to verify quantum chromodynamics" (10 Gflops, '92)
CP-PACS Japanese purpose made machine (Hitachi 614 Gflops, '96)

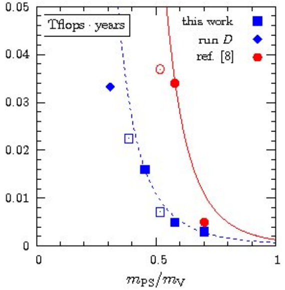


the ≈10% discrepancy was believed to be a quenching effect

Difficulties of full dynamical calculations

though the quenched result can be qualitatively correct
uncontrolled systematics $\Rightarrow$ full “dynamical” studies
by two-three orders of magnitude more expensive (balance)
present day machines offer several Pflops

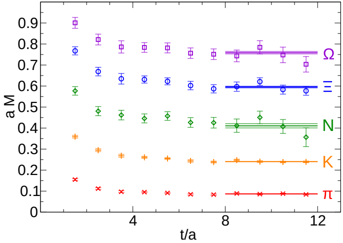
no revolution but evolution in the algorithmic developments
Berlin Wall ’01: it is extremely difficult to reach small quark masses:



Scale setting and masses in lattice QCD

in meteorology, aircraft industry etc. grid spacing is set by hand
in lattice QCD we use g, m_{ud} and m_s in the Lagrangian ('a' not)
measure e.g. the vacuum mass of a hadron in lattice units: $M_\Omega a$
since we know that M_Ω=1672 MeV we obtain 'a'

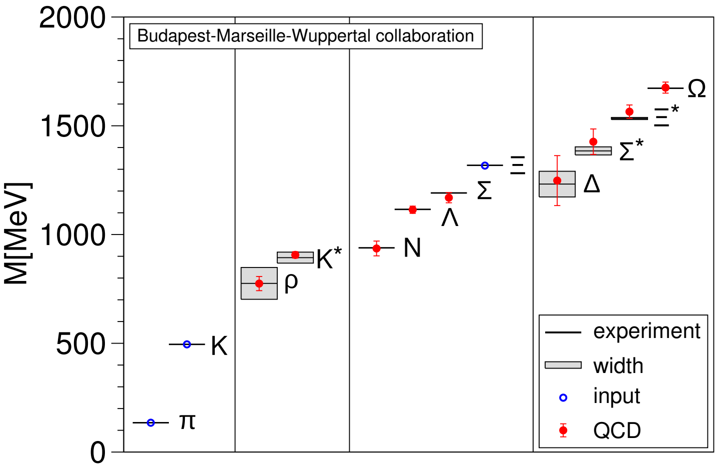
masses are obtained by correlated fits (choice of fitting ranges)
illustration: mass plateaus at the smallest $M_\pi \approx$190 MeV (noisiest)



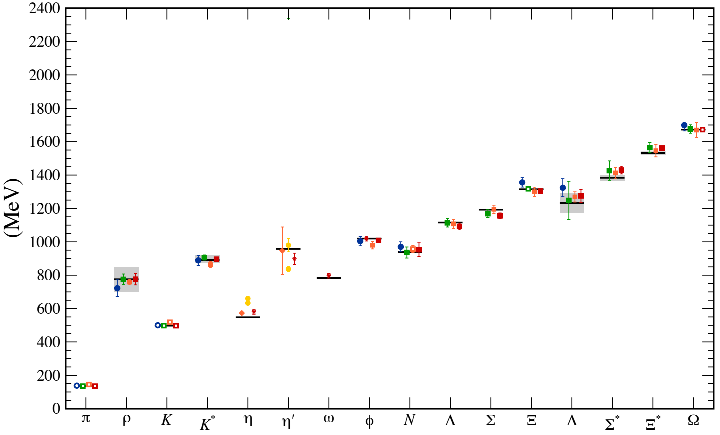
volumes and masses for unstable particles: avoided level crossing
decay phenomena included: in finite V shifts of the energy levels

Final result for the hadron spectrum

S. Durr et al., Science 322 1224 2008



Light hadron spectrum summary: A. Kronfeld 1209.3468

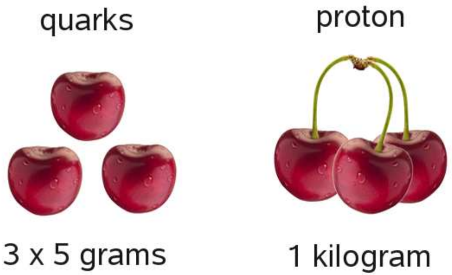


results with various actions and fermion formulations(!) are the same

The mass is not the sum of the constituents' mass

usually the mass of "some ordinary thing" is just
the sum of the mass of its constituents (upto tiny corrections)

origin of the mass of the visible universe: dramatically different
proton is made up of massless gluons and almost massless quarks



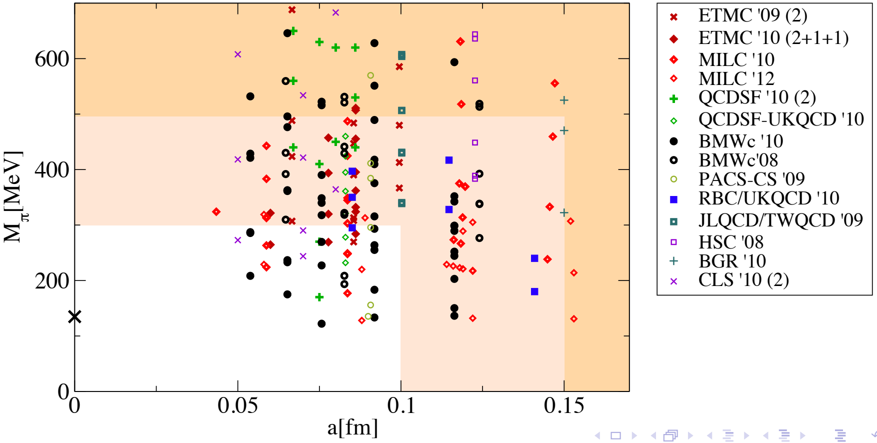
mass of a quark is $\approx$5 MeV, that of a proton (hadron) is $\approx$1000 MeV

The calculation that we have been dreaming of doing

- $N_f = 2 + 1$ all the way down to $M_\pi \lesssim 135$ MeV to allow small interpolation to physical mass point
- Large $L \gtrsim 5 - 6$ fm to have sub percent finite V errors
- At least three $a \le 0.1$ fm for controlled continuum limit
- A reliable determination of the scale with a well measured physical observable
- Full nonperturbative renormalization
- Complete analysis of systematic uncertainties

Where do we stand in lattice QCD?

all simulations with N_f 2,2+1 and 2+1+1 and $M_\pi < 400$ MeV
very first physical mass point simulations: PACS-CS Collaboration



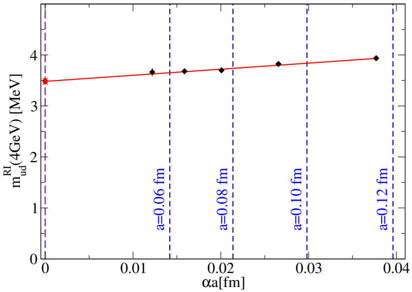
Continuum extrapolation of renormalized masses

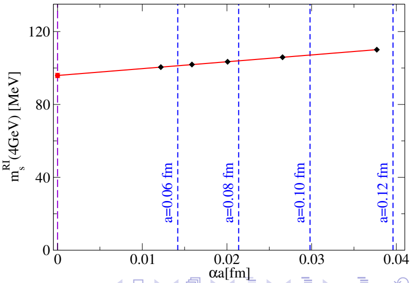
Renormalized quark masses **interpolated** in M_π^2 & M_K^2 to physical point using:

- $SU(2)$ χPT
- or low-order polynomial anszätze
- with cuts on pion mass $M_\pi < 340,\ 380\,\mathrm{MeV}$

Example of continuum extrapolations:

for m_s/m_{ud} the continuum extrapolation is flat





Outline: what has lattice done for the phase diagram

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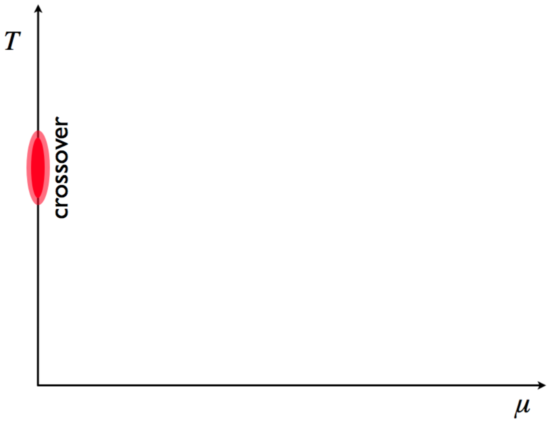
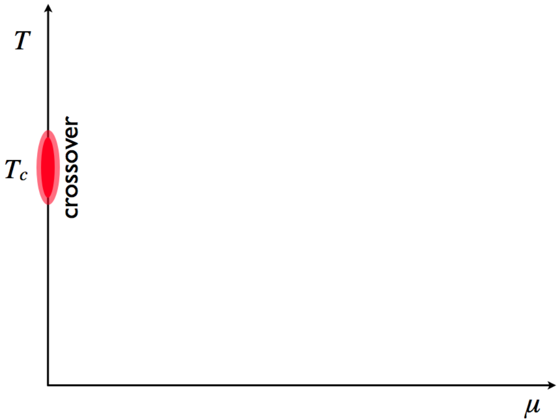


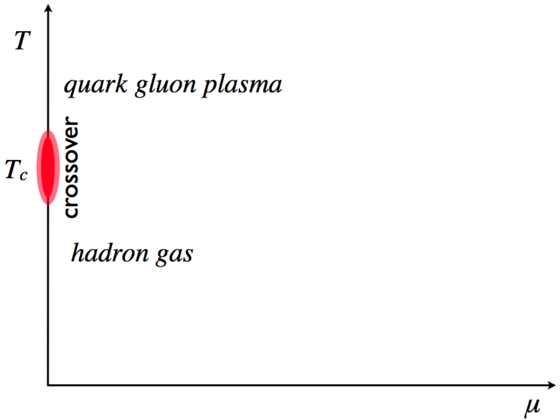
cross-over: Y. Aoki, G. Endrodi, Z. Fodor, S. Katz, K. Szabo, Nature 443 (2006) 675

Outline: what has lattice done for the phase diagram



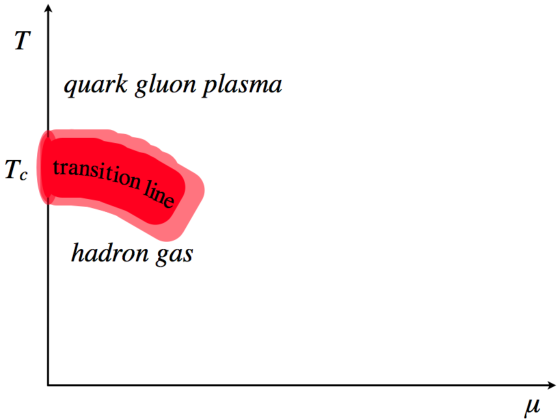
cross-over, absolute scale (T_c)

Outline: what has lattice done for the phase diagram



cross-over, T_c, EoS

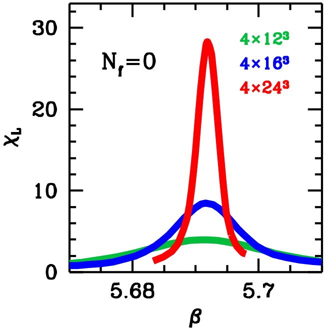
Outline: what has lattice done for the phase diagram



cross-over, T_c, EoS, curvature of phase line, μ>0 EoS, fluct.

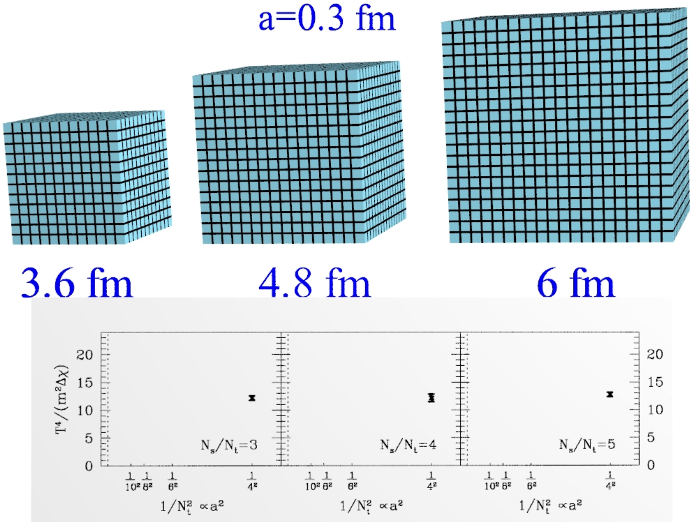
Finite size scaling in the quenched theory

look at the susceptibility of the Polyakov-line
first order transition (Binder) $\Longrightarrow$ peak width $\propto$ 1/V, peak height $\propto$ V

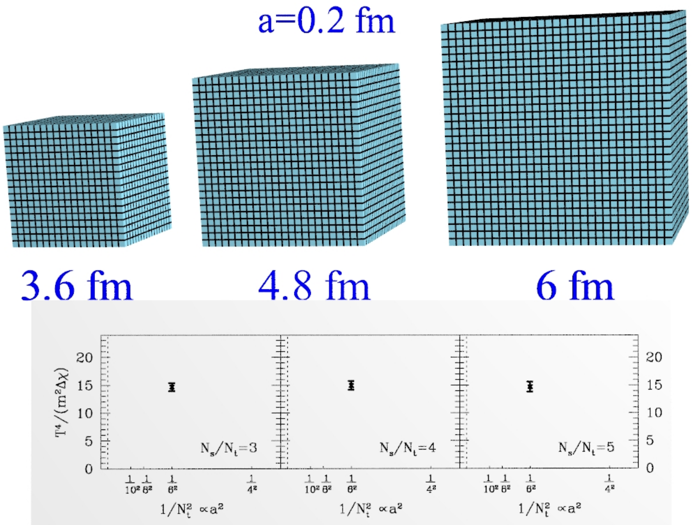


finite size scaling shows: the transition is of first order

Approaching the continuum limuit



Approaching the continuum limuit



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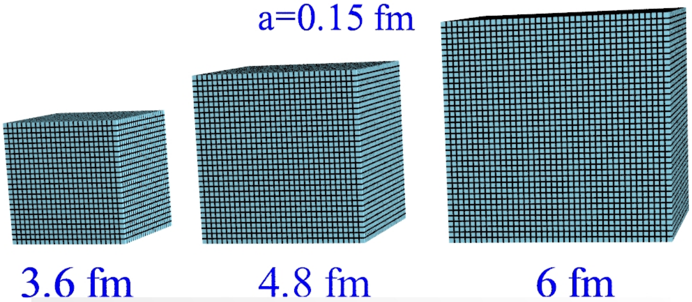

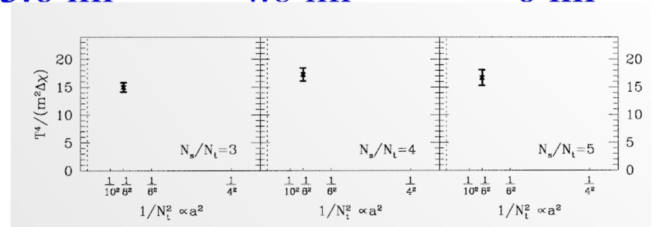

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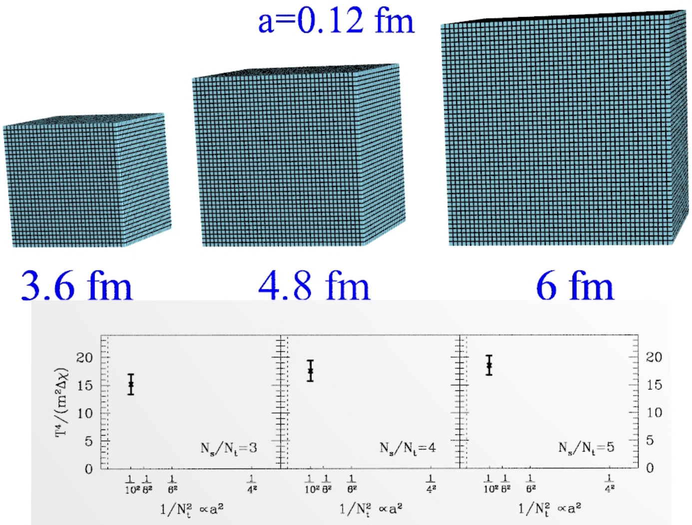

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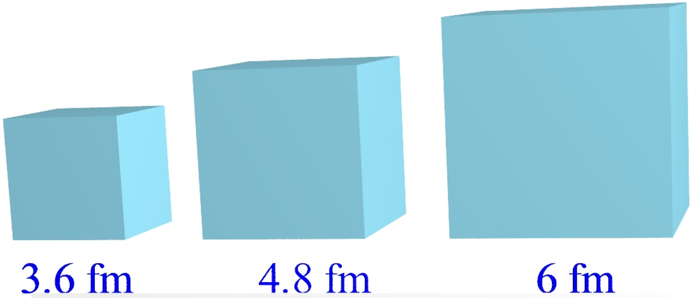
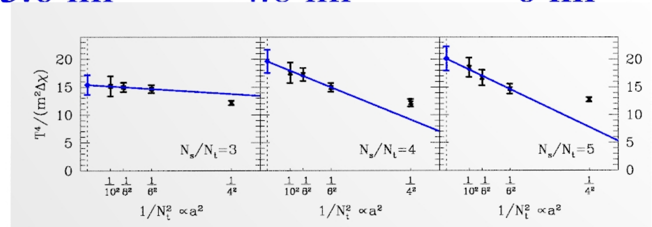
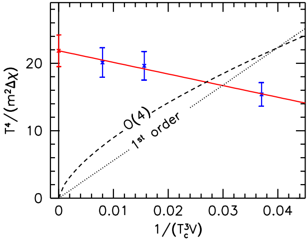




The nature of the QCD transition: analytic

- finite size scaling analysis with continuum extrapolated $T^4/m^2\Delta\chi$



the result is consistent with an approximately constant behavior for a factor of 5 difference within the volume range
chance probability for 1/V is 10^{-19} for O(4) is $7 \cdot 10^{-13}$
continuum result with physical quark masses in staggered QCD:

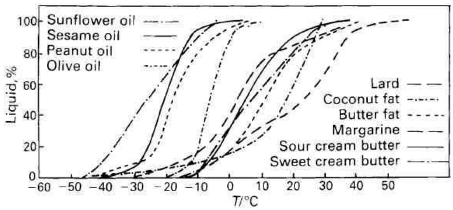
the QCD transition is a cross-over

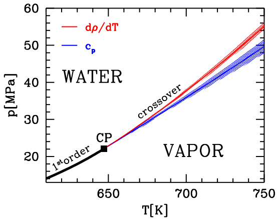
Wuppertal-Budapest Collaboration: Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

analytic transition (cross-over) $\Rightarrow$ it has no unique T_c:
examples: melting of butter (not ice) & water-steam transition





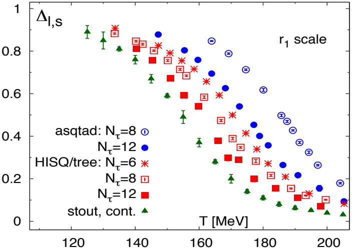
above the critical point c_p and $d\rho/dT$ give different T_cs.
QCD: chiral & quark number susceptibilities or Polyakov loop
they result in different T_c values $\Rightarrow$ physical difference

Wuppertal-Budapest & hotQCD: staggered T_c & eos

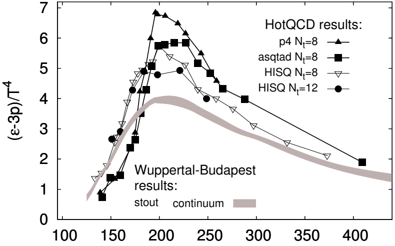
Wuppertal-Budapest: T_c PLB 643 '06 46; JHEP 906 '09 88; 1009 '10 73 eos JHEP 601 '06 89; 1011 '10 77

hotQCD: T_c Phys. Rev. D85 (2012) 054503 eos Phys. Rev. D77 (2008) 014511; D80 (2009) 014504

T_c from chiral condensate



equation of state (eos)



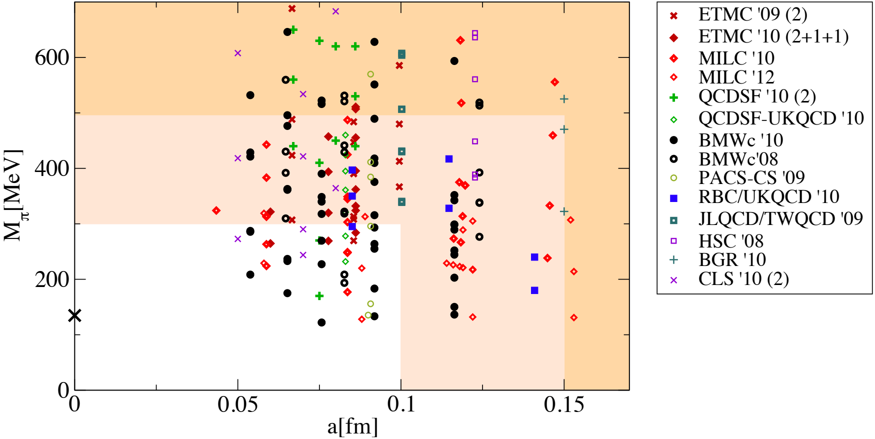
Wuppertal-Budapest: T_c=157(4) MeV; hotQCD: T_c=154(9) MeV

Wuppertal-Budapest: eos-peak ≈4; hotQCD: ≈70,50,40,25% higher

theoretically more solid: Wilson (WHOT-QCD); best: overlap (JLQCD)

Project group A02: HAL-BMW cooperation

NN potential & phase-shift for M_π=300 & 135 MeV (2HEX action)



Project group A03: large baryonic densities

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability $\propto$ its weight

importance sampling, Metropolis algorithm:
(all other algorithms are based on importance sampling)

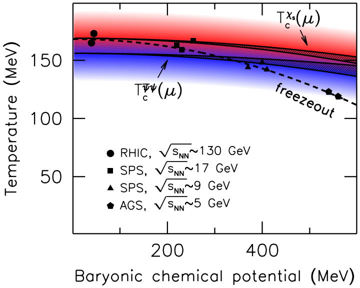
$$P(U \to U') = \min\left[1, \exp(-\Delta S_g) \det(M[U'])/\det(M[U])\right]$$

for $\mu \neq 0$ the determinant is complex $\Rightarrow$ sign problem
no importance sampling is possible

reduction of M: staggered (Fodor-Katz) & Wilson (Nagata-Nakamura)

Continuum prediction for the curvature: full result

G. Endrodi, Z. Fodor, S.D. Katz, K.K. Szabo, JHEP 1104 2011 001



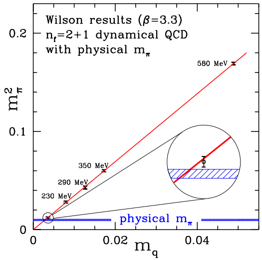
dashed line: freeze-out curve from experiments

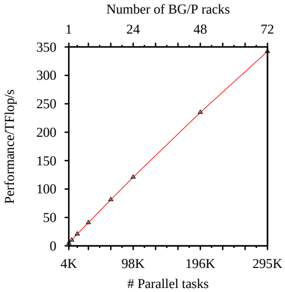
lower solid line: T_c from the chiral condensate
upper solid line: T_c from the strange susceptibility

bands (red and blue) indicate the widths of the transition lines
the widths remain in this order approximately the same

Project group A04: message of computational physics

M's eigenvalues close to 0: CPU demanding (large condition number)





go down to physical pion masses ⇒ algorithmically safe

Blue Gene shows perfect strong scaling from 1 midplane to 72 racks
our sustained performance is as high as 37% of the peak

single K20 GPU card performance upto 570 Gflops (staggered)
(other major source: cell based special purpose machine QPACE)

Summary: physical quark masses and continuum limit

1. Spectrum
2. Quark masses
3. QCD transition
4. T_c & EoS
5. NN interaction
6. High densities
7. CPU-resources