Introduction to and Recent Progress in Lattice QCD

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thermodynamics and T=0 physics
examples to reach the physical limit (physical mass & continuum)

SFB
TR55

Outline

Quantum Chromodynamics (QCD)

QCD: Currently the best known theory to describe the strong interaction.

SU(3) gauge theory with fermions in fundamental representation.

Fundamental degrees of freedom:

- gluons: A^a_μ, $a = 1, \ldots, 8$
- quarks: ψ, 3(color) $\times$ 4(spin) $\times$ 6(flavor) components

$$\mathcal{L}_{\mathrm{QCD}} = \underbrace{-\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu}}_{\text{pure gauge part}} + \underbrace{\overline{\psi}(\mathrm{i} D_\mu \gamma^\mu - m)\psi}_{\text{fermionic part}},$$

where

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu \qquad \text{field strength}$$

$$D_\mu = \partial_\mu + g A^a_\mu \frac{\lambda^a}{2\mathrm{i}} \qquad \text{covariant derivative} \longrightarrow \text{gives quark–gluon interaction}$$

SU(3) group

SU(3): group of 3×3 unitary matrices with unit determinant:

$U \in \mathrm{SU}(3) \quad \Longleftrightarrow$

1. $UU^\dagger = \mathbf{1}_{3\times3}$, that is, $U^{-1} = U^\dagger$,
2. $\det U = 1$.

8 generators: Gell–Mann matrices $\lambda^a \quad (a = 1, \ldots, 8)$

Lie algebra of $SU(3)$: Linear combinations $A = A^a \dfrac{\lambda^a}{2}$

1. Hermitean: $A^\dagger = A$,
2. traceless: $\mathrm{Tr}\, A = 0$.

$$U = \exp(\mathrm{i}A) = \exp\left(\mathrm{i}A^a \frac{\lambda^a}{2}\right): \qquad \text{elements of group SU(3).}$$

$[A, B] = \mathrm{i} f^{abc} A^b B^c \dfrac{\lambda^a}{2}$, $\qquad f^{abc}$: structure coefficients.

Quantum Chromodynamics (cont.)

$\mathcal{L}_{\mathrm{QCD}}$ is invariant under local gauge transformations:

$$A'_\mu(x) = G(x)A_\mu(x)G(x)^\dagger - \frac{\mathrm{i}}{g}\left(\partial_\mu G(x)\right) G(x)^\dagger$$

$$\psi'(x) = G(x)\psi(x)$$

$$\overline{\psi}'(x) = \overline{\psi}(x)G^\dagger(x)$$

Only gauge invariant quantities are physical.

Properties of QCD:

- Asymptotic freedom:
  Coupling constant $g \to 0$ when energy scale $\mu \to \infty$.
  $\Longrightarrow$ Perturbation theory can be used at high energies.
- Confinement:
  Coupling constant is large at low energies.
  $\Longrightarrow$ Nonperturbative methods are required.

Quantum Chromodynamics (cont.)

Quantization using Feynman path integral:

$$\langle 0|\, T[\mathcal{O}_1(x_1)\cdots\mathcal{O}_n(x_n)]\,|0\rangle = \frac{\int [\mathrm{d}\psi]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}A_\mu]\,\mathcal{O}_1(x_1)\cdots\mathcal{O}_n(x_n)\,e^{\mathrm{i}S[\psi,\overline{\psi},A_\mu]}}{\int [\mathrm{d}\psi]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}A_\mu]\,e^{\mathrm{i}S[\psi,\overline{\psi},A_\mu]}}$$

$e^{\mathrm{i}S}$ oscillates $\longrightarrow$ hard to evaluate integrals.
Wick rotation: $t \to -\mathrm{i}t$ analytic continuation to Euclidean spacetime.
$\Longrightarrow \quad e^{\mathrm{i}S} \longrightarrow e^{-S_\mathrm{E}}$, where

$$S_\mathrm{E} = \int \mathrm{d}^4x\ \mathcal{L}_\mathrm{E} = \int \mathrm{d}^4x \left[\frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} + \overline{\psi}(D_\mu\gamma^\mu + m)\psi\right]$$

positive definite Euclidean action.

Quantum Chromodynamics (cont.)

Vector components: $\mu = 0, 1, 2, 3 \quad \longrightarrow \quad \mu = 1, 2, 3, 4$

Euclidean correlator

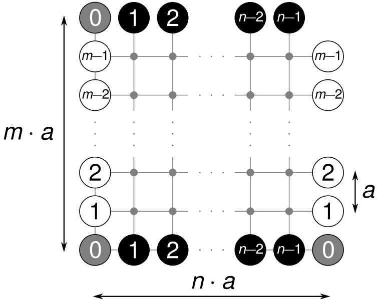
$$\langle 0|\, \mathcal{O}_1(x_1) \cdots \mathcal{O}_n(x_n)\, |0\rangle_{\mathrm{E}} = \frac{\int [\mathrm{d}\psi]\, [\mathrm{d}\overline{\psi}]\, [\mathrm{d}A_\mu]\, \mathcal{O}_1(x_1) \cdots \mathcal{O}_n(x_n)\, e^{-S_{\mathrm{E}}[\psi, \overline{\psi}, A_\mu]}}{\int [\mathrm{d}\psi]\, [\mathrm{d}\overline{\psi}]\, [\mathrm{d}A_\mu]\, e^{-S_{\mathrm{E}}[\psi, \overline{\psi}, A_\mu]}}$$

Expectation value of $\mathcal{O}_1(x_1) \cdots \mathcal{O}_n(x_n)$
with respect to positive definit measure $[\mathrm{d}\psi]\, [\mathrm{d}\overline{\psi}]\, [\mathrm{d}A_\mu]\, e^{-S_{\mathrm{E}}}$.

Lattice regularization

"Most sytematic" nonperturbative approach:
lattice QFT

Take a finite segment of spacetime,
put fields at vertices of hypercubic lattice with lattice spacing a:



Usual boundary conditions:
Bosons:

Periodic in all directions

Fermions:

Time direction: antiperiodic

Space directions: periodic

Lattice regularization (2)

We have to discretize the action:

intagral over spacetime	$\int \mathrm{d}^4 x$	$\longrightarrow$	sum over sites	$a^4 \sum_x$
derivatives ∂_μ		$\longrightarrow$	finite differences	

Momentum $p \leq \frac{\pi}{a}$ $\Longrightarrow$ natural UV cutoff.

At finite "a" results differ from the continuum value.

$$R^{\text{latt.}} = R^{\text{cont.}} + O(a^\nu)$$

for some dimensionless quantity R.

To get physical results, need to perform:

1. Infinite volume limit $(V \to \infty)$,
2. Continuum limit $(a \to 0)$.

Example: scalar field

Continuum action:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 + \frac{1}{2} m^2 \phi^2 + \lambda \phi^4$$

Simplest lattice action:

$$S = \sum_x a^4 \left(\frac{1}{2} \sum_{\mu=1}^{4} \left[\frac{\phi_{x+\hat{\mu}} - \phi_{x-\hat{\mu}}}{2a} \right]^2 + \frac{1}{2} m^2 \phi_x^2 + \lambda \phi_x^4 \right)$$

where $\hat{\mu}$: unit vector in direction μ.

Introduce dimensionless quantities: $\phi' = \phi a, \quad m' = ma, \quad \lambda' = \lambda$

$$S = \sum_x \left(\phi_x'^2 \left[2 + \frac{1}{2} m'^2 \right] + \lambda' \phi_x'^4 - \frac{1}{2} \sum_{\mu=1}^{4} \phi'_{x+\hat{\mu}} \phi'_{x-\hat{\mu}} \right)$$

Lattice spacing a does not appear explicitly in the calculations.

Example: scalar field

the ϕ^4 theory is trivial

it does not exist as an interactive continuum theory
it exists (as an interactive model) only as a cutoff theory
$\Longrightarrow$ the Higgs mass can not be larger than about 600 GeV

analytic & numerical works provide the evidence (Luscher, Weisz ...)
goes far beyond the perturbative unitarity arguments

in each point of the two dimensional parameter-space: m' and λ'
one can determine the renormalized mass and quartic coupling
high order hopping parameter expansion for $m_R a \gtrsim 0.5$
renormalization group equation techniques for $m_R a \lesssim 0.5$
(the latter approaches the infinite cutoff or continuum limit)

$m_R a$=0 defines the critical line (continuum limit)

construct lines of constant physics (LCP):

a$\to$0 but m_R=const., λ_R=const.

as "a" gets smaller along these LCPs the bare λ' gets larger
actually before the LCPs reach the critical line one gets $\lambda' = \infty$
(only the trivial theory $\lambda' = 0$ reaches the critical line)

assume that the maximum momenta are a few times larger than M_H
maximal renormalized self-coupling, thus maximal Higgs mass
is obtained at the maximal bare coupling $\lambda' = \infty$
using the Higgs vacuum expectation value (overall scale)
one obtains $M_H \lesssim$600 GeV

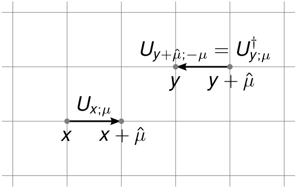
for even higher cutoffs (more than a few times) $\Rightarrow$ smaller M_H
for M_H=126 GeV one can go up to the Planck scale
(we called it in the 1990-ies: the nightmare scenario)

Yang–Mills theories on the lattice

Regularization has to maintain lattice version of gauge invariance.

Gauge fields $\longrightarrow$ on links connecting neighboring sites.

- Continuum: A_μ, elements of Lie algebra of SU(3).
- Lattice: $U_\mu = e^{iagA_\mu}$, elements of group SU(3) itself.



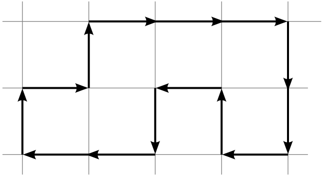
$$U_{x+\hat{\mu};-\mu} = U^{-1}_{x;\mu} = U^\dagger_{x;\mu}$$

Lattice gauge transformation:

$$U'_{x;\mu} = G_x U_{x;\mu} G^\dagger_{x+\hat{\mu}}$$
$$\psi'_x = G_x \psi_x$$
$$\overline{\psi}'_x = \overline{\psi}_x G^\dagger_x$$

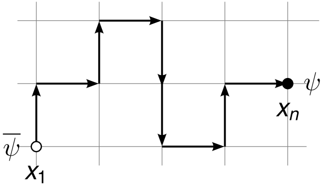
Gauge invariant quantities on the lattice

- Gluon loops



$$\mathrm{Tr}\left[U_{x_1;\mu}\, U_{x_1+\hat{\mu};\nu} \cdots U_{x_1-\hat{\epsilon};\epsilon}\right]$$

- Gluon lines connecting q and $\overline{q}$



$$\overline{\psi}_{x_1} U_{x_1;\mu}\, U_{x_1+\hat{\mu};\nu} \cdots U_{x_n-\hat{\epsilon};\epsilon} \psi_{x_n}$$

Gauge action

Continuum gauge action:

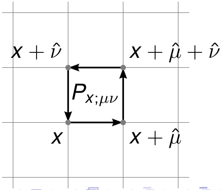
$$S_{\rm g}^{\rm cont.} = -\int \mathrm{d}^4 x \, \frac{1}{4} F_{\mu\nu} F_{\mu\nu}$$

Simplest gauge invariant lattice action: Wilson action

$$S_{\rm g}^{\rm Wilson} = \beta \sum_{\substack{x \\ \nu<\mu}} \left(1 - \frac{1}{3} \mathrm{Re}\left[P_{x;\mu\nu} \right] \right), \quad \beta = \frac{6}{g^2}, \quad S_g^{latt.} = S_g^{cont} + O(a^2),$$

where $P_{x;\mu\nu}$ is the plaquette:

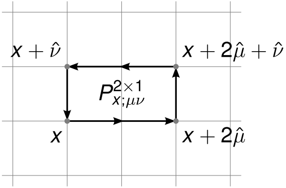
$$P_{x;\mu\nu} = \mathrm{Tr}\left[U_{x;\mu}\, U_{x+\hat{\mu};\nu}\, U^\dagger_{x+\hat{\nu};\mu}\, U^\dagger_{x;\nu} \right]$$



Gauge action – Symanzik improvement

Add 2×1 gluon loops to Wilson action:

$$S_g^{\text{Symanzik}} = \beta \sum_{\substack{x \\ \nu<\mu}} \left\{ 1 - \frac{1}{3} \left(c_0 \, \mathrm{Re}[P_{x;\mu\nu}] + c_1 \, \mathrm{Re}\left[P^{2\times 1}_{x;\mu\nu}\right] + c_1 \, \mathrm{Re}\left[P^{2\times 1}_{x;\nu\mu}\right] \right) \right\}$$



Consistency condition: $c_0 + 8c_1 = 1$.

$c_1 = -\dfrac{1}{12}$ gives tree level improvement $\Longrightarrow S_g^{latt.} = S_g^{cont.} + O(a^4)$

Fermion doubling

Continuum fermion action

$$S_{\rm f} = \int d^4x\, \overline{\psi}(\gamma^\mu \partial_\mu + m)\psi.$$

Naively discretized:

$$S_{\rm f}^{\rm naive} = a^4 \sum_x \left[\overline{\psi}_x \sum_{\mu=1}^{4} \gamma_\mu \frac{\psi_{x+\hat{\mu}} - \psi_{x-\hat{\mu}}}{2a} + m\overline{\psi}_x \psi_x \right]$$

Inverse propagator:

$$G^{-1}_{\rm naive}(p) = {\rm i}\gamma_\mu \frac{\sin p_\mu a}{a} + m.$$

Extra zeros at $p_\mu = 0, \pm\frac{\pi}{a}$ $\implies$ 16 zeros in 1st Brillouin zone. In d dimensions 2^d fermions instead of 1 $\implies$ fermion doubling.
Wilson, staggered (domain wall, overlap) solves it “somehow”

Wilson fermions

$$S_f^W = S_f^{\text{naive}} \underbrace{- a \cdot \frac{r}{2} a^4 \sum_x \overline{\psi}_x \Box \psi_x}_{\text{Wilson term}},$$

where

$$\Box \psi_x = \sum_{\mu=1}^{4} \frac{\psi_{x+\hat{\mu}} - 2\psi_x + \psi_{x-\hat{\mu}}}{a^2}.$$

$0 < r \leq 1$ Wilson parameter, usually $r = 1$.

$$G_W^{-1}(p) = G_{\text{naive}}^{-1}(p) + \frac{2r}{a} \sum_{\mu=1}^{4} \sin^2 (p_\mu a/2)$$

$m_{\text{doublers}} = O(a^{-1}) \quad \Longrightarrow \quad$ doublers disappear in continuum limit.

Wilson fermions (cont.)

Work with dimensionless quantities: $a^{3/2}\psi \to \psi$

$$S_f^W = \sum_x \left\{ \overline{\psi}_x \sum_\mu \left[(\gamma_\mu - r)\, \psi_{x+\hat{\mu}} - (\gamma_\mu + r)\, \psi_{x-\hat{\mu}} \right] + (ma + 4r)\, \overline{\psi}_x \psi_x \right\}$$

Rescale ψ by $\sqrt{2\kappa}$, $\kappa = \dfrac{1}{2ma + 8r}$ hopping parameter.

Action including gauge fields:

$$S_f^W = \sum_x \left\{ \kappa \left[\sum_\mu \overline{\psi}_x\, (\gamma_\mu - r)\, U_{x;\mu} \psi_{x+\hat{\mu}} - \overline{\psi}_{x+\hat{\mu}}\, (\gamma_\mu + r)\, U^\dagger_{x;\mu} \psi_x \right] + \overline{\psi}_x \psi_x \right\}$$

Wilson fermions (cont.)

- Advantages
  1. Kills all doublers.
- Disadvantages
  1. No chiral symmetry at $a \neq 0$.

     $\Longrightarrow$ Massless pions at $\kappa_c \neq \frac{1}{8r}$.

     Additive quark mass renormalization.
  2. Large discretization errors:

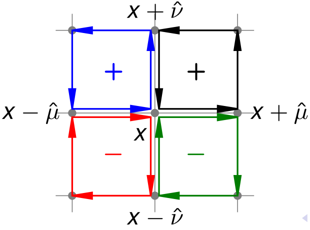
     $S_f^W = S_f^{\text{cont.}} + O(a)$

Wilson fermions – Clover improvement

$$S_f^{\text{clover}} = S_f^{W} - \underbrace{\frac{iac\kappa r}{4} \sum_x \overline{\psi}_x \sigma_{\mu\nu} \mathcal{F}_{x;\mu\nu} \psi_x}_{\text{clover term}} = S_f^{\text{cont.}} + O(a^2), \qquad \sigma_{\mu\nu} = \frac{i}{4} [\gamma_\mu, \gamma_\nu]$$

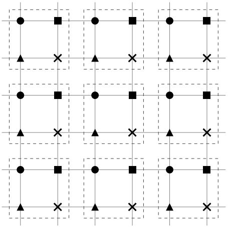
$$\mathcal{F}_{x;\mu\nu} = \frac{1}{4} \Big(U_{x;\mu} U_{x+\hat\mu;\nu} U^\dagger_{x+\hat\nu;\mu} U^\dagger_{x;\nu} - U^\dagger_{x-\hat\nu;\nu} U^\dagger_{x-\hat\mu-\hat\nu;\mu} U_{x-\hat\mu-\hat\nu;\nu} U_{x-\hat\nu;\nu} + \\ + U_{x;\nu} U^\dagger_{x-\hat\mu+\hat\nu;\mu} U^\dagger_{x-\hat\mu;\nu} U_{x-\hat\mu;\mu} - U_{x;\mu} U^\dagger_{x+\hat\mu-\hat\nu;\nu} U^\dagger_{x-\hat\nu;\mu} U_{x-\hat\nu;\nu} \Big)$$

discretized version of field strength $F_{\mu\nu}$.



Kogut–Susskind (staggered) fermions

Fermion degrees of freedom $\longrightarrow$ corners of hypercube.



In d dimensions:

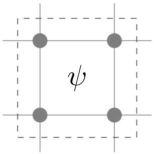
$2^{d/2}$ spinor components of Dirac spinors

2^d corners of hypercube

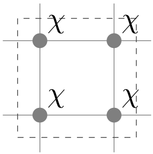
$\Longrightarrow$ describes $2^d/2^{d/2} = 2^{d/2}$ flavors (tastes).

If $d = 4$ $\Longrightarrow$ 4 flavors (tastes) $\Longrightarrow$ 4^{th} rooting required.

Kogut–Susskind (staggered) fermions (cont.)



$\longrightarrow$



3(color) $\times$ 4(spin) components

3(color) $\times$ 1(spin) components

$$S_{\mathrm{f}}^{\mathrm{S}} = \sum_x \overline{\chi}_x \left\{ \frac{1}{2} \sum_\mu \eta_{x,\mu} \left(U_{x;\mu} \chi_{x+\hat{\mu}} - U^\dagger_{x-\hat{\mu};\mu} \chi_{x-\hat{\mu}} \right) + ma \chi_x \right\},$$

where

$$\eta_{x,\mu} = (-1)^{\sum_{\nu=1}^{\mu-1} x_\nu}$$ staggered phase.

Kogut–Susskind (staggered) fermions (cont.)

- Advantages
  1. Remnant chiral symmetry at $a \neq 0$

     $\Longrightarrow$ no additive quark mass renormalization.
  2. $O(a^2)$ discretization errors.
  3. Fast.
- Disadvantages
  1. 4 tastes (flavors) instead of 1

     $\Longrightarrow$ rooting trick required.
  2. Taste symmetry breaking: links within hypercube are not identical.

Finite temperature QFT

Partition function of a quantum system with Hamiltonian H at temperature T:

$$Z = \mathrm{Tr}\left[e^{-H/T}\right]$$

Bosonic QFT $\longrightarrow$ integral over 3d field configurations φ.

$$\mathrm{Tr}\left[e^{-H/T}\right] = \int [\mathrm{d}\varphi]\ \langle\varphi|\, e^{-H/T}\, |\varphi\rangle$$

Integrand: $|\varphi\rangle \to |\varphi\rangle$ transition probability amplitude after imaginary time $t = -\mathrm{i}/T$.

$$\langle\varphi|\, e^{-H/T}\, |\varphi\rangle = \int\limits_{\substack{\phi|_{t=0}=\varphi \\ \phi|_{t=-\mathrm{i}/T}=\varphi}} [\mathrm{d}\phi]\ \exp\left[\mathrm{i}\int_{t=0}^{t=-\mathrm{i}/T} \mathrm{d}t\ L\left(\phi, \frac{\partial\phi}{\partial \mathrm{i}t}\right)\right]$$

Finite temperature QCD (cont.)

$$Z_{\mathrm{QCD}} = \int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\, e^{-S_{\mathrm{E}}(U,\psi,\overline{\psi})}$$
$$= \int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\, \exp\left[\int_0^{1/T} \mathrm{d}x_4 \int \mathrm{d}^3\mathbf{x}\;\; \mathcal{L}_{\mathrm{E}}(U,\psi,\overline{\psi})\right]$$

Boundary condition in the imaginary time (temperature) direction:

Gluons: periodic,

Quarks: antiperiodic.

Temperature of lattice with temporal extension N_t:

$$T = \frac{1}{a \cdot N_{\mathrm{t}}}.$$

Increase of β $\xRightarrow{\text{asymptotic freedom}}$ decrease of a $\Longrightarrow$ increase of T.

Integral over fermions

Full lattice QCD action

$$S(U,\psi,\overline{\psi}) = \underbrace{S_{\mathrm{g}}(U)}_{\text{gluonic part}} - \underbrace{\overline{\psi}\, M(U)\, \psi}_{\text{fermionic part}}$$

Fermions are described by Grassmann variables $\longrightarrow$ have to integrate out analytically.

$$\int [\mathrm{d}U]\, [\mathrm{d}\overline{\psi}]\, [\mathrm{d}\psi]\, e^{-S_{\mathrm{g}}(U)+\overline{\psi}\, M(U)\, \psi} = \int [\mathrm{d}U]\, e^{-S_{\mathrm{g}}(U)} \det M(U)$$

$\Longrightarrow$ Effective action for gluons

$$S_{\mathrm{eff.}}(U) = S_{\mathrm{g}}(U) - \ln\left(\det M(U)\right).$$

Staggered fermion matrix describes 4 tastes.
Rooting trick: for n_f flavors, take power $\frac{n_f}{4}$ of determinant:

$$S^{\mathrm{S}}_{\mathrm{eff.}}(U) = S_{\mathrm{g}}(U) - \ln\left(\det M(U)^{n_f/4}\right) = S_{\mathrm{g}}(U) - \frac{n_f}{4} \ln\left(\det M(U)\right)$$

Expectation values of fermionic quantities

$$\mathcal{O}(x,y) = \left(\overline{\psi}^u \psi^d\right)_y \left(\overline{\psi}^d \psi^u\right)_x \qquad \text{fermionic operator}$$

$$\langle 0|\,\mathcal{O}(x,y)\,|0\rangle = \frac{\int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\,\overline{\psi}_y^{u,a}\,\psi_y^{d,a}\,\overline{\psi}_x^{d,b}\,\psi_x^{u,b}\;e^{-S_g(U)+\overline{\psi}\,M(U)\,\psi}}{\int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\;e^{-S_g(U)+\overline{\psi}\,M(U)\,\psi}} =$$

$$= \frac{\int [\mathrm{d}U]\,\left[M^{-1,u}_{x,y}(U)\right]^{ab}\left[M^{-1,d}_{y,x}(U)\right]^{ba}\,\det M(U)\;e^{-S_g(U)}}{\int [\mathrm{d}U]\,\det M(U)\;e^{-S_g(U)}} =$$

$$= \frac{\int [\mathrm{d}U]\;\mathrm{Tr}_{\text{color,spin}}\left[\left(M^{-1,u}_{x,y}\right)\left(M^{-1,d}_{y,x}\right)\right]\;e^{-S_{\text{eff.}}(U)}}{\int [\mathrm{d}U]\;e^{-S_{\text{eff.}}(U)}}.$$

Expectation values of fermionic quantities (2)

Expectation value of $\mathcal{O} = \left(\overline{\psi}^u \psi^d\right)_y \left(\overline{\psi}^d \psi^u\right)_x$

with respect to action $S(U, \psi, \overline{\psi}) = S_g(U) - \overline{\psi}\, M(U)\, \psi.$

$$\downarrow$$

Expectation value of $\mathcal{O}' = \mathrm{Tr}_{\text{color,spin}} \left[\left(M^{-1,u}_{x,y} \right) \left(M^{-1,d}_{y,x} \right) \right]$

with respect to action $S_{\text{eff.}}(U) = S_g(U) - \ln\left(\det M(U)\right).$

$$\langle 0 | \,\mathcal{O}\, | 0 \rangle = \frac{\int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\,\mathcal{O}\, e^{-S(U,\psi,\overline{\psi})}}{\int [\mathrm{d}U]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}\psi]\, e^{-S(U,\psi,\overline{\psi})}} = \frac{\int [\mathrm{d}U]\,\mathcal{O}'\, e^{-S_{\text{eff.}}(U)}}{\int [\mathrm{d}U]\, e^{-S_{\text{eff.}}(U)}}$$

Importance sampling

Monte Carlo simulation: calculate $\langle 0|\mathcal{O}|0\rangle$ stochastically.

Naive way: take random gauge configurations U_α according to the uniform distribution and calculate the weighed average:

$$\langle 0|\mathcal{O}|0\rangle = \frac{\sum_\alpha \mathcal{O}_\alpha e^{-S_\alpha}}{\sum_\alpha e^{-S_\alpha}}$$

S_α: value of $S_{\text{eff.}}$ at U_α,
$\mathcal{O}_\alpha$: value of $\mathcal{O}$ at U_α.

S_α large for most configurations $\longrightarrow$ small portion of configurations give significant contribution.

Importance sampling: generate configurations with probability based on their importance $\longrightarrow$ probability of U_α is proportional to e^{-S_α}.

Then $\langle 0|\mathcal{O}|0\rangle = \frac{1}{N}\sum_{\alpha=1}^{N}\mathcal{O}_\alpha$ with relative error $\frac{1}{\sqrt{N}}$.

Importance sampling (2)

Simplest method: Metropolis algorithm.
Choose an initial configuration U_0.

1. Generate U_{k+1} from U_k with a small random change.
2. Measure the change ΔS in the action.
3. If $\Delta S \leq 0$, keep U_{k+1}.
4. If $\Delta S > 0$, keep U_{k+1} with a probability of $e^{-\Delta S}$.

- U_0 is far from the region where e^{-S} is significant.
  $\Longrightarrow$ Many steps required to reach equilibrium distribution: Thermalization time.
- $U_k \longrightarrow U_{k+1}$ by small change.
  $\Longrightarrow$ Subsequent configurations are not independent. Number of steps required to reach next independent configuration: Autocorrelation time.

Setting the scale

All quantities in the calculation are in lattice units
$\longrightarrow$ lattice spacing a has to be determined.

Process of obtaining a:

1. Choose physical quantity A such that
   - experimental value $A_{\text{exp.}}$ is well known,
   - easily measurable on the lattice,
   - not sensitive to discretization errors,
   - $[A] = (\mathrm{GeV})^{\nu}$, $\nu \neq 0$.
2. Measure dimensionless $A'_{\text{latt.}} = A_{\text{latt.}} \cdot a^{\nu}$ on the lattice.
3. Setting $A_{\text{latt.}} = A_{\text{exp.}}$ yields $a = \left(\frac{A'_{\text{latt.}}}{A_{\text{exp.}}}\right)^{1/\nu}$.

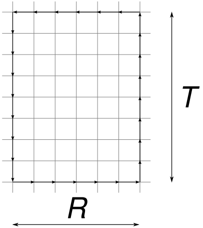
Setting the scale (cont.)

1. $A = \sigma$ string tension

$$\sigma = \lim_{R\to\infty} \frac{\mathrm{d}V(R)}{\mathrm{d}R}$$

Experimental value: $\sqrt{\sigma} = 465\,\mathrm{MeV}$

$$V(R) = -\lim_{T\to\infty} \frac{1}{T} \ln[W(R,T)]\,, \qquad W(R,T) \quad =$$



Static q–$\bar{q}$ potential

Setting the scale (cont.)

2. $A = r_0$ Sommer parameter,

$$R^2 \cdot \left. \frac{\mathrm{d}V(R)}{\mathrm{d}R} \right|_{R=r_0} = 1.65$$

   Experimental value: $r_0 = 0.469(7)\,\mathrm{fm}$

3. $A = F_K$ leptonic decay constant of Kaon
   Experimental value: $f_K = 159.8\,\mathrm{MeV}$

4. A=T can we use the temperature?
   in principle: yes; in practice: not easy at all

Sommer-scale, Omega mass, f_π and f_K

unfortunately, the calculations of r_0 & r_1 are quite involved
far more complicated than fitting the masses of particles

complications are reflected in the literature
MILC: r_1=0.3117(22) fm (better than 1% accuracy)
RBC/UKQCD: r_1=0.3333(93)(1)(2) fm
7% difference and 2.3σ tension between them

another popular way is to use the Omega baryon mass
the experimental value of M_Ω is well known
more CPU demanding & sensititve to the strange quark mass
mismatched strange quark mass leads to a mismatched scale

difficulties with f_π (chiral extrapolation) & f_K (mismatched m_s)

suggestion of M. Luscher: use the Wilson flow to set the scale

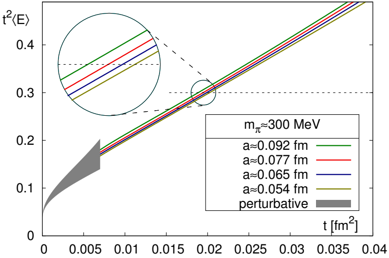
Gauge field flow

flow equation: $\dot{V}_t = Z(V_t)V_t$, where Z is the staple
equivalent to a series of infinitesimal stout smearing steps

M. Luscher, JHEP 1008 (2010) 071

as a representative example $E = G^a_{\mu\nu} G^a_{\mu\nu}/4$ is considered

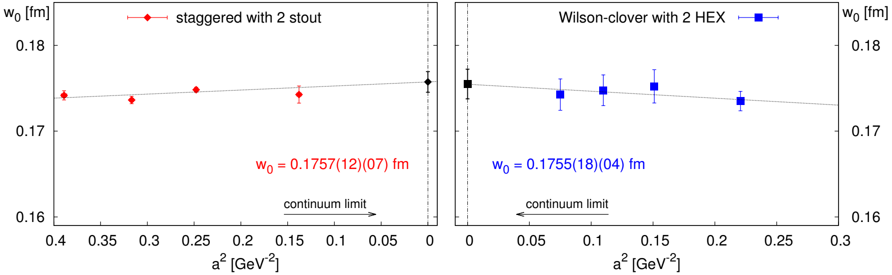
above the cut-off (small t): lattice and continuum quite different



observed "linearity" for $t^2\langle E\rangle$
one can extract it by $t \cdot dt^2\langle E\rangle/dt$
instead $t^2\langle E\rangle$=0.3 (M. Luscher)
$t \cdot dt^2\langle E\rangle/dt$=0.3 ($w_0$ scale)
it should have less scaling violation

the non-universal part (cut-off) shrinks

LCP: Wilson & staggered w_0 S. Borsanyi et al., (BMW-c) JHEP 1209 (2012) 010



the physical scale was obtained by the Omega baryon mass

final result is the Wilson one, staggered (rooting) is a cross check

$$w_0 = 0.1755(18)(04)\ \text{fm}$$

error (dominantly statistical) is 1%
(comes not from the gauge flow itself, but from M_Ω)

User's guide to lattice QCD results

- Full lattice results have three main ingredients

1. (tech.) technically correct: control systematics (users can't prove)
2. (m_q) physical quark masses: $m_s/m_{ud} \approx$28 (and $m_c/m_s \approx$12)
3. (cont.) continuum extrapolated: at least 3 points with $c \cdot a^n$

only few full results (nature, T_c, spectrum, EoS, m_q, curvature, B_K ...)

ad 1: obvious condition, otherwise forget it
ad 2: difficult (CPU demanding) to reach the physical u/d mass
BUT even with non-physical quark masses: meaningful questions
e.g. in a world with M_π=M_ρ/2 what would be M_N/M_π
these results are universal, do not depend on the action/technique
ad 3: non-continuum results contain lattice artefacts
(they are good for methodological studies, they just "inform" you)

FLAG review of lattice results

Colangelo et al. Eur.Phys.J. C71 (2011) 1695

Collaboration	publication status	chiral extrapolation	continuum extrapolation	finite volume	renormalization	running	m_{ud}	m_s
PACS-CS 10	P	★	■	■	★	a	2.78(27)	86.7(2.3)
MILC 10A	C	●	★	★	●	–	3.19(4)(5)(16)	–
HPQCD 10	A	●	★	★	★	–	3.39(6)*	92.2(1.3)
BMW 10AB	P	★	★	★	★	b	3.469(47)(48)	95.5(1.1)(1.5)
RBC/UKQCD	P	●	●	★	★	c	3.59(13)(14)(8)	96.2(1.6)(0.2)(2.1)
Blum et al. 10	P	●	■	●	★	–	3.44(12)(22)	97.6(2.9)(5.5)

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

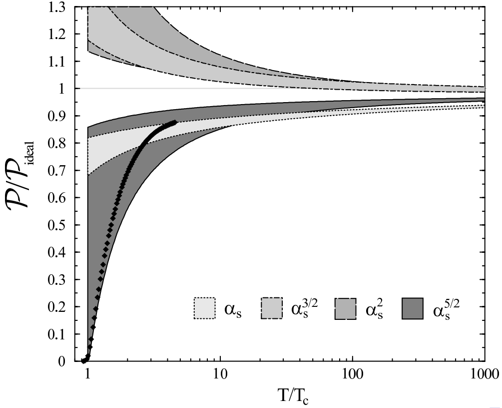
the vast majority (about 95%) comes through another mechanism
$\Longrightarrow$ this mechanism and this 95% will be the main topic of this talk

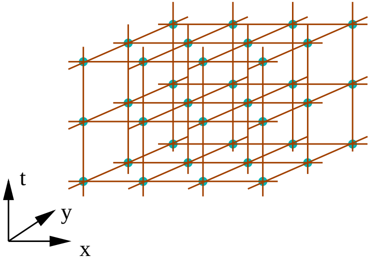
quantum chromodynamics (QCD, strong interaction) on the lattice

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





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
Pflops (10^{15}) is needed

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

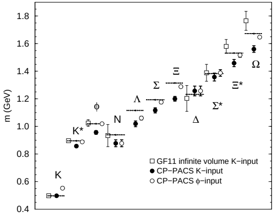
t large $\Rightarrow$ lightest states (created by $\mathcal{O}$) dominate: $C(t) \propto e^{-M\cdot t}$
$\Rightarrow$ exponential fits or mass plateaus M_t=log[C(t)/C(t+1)]

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)

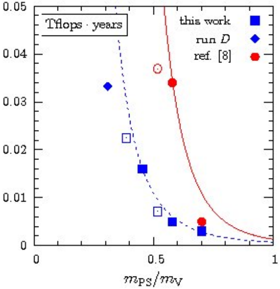


the ≈10% discrepancy was believed to be a quenching effect

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:



Budapest-Marseille-Wuppertal Collaboration

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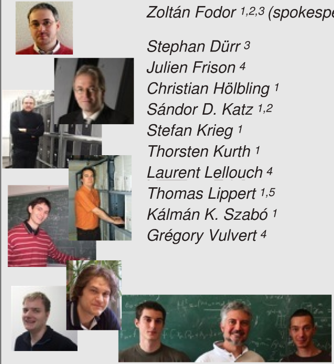
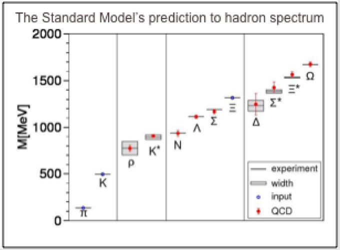


Zoltán Fodor [1,2,3] *(spokesperson)*

Stephan Dürr [3]
Julien Frison [4]
Christian Hölbling [1]
Sándor D. Katz [1,2]
Stefan Krieg [1]
Thorsten Kurth [1]
Laurent Lellouch [4]
Thomas Lippert [1,5]
Kálmán K. Szabó [1]
Grégory Vulvert [4]

Recent results



1 Bergische Universität Wuppertal
2 Eötvös University, Budapest
3 John von Neumann Institute for Computing DESY/FZ-Jülich
4 CNRS, Centre de Physique Theorique UMR 6207
5 FZ-Jülich Supercomputing Centre

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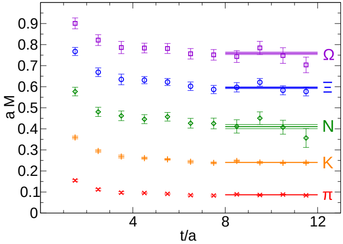
Scale setting and masses in lattice QCD

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'

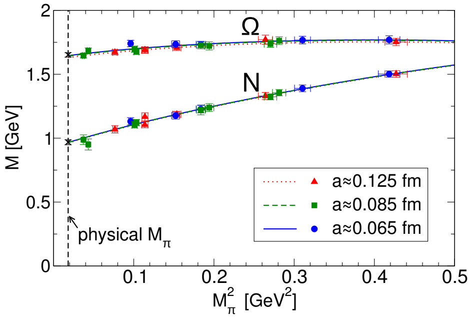
masses are obtained by correlated fits (choice of fitting ranges)
illustration: mass plateaus at the smallest M_π $\approx$190 MeV (noisiest)



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

S. Durr et al., Budapest-Marseille-Wuppertal Collaboration, Science 322 (2008) 1224

altogether 15 points for each hadrons

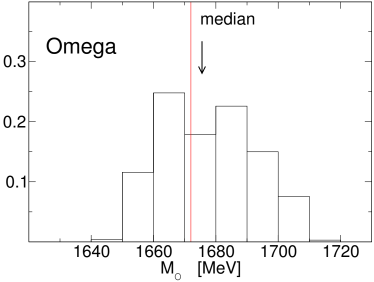


smooth extrapolation to the physical pion mass (or m_{ud})
small discretization effects (three lines barely distinguishable)

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)

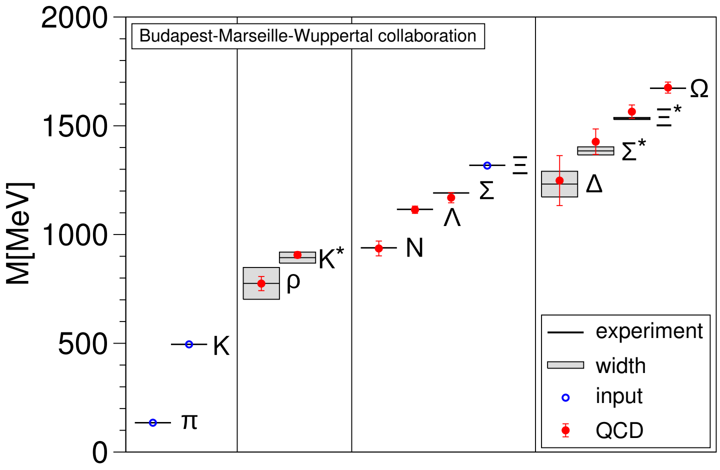
Blind data analysis: avoid any arbitrariness

extended frequentist's method:
2 ways of scale setting, 2 strategies to extrapolate to $M_\pi(phys)$
3 pion mass ranges, 2 different continuum extrapolations
18 time intervals for the fits of two point functions
2·2·3·2·18=432 different results for the mass of each hadron



central value and systematic error is given by the mean and the width
statistical error: distribution of the means for 2000 bootstrap samples

Final result for the hadron spectrum



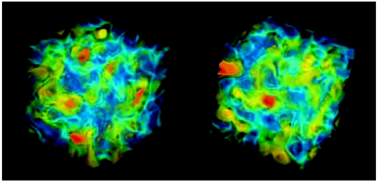
Breakthrough of the Year

Proton's Mass 'Predicted'

STARTING FROM A THEORETICAL DESCRIPTION OF ITS INNARDS, physicists precisely calculated the mass of the proton and other particles 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 quark-antiquark 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.

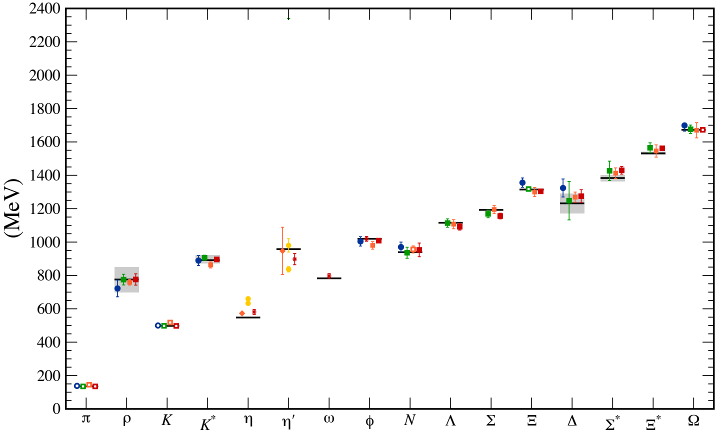
To simplify matters, theorists from France, Germany, and Hungary took an approach known as "lattice quantum chromodynamics."



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.

Light hadron spectrum summary: A. Kronfeld 1209.3468



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

extension steps for a fully realistic theory

1. include dynamical charm:
usually easy since existing codes can include many fermions
since m_c is quite heavy it is computationally cheap
one needs small lattice spacings to have am_c small enough

2. include QED:
difficult, since the action/algorithmic setup must be changed
conceptual difficulties for finite V, since QED is not screened
additional computational costs are almost negligable

3. include $m_u \neq m_d$ (similarly large effect as QED):
usually easy since existing codes can include many fermions
$m_u \approx m_d/2$: more CPU-demanding than 2+1 flavors
since m_u is small larger V needed to stabilize the algorithm:
more CPU but large V (upto 8 fm) is good for other purposes

• immediate consequences/results:

complitely dynamical charm background
unquenching charm is not very significant, but cleaner

determine m_u and m_d separately from first principles
say the final word on $m_u = 0$ or $m_u \neq 0$

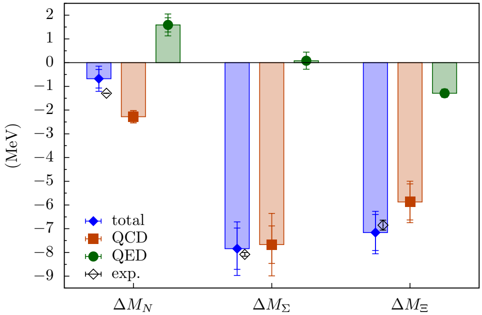
determine the mass difference between neutron and proton:
1 MeV vs. 1000 MeV: the same gap as in nuclear physics

provide configurations for many other relevant questions

sub-MeV accuracy for baryons

S. Borsanyi et al., Phys. Rev. Lett. 111 '13 252001

determine the mass difference between neutron and proton:
1 MeV vs. 1000 MeV: the same gap as in nuclear physics
(finite-V QED corrections are larger than the effect itself)



with new techniques (multigrid) one reaches 5σ accuracy
two-nucleon system with M_π=135 MeV: still not enough (future task)

Summary