Lattice gauge theory: introduction & particle physics phenomenology

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see also RPP review "Lattice QCD" Chin.Phys. C40 (2016) no.10, 100001 and ref.s therein

thanks to N. Tantalo for stimulating discussions and valuable input

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Research field focused on:

- basic laws of Nature in the energy domain $0.1 \, \text{GeV} \leq E \leq 10 \, \text{TeV}$
- strong interactions & non-perturbative Quantum Field Theory

Quantum Field Theory (QFT) $\Leftrightarrow$ Quantum Mechanics + Special Relativity

Non-Perturbative $\Leftrightarrow$ QCD or new forces in Standard Model extensions, which are strong at a scale within $0.1 \, \text{GeV} \leq E \leq 10 \, \text{TeV} \Leftrightarrow 10^{-15} \, \text{m} \geq \ell \geq 10^{-20} \, \text{m}$

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Local collaborators.: G.C. Rossi (honorary prof.), P. Dimopoulos (Centro Fermi)
Domain $0.1 \text{ GeV} \leq E \leq 1 \text{ TeV} \iff \text{Standard Model (SM) of elementary particles: renormalizable QFT based on gauge symmetries } SU(3)_{\text{color}} \times SU(2)_W \times U(1)_Y$

\[
\mathcal{L} = -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{8}tr(W_{\mu\nu}W^{\mu\nu}) - \frac{1}{2}tr(G_{\mu\nu}G^{\mu\nu}) + (\bar{\nu}_L, \bar{e}_L) \tilde{\sigma}^\mu iD_\mu \left( \begin{array}{c} \nu_L \\ e_L \end{array} \right) + \bar{\nu}_R \tilde{\sigma}^\mu iD_\mu e_R + \bar{\nu}_R \tilde{\sigma}^\mu iD_\mu \nu_R + \text{h.c.} \\
-\frac{\sqrt{2}}{v} \left[ (\bar{\nu}_L, \bar{e}_L) \phi M^e e_R + \bar{e}_R \tilde{M}^e \phi \left( \begin{array}{c} \nu_L \\ e_L \end{array} \right) \right] \\
-\frac{\sqrt{2}}{v} \left[ (-\bar{\nu}_L, -\bar{e}_L) \phi^* M^e \nu_R + \bar{\nu}_R \tilde{M}^e \phi^T \left( \begin{array}{c} -e_L \\ -\nu_L \end{array} \right) \right] \\
+ (\bar{u}_L, \bar{d}_L) \tilde{\sigma}^\mu iD_\mu \left( \begin{array}{c} u_L \\ d_L \end{array} \right) + \bar{u}_R \tilde{\sigma}^\mu iD_\mu u_R + \bar{d}_R \tilde{\sigma}^\mu iD_\mu d_R + \text{h.c.} \\
-\frac{\sqrt{2}}{v} \left[ (\bar{u}_L, \bar{d}_L) \phi M^d d_R + \bar{d}_R \tilde{M}^d \phi \left( \begin{array}{c} u_L \\ d_L \end{array} \right) \right] \\
-\frac{\sqrt{2}}{v} \left[ (-\bar{d}_L, -\bar{u}_L) \phi^* M^u u_R + \bar{u}_R \tilde{M}^u \phi^T \left( \begin{array}{c} -d_L \\ -u_L \end{array} \right) \right] \\
+(D_\mu \phi) D^\mu \phi - m_h^2 [\phi \phi - v^2/2]^2/2v^2.
\]

\[SU(2)_W \times U(1)_Y \text{ spontaneously broken to } U(1)_{\text{em}} : \text{fermion and } W/Z \text{ masses } \propto \langle \phi \rangle\]
1. The Standard Model (SM) of elementary particles:

encodes observed gauge symmetries at $E \ll 1$ TeV, is mathematically well defined and highly successful in predicting states and processes of both electroweak (EW) and strong nuclear interaction physics.

Higgs resonance observed at the LHC: $J^{CP} = O^{++}$, $m_h = 125.1 \pm 0.3$ GeV

$h$-couplings still under study → is $h$ elementary (as in SM) or composite?
2. Extension of the SM anyway necessary to account for observed

- neutrino masses and mixings
- dark matter
- baryogenesis (larger CP violation needed)
- dark energy & quantum aspects of gravity

3. SM “paradox”: incomplete but renormalizable (i.e. math.ly sound & highly predictive)

A New Physics completion at some (what?) high energy scale seems required by experimental facts (2) in spite of the nice theoretical self-consistency of the SM (1)

The latter (1) makes hard to guess the former (2) ⇒ different beyond-SM scenarios:

- SM valid up to energies $E \leq 10^{16} \div 10^{19}$ GeV? (big desert)
- SUSY or Non-Perturbative Dynamics at $E \sim$ few TeV?

Low energy ($E < 1$ TeV) description: local QFT not much different from SM
Some SM puzzles & the quest for new physics

- $m_W, Z \sim m_h \sim v \sim 10^{-13} \Lambda_{GUT} \sim 10^{-16} \Lambda_{Planck}$
  
  no extra symmetry when $m_h \sim v$ gets small $\Rightarrow$ un–naturalness

- $m_t \sim 10^5 m_u, \ m_\tau \sim 10^4 m_e, \ m_e > 10^7 m_{\nu_i}$
  
  (even for particles with equal quantum numbers) ... a huge hierarchy

- weak interaction induced flavour mixing – e.g. for quarks encoded in CKM matrix

  $$V_{CKM} = \begin{pmatrix}
  1 - \frac{\lambda^2}{2} & \frac{\lambda}{2} & A\lambda^3 (\rho - i\eta) \\
  -\lambda & 1 - \frac{\lambda^2}{2} & A\lambda^2 \\
  A\lambda^3 (1 - \rho - i\eta) & -A\lambda^2 & 1
  \end{pmatrix} + \mathcal{O}(\lambda^4)$$

  $\lambda = 0.22537 \pm 0.00061, \ A = 0.814^{+0.023}_{-0.024}, \ \bar{\rho} = 0.117 \pm 0.021, \ \bar{\eta} = 0.353 \pm 0.013$

- neutrinos: tiny masses ($< 1 \text{ eV}$) and strong flavour mixing (any CP viol. phase?)

Quest for New Physics (NP) proceeds through direct and indirect searches:

$\Rightarrow$ new particles created via high-E processes in accelerators (few TeV at LHC)

$\Rightarrow$ deviation from SM predictions in processes sensitive to NP via quantum effects:

- EW precision observables, high precision (quark & lepton) flavour physics
Strong interactions & the quest for new physics

★ Accurate (quark & lepton) **flavour physics** requires robust control of **QCD bound states and strong interactions** (from the SM). A few examples:

i) semileptonic hadron decays

![Diagram of semileptonic hadron decay](image)

ii) dark matter particle off nucleon scattering (via exchange of SM bosons)

![Diagram of dark matter scattering](image)
Strong interactions & the quest for new physics

iii) hadron state contributions to muon anomalous magnetic moment $g_\mu - 2$

If strongly interacting states with a few TeV mass are discovered (e.g. at LHC) non-perturbative QFT and lattice computational methods will play a crucial role.

new strong interactions with scale $\sim$ few TeV $\Rightarrow$ resonance $S$ & new mass spectrum
SM in the \((g_Y, g_W) \rightarrow (0, 0)\) limit: QCD

In this limit (recall \(e = g_Y \cos \theta_W\)) and setting \(\phi^t \equiv (0, \nu)\) the \(\mathcal{L}_{SM}\) simplifies to

\[
\mathcal{L}|_{(g_Y, g_W) = (0, 0)} = -\frac{1}{2} \text{tr}\{G_{\mu\nu} G_{\mu\nu}\} + \sum_{f=u,d,s,c,b,...} \bar{q}_f [i\gamma_\mu (\partial_\mu + ig_S A_\mu) - m_f] q_f + \\
+ \sum_{f=e,\nu_e,\mu,\nu_\mu,\tau,\nu_\tau} \bar{\ell}_f [i\gamma_\mu \partial_\mu - m_f] \ell_f
\]

Apart from free lepton terms (2nd line) we get the QCD Lagrangian with

\[
G_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig_S [A_\mu, A_\nu], \quad A_\mu \equiv A_\mu^c t^c, \quad c = 1, ..., 8 = 3^2 - 1
\]

Physicewise: neglecting \(h, t, W/Z\) d.o.f.’s makes sense (\(\Leftrightarrow\) “effective theory”)

★ for processes involving states with external momenta \(|p_\mu| \ll M_W < m_h < m_t\)

★ as starting point to include electroweak effects as \(O(\alpha_{em}, \alpha_W)\) perturbations

while treating almost exactly light “coloured” d.o.f.’s because

★ gluon self-interaction makes QCD interaction strong at scale \(\Lambda_{QCD} \sim 250\) MeV

★ strong QCD forces confine quark & gluons into hadrons \(\Leftrightarrow\) physical states
QCD vs QED: non-perturbative mass scale \( \Lambda_{QCD} \)

QED

- Hydrogen Atom
  - Proton (Strong force)
  - Electron
  - \( M_e = 0.5 \text{ MeV} \)
  - \( M_p = 938 \text{ MeV} \)
  - \( E_{binding} = 13.6 \text{ eV} \)
  - (EM force)

QCD

- Proton
  - Quarks (u, d)
  - \( M_u \sim 3 \text{ MeV} \)
  - \( M_d \sim 6 \text{ MeV} \)
  - \( M_p = 938 \text{ MeV} \)
  - (Strong force)
Non-perturbative QCD and confinement/complexity

Quantum effects $\Rightarrow$ scale-dependent renormalized param.s $\alpha_s \equiv \frac{g_s^2}{4\pi}$ & $m_f$'s

(see e.g. PT analysis of $A_\mu$- & $q_f$-propagators in fixed gauge)

$\star$ at scale $\mu$ renormalized coupling $\alpha_s(\mu) \mu \gg \Lambda_{QCD} \approx \frac{2\pi}{b_0 \log(\mu/\Lambda_{QCD})}, \quad b_0 = 11 - 2\frac{n_f}{3}$

$\star$ $\Lambda_{QCD} \mu \to \infty \mu \exp[-\frac{2\pi}{b_0 \alpha_s(\mu^2)}]$ dynamically generated mass scale $\sim 250$ MeV

weak interaction at $\mu \gg \Lambda_{QCD}$ (DIS and collider exp.'s): perturbative regime

strong interaction at $\mu \lesssim \Lambda_{QCD}$ (hadronic scales): non-perturbative (n.p.) QCD

• strong force at the fm-scale leads to quark&gluon confinement in hadrons!

• emergence of $\Lambda_{QCD}$: intrinsic scale invariance breaking (even as $m_\pi^2 \sim m_{u/d} \to 0$)
### Hadron Spectrum from QCD Lagrangian (ab initio)

**Hadron masses:**

\[
m_H = c_H \Lambda_{QCD} \approx c_H \mu_{\text{ren}} \exp \left[-\frac{2\pi}{b_0 \alpha_s(\mu_{\text{ren}})}\right]
\]

Singularity at \(\alpha_s = 0\) \(\Rightarrow\) PT in \(\alpha_s\) not useful, ... non-perturbative methods needed

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<th>Strangeness</th>
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<th>(N^+)</th>
<th>(\Sigma)</th>
<th>(\Sigma^+)</th>
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**Baryon Spectrum from lattice QCD:**

- \(n_f = 2\) (ETMC) & \(n_f = 2 + 1\) (BMW) sea quarks
Euclidean QCD: building hadronic states

Minkowsky $g_{\mu\nu} = \text{diag}(1,1,1,-1) \Rightarrow$ Euclidean $\delta_{\mu\nu} = \text{diag}(1,1,1,1)$

spacetime metrics. In Euclidean case: $x_4 = -ix_0$, $\gamma^\dagger_\mu = \gamma_\mu$ so that

$$\mathcal{L}_{QCD}^E = \frac{1}{2} \text{tr}\{G_{\mu\nu}G_{\mu\nu}\} + \sum_{f=u,d,s,c,b,...} \bar{q}_f[\gamma_\mu(\partial_\mu + ig_SA_\mu) + m_f]q_f$$

Physical info from $\mathcal{L}_{QCD}^E$: via analytic continuation ($p_4 = ip_0$) for correlation functions & derived observables known with “no errors”; only energies and directly accessible operator matrix elements otherwise

- in QCD (or any confining QFT) the elementary d.o.f. do not correspond to the physical states
- in order to compute an hadronic matrix element of the local operator $J$, say $|\langle 0 | J | h \rangle |$, one needs to “build” the hadronic state $| h \rangle$
- this can be done via a mapping: time-localized interpolating operators $\leftrightarrow$ physical states
- the local operator $J$ is made out of elementary fields, e.g. $J = \bar{u}\gamma_5 d$, and its matrix elements can be extracted from suitable correlators
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$$C(x) = T \langle 0 | J(x) J^\dagger (0) | 0 \rangle =$$

$$= \langle 0 | J(0) e^{-Ht - i \vec{P} \cdot \vec{x}} \sum_n \frac{|E_n\rangle \langle E_n|}{2E_n} J^\dagger (0) | 0 \rangle =$$

$$= \frac{|\langle 0 | J(0) | h \rangle|^2}{2M_h} e^{-M_h t} + O \left( e^{-\Delta E_h t} \right)$$

formulae assume that $t > 0$, the spectrum is discrete with $E_{n+1} > E_n$ and the hadron $| h \rangle$ at zero spatial momentum is the lightest state with the same quantum numbers as $J^\dagger | 0 \rangle$, s. t. $\langle 0 | J | h \rangle \neq 0$

ideally, with infinite precision, one can extract the physical information for all the relevant states

in practice, with non-zero errors and a discrete spectrum (as in a finite volume, see below), only the first lowest-lying states can be resolved
Euclidean QCD: computing correlators

- In the previous slide, we have seen an example of a non-perturbative reduction formula.

- Physics is extracted from Euclidean correlators (l.h.s) analyzed in the Hamiltonian formalism.

- In order to compute correlators, one employs the equivalent path-integral Lagrangian formalism (r.h.s) introduced by Feynman, v.i.z.

\[
T \langle 0 | J(x) J^\dagger(0) | 0 \rangle \equiv \frac{\int DA_\mu \, D\bar{q}_f \, Dq_f \, e^{-\int d^4z \, L_{\text{QCD}}^E[A_\mu, \bar{q}_f, q_f]} \, J[A_\mu, \bar{q}_f, q_f](x) \, J^\dagger[A_\mu, \bar{q}_f, q_f](0)}{\int DA_\mu \, D\bar{q}_f \, Dq_f \, e^{-\int d^4z \, L_{\text{QCD}}^E[A_\mu, \bar{q}_f, q_f]}}
\]

- Mathematically, the functional integral is defined as the (well understood) continuum and infinite-volume limits of an ordinary integral over a (huge but finite) number of variables (for QCD: $[2^3 + \frac{3}{4} N_f^2 N_f]$).

- The UV and IR finite theory “lives” on a four-dimensional lattice: $N_s^3 N_t$ points on a grid with linear spacing $a$.

- The lattice path-integral is equivalent to the canonical partition function of a statistical system, hence it can be computed numerically via “importance sampling” and Monte Carlo methods (see below).
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$$T \langle 0 | J(x) J^\dagger(0) | 0 \rangle \equiv \frac{\int \mathcal{D}A_\mu \mathcal{D}\bar{q}_f \mathcal{D}q_f \, e^{-\int d^4z \, \mathcal{L}^{QCD}_E[A_\mu, \bar{q}_f, q_f]} J[A_\mu, \bar{q}_f, q_f](x) J^\dagger[A_\mu, \bar{q}_f, q_f](0)}{\int \mathcal{D}A_\mu \mathcal{D}\bar{q}_f \mathcal{D}q_f \, e^{-\int d^4z \, \mathcal{L}^{QCD}_E[A_\mu, \bar{q}_f, q_f]}}$$

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The lattice path-integral is equivalent to the canonical partition function of a statistical system, hence it can be computed numerically via “importance sampling” and Monte Carlo methods (see below).
The lattice approach to QCD – I

- Lattice grid: $N_s^3 N_T = \frac{l^3 T}{a^4}$ sites, spacing $a$ & suitable field boundary conditions

- Compute Euclidean QCD expectation values of $O = O[q_f, \bar{q}_f, A](x, y, ...)$

- Lattice action in terms of quark fields on sites and gauge fields $U_{\ell(n,n+\hat{\mu})}$ on links

$$\langle O \rangle = Z^{-1} \int \mathcal{D}[q, \bar{q}, A] e^{-S_E} O \ , \ Z = \int \mathcal{D}[q, \bar{q}, A] e^{-S_E} \ , \ S_E = S_E[q, \bar{q}, A]$$

$$S^L_E = a^4 \sum_n \left\{ \frac{1}{2} \text{tr}[G(U)G(U)]|_n + \sum_f [\bar{q}_f(D(U) + m_f)q_f]|_n \right\} , \quad n_\mu = (\vec{n}, n_4)$$

$$\frac{1}{2} \text{tr}[G(U)G(U)]|_n = \frac{g_0^2}{2} \sum_{\mu<\nu} \text{Re} \text{tr}[1 - U_{n,\mu\nu}] \ , \quad U_{n,\mu\nu} = \prod_{\ell \in P(n,\mu\nu)} U_{\ell(n,n+\hat{\mu})}$$

$$[\bar{q}_f D(U) q_f]|_n = \bar{q}_f|_n \left[ \gamma \cdot \nabla^S(U) + e^{-i\omega_f \gamma_5 / 2} a(-\frac{1}{2} \nabla^B(U) \nabla^F(U) + M_{cr}) \right] q_f|_n$$

$$U_{\ell(n,n+\hat{\mu})} = e^{ig_0 a A_{\mu}(n+\hat{\mu}/2)} \quad \text{so that} \quad S^L_E[q, \bar{q}, U] \xrightarrow{a \to 0} S^{QCD}_E[q, \bar{q}, A] \quad \text{for smooth fields}$$

- physical observables finite as $a \to 0$ once $N_f + 1$ renormalization conditions are imposed

- gauge-invariant formulation (Wilson '74): $a(-\frac{1}{2} \nabla^B \nabla^F + M_{cr})$ avoids fermion doubling; upon clever choice of $\omega_f$ angles: only $O(a^2)$ artifacts in physical quantities (RF - G.Rossi '04)
Quarks and gluons on a lattice ...
The lattice approach to QCD – II

Path integral $\langle O(n, j) \rangle$ with $O(n, j) = (\bar{q}_1 \Gamma q_2)(n)(\bar{q}_2 \Gamma q_1)(j)$ localized at sites $j_\mu, n_\mu$

Fermion d.o.f. ↔ Grassman variables obeying $dq_i q_j = d\bar{q}_i \bar{q}_j = \delta_{ij}$

→ sum over fermionic paths involves $O(N^N)$ terms, $N = 12N_f N_S^3 N_T$.

Way out: $\langle O \rangle = Z^{-1} \int dU e^{-\{G,G\}(U)/2} \prod_f \det[D(U) + m_f] \cdot \text{tr}_{col, spin}([D(U) + m_2]^{-1}_{nj} \Gamma[D(U) + m_1]^{-1}_{jn} \Gamma)$ (Wick theorem on given U)

Valence fermions: quark propagators

Sea fermions: virtual quark effects in $\prod_f \det[D(U) + m_f]$ (non-local)

Importance sampling: $U$-configurations are generated by HMC-like algo’s with probability distribution $\propto e^{-\{G,G\}(U)/2} \prod_f \det[D(U) + m_f]$

Importance sampling for $E_p(O) = \int dx w(x) O(x) = \int dx \frac{dp(x)}{dx} O(x) = \int dp(x) O(x)$

generate sample $\{x_j, j = 1, 2, ..., M\}$ with probability $w(x)$ ($\int dx w(x) = 1$) ⇒

$E_p(O) = \frac{1}{M} \sum_j O(x_j) + \sigma_M(O)$ from sample average with statistical error $\sigma_M(O) = \frac{\sigma_1(O)}{\sqrt{M}}$
Valence and sea quarks in LQCD computations

Valence quark propagators: solve \[ [D(U) + m_f]_{ji} G^f_{ik} = \eta_{jk} \] by CG-like inverters
Get \( G^f_{ik} = \langle q_i \bar{q}_k \rangle \): in practice just one vector \( i \) for fixed \( \bar{k} = \{ \bar{n}, \bar{\alpha}, \bar{c} \} \) in source

CPU cost per HMC traj. vs. \( m_\pi \) [MeV]

Dirac matrix code on BlueGene/P

MultiGrid (DD\( \alpha \)AMG) vs CG linear solvers

\( U \)-ensembles: few \( 10^3 \) MDU's @ \( m_\pi \sim 140 \) MeV, \( m_\pi L \geq 4 \) need \( O(10) \) Tflops·year
Huge configuration space: numerical path integral only feasible by sampling $U$'s with probability distribution $w[U] = e^{-S_{\text{eff}}[U]} \propto e^{-\{G,G\}(U)/2} \prod_f \det[D(U) + m_f] > 0$

Task realized via a Markov chain: using a random number generator set up a stochastic update process $U_0 \to U_1 \to U_2 \to \ldots \to U_n \to \ldots$

characterized by a conditional transition probability $T(U' \mid U) = \text{prob}(U_n = U' \mid U_{n-1} = U)$, s.t. $0 \leq T(U' \mid U)$, $\sum_{U'} T(U' \mid U) = 1$

satisfying after $n \gg 1$ updates (equilibrium wrt $w[U]$) the balance condition $\sum_U T(U' \mid U)w[U] = \sum_U T(U \mid U')w[U'] \equiv w[U'] \quad (\star)$
or the stronger detailed balance condition: $T(U' \mid U)w[U] = T(U \mid U')w[U']$

($\star$) implies that $w[U]$ is the unique fixed point of $T(U' \mid U)$ \Rightarrow starting from an initial distribution $w^{(0)}[U] = \delta(U - U_0)$ the process eventually converges to the desired $w = \lim_{n \to \infty} T^n w^{(0)}$ ... In practice $U_j$ thermalized for $j > N_{\text{equil.}} = O(10^{2})$
Hybrid Monte Carlo (HMC) based Markov chains

In LQCD we estimate \( \langle O \rangle = \langle \tilde{O}_{\text{Wick}} \rangle \) via

\[
N^{-1} \sum_{j=N_{\text{equil}}+1}^{N_{\text{equil}}+N} \tilde{O}_{\text{Wick}}[U_j],
\]

with \( U \)'s produced through a Markov chain – typically based on a HMC-like algo.

HMC basics: illustrated here in terms of \( A \leftrightarrow U = e^{iA} \) s.t. \( w[A] = e^{-S_{\text{eff}}[A]} \)

- \( T(A'|A) = \int dP dP' T_{\text{Acc}}(P', A'|P, A) T_{\text{MD}}(P', A'|P, A) e^{-\{P,P\}/2} \)
  
  with auxiliary \( P \) extracted randomly with prob. \( \propto e^{-\{P,P\}/2} \)

- MD trajectory with \( H_{\text{MD}} = \frac{1}{2}\{P, P\} + S_{\text{eff}}[A] \) in fictitious MD-time implies
  
  \( T_{\text{MD}}(P', A'|P, A) = \delta[(P', A') - K_{\text{MD}}(P, A; \tau, \epsilon)] \)

  as dictated by Newton eq.s discretized (\( \tau/\epsilon \) time steps) so as to preserve i) integration measure \( dP dA \)
  
  and ii) trajectory reversibility \[ T_{\text{MD}}(P', A'|P, A) = T_{\text{MD}}(-P, A| -P', A') \]

- end-trajectory trial \( (P', A') \) accepted or rejected in favour of initial \( (P, A) \) with

\[
T_{\text{Acc}}(P', A'|P, A) = \min \left( 1, \frac{\exp(-H_{\text{MD}}(P', A'))}{\exp(-H_{\text{MD}}(P, A))} \right)
\]

Owing to i) and ii), detailed balance \( T(A'|A) w[A] = T(A|A') w[A'] \) holds.
we argued that in order to “compute correlators ↔ solve QFT” one can conveniently use the path-integral formalism

to non-perturbative level this has to be done by starting from the mathematical definition of the path-integral, the lattice regulated theory, and using numerical techniques: importance sampling, Markov chains, linear solvers

to perturbative level the path-integral is analytically computable by expanding the full around the Gaussian free theory

\[
T \langle 0 | \phi(x) \phi(0) | 0 \rangle = \frac{\int \mathcal{D} \phi \ e^{-\int d^4 z \left\{ \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + \frac{\lambda}{4!} \phi^4 \right\}(z)} \phi(x) \phi(0)}{\int \mathcal{D} \phi \ e^{-\int d^4 z \left\{ \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + \frac{\lambda}{4!} \phi^4 \right\}(z)}} \\
= \frac{\int \mathcal{D} \phi \ e^{-\int d^4 z \left( \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + \frac{\lambda}{4!} \int d^4 z \phi^4(z) + \cdots \right)} \phi(x) \phi(0)}{\int \mathcal{D} \phi \ e^{-\frac{1}{2} \int d^4 z \left( \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi \right) + \cdots}} \\
= \frac{\int \mathcal{D} \phi \ e^{-\int d^4 z \left( \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + j \phi \right)}(z)}{\int \mathcal{D} \phi \ e^{-\frac{1}{2} \int d^4 z \phi \left( -\partial^2 + m^2 \right) \phi(z)}} = e^{\frac{1}{2} \int d^4 z \left\{ j(z) \frac{1}{-\partial^2 + m^2} j(z) \right\}}
\]

and Gaussian integrals can easily be evaluated
Quantization via path integral & the perturbative limit

we argued that in order to “compute correlators ↔ solve QFT” one can conveniently use the path-integral formalism.

to non-perturbative level this has to be done by starting from the mathematical definition of the path-integral, the lattice regulated theory, and using numerical techniques: importance sampling, Markov chains, linear solvers.

to perturbative level the path-integral is analytically computable by expanding the full around the Gaussian free theory.

\[
T \langle 0 | \phi(x) \phi(0) | 0 \rangle = \frac{\int \mathcal{D} \phi \ e^{-\frac{1}{2} \int d^4 z \left\{ \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + \frac{\lambda}{4!} \phi^4 \right\}(z)} \phi(x) \phi(0)}{\int \mathcal{D} \phi \ e^{-\frac{1}{2} \int d^4 z \left\{ \frac{1}{2} \phi \left( -\partial^2 + m^2 \right) \phi + \frac{\lambda}{4!} \phi^4 \right\}(z)}}
\]

the perturbative expansion is usually represented in terms of Feynman’s diagrams

\[
\begin{align*}
\text{---} & \quad = \quad \text{---} & \quad - \frac{\lambda}{2} & \quad \text{---} & \quad + \cdots
\end{align*}
\]

analogously one can perturbatively calculate \( T \langle 0 | \phi(x) \phi^2(y) \phi(0) | 0 \rangle \), etc.
MC histories, data analysis, lowest state(s) signal

LQCD with $u$, $d$, $s$, $c$ sea quarks at physical $\pi$-mass & $N_s = N_t/2 = 64$, $a \sim 0.08$ fm

C.F.'s

\[ -\sum \langle P^{ud}(x)P^{du}(0) \rangle = \frac{G^2}{2M_\pi} \cosh(M_\pi(x_0 - T/2)) \] , with $G_\pi = |\langle 0|\bar{q}u\gamma_5q_d|\pi^+\rangle|$

and

\[ \sum \langle A^{ud}_0(x)P^{du}(0) \rangle = \frac{M_\pi f_\pi G_\pi}{2M_\pi} \sinh(M_\pi(x_0 - T/2)) \] , with $f_\pi M_\pi = |\langle 0|\bar{q}u\gamma_0\gamma_5q_d|\pi^+\rangle|$

Above: $aM_\pi^{\text{plat}}$ (left) and $(M_\pi/f_\pi)^{\text{plat}}$ (right) vs. HMC fictitious time $\tau_{MD}$

Below: $aM_\pi^{\text{aver}}$ and $aM_{\text{nucl}}^{\text{aver}}$ vs. $x_0/a$

ETMC ’17 preliminary: using 1000 HMC traj. for $aM_\pi^{\text{aver}}$ and 64 traj. $\times$ 8 sources for $aM_{\text{nucl}}^{\text{aver}}$
SM hadron physics to LO in EW interactions

SM description of electroweak (EW) corrections to hadronic processes at LO

• \( \pi^+ \rightarrow \mu^+ \nu \Rightarrow \langle \Phi_\pi(x_0) \Phi_{\mu+\nu}(y_0) \rangle = \langle \Phi_\pi(x_0)[i \int_z L_{int}^{EW}(z)]^2 \Phi_{\mu+\nu}(y_0) \rangle^{(QCD+LOEW)} + ... \)

\[ D^0 \rightarrow K^- \mu^+ \nu \Rightarrow \]

\( \Rightarrow \langle \Phi_D(x_0) \Phi_K(y_0) \Phi_{\mu+\nu}(y_0) \rangle = \langle \Phi_\pi(x_0)[i \int_z L_{int}^{EW}(z)]^2 \Phi_K(y_0) \Phi_{\mu+\nu}(y_0) \rangle^{(QCD+LOEW)} + ... \)

where the inserted EW interaction Lagrangian reads

\[ L_{int}^{EW} = -\frac{1}{\sqrt{8}} g_w \left( W^+ \mu J_{\mu_{ch}} + W^- \mu J_{\mu_{ch}}^\dagger \right) - e A_\mu J_{\mu_{em}} + L_{Z \text{ exc}} , \]

\[ J_{\mu_{ch}} = (\bar{u}, \bar{c}, \bar{t}) V_{CKM} \gamma^\mu (1 + \gamma^5) \left( \begin{array}{c} d \\ s \\ b \end{array} \right) + (\bar{\nu}_e, \bar{\nu}_\mu, \bar{\nu}_\tau) \gamma^\mu (1 + \gamma^5) \left( \begin{array}{c} e \\ \mu \\ \tau \end{array} \right) \]

\[ \uparrow \ \text{fermion mass eigenstates} \quad \rightarrow (\bar{\nu}_1, \bar{\nu}_2, \bar{\nu}_3) V_{lep} \gamma^\mu (1 + \gamma^5) \left( \begin{array}{c} \ell_1 \\ \ell_2 \\ \ell_3 \end{array} \right) \]

[ For leptonic & semileptonic decays: LO EW correction ⇔ tree level ... ]
SM hadron physics to LO in EW interactions

- $K^0(B^0) \leftrightarrow \bar{K}^0(\bar{B}^0)$ oscillation (LO EW correction $\leftrightarrow$ 1 loop) $\Rightarrow$

\[
\langle \Phi_{K(B)}(x_0) \Phi_{K(B)}(y_0) \rangle = \langle \Phi_{K(B)}(x_0) [i \int_z L^\text{EW}_{\text{int}}(z) i \int_{z'} L^\text{EW}_{\text{int}}(z')]^2 \Phi_{K(B)}(y_0) \rangle^{(\text{QCD}+\text{LOEW})} + \ldots
\]

\[
= \langle \Phi_{K(B)}(x_0) \int_z \mathcal{H}_{\text{eff}}^{\Delta F=2}(z) \Phi_{K(B)}(y_0) \rangle^{(\text{QCD}+\text{LOEW})} + \ldots
\]

\[
J_{em}^\mu = \sum_f Q^{(f)}_{em} \bar{f} \gamma^\mu f = -\bar{e} \gamma^\mu e + \frac{2}{3} \bar{u} \gamma^\mu u - \frac{1}{3} \bar{d} \gamma^\mu d + \ldots \text{(further 2 generations)}
\]

\[
\mathcal{L}_{Z \text{ exc}} = \frac{-1}{2 \cos^2 \theta_w} g_w Z^\mu \sum_f \left[ \bar{q}_f (g^{(f)}_V \gamma^\mu + g^{(f)}_A \gamma^\mu \gamma_5) q_f + \bar{\ell}_f (g^{(f)}_V \gamma^\mu + g^{(f)}_A \gamma^\mu \gamma_5) \ell_f \right]
\]

\[
g^{(f)}_A = T^{(f)}_3, \quad g^{(f)}_V = T^{(f)}_3 - 2 \sin^2 \theta_w Q^{(f)}_{em} \quad \text{(accidentally small for e, } \mu, \tau)
\]

\[
\mathcal{H}_{\text{eff}}^{\Delta F=2}(Z) = \left[ \frac{1}{8M_w^2} g_w^2 \right]^2 \frac{1}{16\pi^2} \sum_i V^{(i)}_{\text{CKM}} c^{(i)}_W(\mu_r) \hat{O}_i(Z; \mu_r) + \mathcal{O}(\frac{1}{M_W^6})
\]

Effective theory for momenta $\ll M_W$ (approx. good for $B - \bar{B}$; modulo charm exchange corrections for $K - \bar{K}$)
Flavour physics & CP-violation: unitarity triangle

The Wolfenstein Parametrization

<table>
<thead>
<tr>
<th>$1 - 1/2 \lambda^2$</th>
<th>$\lambda$</th>
<th>$A \lambda^3 (\rho - i \eta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$- \lambda$</td>
<td>$1 - 1/2 \lambda^2$</td>
<td>$A \lambda^3$</td>
</tr>
<tr>
<td>$A \lambda^2 \times (1 - \rho - i \eta)$</td>
<td>$-A \lambda^2$</td>
<td>$1$</td>
</tr>
</tbody>
</table>

$V_{ub}$

$\lambda \sim 0.2$ $A \sim 0.8$

$\eta \sim 0.2$ $\rho \sim 0.3$

Sin $\theta_{12} = \lambda$

Sin $\theta_{23} = A \lambda^2$

Sin $\theta_{13} = A \lambda^2 (\rho - i \eta)$
LQCD, $K-\bar{K}$ oscillations and BSM-models

Meson - antimeson matrix elements of $d = 6$ operators in $\mathcal{H}_{\text{eff}}^{\Delta S=2} = \frac{1}{4} \sum_j C_j O_j$

expressed via $B_j$-parameters:  

$$
\langle \bar{K}^0 | O_1(\mu_r) | K^0 \rangle = \frac{8}{3} B_1(\mu_r) m_K^2 f_K^2,
$$

$$
\langle \bar{K}^0 | O_i(\mu_r) | K^0 \rangle = \xi_i B_i(\mu_r) \left[ (m_K^2 f_K) (m_s(\mu_r) + m_d(\mu_r))^{-1} \right]^2, \quad i = 2, 3, 4, 5
$$

Comparing exp. data for $\langle \bar{K}^0 | \mathcal{H}_{\text{eff}}^{\Delta S=2} | K^0 \rangle$ with $\langle \bar{K}^0 | O_j | K^0 \rangle$ for each $j$ constrains

$$C_j = F_j L_j \Lambda_{\text{NP}}^{-2} \Rightarrow \text{lower bounds on } \Lambda_{\text{NP}}^{-2} \text{ for } j = 1, \ldots, 5 \text{ (see table for } F_j = L_j = 1)$$

with $F_j$ the relevant NP coupling, $L_j$ a loop factor depending on interactions for $O_j$

<table>
<thead>
<tr>
<th>95% allowed range (GeV$^{-2}$)</th>
<th>Lower limit on $\Lambda$ (TeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Im } C^K_1$ [-2.1, 3.4] $\cdot 10^{-15}$</td>
<td>1.7 $\cdot 10^4$</td>
</tr>
<tr>
<td>$\text{Im } C^K_2$ [-2.1, 1.4] $\cdot 10^{-17}$</td>
<td>22 $\cdot 10^4$</td>
</tr>
<tr>
<td>$\text{Im } C^K_3$ [-5.1, 7.8] $\cdot 10^{-17}$</td>
<td>11 $\cdot 10^4$</td>
</tr>
<tr>
<td>$\text{Im } C^K_4$ [-3.0, 4.7] $\cdot 10^{-18}$</td>
<td>46 $\cdot 10^4$</td>
</tr>
<tr>
<td>$\text{Im } C^K_5$ [-0.9, 1.4] $\cdot 10^{-17}$</td>
<td>27 $\cdot 10^4$</td>
</tr>
</tbody>
</table>

$O_1 = [s^a \gamma_\mu (1-\gamma_5) d^a][s^b \gamma_\mu (1-\gamma_5) d^b]$

$O_2 = [s^a (1-\gamma_5) d^a][s^b (1-\gamma_5) d^b]$

$O_3 = [s^a (1-\gamma_5) d^a][s^b (1-\gamma_5) d^a]$

$O_4 = [s^a (1-\gamma_5) d^a][s^b (1+\gamma_5) d^b]$

$O_5 = [s^a (1-\gamma_5) d^a][s^b (1+\gamma_5) d^a]$
LQCD observables with heavy quarks \((h)\) display large lattice artifacts \(O(a^2 m_h^2)\), which actually get reduced if \(m_h\) is multiplicatively renormalizable. A way to control them is known as the “ratio method” (ETMC ’10): one uses quarks with masses lying at, and up to 2–3 times above, \(m_c\). Ratios of observables at nearby heavy quark masses show controllable lattice artifacts and can be extrapolated to \(m_b\) incorporating the behavior predicted by Heavy Quark Effective Theory.

Heavy flavour physics results from twisted mass LQCD + ratio method & other approaches
Chiral & isospin symmetry in the \((u,d)\) quark sector

1. Pure \(N_f = 2\) QCD with \(m_u = m_d = m\) i.e.

\[
L^\text{QCDud}_E = \frac{1}{2} \text{tr}\{G_{\mu\nu} G^{\mu\nu}\} + \sum_{f=u,d} \bar{q}_f [\gamma_\mu (\partial_\mu + ig S A_\mu) + m] q_f
\]

obeys simple flavour chiral Ward–Takahashi (WT) ↔ symmetry identities

\[
\partial_\mu V_i^\mu = 0 \quad (\text{exact isospin}), \quad \partial_\mu A_i^\mu - 2mP^i = 0, \quad i = 1, 2, 3,
\]

axial generators dynamically broken (SSB) by

\[
-\langle (\bar{u}u + \bar{d}d)_r \rangle = \Sigma = 2G_\pi f_\pi = O(\Lambda_{QCD}^3)
\]

and \(m_\pi^2 = 2G_\pi f_\pi^{-1} m + O(m^2)\) with \(g_A(q^2 = 0) M_N/f_\pi \sim g_{NN\pi} = O(10)\)

Notation: \(\psi = (u,d)^t\) and \(A_i^\mu = \bar{\psi} \gamma_\mu \gamma_5 \frac{1}{2} \tau_i \psi\), \(P^i = \bar{\psi} \gamma_5 \frac{1}{2} \tau_i \psi\), etc.

2. (Formal) QCD + QED with mass non-degenerate \((u,d)\) quark flavours obeys

WT identities with isospin symmetry broken by \(\delta q = q_u - q_d\) and \(\epsilon = m_u - m_d\)

\[
\begin{align*}
\partial_\mu V_\mu^3 &= 0 \\
\partial_\mu V_\mu^1 + e \delta q A_\mu V_\mu^2 - 2\epsilon i S^2 &= 0 \\
\partial_\mu V_\mu^2 - e \delta q A_\mu V_\mu^1 + 2\epsilon i S^1 &= 0 \\
\partial_\mu A_\mu^3 - 2mP^3 - 2\epsilon P^0 &= 0 \\
\partial_\mu A_\mu^1 + e \delta q A_\mu A_\mu^2 - 2mP^1 &= 0 \\
\partial_\mu A_\mu^2 + e \delta q A_\mu A_\mu^1 - 2mP^2 &= 0
\end{align*}
\]

where \(A_\mu\) = photon field... In physical observables isospin breaking (IB) is \(O(\alpha_{em}, \epsilon/\Lambda_{QCD})\)
**QCD+QED on the lattice: why?**

- *Isospin* symmetry is a very good approximation…

\[
\frac{m_u - m_d}{M_p} \ll 1, \quad \alpha_{em}(M_p) \ll \alpha_s(M_p), \quad \frac{M_n - M_p}{M_p} \approx 0.1\%
\]

- yes, but *isospin breaking* explains chemistry…

- Hydrogen is stable because the electron capture reaction 
  \( p + e \rightarrow n + \nu \) is forbidden

\[
M_n - M_p = [M_n - M_p]^{\text{QCD}} + [M_n - M_p]^{\text{QED}} > m_e
\]

- *Caveat*: the separation of QED and QCD isospin breaking effects is not necessary, although it may be useful in phenomenological applications, and is a *subtle issue*!
concerning flavour physics (i.e. *precision* tests of the Standard Model),
leptonic and semileptonic decays of the pions and of the kaons are our
main source of information on the Cabibbo angle (or $V_{us}$)

QCD lattice simulations in the isosymmetric limit give *(FLAG)*

\[
\frac{F_K}{F_\pi} = 1.194(5) \sim 0.4\%
\]

\[
F_{\pi}^K(0) = 0.9661(32) \sim 0.3\%
\]

isospin breaking corrections are calculated in chiral perturbation theory
V Cirigliano et al., Rev.Mod.Phys. 84 (2012)

\[
\Delta_{QED+QCD} \left( \frac{F_K}{F_\pi} \right) \sim 1\%
\]

\[
\Delta_{QED+QCD} \left[ F_{\pi}^K(0) \right] \sim [0.5, 3]\%
\]

it's time to put QED+QCD on the lattice...
Leading Isospin Breaking (LIB) effects can be calculated directly or by expanding the lattice path-integral w.r.t. $\alpha_{em} \sim (m_d - m_u)/\Lambda_{QCD}$

\[ \mathcal{O}(\bar{g}) = \frac{\langle R[U, A; \bar{g}] O[U, A; \bar{g}] \rangle^A, \bar{g}^0}{\langle R[U, A; \bar{g}] \rangle^A, \bar{g}^0} = \frac{\langle (1 + \hat{R} + \cdots) (O + \dot{O} + \cdots) \rangle}{\langle 1 + \hat{R} + \cdots \rangle} = \mathcal{O}(\bar{g}^0) + \Delta \mathcal{O} \]

The building blocks for the graphical notation, used as a device to do calculations, are the corrections to the quark propagator

\[ \Delta \rightarrow \pm = \]

\[
\begin{align*}
(e_f e)^2 & \quad + (e_f e)^2 & \quad - [m_f - m_f^0] & \quad \mp [m_f^r - m_f^r] \\
-e^2 e_f \sum_{f_1} e_{f_1} & \quad - e^2 \sum_{f_1} e_{f_1}^2 & \quad - e^2 \sum_{f_1} e_{f_1}^2 & \quad + e^2 \sum_{f_1} e_{f_1} e_{f_2} \\
\sum_{f_1} \pm [m_{f_1}^r - m_{f_1}^r] & \quad + \sum_{f_1} [m_{f_1} - m_{f_1}^0] & \quad + [g_s^2 - (g_s^0)^2] & \quad \text{G}_{\mu
u} G^{\mu\nu} 
\end{align*}
\]
with our method we have calculated LIB on pseudoscalar mesons mass splittings

\[ M_{\pi^+} - M_{\pi^0} = \frac{(e_u - e_d)^2}{2} e^2 \partial_t - \text{connected diagram} \]

we have also computed the QED radiative corrections to the leptonic decay rates of the processes $\pi \rightarrow \ell \nu(\gamma)$ and $K \rightarrow \ell \nu(\gamma)$

this is a very complicated problem, much more involved than in the case of the corrections to hadron masses, because of the appearance of infrared divergences at intermediate stages of the calculations

in all calculations we evaluated analytically the leading finite size effects (large & power-like in $L^{-1}$ due to massless $\gamma$)


on the theoretical side, using $C$-periodic boundary conditions in space we solved a long standing problem in QFT: the proper finite volume definition of the quantum state of electrically charged particles