Lattice QCD: a numerical tool for precision physics in the Standard Model and beyond

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Interpreting data needs precise background estimation

Double Drell-Yan process

An interesting observation on the impact of lack of precise QCD background knowledge [Krasny, Placzek '15]:



Two conclusions:

- precise knowledge of QCD background crucial in correctly interpreting collider data!
- but there is not enough experimental data to constrain Double Parton Distributions ⇒ Lattice QCD!

Lattice QCD in two slides

Basics

Lattice QCD is based on analytic continuation to imaginary time:

$$it
ightarrow au$$

 $S = \int dx^4 (T - V)
ightarrow i \int dx_E^4 (T + V) \equiv iS_E$
 $e^{iS}
ightarrow e^{-S_E}$
QFT $ightarrow$ statistical system

Baryons

One needs combinations of field operators which have the wanted quantum numbers, e.g. for the nucleon

$$\hat{B}_{\alpha}(t,\vec{p}) = \sum_{\vec{x}} e^{i\vec{p}\vec{x}} \epsilon_{ijk} \hat{u}^{i}_{\alpha}(x) \hat{u}^{j}_{\beta}(x) (C^{-1}\gamma_{5})_{\beta\gamma} \hat{d}^{k}_{\gamma}(x)$$

Lattice QCD in two slides

Hadronic matrix elements

Compute correlation functions

$$\langle N(P) | \bar{\psi}_{q} \gamma^{\{\mu} i D^{\mu_{1}\}} \psi_{q} | N(P') \rangle = \\ = \bar{\psi}_{q} \Big\{ \sum_{i} \alpha_{i}^{\mu,\mu_{1}} A_{2,i}^{q}(Q^{2}) + \sum_{i} \beta_{i}^{\mu,\mu_{1}} B_{2,i}^{q}(Q^{2}) \Big\} \psi_{q}$$

which allow to estimate the Generalized Form Factors $A_{2,i}^q$ and $B_{2,i}^q$. \Rightarrow nucleon's total angular momentum

$$J^{u-d} = \frac{1}{2} \big(A^{u-d}_{2,0}(Q^2 = 0) + B^{u-d}_{2,0}(Q^2 = 0) \big).$$

Hand on actual work to supercomputers

- use Monte Carlo methods to estimate path integrals
- use Markov chains to generate representative configurations with Boltzmann probability distribution
- \Rightarrow rough idea of the cost: 100 M core \times hours \approx 1 core \times 11500 years

Computing resources

Overview of the usage of Europe's largest supercomputers



JUQUEEN is an IBM BlueGene/Q installation in Juelich Supercomputing Center: 458000 cores with peak performance 5.8 PFlops/s. \Rightarrow 11th place on TOP500 @ Nov. 2015, 3rd in Europe Lattice QCD became a precision tool for QCD, since today we have at our disposal:

- better computer architectures
- better algorithms
- better observables
- better control over the systematics

 \Rightarrow LQCD provides precise results for QCD processes with all systematics under control!

6/24

Ingredients of precision

New computer architectures



Intel Xeon Phi processor (codename Knights Landing):

64 cores, 256 hardware threads, shared L2 cache, AVX512 instruction set, 2 vector units/core, 16 GB MCDRAM $\Rightarrow>$ 3 TFlops/s double precision

Ingredients of precision

New algorithms

Invertions of the Dirac operator contribute significantly to the total numerical cost.



Domain Decomposition Adaptive Algebraic Multigrid Solver (DD- α AMG) is the state-of-the-art solver developed and implemented by mathematicians and physicists from Univ. of Wuppertal and Regensburg.

New observables

Observables defined with Wilson flow [Lüscher '13-'15] provide excellent statistical precision. Wilson flow is defined by introducing a fictitious time dimension and along which the gauge fields are evolved according to

$$rac{d}{dt}B_\mu(x,t)=D_
u\, G_{\mu
u}(x,t)=-rac{\delta S_{
m YM}[B]}{\delta B_\mu(x,t)}, \qquad B_\mu(x,0)=A_\mu(x)$$

For example one can define the renormalized coupling constant in a finite volume scheme [ALPHA '16] and compute the Λ parameter in a theory with 3 dynamical quarks with a 2% precision

 $L_0 \Lambda = 0.0303(8)$

The scale L_0 will be linked to dimensionfull quantities in the upcoming simulations.

In order to get the final number:

Translating a hadron matrix element obtained from a numerical simulation to the continuum MS scheme involves the following systematic effects:

List of systematics

- finite volume, nowadays $m_{\pi}L > 4$
- chiral extrapolation, nowadays $m_{u,d} = m_{u,d}^{\text{physical}}$
- $\bullet\,$ continuum extrapolation, nowadays $a\approx 0.045 {\rm fm}-0.05 {\rm fm}$
- renormalization, nowadays fully non-perturbative

 \Rightarrow perturbative estimates of the renormalization constants contribute the most significant part to the final result's uncertainty!

Non-perturbative renormalization of lattice QCD

To define QCD as a QFT beyond perturbation theory it is not enough to write down its classical Lagrangian:

$$\mathcal{L}_{\text{QCD}}(x) = \frac{1}{2g^2} \text{tr} \big\{ F_{\mu\nu}(x) F_{\mu\nu}(x) \big\} + \sum_{i=1}^{N_r} \overline{\psi}_i \big(\not D + m_i \big) \psi_i(x)$$

One needs to define the functional integral:

- Introduce a Euclidean space-time lattice and discretise the continuum action such that the doubling problem is solved
- Consider a finite space-time volume ⇒ the functional integral becomes a finite dimensional ordinary or Grassmann integral
- Take the infinite volume limit L
 ightarrow 1
- Take the continuum limit $a \rightarrow 0$

From asymptotic freedom expect

$$g_0^2 = g_0^2(a) \stackrel{a \to 0}{\sim} \frac{-1}{2b_0 \ln a}$$

Non-perturbative renormalization of lattice QCD

$$\mathcal{L}_{\text{QCD}}(x) = rac{1}{2g^2} ext{tr} \left\{ F_{\mu
u}(x) F_{\mu
u}(x)
ight\} + \sum_{i=1}^{N_f} ar{\psi}_i ig(D \!\!\!/ + m_i ig) \psi_i(x)$$

- The basic parameters of QCD are g_0 and $m_{0,i}$, i = u, d, ...
- To renormalise QCD one must impose a corresponding number of renormalisation conditions
- If we only consider gauge invariant observables \Rightarrow no need to renormalize quark, gluon, ghost field and gauge parameter.
- All physical information (particle masses and energies, particle interactions) is contained in the (Euclidean) correlation functions of gauge invariant composite, local fields \(\phi_i(x)\)

$$\langle \phi_1(x_1) \dots \phi_n(x_n) \rangle$$

 a priori each \u03c6_i requires renormalisation, and thus further renormalisation conditions.

How to renormalize QCD in a hadronic scheme?

Sketch of the procedure, using e.g. hadronic observables F_{π} , m_{π} , m_{K} , m_{D} :

- Choose a value of the bare coupling g₀² = 6/β; this determines the lattice spacing (i.e. mass independent scheme); choose some initial values for the bare quark mass parameters and a spatial lattice volume (L/a)³ that is large enough to contain the hadrons;
- 3 tune the bare quark mass parameters such that m_{π}/F_{π} , m_{K}/F_{π} , m_{D}/F_{π} take their desired values (e.g. experimental)
- **③** the lattice spacing is obtained from $a(\beta) = (aF_{\pi})(\beta)/F_{\pi}|_{exp.}$
- reduce the value of g_0^2 (i.e. increase β) and increase L/a accordingly

13/24

• for g_0^2 (or β) in some interval one obtains:

 $F_{\pi}, m_{\pi}, m_{K}, m_{D} \Rightarrow g_{0}, am_{0,l}(g_{0}), am_{0,s}(g_{0}), \ldots$

- these are bare parameters
- SM for energies ≪ m_W reduces to QCD + QED + tower of effective weak interaction vertices (4-quark operators, 6-quark operators, ...)
- \bullet the structure of this effective "weak hamiltonian" is obtained perturbatively e.g. in the $\overline{\rm MS}$ scheme
- $\bullet\,$ How can we relate the bare lattice parameters to the renormalized ones in, say, the $\overline{\rm MS}$ scheme
- ⇒ introduce an intermediate renormalization scheme which can be evaluated both perturbatively and non-perturbatively

We have a hierarchy of scales

- The renormalization scale μ must reach the perturbative regime: $\mu \gg \Lambda_{\rm QCD}$
- the lattice cutoff must still be larger: $\mu \ll a^{-1}$
- The volume must be large enough to contain pions: $L \gg 1/m_\pi$

$$L/a \gg \mu L \gg m_{\pi}L \gg 1 \Rightarrow L/a \approx \mathcal{O}(10^3)$$

 \Rightarrow widely different scales cannot be resolved simultaneously on a finite lattice! \Rightarrow window problem

Method

Consider the correlation functions of flavor non-singlet bilinear quark operators of the form $\langle \mathcal{O}_{\Gamma}(x)\mathcal{O}_{\Gamma}(0)\rangle$, where:

 $\mathcal{O}_{\Gamma}(x) = \overline{\psi}(x)\Gamma\psi(x), \qquad \Gamma = \{1, \gamma_5, \gamma_{\mu}, \gamma_{\mu}\gamma_5\}.$

Impose the following coordinate space conditions in the chiral limit:

 $\lim_{a\to 0} \langle \mathcal{O}_{\Gamma}^{X}(x) \mathcal{O}_{\Gamma}^{X}(0) \rangle \big|_{x^{2}=x_{0}^{2}} = \langle \mathcal{O}_{\Gamma}(x_{0}) \mathcal{O}_{\Gamma}(0) \rangle_{\mathrm{cont}}^{\mathrm{free},\mathrm{massless}}.$

The renormalized operator is

$$\mathcal{O}_{\Gamma}^{X}(x, x_{0}) = Z_{\Gamma}^{X}(x_{0})\mathcal{O}_{\Gamma}(x),$$

 x_0 is the renormalization point, which must satisfy:

$$a \ll x_0 \ll \Lambda_{\rm QCD}^{-1}$$

to keep the discretization & non-perturbative effects under control.

 $Z_P^{\overline{\text{MS}}}(\mu = 2 \,\text{GeV}) = 0.503(1)(3)(2) = 0.503(6)$



The running of the renormalization constants can be estimated non-perturbatively on the lattice by calculating the step scaling function, i.e. the ratio

$$\Sigma_{\Gamma}(\mu, 2\mu) = \lim_{a o 0} rac{Z_{\Gamma}(2\mu, a)}{Z_{\Gamma}(\mu, a)}$$

Example:

$$\frac{Z_{\Gamma}(\sqrt{X^2} = 0.0196 \text{fm})}{Z_{\Gamma}(\sqrt{X^2} = 0.0392 \text{fm})} = \frac{Z_{\Gamma}(\mu = 10 \text{GeV})}{Z_{\Gamma}(\mu = 5 \text{GeV})}\Big|_{\beta = 7.90}, \ \Big|_{\beta = 8.62}, \ \Big|_{\beta = 9.00}, \ \Big|_{\beta = 9.50}$$

On the lattice this corresponds to the ratios:

$$\frac{Z_{\Gamma}(X = \{1, 1, 1, 1\})}{Z_{\Gamma}(X = \{2, 2, 2, 2\})}\Big|_{\beta=7.90}, \qquad \frac{Z_{\Gamma}(X = \{2, 2, 2, 2\})}{Z_{\Gamma}(X = \{4, 4, 4, 4\})}\Big|_{\beta=8.62}, \\
\frac{Z_{\Gamma}(X = \{3, 3, 3, 3\})}{Z_{\Gamma}(X = \{6, 6, 6, 6\})}\Big|_{\beta=9.00}, \qquad \frac{Z_{\Gamma}(X = \{4, 4, 4, 4\})}{Z_{\Gamma}(X = \{8, 8, 8, 8\})}\Big|_{\beta=9.50}$$

Non-perturbative running of Z_S



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Suppose we have renormalised lattice QCD non-perturbatively, how is the the continuuum limit approached?

Symanzik's effective continuum theory:

- purpose: render the *a*-dependence of lattice correlation functions explicit. ⇒ structural insight into the nature of cutoff effects
- at scales far below the cutoff a^{-1} , the lattice theory is effectively continuum like, the influence of cutoff effects is expanded in powers of *a*:

$$egin{aligned} S_{ ext{eff}} &= S_0 + aS_1 + a^2S_2 + \dots, S_0 = S_{ ext{QCD}}^{ ext{cont}} \ S_k &= \int d^4x \mathcal{L}_k(x) \end{aligned}$$

At small distances one expects that there is neither explicit nor spontaneous chiral symmetry breaking: the dominant effects are the discretization errors \Rightarrow difference between the massless and massive correlation functions are the mass dependent discretization errors.

b_P coefficient

$$\left(\bar{\psi}(x)\gamma_5\psi(x)
ight)^{\mathrm{R,\ impr}} = Z_P \left(1 + b_P m\right) \bar{\psi}(x)\gamma_5\psi(x)$$



[P.K., G. Bali, in prep]

Nucleons mass splittings [BMW collab. '16]



 \Rightarrow simulations of QCD + QED!



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Lattice QCD is a precision tool!

- Lattice QCD allows to compute hadronic matrix elements with all systematic errors under control
- With more computer resources and improved algorithms more challenging problems can be now addressed

Stay tuned! Even more interesting results will come! \Rightarrow LATTICE'16 @ Southampton

Thank you for your attention!