Recent Progress in Lattice QCD

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24 September 2010, Antwerpen, Belgium

lattice field theory talk

examples to reach the physical limit (physical mass & continuum)



Outline





3 Nonvanishing temperature



Z. Fodor Recent Progress in Lattice QCD

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The origin of mass of the visible Universe

source of the mass for ordinary matter (not a dark matter talk)

basic goal of LHC (Large Hadron Collider, Geneva Switzerland):

"to clarify the origin of mass"

e.g. by finding the Higgs particle, or by alternative mechanisms order of magnitudes: 27 km tunnel and O(10) billion dollars



The vast majority of the mass of ordinary matter

ultimate (Higgs or alternative) mechanism: responsible for the mass of the leptons and for the mass of the quarks

interestingly enough: just a tiny fraction of the visible mass (such as stars, the earth, the audience, atoms) electron: almost massless, $\approx 1/2000$ of the mass of a proton quarks (in ordinary matter): also almost massless particles

the vast majority (about 95%) comes through another mechanism \implies this mechanism and this 95% will be the main topic of this talk

quantum chromodynamics (QCD, strong interaction) on the lattice

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QCD: need for a systematic non-perturbative method

in some cases: good perturbative convergence; in other cases: bad pressure at high temperatures converges at $T=10^{300}$ MeV



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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 \Rightarrow two restrictions

- a. put it on a space-time grid (proper approach: asymptotic freedom) formally: four-dimensional statistical systemb. finite size of the system (can be also controlled)
- \Rightarrow stochastic approach, with reasonable spacing/size: solvable

Importance sampling

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

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)

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

gauge part: trace of 3×3 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 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 O) dominate: $C(t) \propto e^{-M \cdot t}$

t large \Rightarrow exponential fits or mass plateaus $M_t = \log[C(t)/C(t+1)]$

Quenched results

QCD is 35 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 \approx 10% discrepancy was believed to be a quenching effect \rightarrow

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Ingredients to control systematics

BMW Collaboration, Science 322:1224-1227,2008

- inclusion of det[M] with an exact n_f=2+1 algorithm action: universality class is known to be QCD (Wilson-quarks)
- spectrum: light mesons, octet & decuplet baryons (resonances) (three of these fix the averaged m_{ud}, m_s and the cutoff)
- large volumes to guarantee small finite-size effects rule of thumb: $M_{\pi}L\gtrsim4$ is usually used (correct for that)
- controlled interpolations & extrapolations to physical m_s and m_{ud} (or eventually simulating directly at these masses) since $M_{\pi} \simeq 135$ MeV extrapolations for m_{ud} are difficult CPU-intensive calculations with M_{π} reaching down to ≈ 200 MeV
- controlled extrapolations to the continuum limit (*a* → 0) calculations are performed at no less than 3 lattice spacings

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_{Ω} 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 $M_{\pi} \approx 190 \text{ MeV}$ (noisiest)



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

altogether 15 points for each hadrons



smooth extrapolation to the physical pion mass (or m_{ud}) small discretization effects (three lines barely distinguishable)

continuum extrapolation goes as $c \cdot a^n$ and it depends on the action in principle many ways to discretize (derivative by 2,3... points) goal: have large *n* and small *c* (in this case n = 2 and *c* is small)

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Final result for the hadron spectrum



Breakthrough of the Year

Proton's Mass 'Predicted'

STARTING FROM A THEORETICAL DESCRIPTION OF ITS INNARDS, physicists precisely calculated the mass of the proton and other parti-

cles made of quarks and gluons. The numbers aren't new; experimenters have been able to weigh the proton for nearly a century. But the new results show that physicists can at last make accurate calculations of the ultracomplex strong force that binds quarks.

In simplest terms, the proton comprises three quarks with gluons zipping between them to convey the strong force. Thanks to the uncertainties of quantum mechanics, however, myriad gluons and quarkantiquark pairs flit into and out of existence within a proton in a frenzy that's nearly impossible to analyze but that produces 95% of the particle's mass.

To simplify matters, theorists from France, Germany, and Hungary took an approach known as "lattice quantum chromodynamics."



They modeled continuous space and time as a four-dimensional array of points—the lattice and confined the quarks to the points and the gluons to the links between them. Using supercomputers, they reckoned the masses of

the proton and other particles to a precision of about 2%—a tenth of the uncertainties a decade ago—as they reported in November.

In 2003, others reported equally precise calculations of more-esoteric quantities. But by calculating the familiar proton mass, the new work signals more broadly that physicists finally have a handle on the strong force.

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Finite-size scaling theory

problem with phase transitions in Monte-Carlo studies Monte-Carlo applications for pure gauge theories ($V = 24^3 \cdot 4$) existence of a transition between confining and deconfining phases: Polyakov loop exhibits rapid variation in a narrow range of β



• theoretical prediction: SU(2) second order, SU(3) first order \implies Polyakov loop behavior: SU(2) singular power, SU(3) jump

data do not show such characteristics!

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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

The nature of the QCD transition

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

finite size scaling study of the chiral condensate (susceptibility)

$\chi = (T/V)\partial^2 \log Z/\partial m^2$

phase transition: finite V analyticity $V \rightarrow \infty$ increasingly singular (e.g. first order phase transition: height $\propto V$, width $\propto 1/V$) for an analytic cross-over χ does not grow with V

two steps (three volumes, four lattice spacings): a. fix V and determine χ in the continuum limit: a=0.3,0.2,0.15,0.1fm b. using the continuum extrapolated χ_{max} : finite size scaling

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Approaching the continuum limuit



Approaching the continuum limuit



Approaching the continuum limuit



Approaching the continuum limuit



Approaching the continuum limuit



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

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675 🔹 🖉 🕨 🗸 🚍 🕨 🤻 🚍 🕨

Possible first order scenario with critical bubbles



Reality: smooth analytic transition (cross-over)



Literature: discrepancies between T_c

Bielefeld-Brookhaven-Riken-Columbia Collaboration:

M. Cheng et.al, Phys. Rev. D74 (2006) 054507

 T_c from $\chi_{\bar{\psi}\psi}$ and Polyakov loop, from both quantities:

 $T_c = 192(7)(4) \text{ MeV}$

Bielefeld-Brookhaven-Riken-Columbia merged with MILC: 'hotQCD'

Wuppertal-Budapest group: WB

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46

chiral susceptibility: Polyakov and strange susceptibility: $T_c = 151(3)(3) \text{ MeV}$ $T_c = 175(2)(4) \text{ MeV}$

'chiral T_c ': \approx 40 MeV; 'confinement T_c ': \approx 15 MeV difference

both groups give continuum extrapolated results with physical m_{π}

Literature: discrepancies between T dependencies

Reason: shoulders, inflection points are difficult to define? Answer: no, the whole temperature dependence is shifted



for $\Delta_{I,s} \approx 35$ MeV; for the strange susceptibility ≈ 15 MeV this discrepancy would appear in all quantities (eos, fluctuations)

Examples for improvements, consequences

how fast can we reach the continuum pressure at $T=\infty$?



p4 action is essentially designed for this quantity $T \gg T_c$

asqtad designed mostly for T=0 physics (but good at high T, too)

stout-smeared one-link converges slower but in the a^2 scaling regime (e.g. extrapolation from N_t =8,10 provides a result within about 1%)

Choice of the action

no consensus: which action offers the most cost effective approach

Aoki, Fodor, Katz, Szabo, JHEP 0601, 089 (2006) [arXiv:hep-lat/0510084]

our choice: tree-level $O(a^2)$ -improved Symanzik gauge action



2-level (stout) smeared improved staggered fermions



best known way to improve on taste symmetry violation

Chiral symmetry breaking and pions

transition temperature for remnant of the chiral transition: balance between the f's of the chirally broken & symmetric sectors chiral symmetry breaking: 3 pions are the pseudo-Goldstone bosons

staggered QCD: 1 $(\frac{3}{16})$ pseudo-Goldstone instead of 3 (taste violation) staggered lattice artefact \Rightarrow disappears in the continuum limit WB: stout-smeared improvement is designed to reduce this artefact



strange quark number susceptibility and Polyakov-loop

strange susceptibility: $\chi_2^s = (T/V) \cdot \partial^2 \ln Z / \partial \mu_s^2$ Polyakov-loop renormalization procedure: Acki, Fodor, Katz, Szabo: PLB643 46 (2006)

continuum behaviour can be given for both observables



overall scale (lattice spacing, thus also T) is set by $f_{\mathcal{K}}$

renormalized chiral condensate

$$\langle \bar{\psi}\psi\rangle_{\mathsf{R}} = -\left[\langle \bar{\psi}\psi\rangle_{\mathsf{I},\mathsf{T}} - \langle \bar{\psi}\psi\rangle_{\mathsf{I},\mathsf{0}}\right]\frac{m_{\mathsf{I}}}{\mathsf{X}^{\mathsf{4}}}$$

X can be chosen as m_{π}

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

 $\Delta_{I,s}$ (strange subtraction)



T_c summary of the Wuppertal-Budapest group

list of pseudocritical temperatures (various observables)

	$\chi_{ar\psi\psi}/T^4$	$\Delta_{l,s}$	$\langle \bar{\psi}\psi \rangle_{R}$	$\chi^{s}_{ m 2}/T^{ m 2}$	ϵ/T^4	(<i>ϵ</i> -3p)/T ⁴
WB'10	147(2)(3)	157(3)(3)	155(3)(3)	165(5)(3)	157(4)(3)	154(4)(3)
WB'09	146(2)(3)	155(2)(3)	-	169(3)(3)	-	-
WB'06	151(3)(3)	-	-	175(2)(4)	-	-

all numbers (in a given coloumn) are in complete agreement different variables give different pseudocritical T_c -s: 147–165 MeV reason: the transition is a broad one with 30-40 MeV broadness

3% shift to lower values between 2006 and 2009 reason: 3% experimental change in f_K (no change in lattice results)

Wuppertal-Budapest: physical quark masses ($m_s/m_{ud} \approx 28$) gauge configs: N_t =8,10 in 2006 $\Rightarrow N_t$ =12 in 2009 $\Rightarrow N_t$ =16 in 2010



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Equation of state: integral method

J. Engels et al., Phys. Lett. B252 (1990) 625

on the lattice the dimensionless pressure is given by

$$p^{\text{lat}}(\beta, m_q) = (N_t N_s^3)^{-1} \log \mathcal{Z}(\beta, m_q)$$

not accessible using conventional algorithms, only its derivatives

$$p^{\text{lat}}(\beta, m_q) - p^{\text{lat}}(\beta^0, m_q^0) = (N_t N_s^3)^{-1} \int_{(\beta^0, m_q^0)}^{(\beta, m_q)} \left(d\beta \frac{\partial \log \mathcal{Z}}{\partial \beta} + dm_q \frac{\partial \log \mathcal{Z}}{\partial m_q} \right)$$

first term: gauge action & second term: chiral condensate

the pressure has to be renormalized: subtraction at T=0 (or T>0)

T≠0 simulations can't go below T≈100 MeV (lattice spacing is large) physical HRG gives here 5% contribution of SB \Rightarrow path of M_{π} =720 MeV \Rightarrow distorted HRG no contribution at T=100 MeV_{2,0}

Finite volume and discretization effects



finite V: $N_s/N_t=3$ and 6 (8 times larger volume): no sizable difference

finite a: improvement program of lattice QCD (action & observables) tree-level improvement for p (thermodynamic relations fix the others) trace anomaly for three T-s: high T, transition T, low T continuum limit N_t =6,8,10,12: same with or without improvement

improvement strongly reduces cutoff effects: slope ≈ 0 (1-2 σ level)

Pressure and energy density



 ϵ normalized to the Stefan-Boltzmann limit: $\epsilon(T \rightarrow \infty)=15.7$ at 1000 MeV still 20% difference to the Stefan-Boltzmann value essentially perfect scaling, lines/points are lying on top of each other

Entropy and trace anomaly



good agreement with the HRG model up to the transition region T_c can be defined as the inflection point of the trace anomaly

Inflection point of $I(T)/T^4$	154(4) MeV
T at the maximum of $I(T)/T^4$	187(5) MeV
Maximum value of $I(T)/T^4$	4.1(1)

agreement with Aoki, Fodor, Katz, Szabo, JHEP 0601, 089 (2006) [arXiv:hep-lat/0510084]

Speed of sound & parametrization



 c_s minimum value is about 0.13 at T \approx 145 MeV 'smaller than error' parametrization T=100...1000 MeV (t=T/200 MeV)

$$\frac{l(T)}{T^4} = \exp(-h_1/t - h_2/t^2) \cdot \left(h_0 + \frac{f_0 \cdot [\tanh(f_1 \cdot t + f_2) + 1]}{1 + g_1 \cdot t + g_2 \cdot t^2}\right)$$

$$\frac{h_0}{0.1396} + \frac{h_1}{0.1396} + \frac{h_2}{0.0350} + \frac{f_0}{2.76} + \frac{f_1}{6.79} + \frac{f_2}{5.29} + \frac{g_1}{6.47} + \frac{g_2}{1.04}$$

$$2.Fodor = \frac{1}{2} \operatorname{Recent Progress in Lattice QCD}$$

Equation of state: $I(T) = \epsilon - 3p$



two pion masses: $M_{\pi} \approx 720 \text{ MeV} (\text{R=1})$ and $M_{\pi} = 135 \text{ MeV} (\text{R}^{phys})$ good agreement with the HRG model up to the transition region quark mass dependence disappears for high T good agreement with perturbation theory

comparison with the published results of the hotQCD collaboration discrepancy: peak at ${\approx}20$ MeV larger T and ${\approx}50\%$ higher

- lattice QCD arrived to the "productive phase" algorithmic developments: Berlin Wall has fallen physical m_q (M_π) are possible with a=0.05 fm & L=6 fm we can control all systematic uncertainites
- full result for the light hadron spectrum all systematic uncertainties are controlled: action, algorithm, a→0, L→∞, M_π→135 MeV both stable particles & resonances can be appropriately treated
- QCD at nonvanishing temperatures: analytic cross-over long standing discrepancy in the literature overall scale clarified (equation of state needs more time)

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fine lattice to resolve the structure of the proton (≤ 0.1 fm) few fm size is needed 50-100 points in 'xyz/t' directions $a \Rightarrow a/2$ means 100-200×CPU mathematically 10⁹ dimensional integrals

advanced techniques, good balance and several Tflops are needed

Image: A image: A

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 hundreds of Tflops

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



Discretization errors in the transition region

we always have discretization errors: nothing wrong with it as long as

a. result: close enough to the continuum value (error subdominant) b. we are in the scaling regime (a^2 in staggered)

various types of discretization errors \Rightarrow we improve on them (costs)

we are speaking about the transition temperature region interplay between hadronic and quark-gluon plasma physics smooth cross-over: one of them takes over the other around T_c

both regimes (low T and high T) are equally important improving for one: $T \gg T_c$, doesn't mean improving for the other: $T < T_c$

example: 'expansion' around a Stefan-Boltzman gas (van der Waals) for water: it is a fairly good description for T \gtrsim 300^o claculate the boiling point: more accuracy needed for the liquid phase

Further advantages of the action

smallest eigenvalue of M: small fluctuations

 \Rightarrow simulations are stable (major issue of Wilson fermions & speedup)

non-perturbative improvement coefficient: \approx tree-level (smearing)

R. Hoffmann, A. Hasenfratz, S. Schaefer, PoS LAT2007 (2007) 1 04

good a^2 scaling of hadron masses (M_{π}/M_{ρ} =2/3) up to $a\approx$ 0.2 fm

S. Dürr et al. [Budapest-Marseille-Wuppertal Collaboration] Phys. Rev. D79, 014501 (2009)



Scaling for the pion splitting



scaling regime is reached if a^2 scaling is observed asymptotic scaling starts only for $N_t \gtrsim 8$ (a ≤ 0.15 fm): two messages a. $N_t=8,10$ extrapolation gives 'p' on the $\approx 1\%$ level: good balance b. stout-smeared improvement is designed to reduce this artefact most other actions need even smaller 'a' to reach scaling

Consequences of the non-scaling behaviour

for large '*a*' no proper a^2 scaling (e.g. due to large m_{π} splitting) how do we monitor it, how to be sure being in the scaling regime? dimensionless combinations in the $a \rightarrow 0$ limit:

 $T_c r_0$ or T_c / f_K for the remnant of the chiral transition



 N_t =4,6: inconsistent continuum limit

*N*_t=6,8,10: consistent continuum limit (stout-link improvement)

independently which quantity is taken one obtains the same T_c signal: extrapolation is safe, we are in the a^2 scaling regime

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Setting the scale 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 $M_{\Omega}=1672$ MeV we obtain 'a' and T=1/ N_ta

Y.Aoki et al. [Wuppertal-Budapest Collaboration] arXiv:0903.4155



independently which quantity is taken (we used physical masses)

 \Rightarrow one obtains the same 'a' and T, result is safe

compare with the hadron resonance gas model: HRG



temperature dependence of the chiral condensate



Wuppertal-Budapest: good agreement with the physical HRG

Borsanyi, Fodor, Hoelbling, Katz, Krieg, Ratti, Szabo, arXiv:1005.3508

hotQCD: agreement only with the distorted spectrum though their results are gradually getting closer to ours

Illustration: lattice artefacts due to pion splitting

we have seen: our action (WB) has less unphysical pion splitting than the asqtad (MILC) and far less than the p4 (Bielefeld) action

in the continuum limit: no problem; at $a \neq 0$ it mimics larger M_{π} "reproduce" the result of hotQCD with larger M_{π} (asqtad is better)



 $M_{\pi} \approx 220 \text{ MeV}$ (hotQCD) "corresponds" to $M_{\pi} \approx 410 \text{ MeV}$ (WB) asqtad (MILC) needs finer p4 (Bielefeld) needs much finer lattices in order to handle physical quark masses

All path approach

goal: determine the equation of state for several pion masses reduce the uncertainty related to the choice of β^0 give the uncertainty related to the integration path



conventional path: A, though B, C or any other paths are possible generalize: take all paths into account (use derivatives of p) two-dimensional spline function gives p for any $(\beta, R=m_s/m_{ud})$ technically: solution of a large system of linear equations $\beta \in \mathbb{R}$

Charm contribution

perturbative indications: important already at $2 \cdot T_c$

M. Laine and Y. Schroder, Phys. Rev. D73 (2006) 085009

determine it within the partially quenched framwork: $m_c/m_s=11.85$



charm contribution is indeed non-negligeble from 200 MeV one has to extend this observation to the dynamical case