ETH zürich

Institute for Theoretical
Physics, HPCP lab

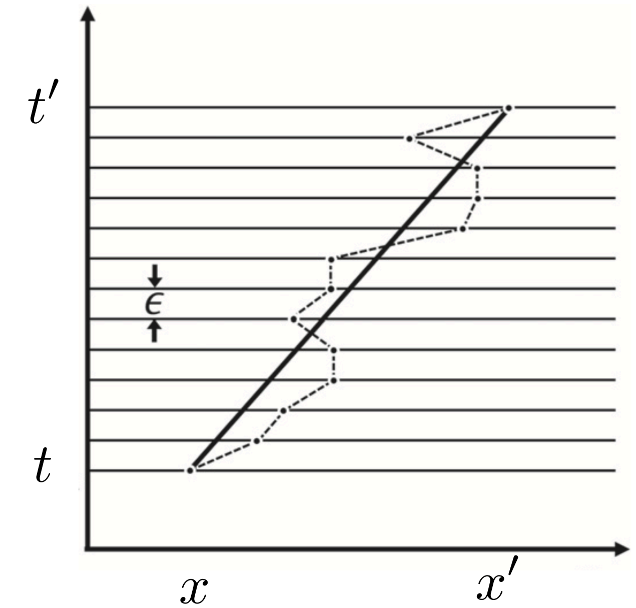
QCD+QED on the lattice

Prof. Marina Krstic Marinkovic, ETH Zürich

10-21 July 2023, Bad Honnef Physics School, Methods of effective field theory and lattice field theory

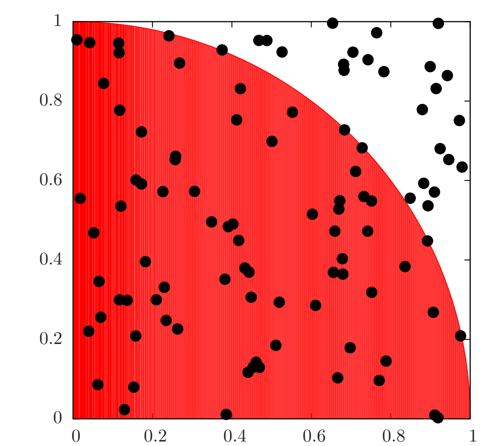
In the first lecture:

- We have learned/reminded ourselves how to quantize:



  - ➡ Quantum Mechanics
  - ➡ Scalar Field Theory

- Mapping to Classical Statistical Mechanics

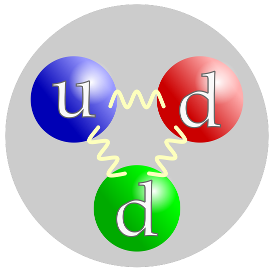


- Monte Carlo Sampling of Spin Systems $\longrightarrow$ Quantum Fields

- Monte Carlo Errors, other sources of errors

In the second part:

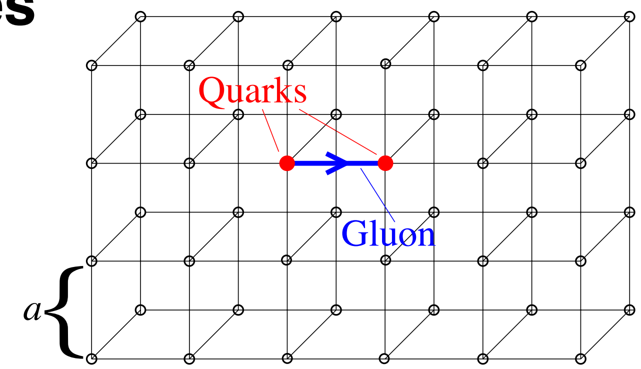
- We shall generalize this approach to Quantum Chromodynamics (QCD)

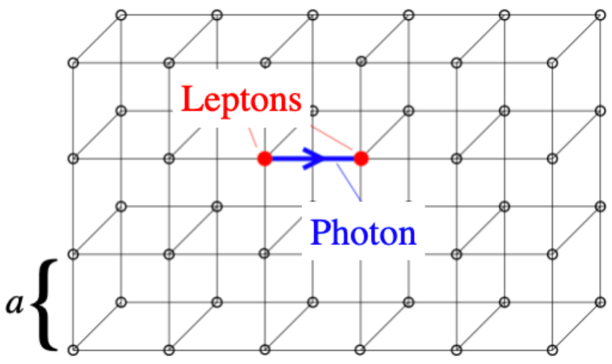


- We shall see how the numerical sampling is done in practice
    - for scalar field theory
    - for QCD

- Why is QCD numerically so expensive?

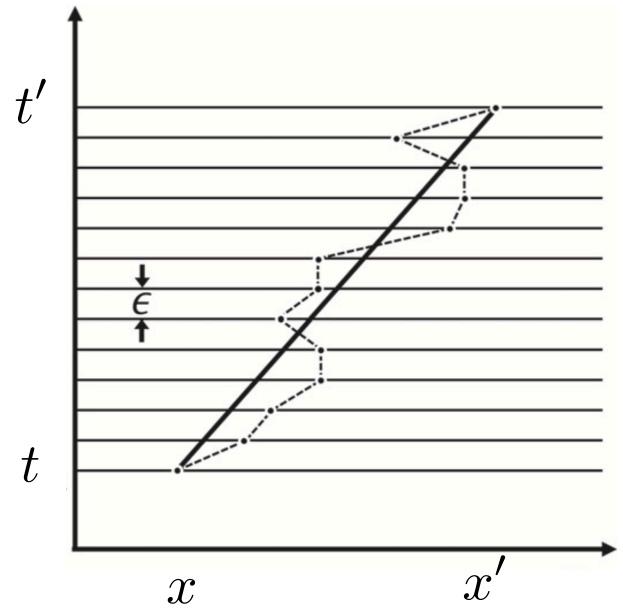
- QED corrections to hadronic observables





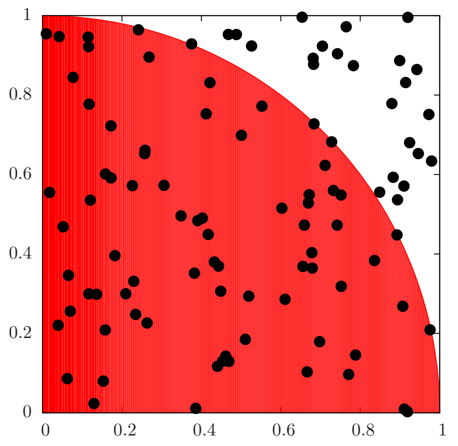
Recap.

- We have learned/reminded ourselves how to quantize:



  - ➡ Quantum Mechanics
  - ➡ Scalar Field Theory

- Mapping to Classical Statistical Mechanics



- Monte Carlo Sampling of Spin Systems $\longrightarrow$ Quantum Fields

- Monte Carlo Errors, other sources of errors

Expectation values in the MC approach: QFT

- **Numerical approach exploits the analogy:**

Euclidean QFT ⟷ **Statistical Mechanics**

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

- **Path integrals are computed by importance sampling**

$$\mathcal{P}[\phi_i] \propto e^{-S_E[\phi]}$$

- **Generate ensemble of field configurations** $\{\phi_i\}$

- **Expectation values** $\langle O[\phi]\rangle$ **are averages over the ensemble**

$$\langle O\rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[\phi] + \mathcal{O}\left(\frac{1}{\sqrt{N_{cnfg}}}\right)$$

- **How do we generate ensemble** $\{\phi_i\}$ **with the correct probability distribution?**

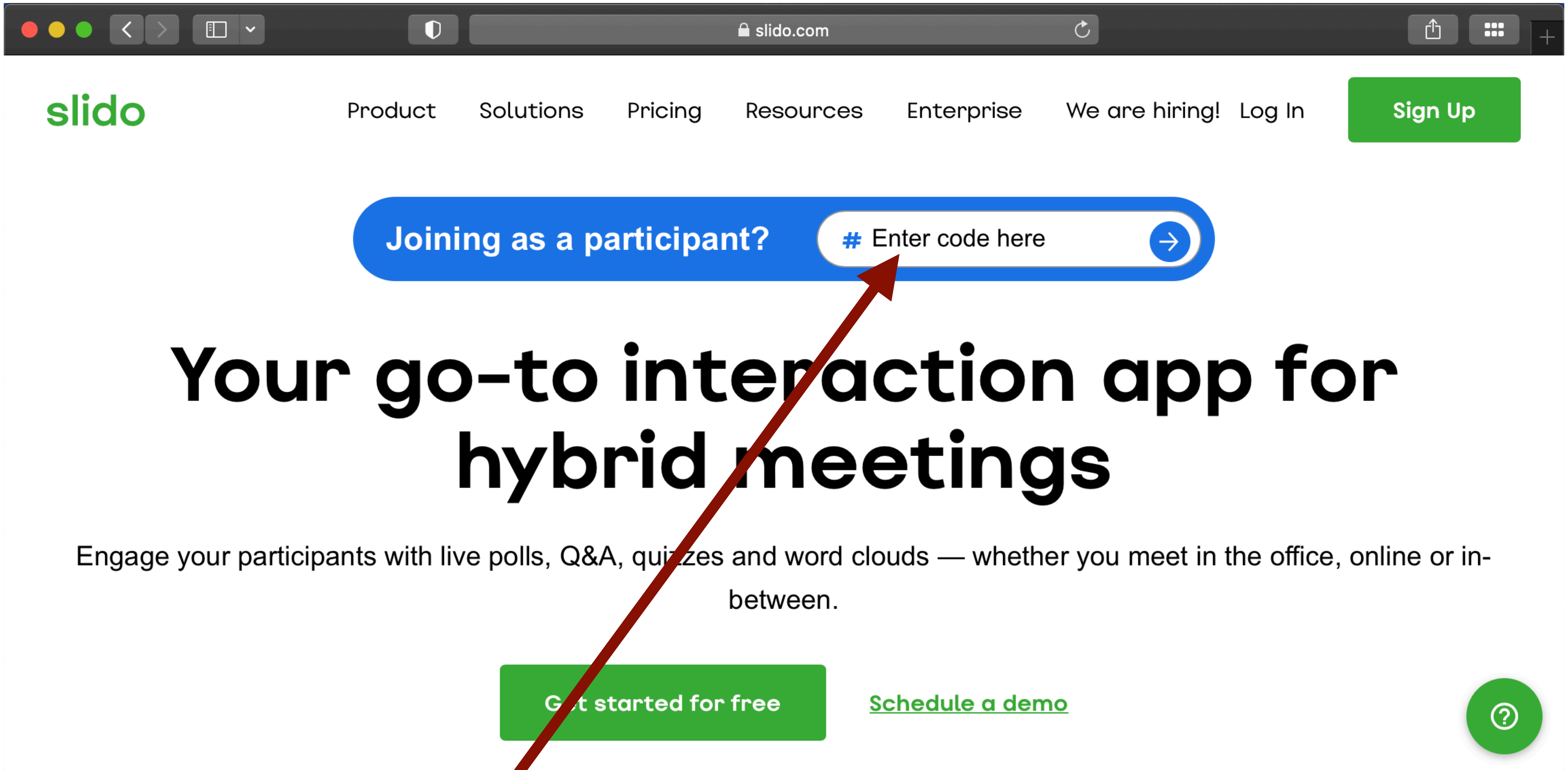
Markov processes

- Recursive procedure that generates $\{\phi_i\}$ with specific algorithm s.t. aimed distribution is asymptotically obtained

$$\{\phi_0\} \longrightarrow \{\phi_1\} \longrightarrow \{\phi_2\} \longrightarrow \cdots \longrightarrow \{\phi_i\} \longrightarrow \{\phi_{i+1}\} \longrightarrow \ldots$$

- Markov chains that converge exponentially to the equilibrium distr.

Go to slido.com



- **Poll 2: #lattice2**

Markov processes

- **Recursive procedure that generates $\{\phi_i\}$ with specific algorithm s.t. aimed distribution is asymptotically obtained**

$$\{\phi_0\} \longrightarrow \{\phi_1\} \longrightarrow \{\phi_2\} \longrightarrow \cdots \longrightarrow \{\phi_i\} \longrightarrow \{\phi_{i+1}\} \longrightarrow \ldots$$

- **Markov chains that converge exponentially to the equilibrium distr.**

- **The configurations $\{\phi_i\}$ are correlated by construction**

$$Var\,[\bar{O}] \;=\; Var[O]\,\Big(\frac{2\tau_O}{N_{cnfg}}\Big)$$

τ_O– **integrated autocorrelation time**

- **The error of the estimator scales as $\dfrac{1}{\sqrt{N_{cnfg}}}$ (Monte Carlo)**

- **The variance of the actual observable**

$$Var\,[O] \;=\; \langle \big(O - \langle O \rangle\big)^2 \rangle$$

↳ **property of QFT itself, should not depend of the Markov chain.**

The MR²T² algorithm

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- **The Metropolis Algorithm:**
- **Given ϕ, propose ϕ' in a reversible, area-preserving way**
- **Accept the proposal as new entry with probability p, otherwise add ϕ to the chain again.**
- $\mathrm{p} = \min(1, \frac{\pi(\phi')}{\pi(\phi)})$

The MR²T² algorithm

- The Metropolis Algorithm for Scalar F.T.:
- Given ϕ propose ϕ'
- Choose a random number $r \in [0,1]$
- If $S_E(\phi') < S_E(\phi)$, always accept, otherwise add ϕ' to the chain again if

$$e^{-\Delta S} > r; \Delta S = S_E(\phi') - S_E(\phi)$$

- The Metropolis Algorithm:
- Given ϕ, propose ϕ' in a reversible, area-preserving way
- Accept the proposal as new entry with probability p, otherwise add ϕ to the chain again.
- $\mathrm{p} = \min(1, \frac{\pi(\phi')}{\pi(\phi)})$

Quantum Chromodynamics

COLOUR: SU(3) symmetry

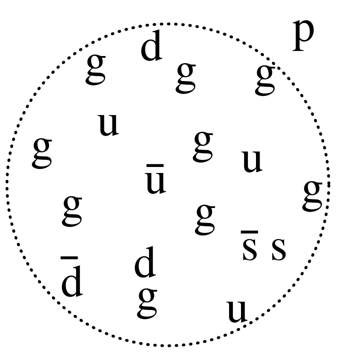
- QCD Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\dots} \overline{\psi}_f \left\{ i\gamma_\mu \left(\partial_\mu - i g_s A^a_\mu T^a\right) - m_f \right\} \psi_f$$

$$S = \int d^4x \, \mathcal{L}_{QCD}$$

- Covariant derivative: $D_\mu = \partial_\mu - i g_s A_\mu$

- Bare QCD parameters ($N_f + 1$)
  - gauge coupling g_s
  - quark masses m_u, m_d, ...

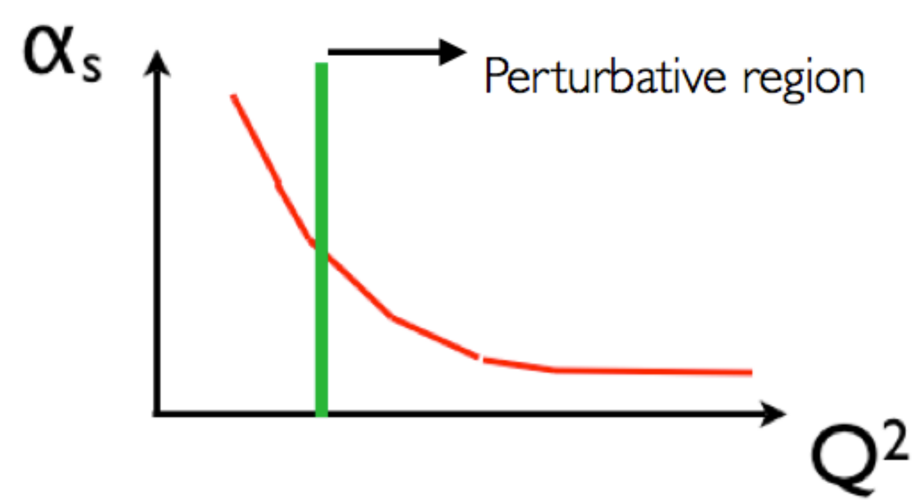


Quantum Chromodynamics

- QCD Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f \left\{ i\gamma_\mu \left(\partial_\mu - i g_s A^a_\mu T^a\right) - m_f \right\} \psi_f$$

$$S = \int d^4x \, \mathcal{L}_{QCD}$$



- Euclidean QCD Lagrangian ($t \equiv x^E \leftrightarrow -ix_0$)

$$\mathcal{L}_{QCD} = \frac{1}{2g^2} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f \left\{ \gamma_\mu \left(\partial_\mu + i A^a_\mu T^a\right) + m_f \right\} \psi_f$$

$$S_{QCD} = \int d^4x \, \mathcal{L}_{QCD}$$

Path Integrals in Quantum Chromodynamics

- Each specific field configuration:

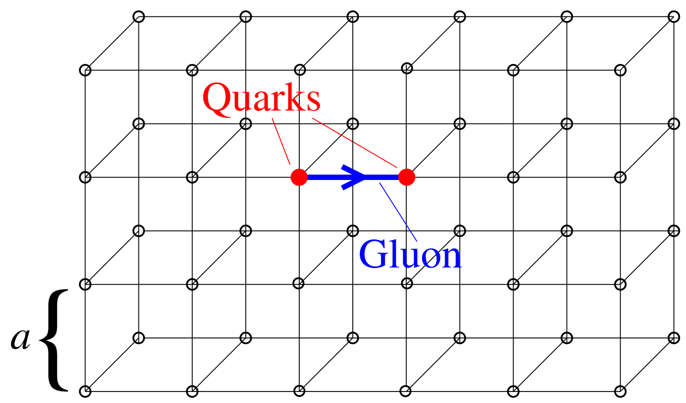
$$P(\psi, \overline{\psi}, A) \sim e^{-S(\psi, \overline{\psi}, A)}$$

- Expectation value of an operator $O(\psi, \overline{\psi}, A)$:

$$\begin{aligned}
\langle O(\psi, \overline{\psi}, A) \rangle &= \langle \langle O(\psi, \overline{\psi}, A) \rangle_F \rangle_G \\
&= \frac{1}{Z} \int \mathcal{D}[A] \mathcal{D}[\overline{\psi}, \psi] \, e^{-S(\psi, \overline{\psi}, A)} O(\psi, \overline{\psi}, A) \\
Z &= \int \mathcal{D}[A] \mathcal{D}[\overline{\psi}, \psi] \, e^{-S(\psi, \overline{\psi}, A)}
\end{aligned}$$

Lattice regularization of QCD

$$\Lambda_{\text{cut}} \sim \frac{1}{a}$$



- Divergencies in continuum QCD $\rightarrow$ **regularization** is necessary!
- One possible regularization:
  Introduce **momentum ultraviolet-cutoff** $\Leftrightarrow$ minimum distance (FT)
- If required also: **local gauge symmetry** $\rightarrow$ **Lattice QCD**
- Finite number of integrals over fields ($\int d^4x \;\rightarrow\; a^4 \sum_n$)
- Computable with the help of Monte Carlo techniques

Lattice regularization of QCD

$$S_{QCD}[\psi,\bar\psi,A] = S_G + S_F$$
$$= \frac{1}{2g} F_{\mu\nu}F_{\mu\nu} + \int d^4x\ \bar\psi(x)\ [\gamma_\mu\ (\partial_\mu + iA_\mu(x)) + m]\ \psi(x)$$

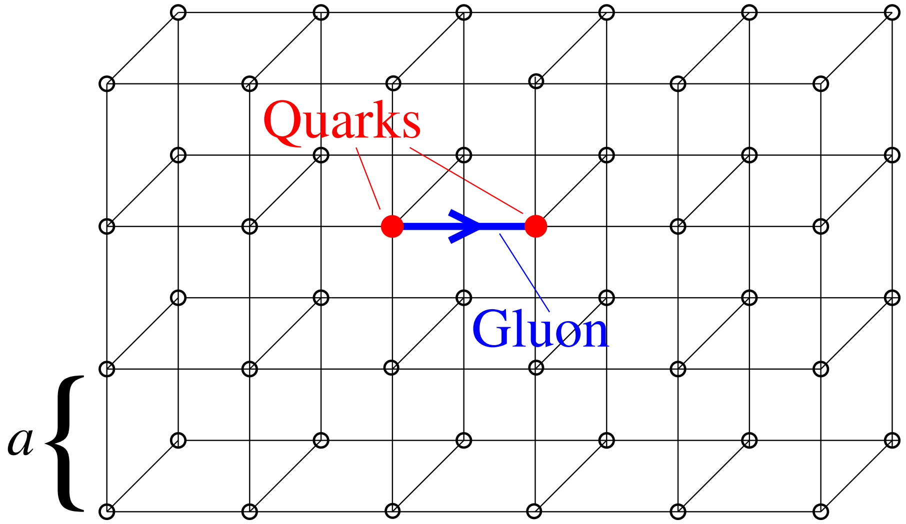
- Discretization prescription:

$$x \longrightarrow n = (n_1, n_2, n_3, n_4)\ n_1 = 0,\ldots,N-1$$

$$\psi(x),\bar\psi(x) \longrightarrow \psi(n),\bar\psi(n)$$

$$\int d^4x \ldots \longrightarrow a^4 \sum_n \ldots$$

$$\partial_\mu\ \psi(x) \longrightarrow \frac{\psi(n+\hat\mu)-\psi(n-\hat\mu)}{2a} + \mathcal{O}(a^2)$$



Naive Lattice Fermion Action

- Simple example - free fermion field ($A_\mu = 0$):

  $S_F^0[\psi,\bar{\psi}] = \int d^4x\ \bar{\psi}(x)\ (\gamma_\mu\ \partial_\mu + m)\ \psi(x)$

- Symmetrically discretized partial derivative:

$$\partial_\mu \psi(na) = \frac{\psi((n+\hat{\mu}))-\psi((n-\hat{\mu}))}{2a} + \mathcal{O}(a^2)$$

- Naive lattice ansatz for free fermion action:

$$S_F\left[\psi,\overline{\psi}\right] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\psi(n+\hat{\mu})-\psi(n-\hat{\mu})}{2a} + m\psi(n) \right)$$

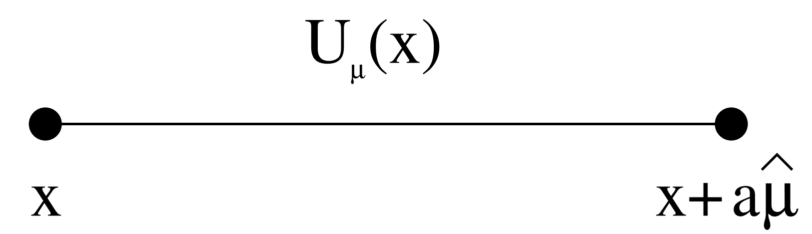
- **Let us examine gauge invariance** $\rightarrow$

Gauge Invariance

- $\Omega(n) \in SU(3)$:

$$\begin{aligned} \psi'(n) &= \Omega(n)\psi(n) \\ \overline{\psi}'(n) &= \overline{\psi}(n)\Omega(n)^\dagger \\ \overline{\psi}'(n)\psi'(n+\hat{\mu}) &= \overline{\psi}(n)\Omega(n)^\dagger\Omega(n+\hat{\mu})\psi(n+\hat{\mu}) \quad (!) \end{aligned}$$

- (!) not gauge invariant

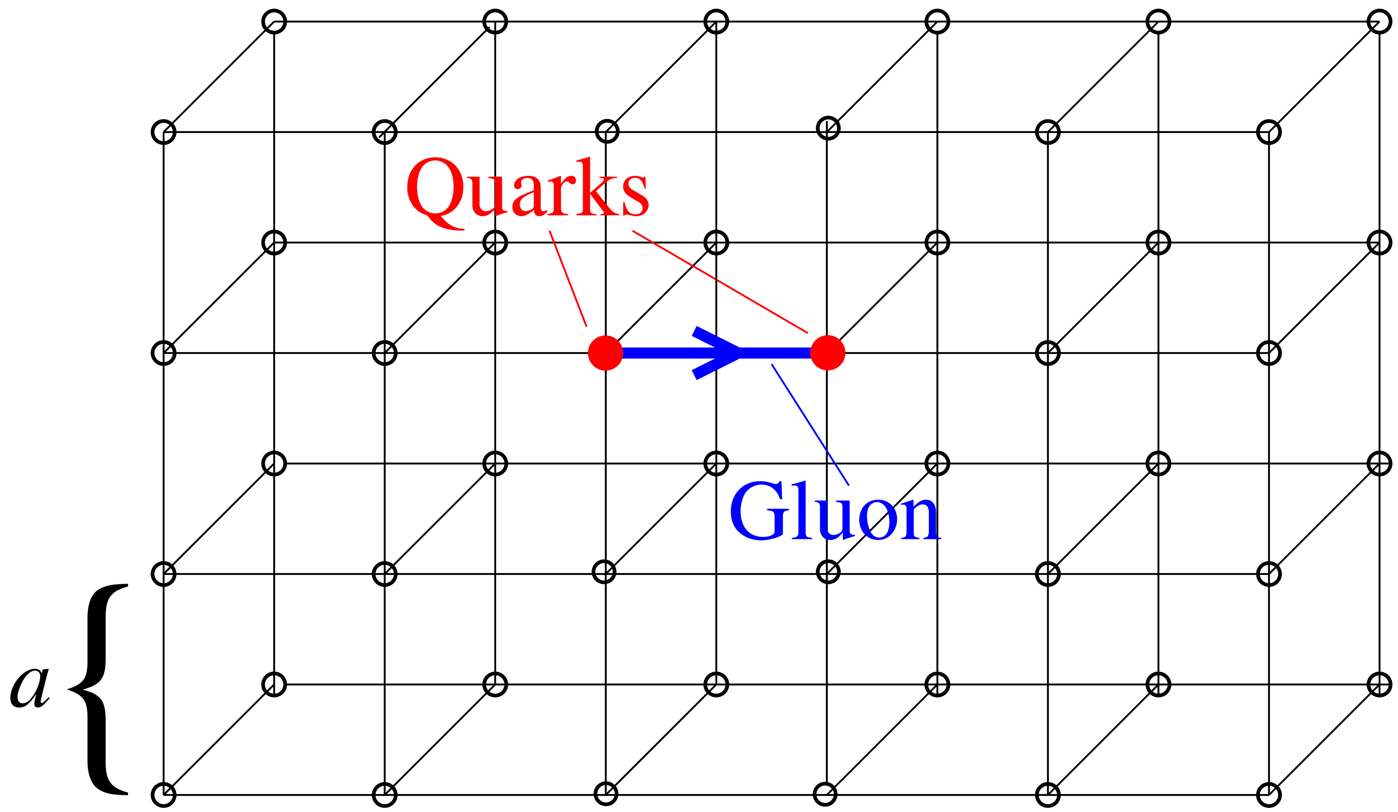


- Introduce **link variables $\mathbf{U_\mu(n)}$**:

$$\begin{aligned} U'_\mu(n) &= \Omega(n)U_\mu(n)\Omega(n+\hat{\mu})^\dagger \\ \overline{\psi}'(n)U'_\mu(n)\psi'(n+\hat{\mu}) &= \overline{\psi}(n)U_\mu(n)\psi(n+\hat{\mu}) \end{aligned}$$

- $U_\mu(n) \rightarrow$ fundamental gluonic variables on the lattice

Quark and gluon fields on the lattice



Quarks $\sim \overline{\psi}(n), \psi(n)$

Gluons $\sim$ "Link variables" $\sim$ Parallel transporter $\sim U_\mu(n) = e^{iagA_\mu}$

Lattice fermion action (I)

- Fermionic action: $S_F = a^4 \sum_f \overline{\psi}(n)\, D(n,m)\, \psi(m)$
- Naive fermion action

$$D(n,m) = m\delta_{n,m} + \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} \gamma_\mu U_\mu(n)\, \delta_{n+\hat{\mu},m}$$

- Propagator in momentum space:

$$\tilde{D}(p)^{-1} = \frac{m\mathbf{1} - ia^{-1} \sum_{\mu=\pm 1}^{\pm 4} \gamma_\mu sin(p_\mu a)}{m^2 + a^{-2} \sum_{\mu=\pm 1}^{\pm 4} sin(p_\mu a)^2}$$

- Important: case of massless fermions, $m = 0$:

$$\tilde{D}(p)^{-1}|_{m=0} = \frac{-ia^{-1} \sum_\mu \gamma_\mu sin(p_\mu a)}{a^{-2} \sum_\mu sin(p_\mu a)^2}$$

- Unphysical poles at $p_\mu = \frac{\pi}{a}$
- Unwanted **doublers**: obtainded 16 instead of 1 fermionic particles!

Lattice fermion action (II)

- **Wilson Dirac matrix** D_W

$$D_W(n,m) = \left(m + \tfrac{4}{a}\right)\delta_{n,m} - \tfrac{1}{2a}\sum_{\mu=\pm 1}^{\pm 4} \left(1-\gamma_\mu\right) U_\mu(n)\,\delta_{n+\hat{\mu},m}$$

- Wilson term: shifting the mass of the doublers to infinity, as $a \to 0$
- Only the physical pole, no doublers!
- Problem: Additional term **breaks chiral symmetry** explicitly
- **No-Go Theorem** on the lattice [Nielsen & Ninomiya, 1981]: simple action without doublers $\leftrightarrow$ broken chiral symmetry
- Different choices of lattice derivatives
  $\rightarrow$ $O(a), O(a^2), \ldots$ discretization errors
  $\rightarrow$ different rates to approach continuum limit

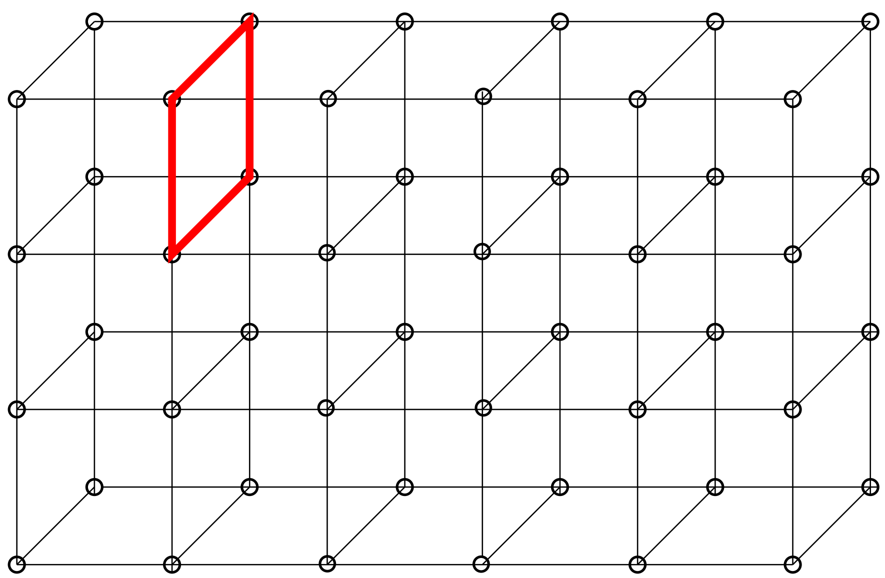
Lattice gauge action (I)

- $S_G = \frac{1}{2g} Tr\ F_{\mu\nu}(x)\ F_{\mu\nu}(x)$
- Need gauge invariant object: trace over closed loop of gauge links
- Smallest possible closed loop: **Plaquette**

$$U_{\mu\nu}(n) = U_\mu(n) U_\nu(n+\hat{\mu}) U_{-\mu}(n+\hat{\mu}+\hat{\nu}) U_{-\nu}(n+\hat{\nu})$$
$$= U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger$$

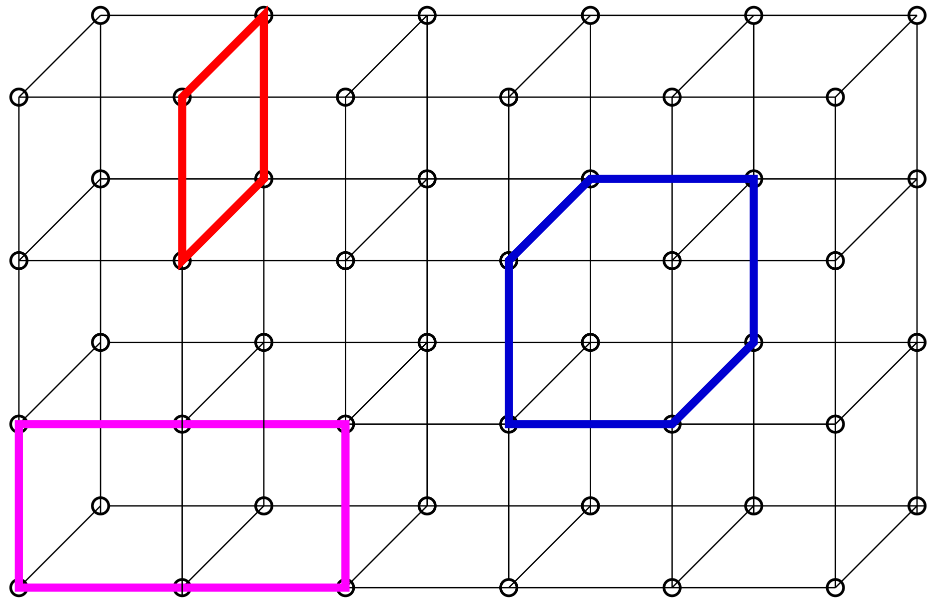
- **Wilson gauge action:**

$$S_g \sim \sum_n \sum_{\mu<\nu} \ \mathrm{Re\ tr}\left[1 - U_{\mu\nu}(n)\right]$$



Lattice gauge action (II)

- Improvement: taking into account larger Wilson loops



- All in the same universality class:

  $\longrightarrow$ converge to $\text{tr}\,\left[F_{\mu\nu}(x)F_{\mu\nu}(x)\right]$ in the continuum limit

  $\longrightarrow$ improvement reduces the discretization errors!

- Lattice artefacts in scaling behaviour:

  $\longrightarrow$ Wilson gauge action: $O(a^2)$

  $\longrightarrow$ Luscher-Weisz: $O(a^4)$ [K. Symanzik, 1981; Luscher and Weisz, 1985]

Recipe for Lattice QCD Computation

(1) Generate ensembles of field configurations using Monte Carlo $\mathcal{P}[U_i] \propto e^{-S_E[U]}$

(2) Average over a set of configurations: $\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[U] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$

- Compute correlation function of fields, extract Euclidean matrix elements or amplitudes
- Computational cost dominated by quarks: inverses of large, sparse matrix

(3) Extrapolate to continuum, infinite volume, physical quark masses (now directly accessible)

Recipe for Lattice QCD Computation

(1) Generate ensembles of field configurations using Monte Carlo $\mathcal{P}[U_i] \propto e^{-S_E[U]}$

(2) Average over a set of configurations: $\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[U] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$

- Compute correlation function of fields, extract Euclidean matrix elements or amplitudes
- Computational cost dominated by quarks: inverses of large, sparse matrix

(3) Extrapolate to continuum, infinite volume, physical quark masses (now directly accessible)

- Lattice QCD path integrals are computed by **importance sampling**: $\mathcal{P}[U_i] \propto e^{-S_E[U]}$
- Markov chain: $\{U_0\} \longrightarrow \{U_1\} \longrightarrow \{U_2\} \longrightarrow \cdots \longrightarrow \{U_i\} \longrightarrow \{U_{i+1}\} \longrightarrow \ldots$
- The configurations are correlated by construction: $Var\,[\bar{O}] = Var[O]\,(\frac{2\tau_O}{N_{cnfg}})$

The cost of dynamical fermions

$$S^E_{QCD} = S_G[U] + S_f[U, \psi, \overline{\psi}]$$

$$\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\overline{\psi} e^{\underline{-S_G[U]} \underline{-S_f[U,\psi,\overline{\psi}]}} O[\psi, \overline{\psi}, U]$$

$$\int \mathcal{D}\,\psi\;\mathcal{D}\,\overline{\psi}\; e^{-\overline{\psi}\,(\gamma_\mu D_\mu + m_q)\,\psi} \quad \approx \quad det\,(\gamma_\mu D_\mu + m_q)$$

- Fermions represented by Grassmann variables in P.I: expensive to manipulate on a classical computer
- Easy to evaluate integral over fermionic (anti-commuting) fields: $\eta_i \eta_j = -\eta_j \eta_i$
- Integration rules: $\int d\eta = 0; \quad \int d\eta\, \eta = 1$

The cost of dynamical fermions

$$\langle O[\psi,\overline{\psi},U]\rangle = \frac{1}{Z}\int \mathcal{D}\,U\ e^{-S_G[U]}\,[det\,(\gamma_\mu D_\mu + m_q)]^{N_f}\ O[\psi,\overline{\psi},U]$$

$$\int \mathcal{D}\,\phi\ \mathcal{D}\,\phi^\dagger\ e^{-\phi^\dagger\,(D^\dagger(m_q)D(m_q))^{-1}\,\phi} \quad\propto\quad [det\,(\gamma_\mu D_\mu + m_q)]^2$$

- Determinant: non-local object on the lattice —> virtually impossible to compute exactly!

- Computational cost of solving:

$$\chi = (\gamma_\mu D_\mu + m_q)^{-1}\Phi$$

  grows for: small quark masses m_q, and large $\dfrac{L}{a}$

- $k = \mathrm{cond}\,(M) \ \propto\ \dfrac{\lambda_{max}}{\lambda_{min}}$

The cost of dynamical fermions

$$\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}\, U\, \mathcal{D}\, \phi\, \mathcal{D}\, \phi^\dagger \; e^{-S_G[U] - \phi^\dagger\, (D^\dagger(m_q) D(m_q))^{-\frac{N_f}{2}}\, \phi}\, O[U, \phi, \phi^\dagger]$$

$$\int \mathcal{D}\, \phi\, \mathcal{D}\, \phi^\dagger \; e^{-\phi^\dagger\, (D^\dagger(m_q) D(m_q))^{-1}\, \phi} \quad \propto \quad [det\, (\gamma_\mu D_\mu + m_q)]^2$$

- Determinant: non-local object on the lattice —> virtually impossible to compute exactly!

- Computational cost of solving:

$$\chi = (\gamma_\mu D_\mu + m_q)^{-1} \Phi$$

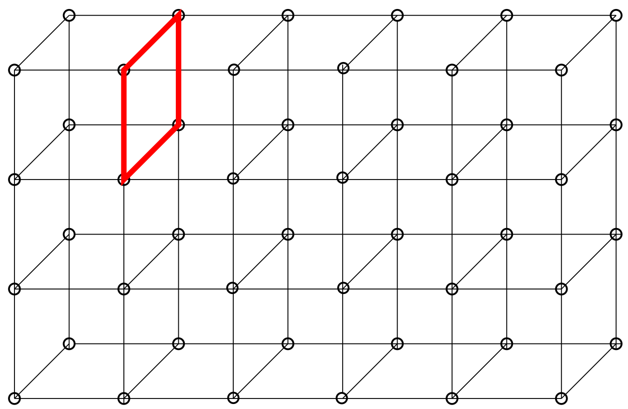
grows for: small quark masses m_q, and large $\frac{L}{a}$

- $k = \text{cond}\,(M) \;\propto\; \frac{\lambda_{max}}{\lambda_{min}}$

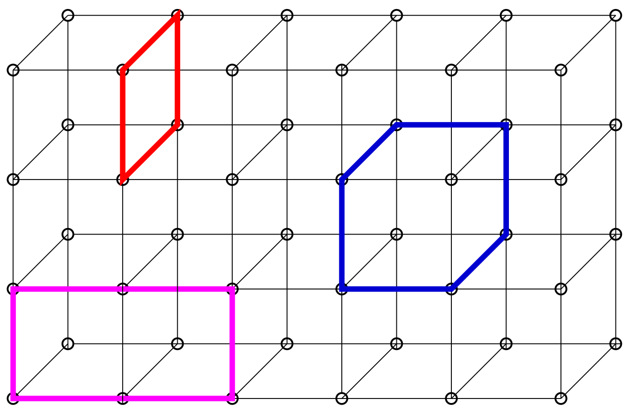
The cost of dynamical fermions

$$\langle O[\psi,\overline{\psi},U]\rangle = \frac{1}{Z}\int \mathcal{D}\,U\ e^{-S_G[U]}\ [det\,(\gamma_\mu D_\mu + m_q)]^{N_f}\ O[\psi,\overline{\psi},U]$$

S_G Wilson



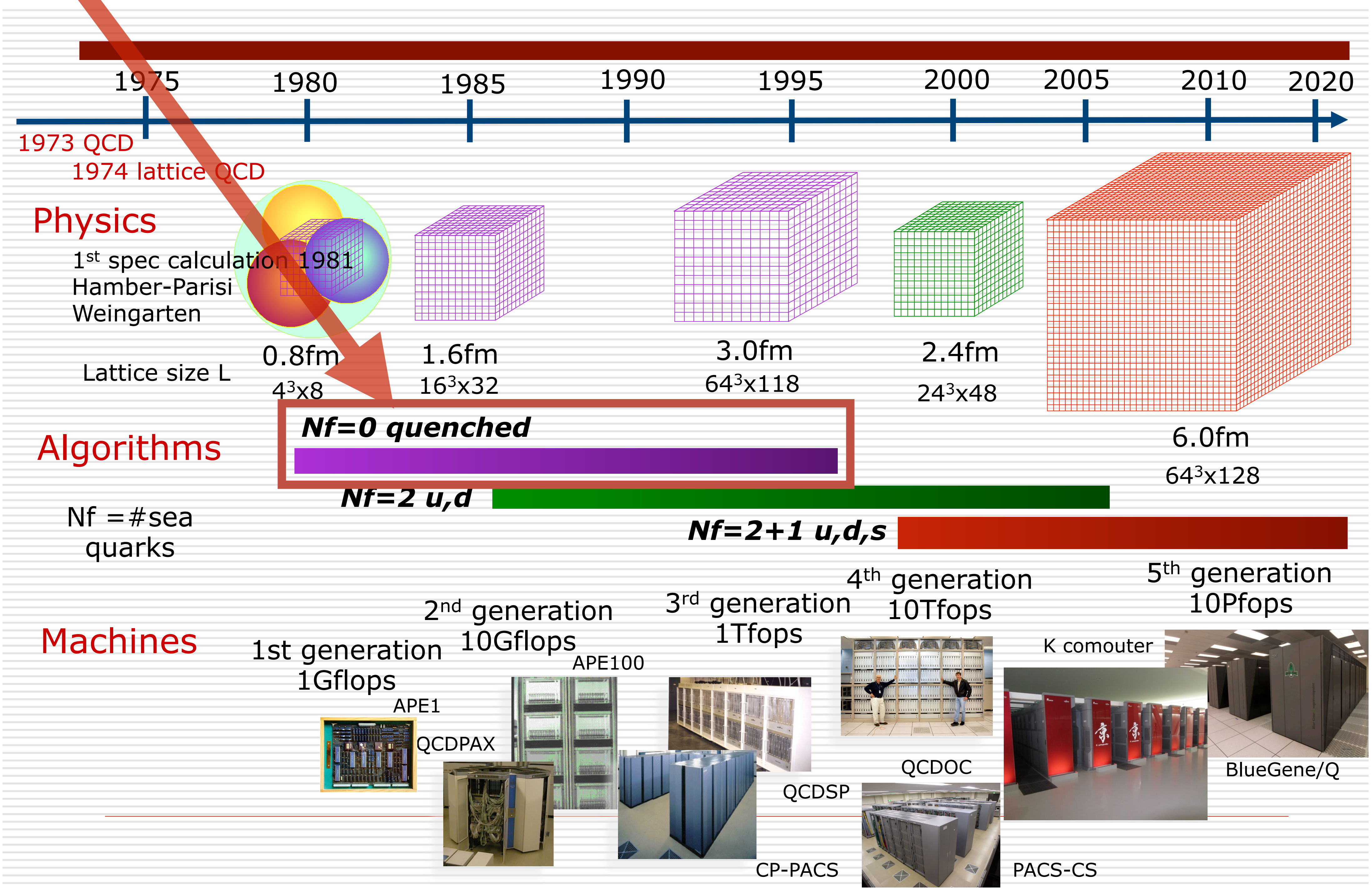
Luscher-Weisz



- Local objects: plaquettes, extended plaquettes (rectangles, chairs …)
- Rate of convergence towards continuum limit: $O(a), O(a^2), \ldots$
- Monte Carlo algorithms with local updates sufficient in the approximation: $\det\,(\gamma_\mu D_\mu + m_q) \equiv 1$

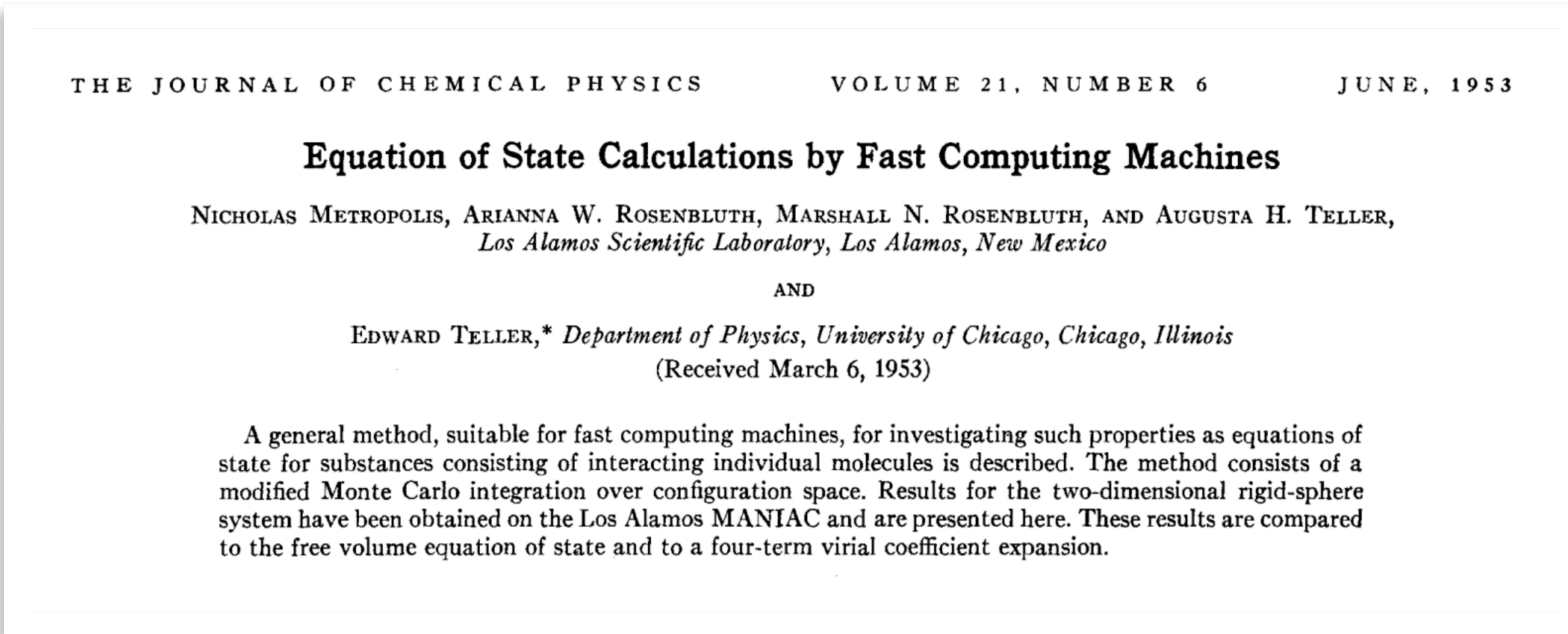
Development of Lattice QCD

$\det\,(\gamma_\mu D_\mu + m_q) \equiv 1$



[Credit: A. Ukawa, HPC Summer School (2013)]

The Metropolis algorithm


THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

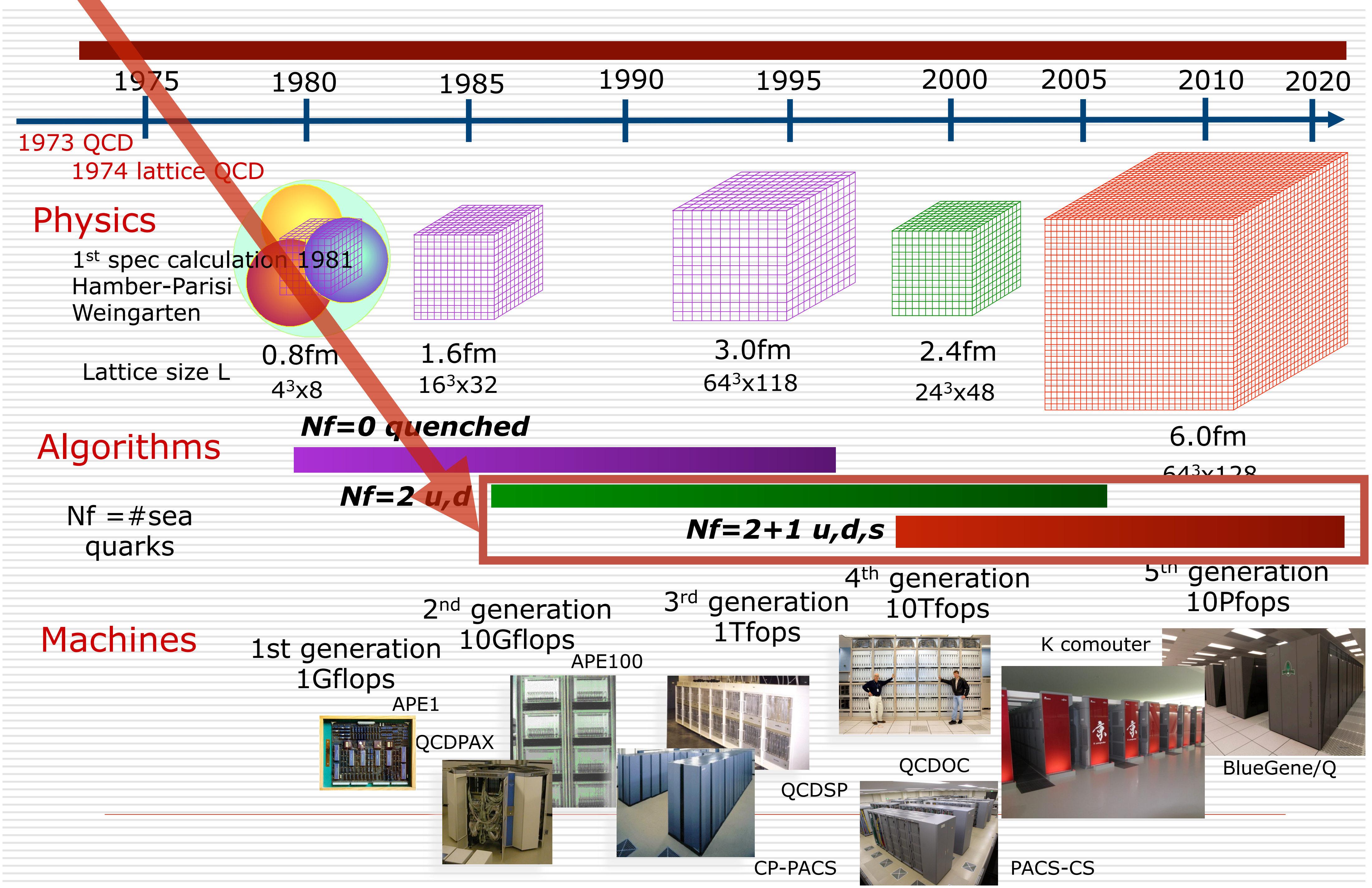
EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- The Metropolis Algorithm:
- Given $\{U\}$, propose $\{U'\}$ in a reversible, area-preserving way
- Accept the proposal as new entry with probability p, otherwise add $\{U\}$ to the chain again.
- $$p = \min\left(1, \frac{\pi(U')}{\pi(U)}\right)$$

Development of Lattice QCD

$$\det(\gamma_\mu D_\mu + m_q) \neq 1$$



[Credit: A. Ukawa, HPC Summer School (2013)]

Hybrid Monte Carlo algorithm for QCD

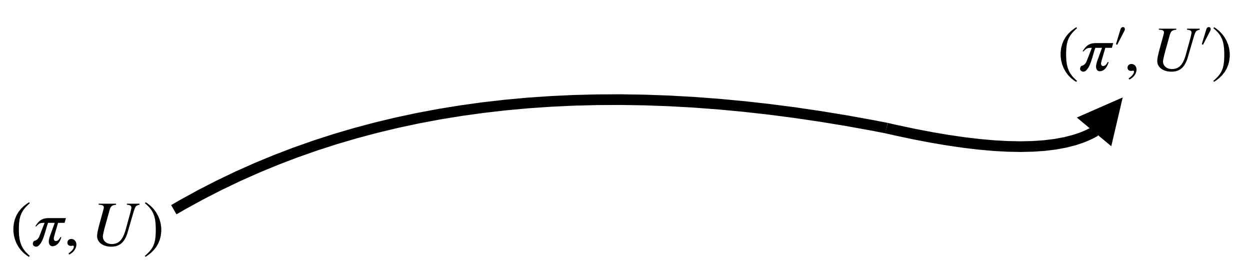
- Most widely used exact method for lattice QCD [Duane, Kennedy, Pendleton, Roweth, Phys. Lett. B, 195 (1987)]

- Introduce momenta $\pi_\mu(n)$ conjugate to fundamental fields $U_\mu(n)$ and the Hamiltonian

$$\mathscr{H} = \frac{1}{2} \sum_{n,\mu} \pi_{n,\mu}^2 + S[U]$$

- **Momentum Heat-bath**: refresh momenta π (Gaussian random numbers)

- **Molecular Dynamics (MD)** evolution of π and U
  - ➡ numerically integrating the corresponding equations of motion (fictitious time τ):

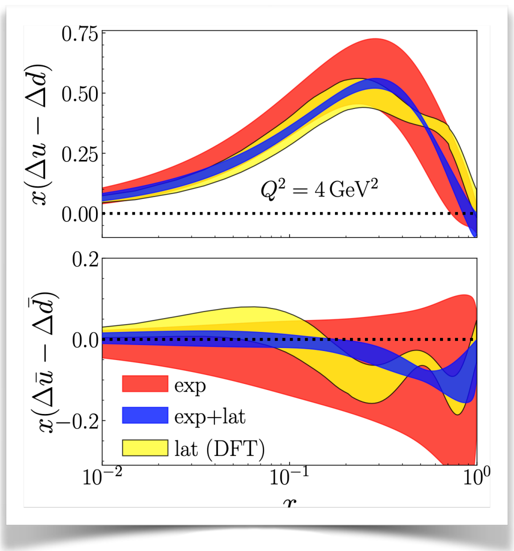


reversible, area-preserving scheme such as leap-frog, Omelyan…

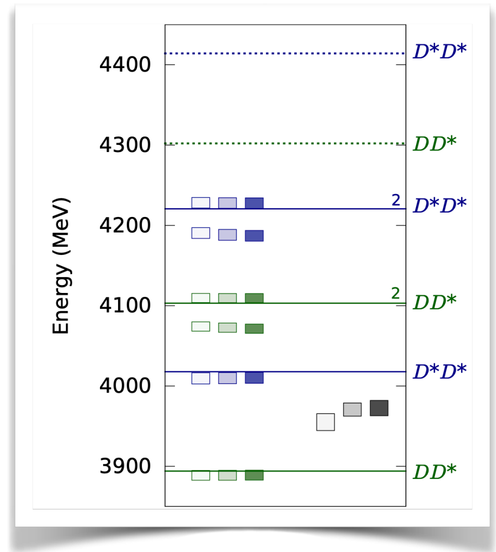
- **Metropolis accept/reject step**
  - ➡ correcting for discretization errors of the numerical integration

$$P_{acc} = min\{1, e^{-(\mathscr{H}(\pi', U') - \mathscr{H}(\pi, U))}\}$$

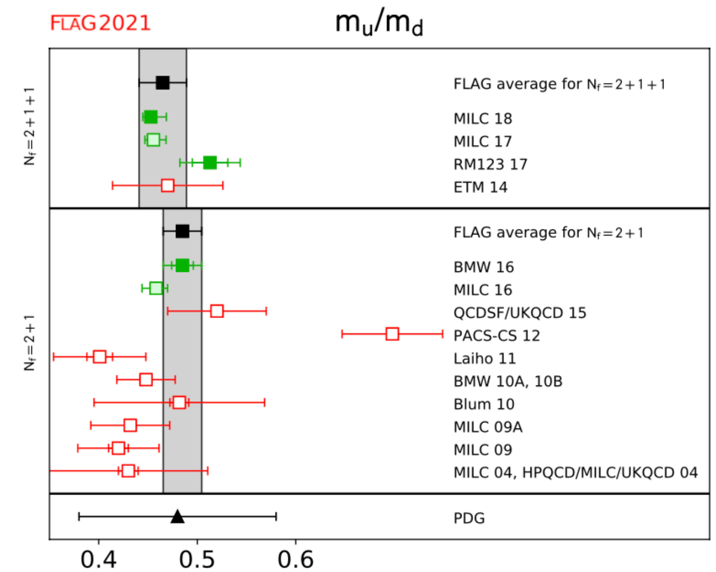
What lattice QCD CAN do?



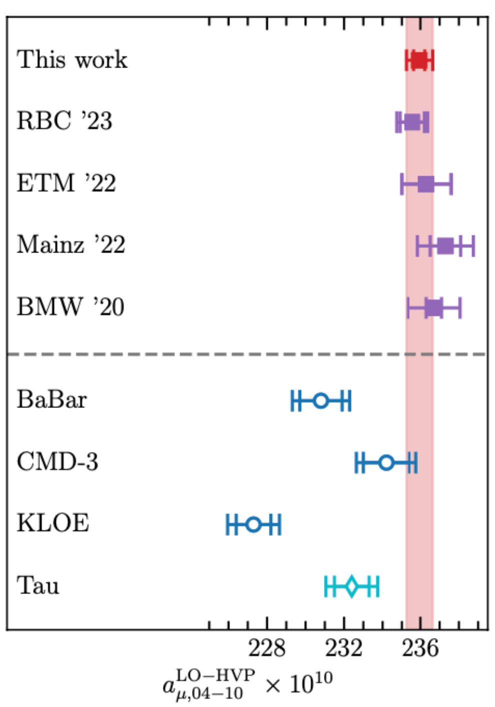
Lattice PDFs [Bringewatt, Sato, Melnitchouk, Qiu, Steffens, Constantinou, 2020]



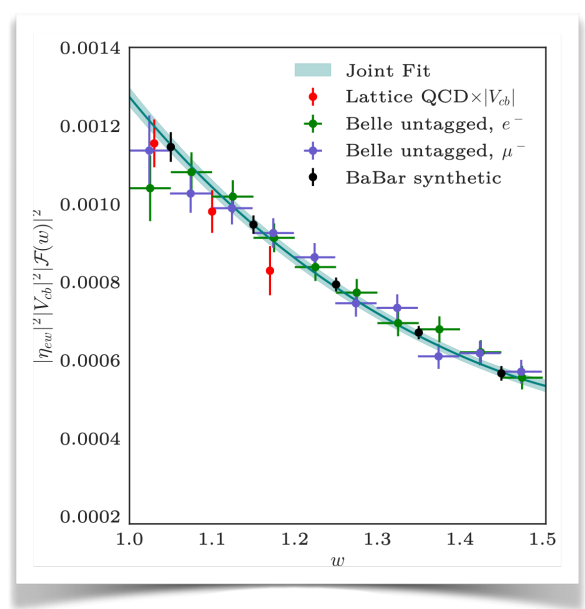
Double-charm FV energy spectrum [Cheung, Thomas, Dudek, Edwards 2017]



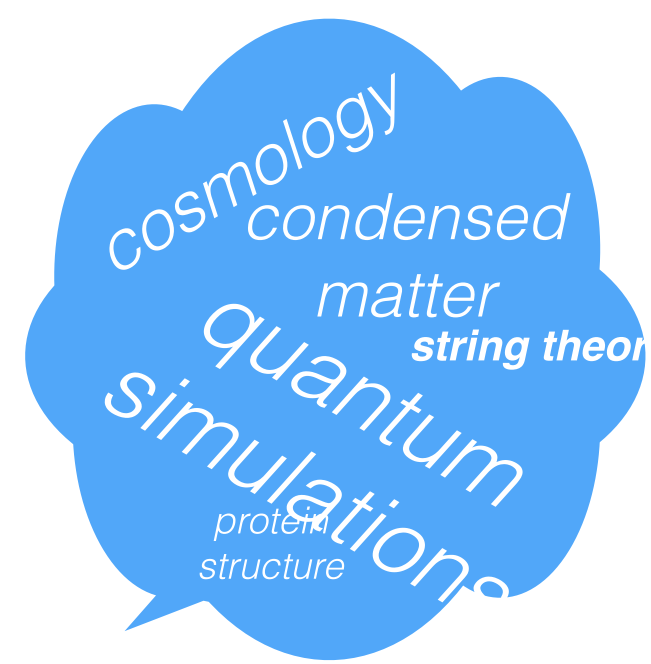
Non-degenerate light quark masses [FLAG 2021]



muon g-2: HVP [BMW Collab. +DMZ Boccaletti et al. 2024]



$|V_{cb}|$ from $B \to D^* l\nu$ [Bazavov et al. 2021]



In this lecture so far:

- QCD can be formulated on a Euclidean space time lattice

- Quantization amounts to summing over all gauge configurations; this can again be computed by Monte Carlo methods

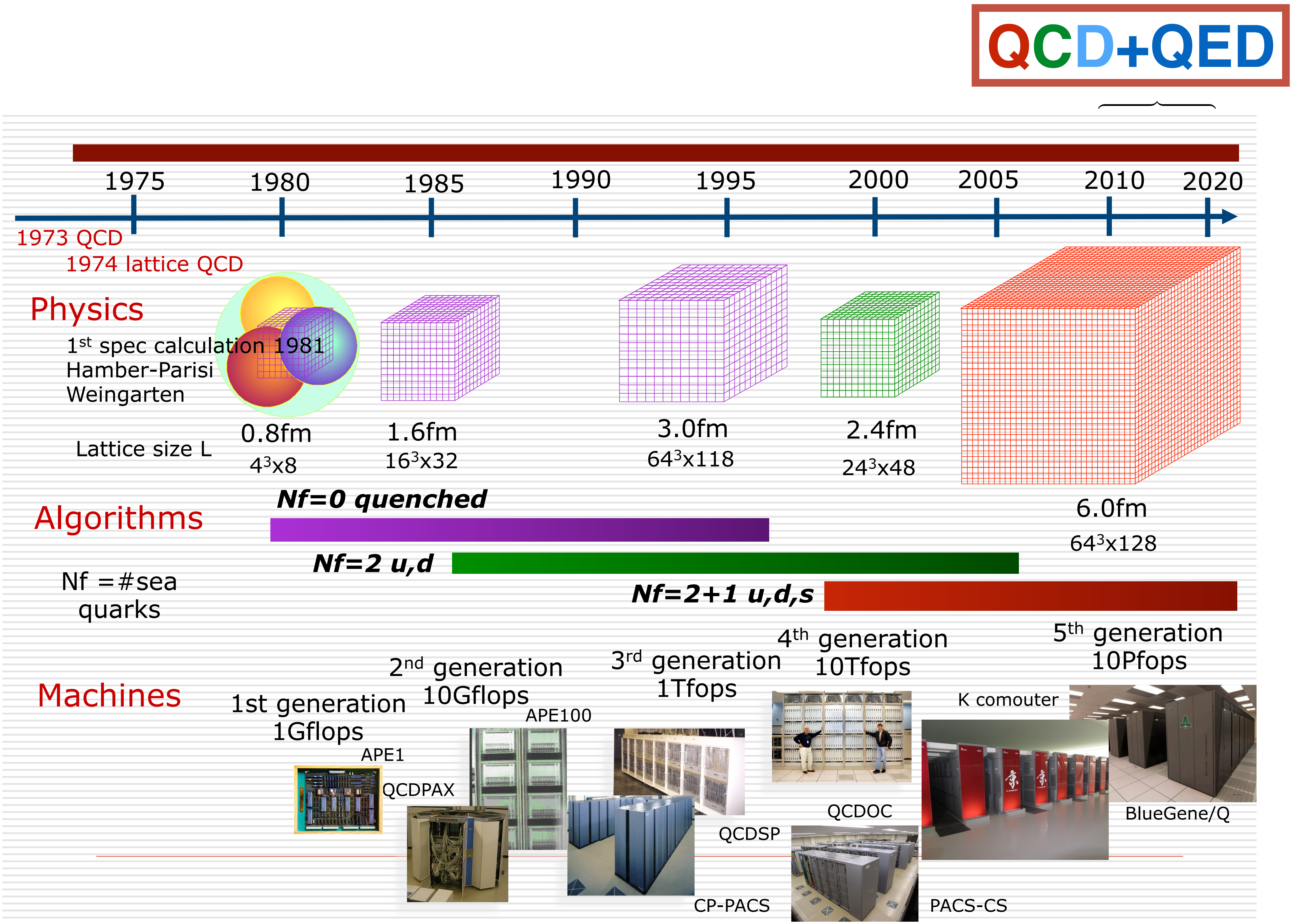
- Different discretizations give different lattice artefacts

  ➡ universal in continuum limit!

- Simulations with dynamical fermions computationally costly; many tricks in algorithms need to be applied

  ➡ precise predictions of hadron spectrum, non-pert. renormalization, muon g-2, CKM matrix elements etc.

Development of Lattice QCD



[Credit: A. Ukawa, HPC Summer School (2013)]

Motivation for Lattice QCD+QED

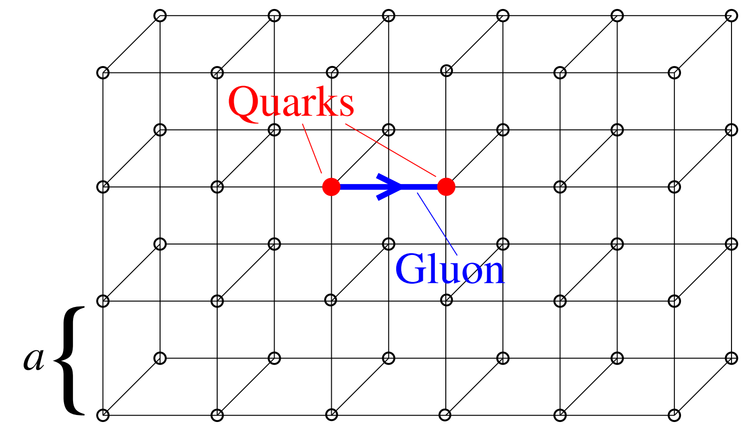
- **QCD on the lattice:**

  ➡ quarks and gluons feel only strong force

  ➡ first decades of lattice QCD with fermions:

  isosymmetric universe: $m_u = m_d$ and $\alpha_{em} = 0$

  ➡ approximate symmetry of QCD

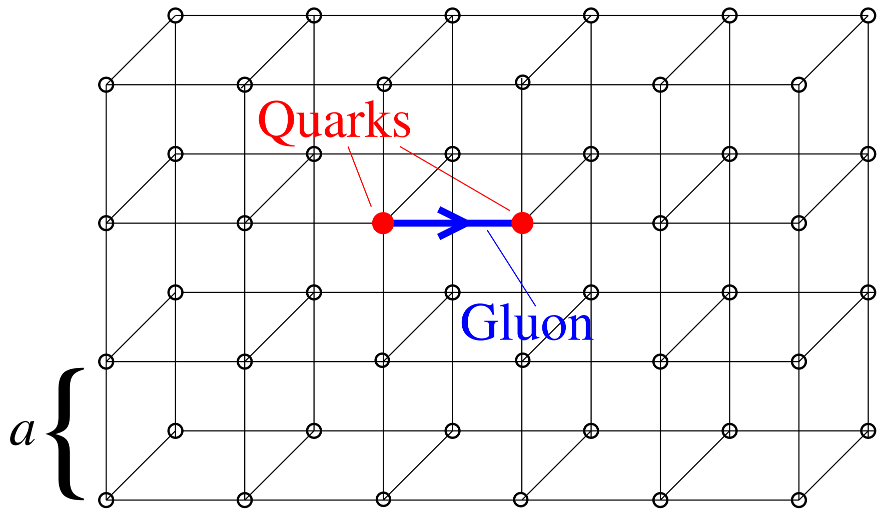


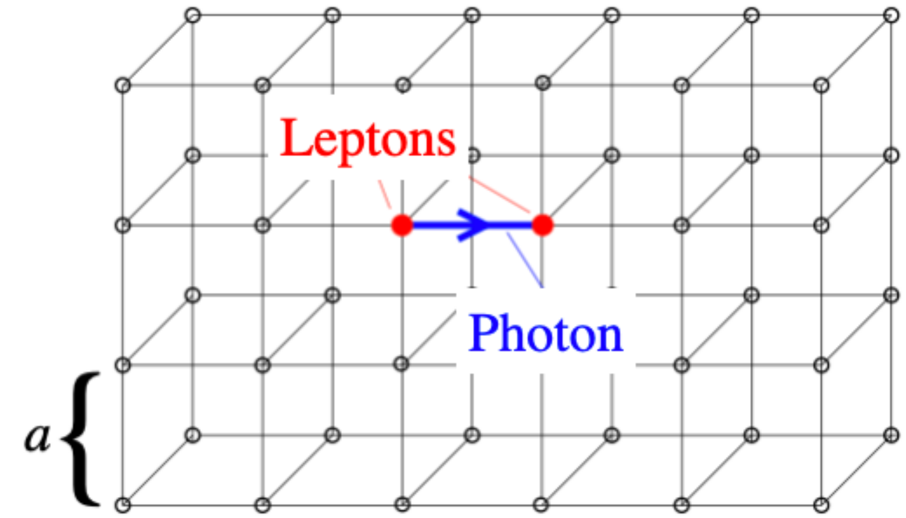
$$\begin{pmatrix} u \\ d \end{pmatrix} \longrightarrow V \begin{pmatrix} u \\ d \end{pmatrix}, \quad V \in SU(2)$$

➡ **Isospin breaking effects**

✳ Have to be taken into account for the **goal precision** of many hadronic observables, e.g. decay rates, HVP $\frac{\delta a_\mu^{HVP}}{a_\mu^{HVP}} < 0.005$

Beyond Isosymmetric Lattice QCD





- **Lattice QCD only**
  - ➡ neglecting/incomplete treatment of **isospin breaking effects**

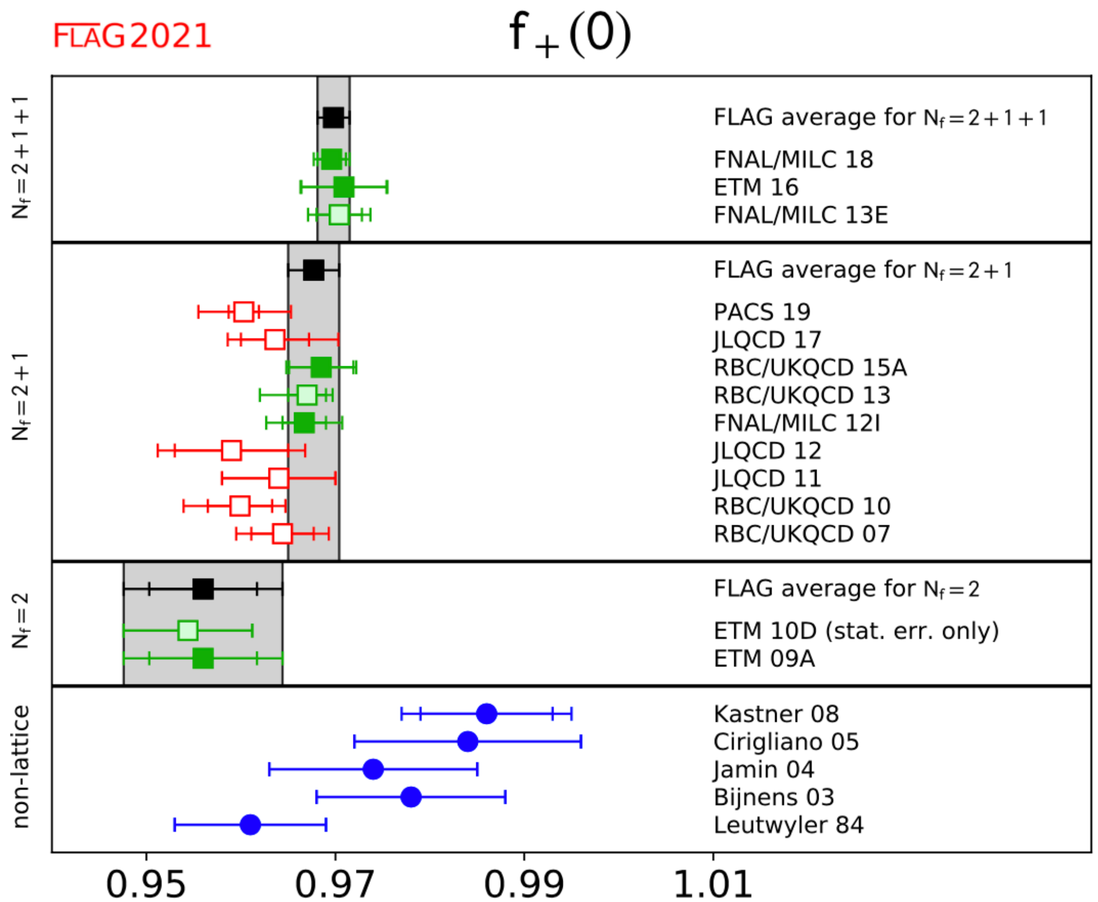
Typically: $m_u = m_d$ **and** $\alpha_{em} = 0$

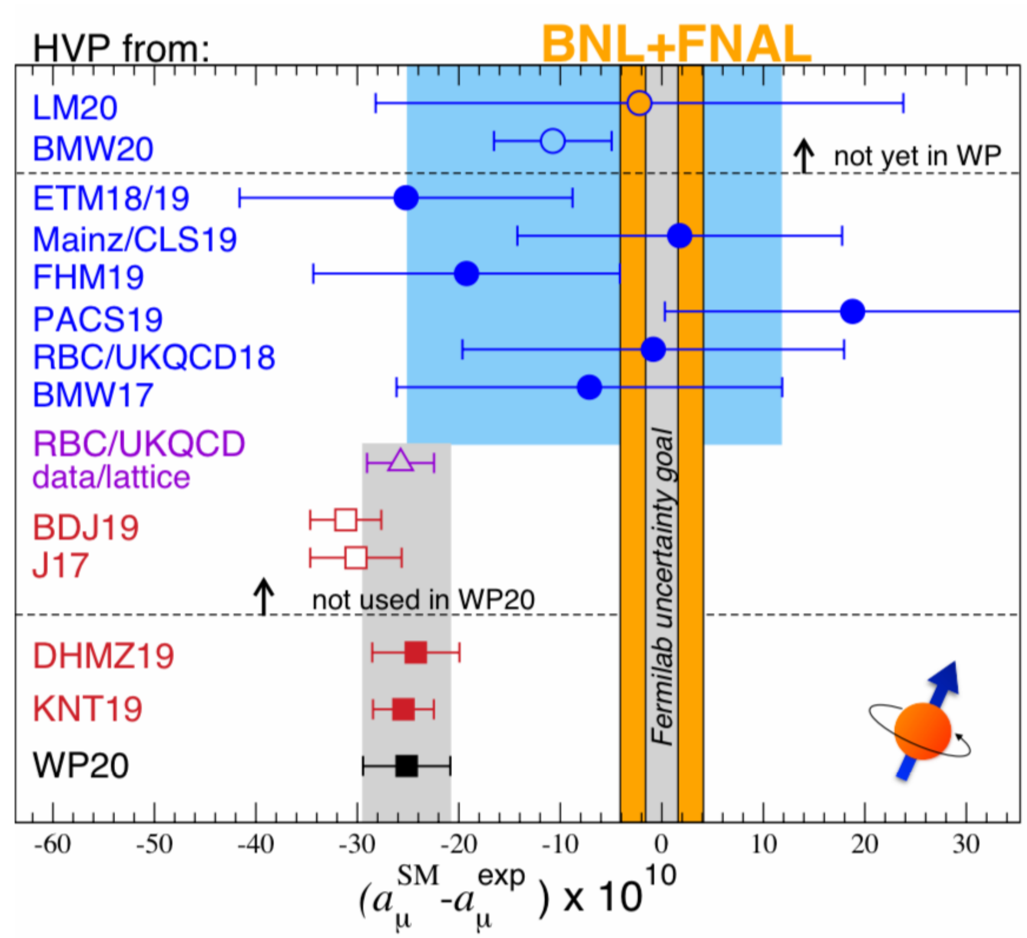
- **Lattice QCD+QED**
  - ➡ Few percent effects: $m_u \neq m_d$ **and** $\alpha_{em} \approx \frac{1}{137}$

$$\frac{m_u - m_d}{M_p} \simeq 0.3\% \qquad \alpha_{\mathrm{EM}} = 0.7\% \qquad \frac{M_n - M_p}{M_n} \simeq 0.1\%$$

Required for precision calculations!

Beyond Isosymmetric Lattice QCD





$$\frac{\Delta f_+(0)}{f_+(0)} \approx 0.002 - 0.003$$

$$\frac{\Delta a_\mu^{HVP}}{a_\mu^{HVP}} \approx 0.005$$

[FLAG21 2111.09849 [hep-lat]]

[Snowmass22 2203.15810 [hep-ph]]

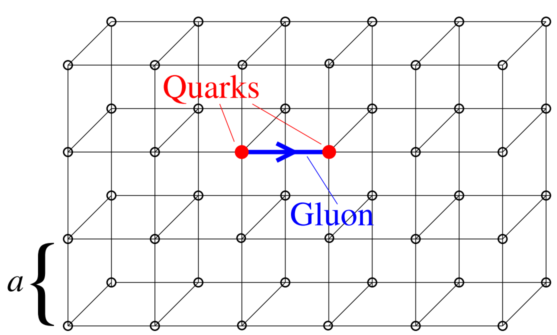
Beyond Isosymmetric Lattice QCD

$m_u \neq m_d$ **and** $\alpha_{em} \neq 0$

➡ expand about isosymmetric theory

QCD TREATED NON-PERTURBATIVELY, α_{em} "SMALL"

[R123: 1303.4896, PRD87(2013)11]

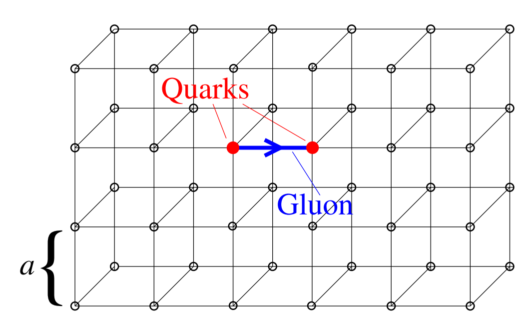


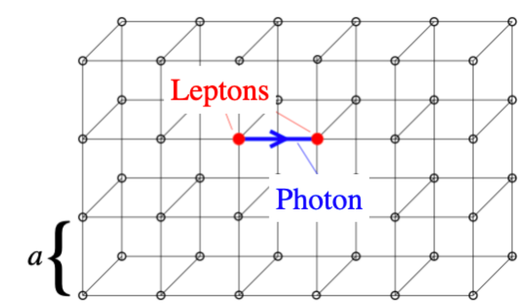
$$O(\alpha_{em}), O(m_u - m_d)$$

➡ simulate QED+QCD

QCD AND QED TREATED NON-PERTURBATIVELY,

[Duncan,Eichten, hep-lat/9602005, PRL76(1996), Blum et al. 0708.0484 *PRD* 76 (2007)114508, …]
[BMW: 1406.4088 Science 347 (2015), QCDSF: 1509.00799, *JHEP* 04(2016) 093, RCstar: 2209.13183 JHEP 03(2023)012, …]





Charged particles don't like boxes

- Challenges with charged particles in a finite box: classical picture

- A solution for gauge invariant interpolating operators of charged particles (C-parity bc's)

- Other prescriptions (pros/cons)

Beyond Isosymmetric Lattice QCD

- QCD+QED action (in continuum):

$$S = \int d^4x \left\{ \frac{1}{2g^2} \mathrm{Tr}\, G_{\mu\nu}G^{\mu\nu} + \frac{1}{4e^2} F_{\mu\nu}F^{\mu\nu} + \sum_f \bar{\psi}_f(\not{D} + m_f)\psi_f \right\} \qquad f = u, d, s, c$$

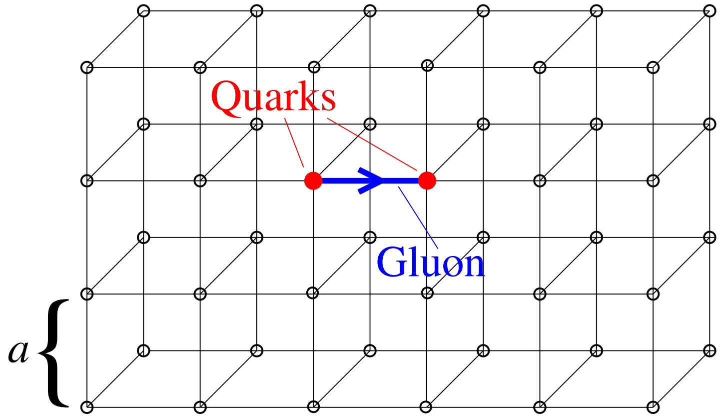
$B_\mu \in SU(3)$ gluon field $\quad A_\mu \in \mathbb{R}$ photon field $\quad D_\mu = \partial_\mu + iB_\mu + iQ_f A_\mu$

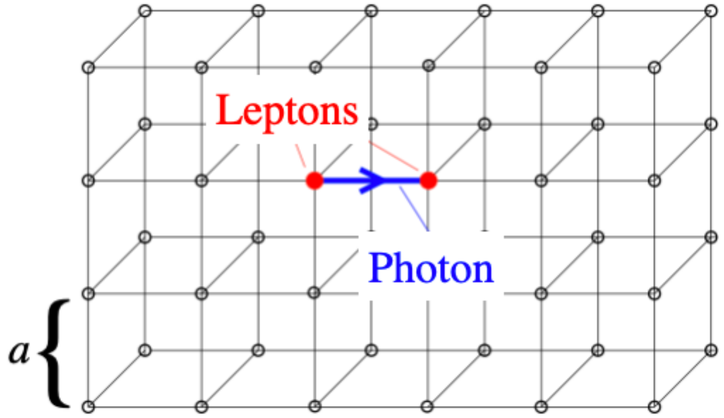
$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \quad Q_u = Q_c = \frac{2}{3} \quad Q_d = Q_s = -\frac{1}{3}$

➡ Gauge symmetries:

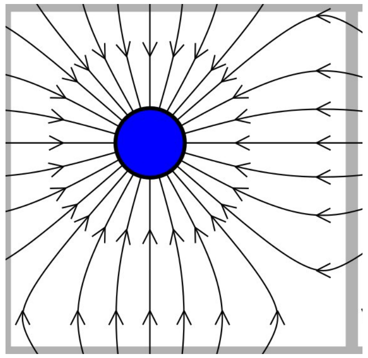
➡ $\Omega(x) \in SU(3): \quad \psi \to \Omega\psi,\ \bar{\psi} \to \bar{\psi}\Omega^\dagger,\ B_\mu \to \Omega B_\mu \Omega^\dagger - i\Omega\partial_\mu\Omega^\dagger$

➡ $\Lambda(x) \in \mathscr{R}: \quad \psi \to e^{iQ\Lambda}\psi,\ \ \bar{\psi} \to \bar{\psi}e^{-iQ\Lambda},\ \ A_\mu \to A_\mu - \partial_\mu\Lambda$





Periodic bc's: classical picture



➡ Maxwell's equations:

$$\vec{\nabla} \cdot \vec{E} = \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \frac{\partial \vec{E}}{\partial t} + \vec{j}$$

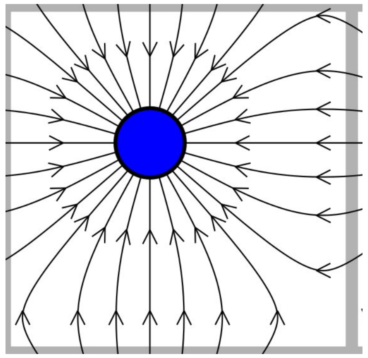
$Q(t)$

Finite (spacial) V:

$\mathbb{R}^4 \longrightarrow \mathbb{R} \times [0,L]^3$, or

$[0,\tau] \times [0,L]^3$

Periodic bc's: classical picture



➡ Maxwell's equations:

$$\vec{\nabla} \cdot \vec{E} = \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \frac{\partial \vec{E}}{\partial t} + \vec{j}$$

$\longrightarrow$ $Q(t)$

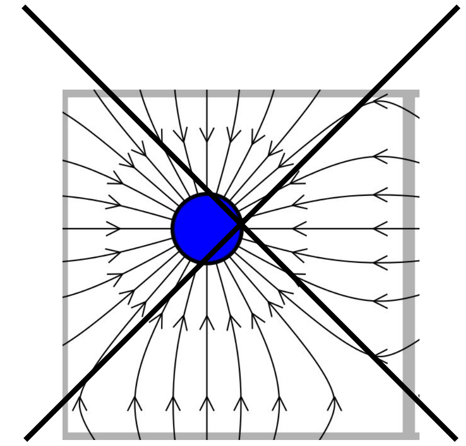
Finite (spacial) V:

$\mathbb{R}^4 \longrightarrow \mathbb{R} \times [0,L]^3$, or

$[0,\tau] \times [0,L]^3$

$$Q(t) = \int_{[0,L]^3} d^3x\, \rho(t, \vec{x}) = \int_{[0,L]^3} d^3x \sum_{k=1}^{3} \partial_k E_k(t, \vec{x}) = \sum_{k=1}^{3} \int_{[0,L]^2} d^2x_\perp^{(k)} \left[E_k(t, \vec{x} + L\hat{k}) - E_k(t, \vec{x})\right]_{x_k=0}$$

Periodic bc's: classical picture



➡ Maxwell's equations:

$$\vec{\nabla} \cdot \vec{E} = \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \frac{\partial \vec{E}}{\partial t} + \vec{j}$$

Finite (spacial) V:

$\mathbb{R}^4 \longrightarrow \mathbb{R} \times [0,L]^3$, or

$[0,\tau] \times [0,L]^3$

$Q(t)$

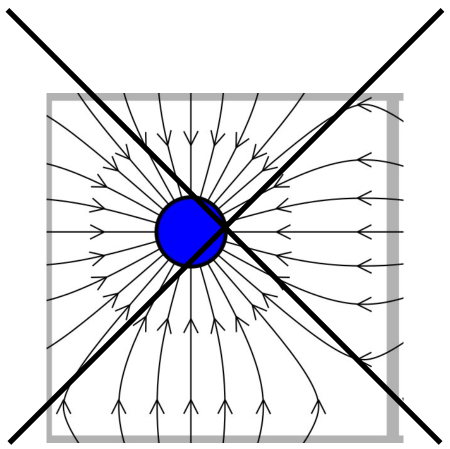
Periodic bc's for $\vec{E}$:

$E_k(t, \vec{x} + L\hat{k}) = E_k(t, \vec{x})$,

thus $Q(t) = 0$

$$Q(t) = \int_{[0,L]^3} d^3x\, \rho(t, \vec{x}) = \int_{[0,L]^3} d^3x \sum_{k=1}^{3} \partial_k E_k(t, \vec{x}) = \sum_{k=1}^{3} \int_{[0,L]^2} d^2x_\perp^{(k)} \left[E_k(t, \vec{x} + L\hat{k}) - E_k(t, \vec{x})\right]_{x_k=0}$$

Periodic bc's: classical picture



➡ Maxwell's equations:

$$\vec{\nabla} \cdot \vec{E} = \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \frac{\partial \vec{E}}{\partial t} + \vec{j}$$

Finite (spacial) V:

$\mathbb{R}^4 \longrightarrow \mathbb{R} \times [0,L]^3$, or

$[0,\tau] \times [0,L]^3$

$Q(t)$

Periodic bc's for $\vec{E}$:

$E_k(t, \vec{x} + L\hat{k}) = E_k(t, \vec{x})$,

thus $Q(t) = 0$

$$Q(t) = \int_{[0,L]^3} d^3x\, \rho(t, \vec{x}) = \int_{[0,L]^3} d^3x \sum_{k=1}^{3} \partial_k E_k(t, \vec{x}) = \sum_{k=1}^{3} \int_{[0,L]^2} d^2x_\perp^{(k)} \left[E_k(t, \vec{x} + L\hat{k}) - E_k(t, \vec{x})\right]_{x_k=0}$$

Alternative bc's: classical picture

- **Non-trivial boundary conditions:** $\varphi(x + L\hat{k}) = B_k(x, \varphi(x), \partial\varphi(x), \partial^2\varphi(x), \ldots)$

- Consistency relation: $\varphi(x + L\hat{j} + L\hat{k}) = \varphi((x + L\hat{j}) + L\hat{k}) = \varphi((x + L\hat{k}) + L\hat{j}) \Rightarrow B_k \circ B_j = B_j \circ B_k$

- The action is translation invariant ⇔ the action is invariant under B_k

- Translational invariance ⇒ B_k can be
  - gauge tranformation
  - flavour transformation
  - charge conjugation

(brace grouping gauge and flavour transformation:) E **is periodic**

Alternative bc's: classical picture

- **Non-trivial boundary conditions:** $\varphi(x + L\hat{k}) = B_k(x, \varphi(x), \partial\varphi(x), \partial^2\varphi(x), \ldots)$

- Consistency relation: $\varphi(x + L\hat{j} + L\hat{k}) = \varphi((x + L\hat{j}) + L\hat{k}) = \varphi((x + L\hat{k}) + L\hat{j}) \Rightarrow B_k \circ B_j = B_j \circ B_k$

- The action is translation invariant ⇔ the action is invariant under B_k

- Translational invariance ⇒ B_k can be
  - gauge tranformation
  - flavour transformation
  - charge conjugation

(gauge tranformation, flavour transformation) } E **is periodic** $\longrightarrow$ **no charged particles in a finite box**

Alternative bc's: classical picture

- **Non-trivial boundary conditions:** $\varphi(x+L\hat{k}) = B_k(x, \varphi(x), \partial\varphi(x), \partial^2\varphi(x), \ldots)$

- Consistency relation: $\varphi(x+L\hat{j}+L\hat{k}) = \varphi((x+L\hat{j})+L\hat{k}) = \varphi((x+L\hat{k})+L\hat{j}) \Rightarrow B_k \circ B_j = B_j \circ B_k$

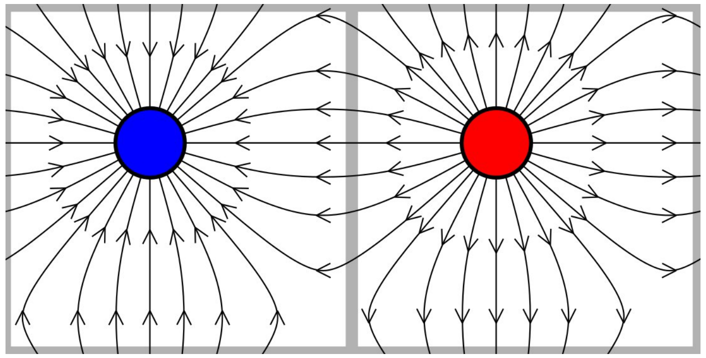
- The action is translation invariant ⇔ the action is invariant under B_k

- Translational invariance ⇒ B_k can be

  - gauge tranformation
  - flavour transformation

  } E **is periodic**

  - charge conjugation (E **is antiperiodic**)



The electic field flux is forced **not to vanish** at the boundary

QCD+QED with C-parity bc's

➡ Photon field: $A_\mu(x+L\hat{k}) = A^{\mathrm{C}}_\mu(x) = -A_\mu(x)$

➡ Quark field: $\Psi(x+L\hat{k}) = \Psi^{\mathrm{C}}(x) = \mathrm{C}\,\overline{\Psi}^{\mathrm{T}}(x)$

$$\overline{\Psi}(x+L\hat{k}) = \overline{\Psi}^{\mathrm{C}}(x) = -\overline{\Psi}^{\mathrm{T}}(x)\,\mathrm{C}^{-1}$$

➡ Gluon field: $B_\mu(x+L\hat{k}) = B^{\mathrm{C}}_\mu(x) = -B^*_\mu(x)$

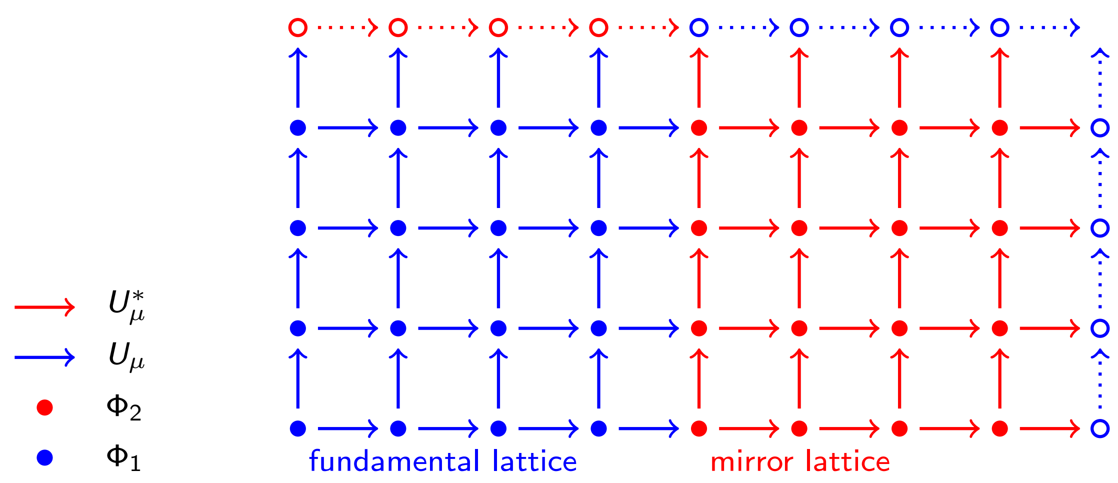
[Wiese, Nucl. Phys. B 375, 45 (1992)]

[Polley, Z. Phys. C 59, 105 (1993)]

[Kronfeld and Wiese, Nucl. Phys. B 357, 521 (1991)]

[Carmona et al., IJMPC 11 (2000) 637-654]

[Lucini et al., JHEP 1602, 076 (2016)]



$$\tilde{U}_\mu(x) = \begin{cases} U_\mu(x) & x \in \text{fundamental lattice} \\ U^*_\mu(x - L\hat{1}) & x \in \text{mirror lattice} \end{cases}$$

$$\tilde{\phi}(x) = \begin{cases} \Phi_1(x) & x \in \text{fundamental lattice} \\ \Phi_2(x - L\hat{1}) & x \in \text{mirror lattice} \end{cases}$$

➡ In Euclidean spacetime: C - charge conjugation matrix, $\mathrm{C}^{\mathrm{T}} = -\mathrm{C}; \quad \mathrm{C}^{-1}\gamma_\mu\mathrm{C} = -\gamma_\mu^T$

➡ Chiral representation of γ-matrices: $\mathrm{C} = -i\gamma_0\gamma_2$

Interpolating operators in QCD

- Interpolating operator for π^+: $P\,(x) = \bar{u}\,\gamma_5\,d\,(x)$
- $P(x)\,|\,0\rangle$ has the same quantum numbers as π^+:

spin: 0 parity: -1 up-number: 1 down-number: -1 strange-number: 0

$$\langle 0\,|\,P^\dagger(x)P(0)\,|\,0\rangle = \langle 0\,|\,P^\dagger e^{-Ht} e^{i\vec{p}\,\vec{x}} P(0)\,|\,0\rangle \underset{t\to\infty}{\simeq} \int d\Omega_P\,|\,\langle \pi^+(\vec{p}\,)\,|\,P(0)\rangle\,|^2\, e^{i\vec{p}\,\vec{x}} e^{-t\sqrt{m_\pi^2 + \vec{p}^{\,2}}}$$

Interpolating operators in QCD (Dirac dressing)

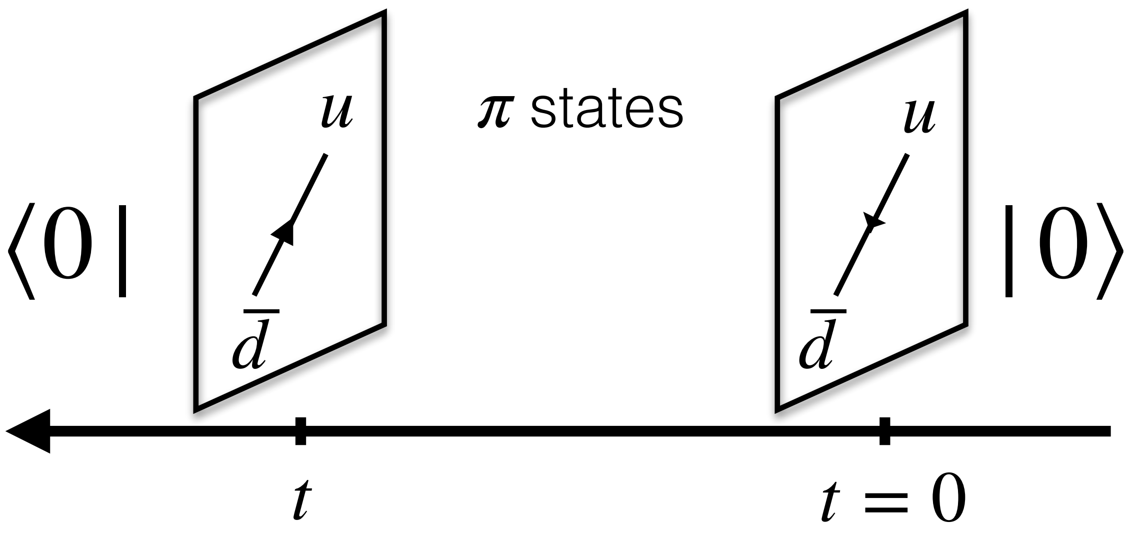
➡ Interpolating operator for π^+: $P\,(x) = \bar{u}\,\gamma_5\,d\,(x)$

➡ $P(x)\,|\,0\rangle$ has the same quantum numbers as π^+:

spin: 0 parity: -1 up-number: 1 down-number: -1 strange-number: 0

➡ Different choice for interpolating operator (Dirac):

$$P\,(x) = \int_{SO(3)} dR\,\bar{u}(t, \vec{x} + R\vec{z})\,\gamma_5\,W(t, \vec{x} + R\vec{z} \leftarrow \vec{x})\,d\,(x)$$



Interpolating operators in QCD (Dirac dressing)

- Interpolating operator for π^+: $P\,(x) = \bar{u}\,\gamma_5\,d\,(x)$
- $P(x)\,|\,0\rangle$ has the same quantum numbers as π^+:

spin: 0   parity: -1   up-number: 1   down-number: -1   strange-number: 0

- Different choice for interpolating operator (Dirac):

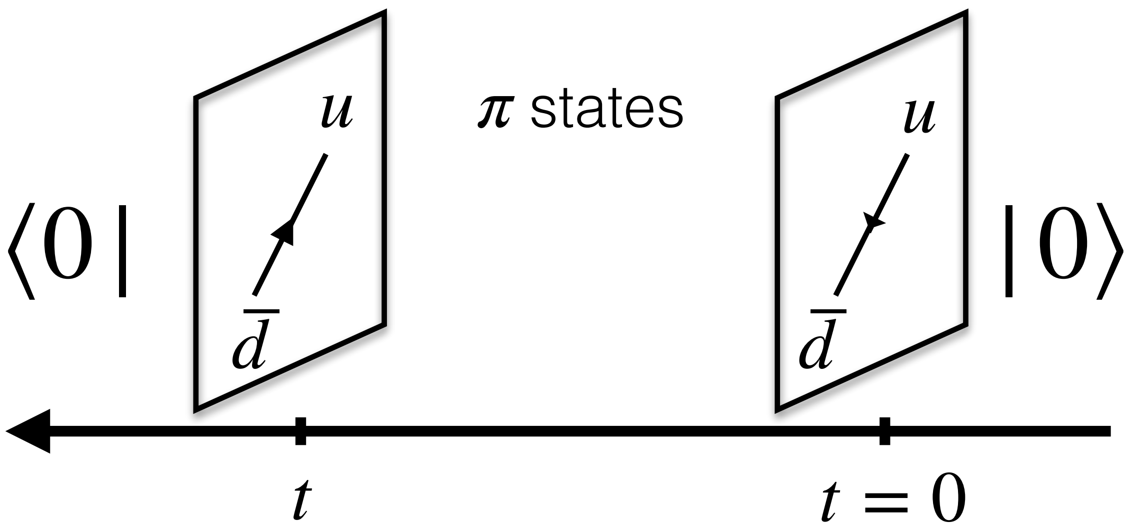
$$P\,(x) = \int_{SO(3)} dR\;\bar{u}(t, \vec{x} + R\vec{z})\,\gamma_5\,W(t, \vec{x} + R\vec{z} \leftarrow \vec{x})\,d\,(x)$$

Main properties:

(1) Desired quantum numbers

(2) Localized on a timeslice

(3) **<u>Invariant under local gauge transformations</u>**



Interpolating operators in QCD+QED

- Interpolating operator for π^+: $P(x) = \bar{u}\,\gamma_5\,d(x)$
- Under $U(1)$ gauge transformation: $\bar{u}(x) \rightarrow e^{-i\frac{2}{3}\Lambda(x)}\,\bar{u}(x)$

$$d(x) \rightarrow e^{-i\frac{1}{3}\Lambda(x)}\,d(x)$$

$$\left.\begin{matrix} \bar{u}(x) \rightarrow e^{-i\frac{2}{3}\Lambda(x)}\,\bar{u}(x) \\ d(x) \rightarrow e^{-i\frac{1}{3}\Lambda(x)}\,d(x) \end{matrix}\right\} \quad P(x) \rightarrow e^{-i\Lambda(x)}\,P(x)$$

Physical observables and physical states are invariant under local gauge transformations!

$$P(x) = e^{-i\int d^3y\, G(\overrightarrow{y}-\overrightarrow{x})\overrightarrow{\nabla}\overrightarrow{A}(x_0,\overrightarrow{y})}\,\bar{u}\,\gamma_5\,d(x), \quad \overrightarrow{\nabla}^2 G(\overrightarrow{x}) = \delta^3(\overrightarrow{x})$$

[P. Dirac 1955]

Interpolating operators in QCD+QED

- Interpolating operator for π^+: $P(x) = \bar{u}\,\gamma_5\,d(x)$
- Under $U(1)$ gauge transformation: $\bar{u}(x) \to e^{-i\frac{2}{3}\Lambda(x)}\,\bar{u}(x)$, $d(x) \to e^{-i\frac{1}{3}\Lambda(x)}\,d(x)$ $\Big\}$ $P(x) \to e^{-i\Lambda(x)}\,P(x)$

Physical observables and physical states are invariant under local gauge transformations!

$$P(x) = e^{-i\int d^3y\, G(\vec{y}-\vec{x})\vec{\nabla}\vec{A}(x_0,\vec{y})}\,\bar{u}\,\gamma_5\,d(x), \quad \vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x})$$

[P. Dirac 1955]

> “It is found that the gauge-invariant operation of creation of an electron involves the simultaneous creation of an electron and of the Coulomb field around it. The requirement of manifest gauge invariance prevents one from using the concept of an electron separated from its Coulomb field.”

Interpolating operators in QCD+QED

- ➡ Interpolating operator for π^+: $P(x) = \bar{u}\,\gamma_5\,d(x)$
- ➡ Under $U(1)$ gauge transformation: $\left.\begin{aligned} \bar{u}(x) &\to e^{-i\frac{2}{3}\Lambda(x)}\,\bar{u}(x) \\ d(x) &\to e^{-i\frac{1}{3}\Lambda(x)}\,d(x) \end{aligned}\right\}\quad P(x) \to e^{-i\Lambda(x)}\,P(x)$

Physical observables and physical states are invariant under local gauge transformations!

$$P(x) = e^{-i\int d^3y\, G(\vec{y}-\vec{x})\vec{\nabla}\vec{A}(x_0,\vec{y})}\,\bar{u}\,\gamma_5\,d(x), \quad \vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x})$$

[P. Dirac 1955]

(1) Desired quantum numbers

(2) Localized on a timeslice

(3) Invariant under local gauge transformations

} not a unique construction!

This construction of the interp. operator. works $\Leftrightarrow$ $\vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x})$ admits a solution. (b.c.'s dependent)

Interpolating operators in QCD+QED

- Interpolating operator for π^+: $P(x) = \bar{u}\,\gamma_5\,d(x)$
- Under $U(1)$ gauge transformation: $\bar{u}(x) \to e^{-i\frac{2}{3}\Lambda(x)}\,\bar{u}(x)$, $d(x) \to e^{-i\frac{1}{3}\Lambda(x)}\,d(x)$ $\Big\}$ $P(x) \to e^{-i\Lambda(x)}\,P(x)$

Physical observables and physical states are invariant under local gauge transformations!

$$P(x) = e^{-i\int d^3y\, G(\vec{y}-\vec{x})\vec{\nabla}\vec{A}(x_0,\vec{y})}\,\bar{u}\,\gamma_5\,d(x), \quad \vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x})$$

[P. Dirac 1955]

(1) Desired quantum numbers

(2) Localized on a timeslice

(3) Invariant under local gauge transformations

$\Big\}$ not a unique construction!

This construction of the interp. operator. works $\Leftrightarrow$ $\vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x})$ admits a solution. (**b.c.'s dependent**)

Interpolating operators in QCD+QED

$$P(x) = e^{-i \int d^3y \, G(\vec{y}-\vec{x}) \vec{\nabla} \vec{A}(x_0,\vec{y})} \, \bar{u} \, \gamma_5 \, d\,(x)$$

such that: $\vec{\nabla}^2 G(\vec{x}) = \delta^3(\vec{x}) \quad \longrightarrow \quad -\vec{p}^{\,2} \hat{G}(\vec{p}) = 1$

(1) Infinite Volume:

$$G(\vec{x}) = -\int \frac{dp^3}{(2\pi)^3} \frac{e^{i\vec{p}\,\vec{x}}}{\vec{p}^{\,2}} = -\frac{1}{4\pi \vec{x}}$$

(2) Finite Volume with periodic b.c.'s

$$\vec{p} = \frac{2\pi}{L}(n_x, n_y, n_z), \qquad n_k \in \mathbb{Z} \quad \longrightarrow \quad \hat{G}(\vec{0}) = -\frac{1}{0} \;!!!$$

} **no solution for** $G(\vec{x})$

(3) Finite Volume with C-parity b.c.'s

$$\vec{p} = \frac{\pi}{L}(2n_x+1, 2n_y+1, 2n_z+1), \quad n_k \in \mathbb{Z} \quad \longrightarrow \quad \hat{G}(\vec{x}) = -\frac{1}{L^3} \underbrace{\sum_{\vec{p}} \frac{e^{i\vec{p}\,\vec{x}}}{\vec{p}^{\,2}}}$$

well defined solution for $G(\vec{x})$

Discussed so far:

- **Motivation for lattice QCD+QED**
- **Challenges with charged particles in a finite box: classical picture**
- **A solution for gauge invariant interpolating operators of charged particles (C-parity bc's)** $[QED_{\mathrm{C}}]$

In the next part:

- Motivation for lattice QCD+QED
- Challenges with charged particles in a finite box: classical picture
- A solution for gauge invariant interpolating operators of charged particles (C-parity bc's) $[QED_{\rm C}]$
- **Other prescriptions (pros/cons):**
  - ➡ $QED_{\rm TL}/QED_{\rm L}$ (pure IB effects, baryon spectrum, mass splittings, HVP IB effects, …)
  - ➡ $QED_{\rm M}$ **massive photon** (decay rates, muon g-2)
  - ➡ QED_{∞} (HLbL, mass splittings)

Many ways to QCD+QED

➡ continuum: $$\alpha_{em} \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2} \cdots$$

➡ lattice: $$\frac{\alpha_{em}}{V} \sum_k \frac{1}{k^2} \cdots$$

- Four perscriptions to go around this:

➡ **Modify gauge filed**: removing the global zero-mode/ spatial zero mode per timeslice ($QED_{\rm TL}/QED_{\rm L}$) [PRL76(1996), Prog. Theor. Phys. 120(2008)413, Science 347 (2015) 1406.4088, …]

➡ **Massive photon** [PRL 117 (2016) 7, PoS LATTICE2021 (2022) 281]

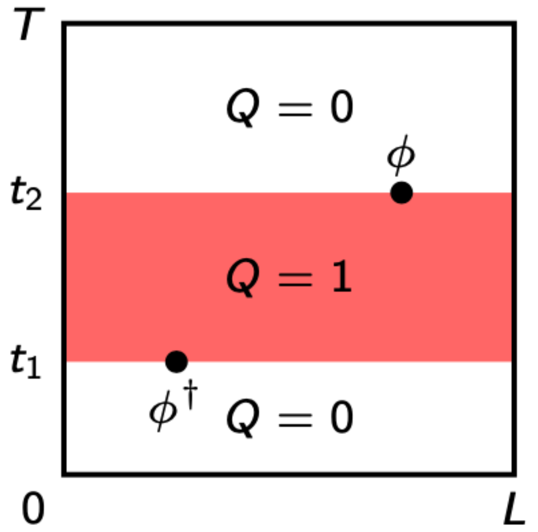
➡ QED_∞ [Phys. Rev. D 96 (2017), Phys. Rev. D 100 (2019) 094509]

➡ **C* boundary conditions** (no zero-mode present) [JHEP 1602, 076, EPJC 80 (2020) 3, JHEP03(2023)012]

Modify gauge field: $QED_{\mathrm{TL}}/QED_{\mathrm{L}}$ approach

- **Removing the global zero-mode**/ spatial zero mode per timeslice ($QED_{\mathrm{TL}}/QED_{\mathrm{L}}$)
  [Duncan,Eichten, PRL76(1996)]

$$z_\mu = eL_\mu \int d^4x A_\mu(x)$$



- QED action: $$S_{QED}\left(\frac{1}{eL_\mu} z_\mu + A'_\mu\right) = S(A'_\mu) + \frac{1}{L_\mu} z_\mu \int d^4 \rho_\mu(x)$$

- Integration over the zero modes:

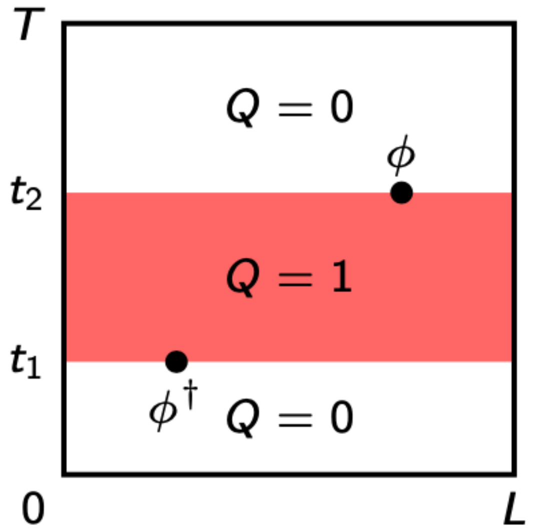
$$T = L_0, \quad \frac{1}{T}\int dx_0 j_0(x) = \frac{t_2 - t_1}{T}$$

$$\int dz_\mu \, e^{-S(z,A')} = e^{-S(0,A')} \prod_\mu \delta\left(\frac{1}{L_\mu}\int d^4x \rho_\mu(x)\right)$$

Modify gauge field: $QED_{\mathrm{TL}}/QED_{\mathrm{L}}$ approach

- **Removing the global zero-mode**/ spatial zero mode per timeslice ($QED_{\mathrm{TL}}/QED_{\mathrm{L}}$)
  [Duncan,Eichten, PRL76(1996)]

$$z_\mu = eL_\mu \int d^4x A_\mu(x)$$



- QED action: $$S_{QED}\left(\frac{1}{eL_\mu} z_\mu + A'_\mu\right) = S(A'_\mu) + \frac{1}{L_\mu} z_\mu \int d^4 \rho_\mu(x)$$

- Integration over the zero modes:

$$\int dz_\mu\, e^{-S(z,A')} = e^{-S(0,A')} \prod_\mu \delta\left(\frac{1}{L_\mu}\int d^4x \rho_\mu(x)\right)$$

$$T = L_0, \quad \frac{1}{T}\int dx_0 j_0(x) = \frac{t_2 - t_1}{T}$$

- Configurations where charged state is created between two interpolating operators are excluded by $\delta\left(\frac{1}{L_\mu}\int d^4x \rho_\mu(x)\right)$

- No transfer matrix, 2-pt. function does not have a spectral decomposition [Borsanyi et al., Science 347 1406.4088]

- In practice: $L, T \longrightarrow \infty$ **limit should be taken before fitting plateaux in effective masses and $a \to 0$ limit**

Modify gauge field: $QED_{\mathrm{TL}}/QED_{\mathrm{L}}$ approach

- **Removing** the global zero-mode/ **spatial zero mode** per timeslice ($QED_{\mathrm{TL}}/QED_{\mathrm{L}}$)
  [Hayakawa and Uno, Prog. Theor. Phys. 120(2008)413, Borsanyi et al., Science 347 1406.4088,]

$$z_\mu(t) = \int d^3x A_\mu(t,x)$$

- Pro: QED_{L} has a transfer matrix

- Cons: it is a nonlocal prescription. Locality is a core property of QFT, and a fundamental assumption behind:
    - Renormalizability by power counting
    - Volume-independence of renormalization constants
    - Operator product expansion
    - Effective-theory description of long-distance physics
    - Symanzik improvement program

- In practice: $L, T \longrightarrow \infty$ **limit should be taken before** $a \to 0$ **limit**

Massive Photon: $QED_{\rm m}$

- **Massive photon** [Endres et al. PRL 117(2016), Bussone et al. EPJ WC:06005(2018), Clark et al. PoS LATTICE2021 (2022) 281]

$$S_\gamma = \int d^4x \frac{1}{e^2}\left\{ \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2\xi}(\partial_\mu A_\mu)^2 + \frac{1}{2}m_\gamma A_\mu^2 \right\}$$

- Landau gauge + mass term for the photon
- Pros: Locality is preserved

  Gauge invariance is broken in a controlled way (soflty broken)
- In practice:
  - **$a \to 0$ limit can be taken before $L, T \to \infty$ limit and $m_\gamma \to 0$ limit**
  - **$L, T \to \infty$ limit must be taken before the $m_\gamma \to 0$ limit**
- Competing effect: suppresses charged states and $L, T \to \infty$
- 2-pt. function: $\lim_{m_\gamma \to 0} \langle \psi(x)\psi(0) \rangle = 0 + \text{ contact terms}$
- In Minkowski spacetime, the theory is not manifestly unitary (negative-norm states)

Infinite-Volume QED: QED_∞

- QED_∞ [Blum et al, Phys. Rev. D 96 (2017), Feng, Jun, Phys. Rev. D 100, 094509 (2019), Feng, Jin, Riberdy, PRL 128 (2022) no.5, 052003, …]
- Original method for HLbL&HVP:
  - QED treated analytically
  - No power-law corrections, FV effects exponentially suppressed by the size of the system
- Stable hadron masses:
  - absolute size exonentially supressed, but
  - corerction still is only power-law suppressed compared with the correction functions
- Gauge fixing needed
- New proposal: allows for exponentially suppressed corrections also for hadron masses [Feng, Jun, Phys. Rev. D 100, 094509 (2019), Feng, Jin, Riberdy, PRL 128 (2022) no.5, 052003]

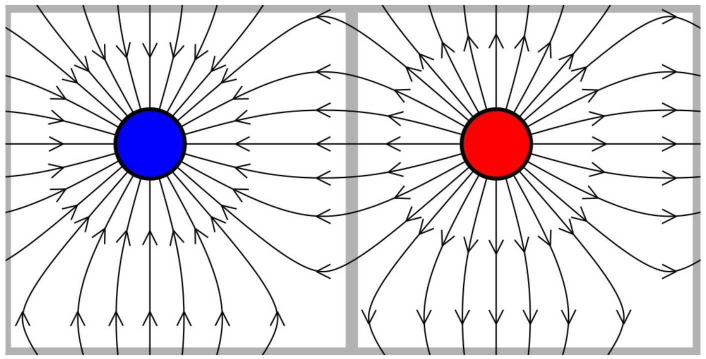
QED with C-parity boundary conditions

[Lucini et al., JHEP 1602, 076 (2016)]

[Campos et al. Eur.Phys.J.C 80 (2020) 3, Bushnaq et al. JHEP03(2023)012]

- **C* boundary conditions**
- Translations: momentum is conserved
- Charge conjugation, parity, **locality**, gauge invariance: preserved
- Flavour and charge conservation are partially violated:

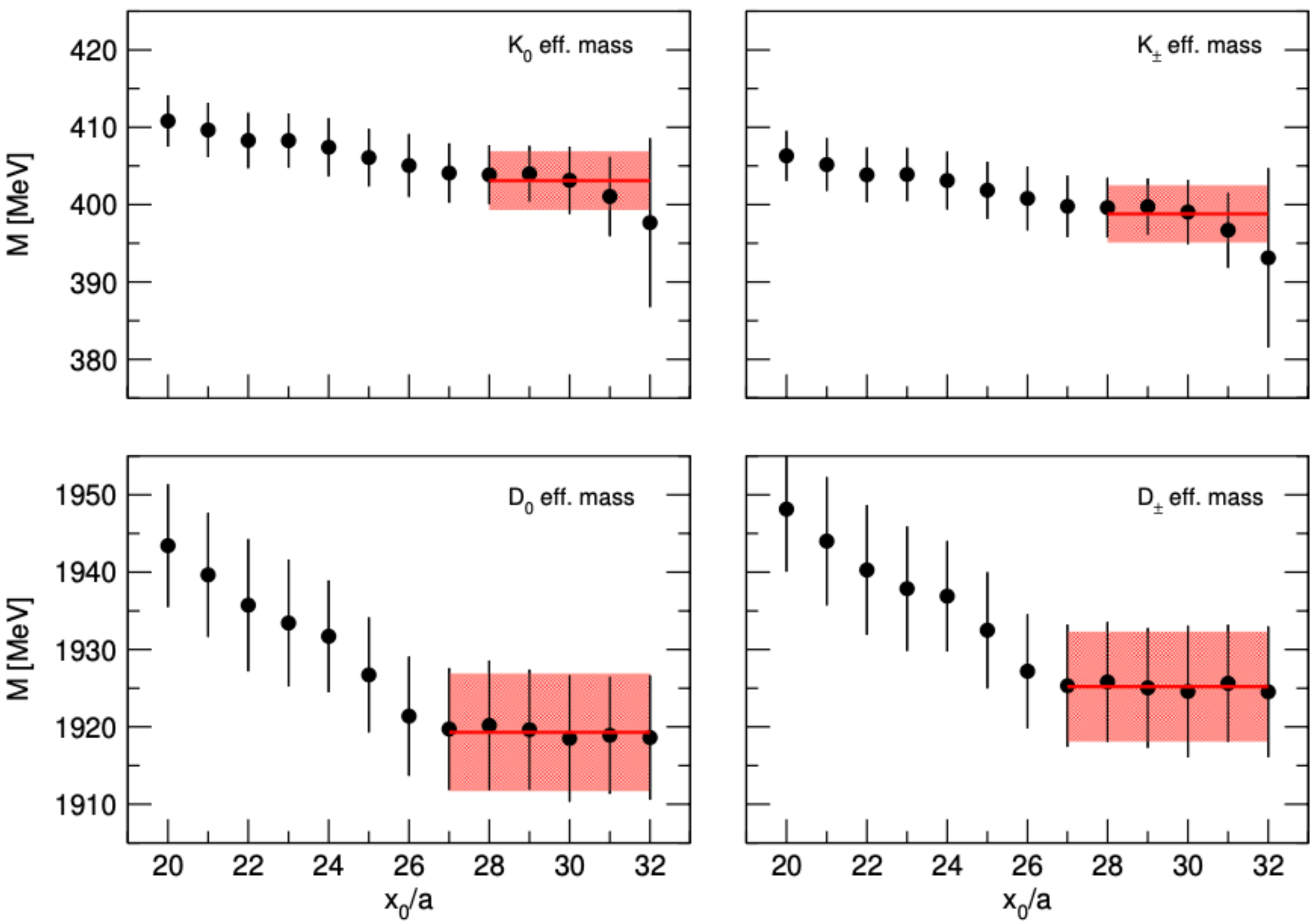
$$\psi_f \to e^{i\alpha}\psi_f, \quad \bar{\psi}_f \to e^{-i\alpha}\bar{\psi}_f, \quad e^{i\alpha} = \pm 1 \qquad [\,(-1)^{F_f} \text{ is conserved }]$$



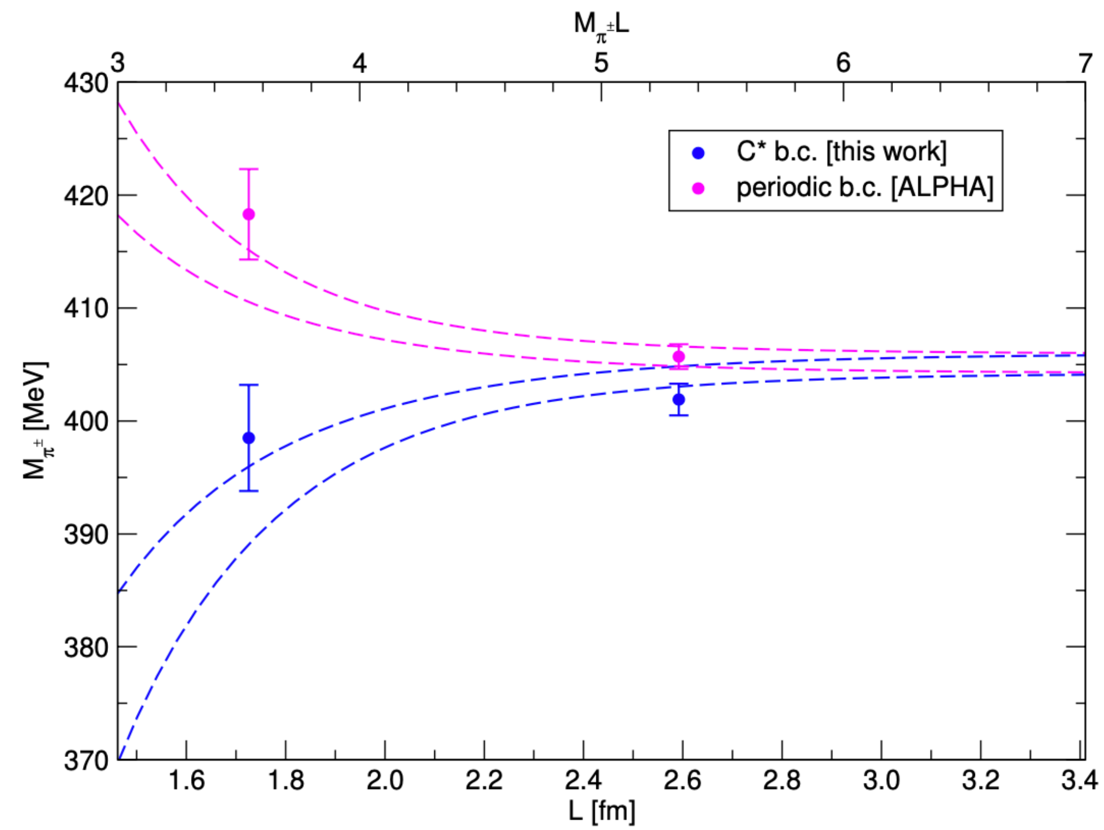
The electic field flux is forced **not to vanish** at the boundary

- In practice:
  - **$a \to 0$ limit can be consistently taken before $L, T \to \infty$ limit**
  - **Electric charge is a linear combination of flavour charges** $Q = \sum_f n_f q_{el} F_f$
    - Unphysical decay of a few hadrons (baryons), but most protected
    - In n-point functions involving the non-protected hadrons, $L \to \infty$ must be taken before the $t \to \infty$ limit

Dynamical QCD+QED with C-parity b.c.'s



[Bushnaq et al. JHEP03(2023)012]



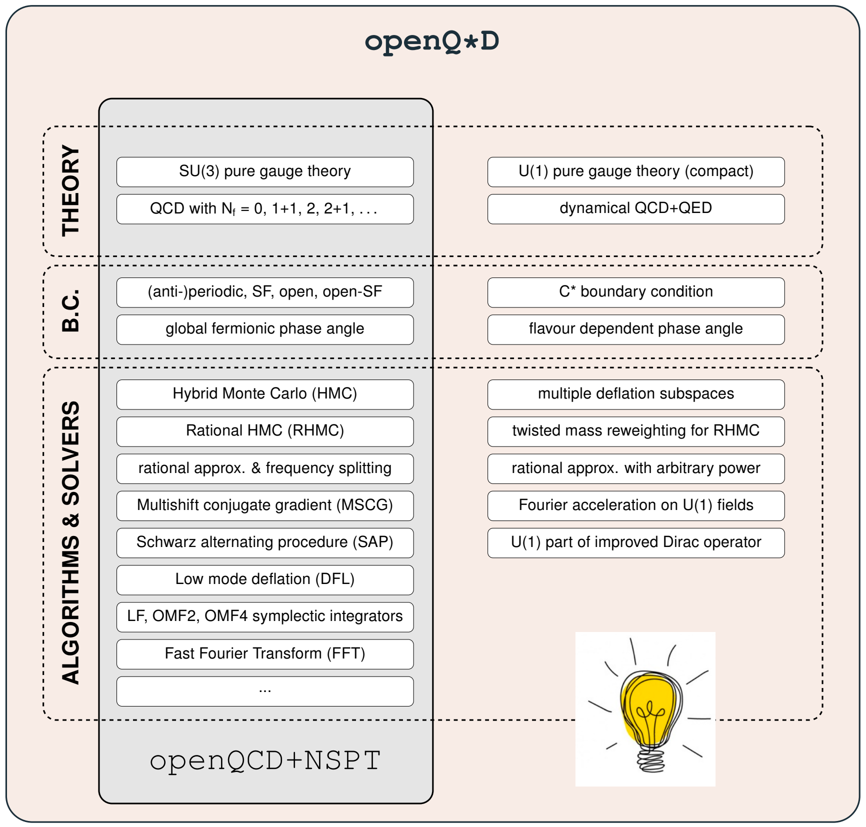
[Campos et al. Eur.Phys.J.C 80 (2020) 3, Bushnaq et al. JHEP03(2023)012]

openQ*D: a versatile code for QCD+QED simulations

[**openQ*D:** https://gitlab.com/rcstar/openQxD]

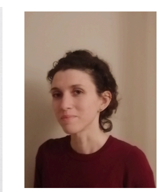
[Campos, Fritzsch, Hansen, MKM, Patella, Ramos, Tantalo Eur.Phys.J.C 80 (2020) 3]

[I. Campos, P. Fritzsch, M. Hansen, MKM, A. Patella, A. Ramos, N. Tantalo EPJ Web Conf. 175 (2018)]

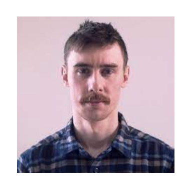
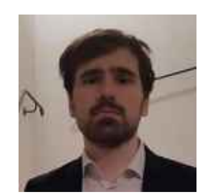


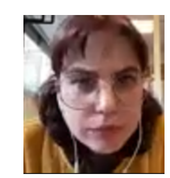




A. Altherr P. Tavella J. Komijani S. Rosso G. Ray L. Parato



R. Gruber T.Harris A. Cotellucci G. La Scala F. Margari A. De Santis

interTwin

Summary of Lattice Q(C+E)D

- **Motivation for lattice QCD+QED**

- **Challenges with charged particles in a finite box: classical picture**

- **A solution for gauge invariant interpolating operators of charged particles (C-parity bc's)** $[QED_{\mathrm{C}}]$

- **Other prescriptions (pros/cons):**

    - ➡ $QED_{\mathrm{TL}}/QED_{\mathrm{L}}$ (pure IB effects, baryon spectrum, mass splittings, HVP IB effects, …)

    - ➡ QED_{M} **massive photon** (decay rates, muon g-2)

    - ➡ QED_{∞} (HLbL, mass splittings)

Not covered in this lecture

- **How to choose the renormalization scheme for QCD+QED** [https://indico.ph.ed.ac.uk/event/257/]
- **Detailed discussion of FV corrections** [A. Patella, arXiv:1702.03857]
- **Applications to HLbL contribution to the muon g-2** [Phys.Rept.887, arXiv:2006.04822] [Snowmass22 2203.15810]
- **Application to decay rates** [see e.g. N. Tantalo 2301.02097 LATT22, M.Di Carlo LATT23]
- ...

High Performance Computational Physics @ ETH zürich


+ A. Altherr


+ P. Tavella


+ R. Gruber


+ J. Pinto Baros

FNSNF

PAULI CENTER for Theoretical Studies

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

European Commission

Google Research

IONQ

AQT

QC QUANTUM CENTER

IBM Quantum

Sandia National Laboratories

ETH AI CENTER

- HPCP lab, July 2024

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

IT Services

Thank you!

Additional slides:

- **Methods for computing IB corrections**

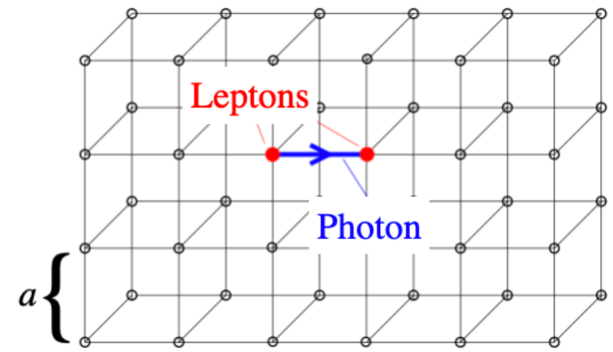
  - **Isospin breaking (IB) effects to hadronic observables** (dynamical $QCD + QED$, $QCD + QED_q$)

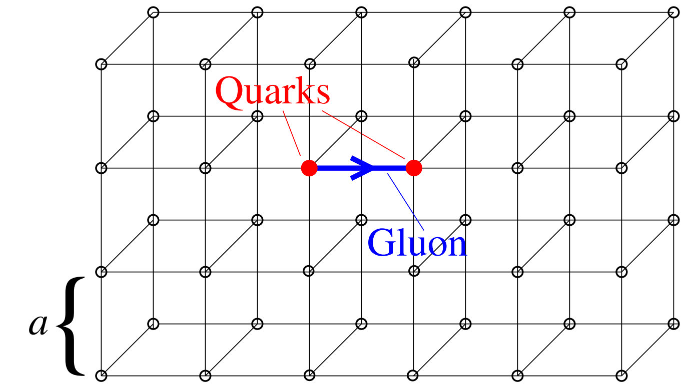
  - **Expanding about isosymmetric QCD** (dynamical QCD + perturbative QED)

- **Numerical results and applications**

- **Open questions and prospects** (what can you do?)

QCD+QED on the lattice





Non compact formulation
(+gauge fixing)

$$S_\gamma = a^4 \sum_{x\mu\nu} \frac{1}{e^2} \left\{ \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{\lambda}{2} (\hat{\partial}^*_\mu A_\mu)^2 \right\}$$

$A_\mu \in \mathbb{R}$ photon field

$$F_{\mu\nu} = \hat{\partial}_\mu A_\nu - \hat{\partial}_\nu A_\mu$$

Compact formulation
(gauge invariant)

$$S_\gamma = \frac{1}{2e^2 q_{el}^2} \sum_{x\mu\nu} \left\{ 1 - U_{\mu\nu}(x) \right\}$$

$v_\mu \in U(1)$ photon link variable

$$v_\mu(x) = e^{iaq_{el}A_\mu(x)}$$

Wilson's Dirac Operator: $D_f = m_f + \frac{1}{2} \sum_\mu \{\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - \nabla^*_\mu \nabla_\mu\}$

$$\nabla_\mu \psi(x) = \frac{1}{a}\left[U_\mu(x)\, e^{iaqA_\mu(x)}\, \psi(x+\hat{\mu}) - \psi(x)\right]$$

q - electric charge

$$\nabla_\mu \psi(x) = \frac{1}{a}\left[U_\mu(x)\, v_\mu^{\hat{q}}(x)\, \psi(x+\hat{\mu}) - \psi(x)\right]$$

$q = \hat{q}\, q_{el}$ - electric charge

Beyond Isosymmetric Lattice QCD

$m_u \neq m_d$ **and** $\alpha_{em} \neq 0$

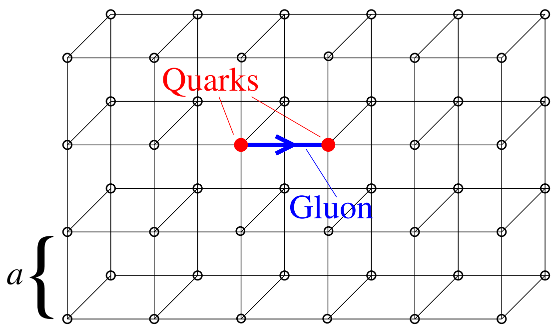
➡ expand about isosymmetric theory

QCD TREATED NON-PERTURBATIVELY, α_{em} "SMALL"

[R123: 1303.4896, PRD87(2013)11]

HVP:
[RBC/UKQCD: JHEP09 (2017) 153, PRL121(2018)022003]
[BMW: Borsanyi et al. Nature 593 (2021)7857]
[Mainz: PRD106(2022)11]

… [decay rates, see e.g. M.Di Carlo LATTICE'23]

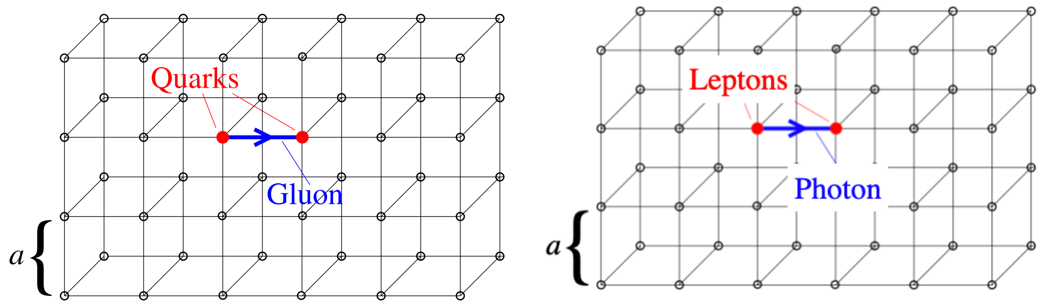


$O(\alpha_{em}), O(m_u - m_d)$

➡ simulate QED+QCD

QCD AND QED TREATED NON-PERTURBATIVELY,

[Duncan,Eichten, hep-lat/9602005, PRL76(1996), Blum et al. 0708.0484 *PRD* 76 (2007)114508, …]
[BMW: 1406.4088 Science 347 (2015), QCDSF: 1509.00799, *JHEP* 04(2016) 093, RCstar: 2209.13183 JHEP 03(2023)012, …]



Prescriptions for lattice QCD+QED

➡ **Modify gauge filed**: removing the global zero-mode/ spatial zero mode per timeslice ($QED_{\rm TL}/QED_{\rm L}$)
[PRL76(1996), Prog. Theor. Phys. 120(2008)413, Science 347 (2015) 1406.4088, …]

➡ **Massive photon** [PRL 117 (2016) 7, PoS LATTICE2021 (2022) 281]

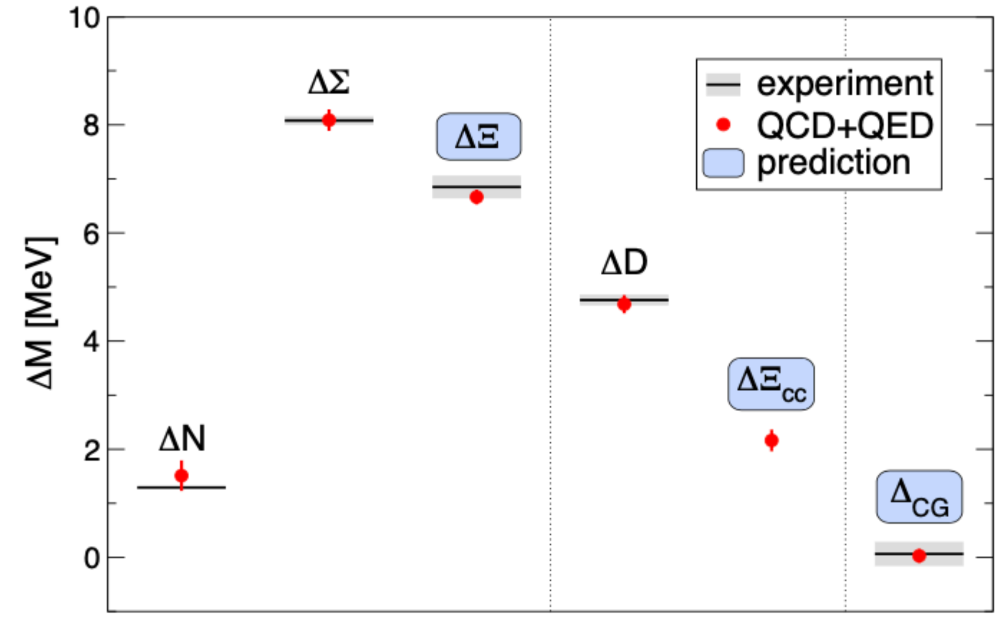
➡ QED_∞ [Phys. Rev. D 96 (2017), Phys. Rev. D 100 (2019) 094509]

➡ **C* boundary conditions** (no zero-mode present) [JHEP 1602, 076, EPJC 80 (2020) 3, JHEP03(2023)012]

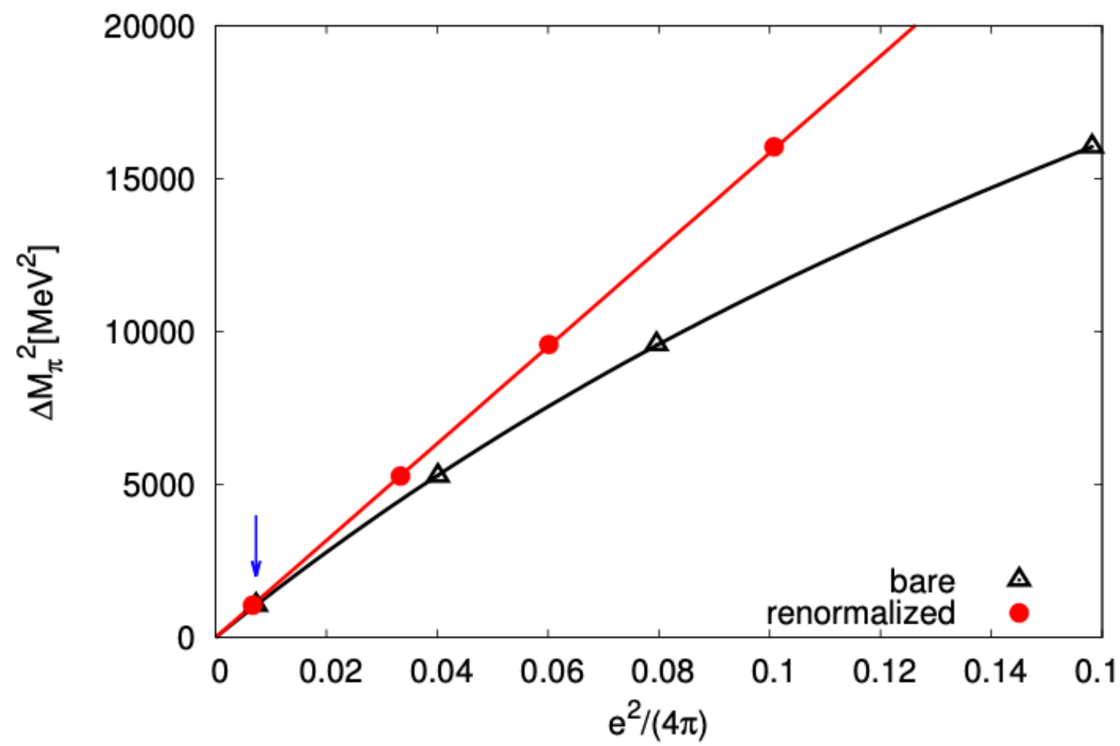
Modified gauge field: QED_{L} in practice

- Power-law finite volume corrections to masses of stable states <u>and HVP</u> understood analytically [Fodor et al. PLB 5 245 (2016), Davoudi, Savage, PRD90 (2014) 054503 , Bijnens et al. *Phys.Rev.D* 100 (2019) 1, 014508]

- Large volume simulations: physical sizes up to $m_\pi L = 8.1$ with a $64^3 \times 80$ lattice already ~a decade ago
  - Wilson fermions $N_f = 1 + 1 + 1 + 1$



Dynamical QED+QCD:



BMW [Borsanyi et al.,Science 347 (2015) 1406.4088
"Ab initio calculation of the neutron-proton mass difference"

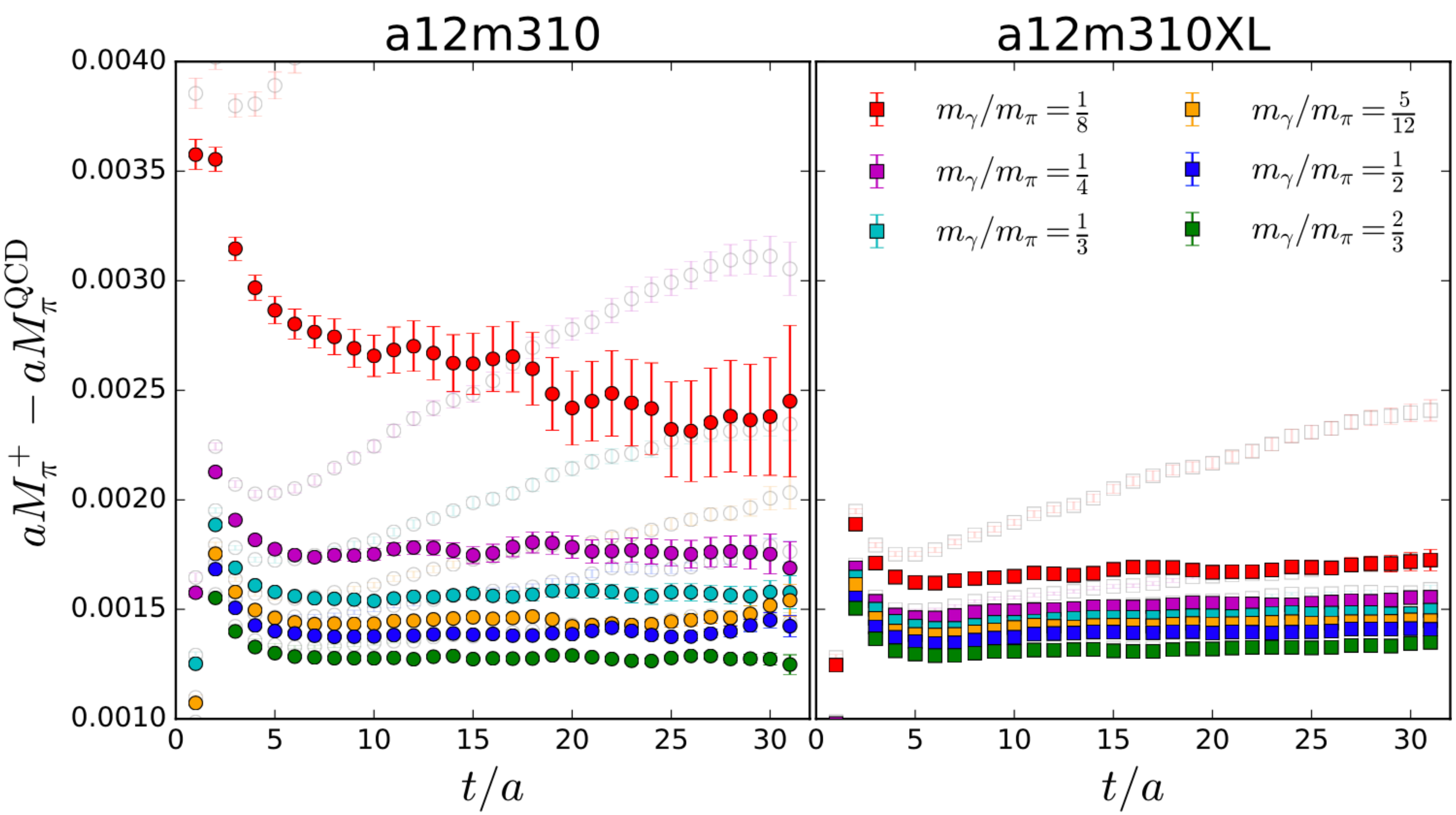
- Pros: simpler observables (e.g. 2-pt for mass correction or 3-pt functions for baryon spectrum)

- Cons: signal is typically $O(\alpha_{em})$

Massive Photon: QED_{M} in practice

[Endres et al. PRL 117(2016),
Bussone et al. EPJ WC:06005(2018),
Clark et al. PoS LATTICE2021 (2022) 281]

- Effective Mass Splittings for Charged Hadrons
- z_μ causes linear rise in the effective mass
- Analytically remove these effects



[Clark et al. PoS LATTICE2021 (2022) 281]

Beyond Isosymmetric Lattice QCD

$m_u \neq m_d$ **and** $\alpha_{em} \neq 0$

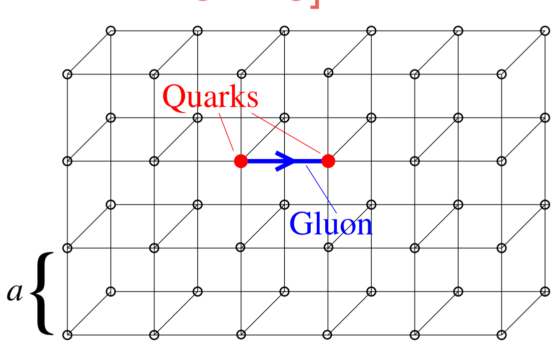
➡ expand about isosymmetric theory

QCD TREATED NON-PERTURBATIVELY, α_{em} "SMALL"

[R123: 1303.4896, PRD87(2013)11]

HVP:
- [RBC/UKQCD: JHEP09 (2017) 153, PRL121(2018)022003]
- [BMW: Borsanyi et al. Nature 593 (2021)7857]
- [Mainz: PRD106(2022)11]

… [decay rates, see e.g. M.Di Carlo LATTICE'23]

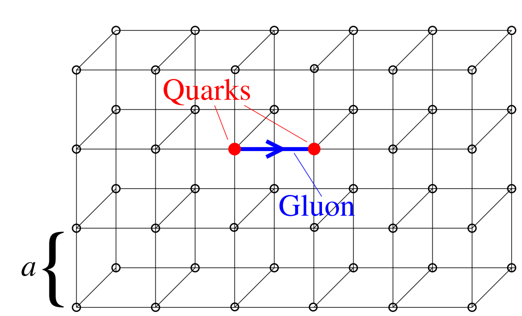


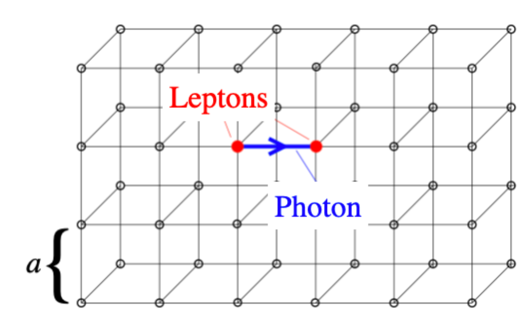
$O(\alpha_{em}), O(m_u - m_d)$

➡ simulate QED+QCD

QCD AND QED TREATED NON-PERTURBATIVELY,

[Duncan,Eichten, hep-lat/9602005, PRL76(1996), Blum et al. 0708.0484 *PRD* 76 (2007)114508, …]
[BMW: 1406.4088 Science 347 (2015), QCDSF: 1509.00799, *JHEP* 04(2016) 093, RCstar: 2209.13183 JHEP 03(2023)012, …]





Beyond Isosymmetric Lattice QCD: à la R123

[R123: 1303.4896, PRD87(2013)11]

- Compute leading isospin breaking corrections (LIBE)
  - ➡ Expanding an observable (in the isospin broken theory) with respect to the isosymmetric QCD result
- Applied to meson mass splitting, and more recently to HVP isospin-breaking corrections
- Main advantage w. respect to simulating QED+QCD:
  - ➡ Correction contributions obtained individually (before multiplying with $O(\alpha_{em})$, $O(m_u - m_d)$ coef.), albeit 3-pt. and 4-pt. functions
  - ➡ No extrapolation in α_{em} needed

Beyond Isosymmetric Lattice QCD: R123

- Pros: reuse the gauge configurations generated in the isosymmetric theory
- Reweighting:

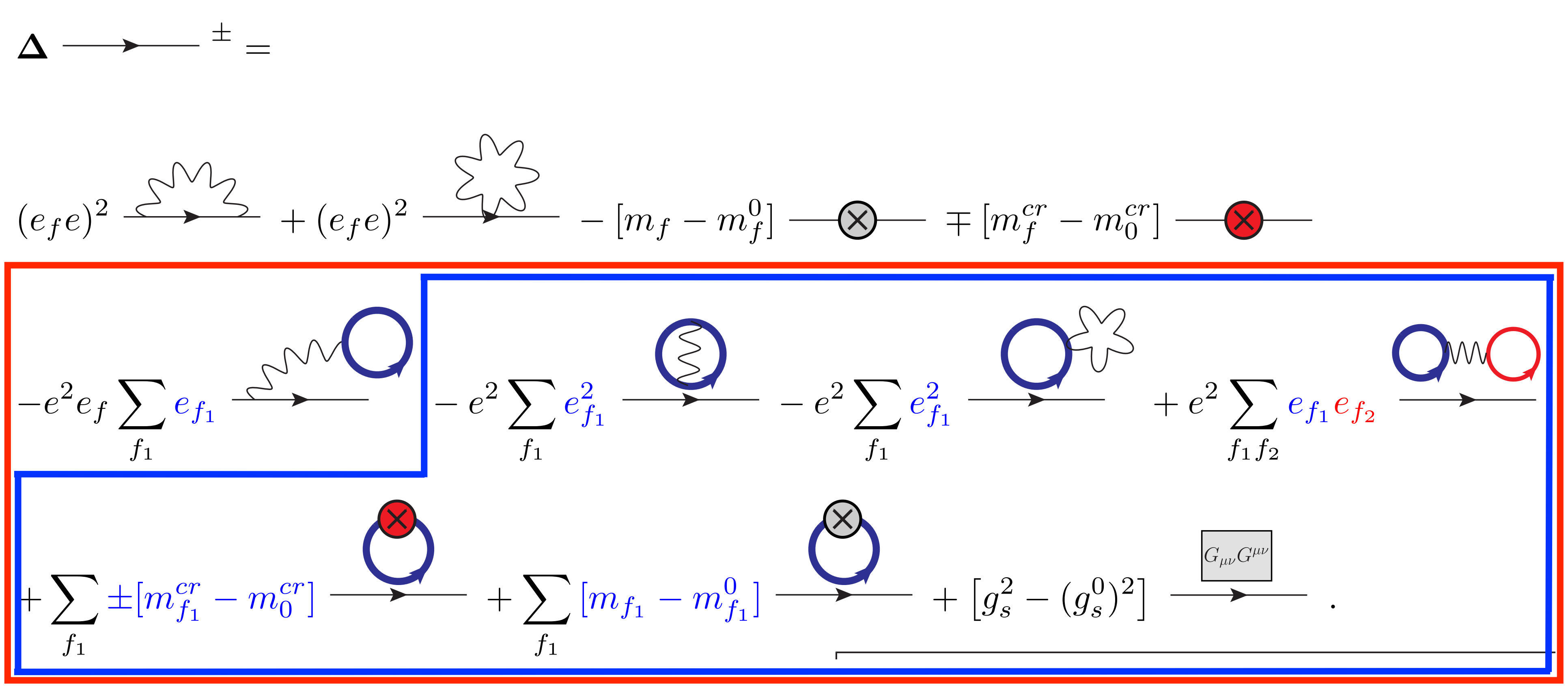
$$\langle O \rangle^{\vec{g}} = \frac{\left\langle\, R[U,A;\vec{g},\vec{g}^{0}]\; O[U,A;\vec{g}] \,\right\rangle^{A,\vec{g}^{0}}}{\left\langle\, R[U,A;\vec{g},\vec{g}^{0}] \,\right\rangle^{A,\vec{g}^{0}}}$$

$\vec{g}^{0}$ - bare param. of isosymm. th

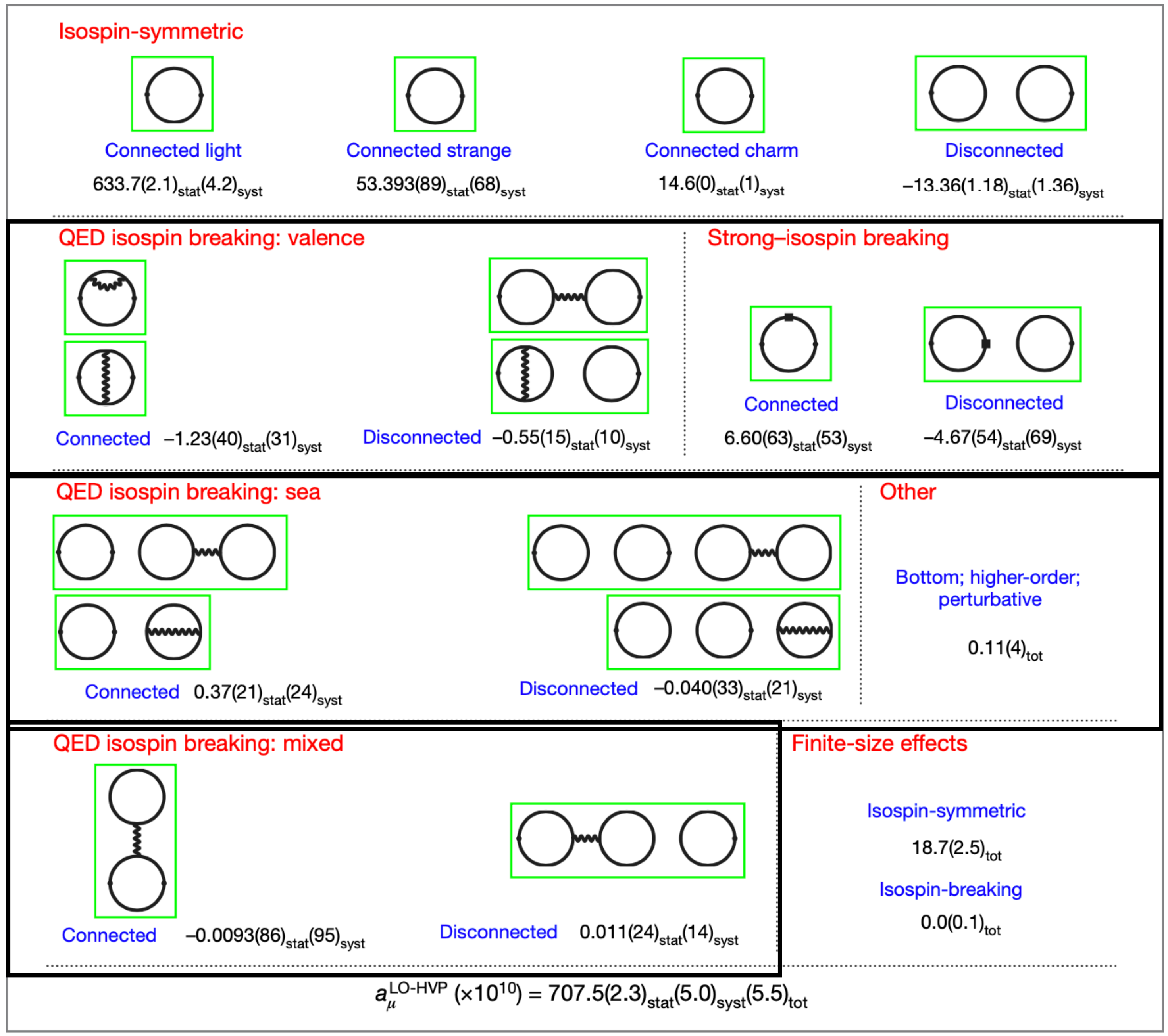
$\vec{g}$ - bare param. of the full th

- For simplicity, approximate sea quarks as electrically neutral: $R[U,A;\vec{g},\vec{g}^{0}] = 1$
- Once an appropriate renormalisation procedure is applied: $\Delta O = O(\vec{g}) - O(\vec{g}^{0})$

- Example:



Beyond Isosymmetric Lattice QCD: R123



BMW [Borsanyi et al. Nature 2021, arxiv:2002.12347]

➡ Staggered fermions $N_f = 2 + 1 + 1$

Beyond Isosymmetric Lattice QCD

$m_u \neq m_d$ **and** $\alpha_{em} \neq 0$

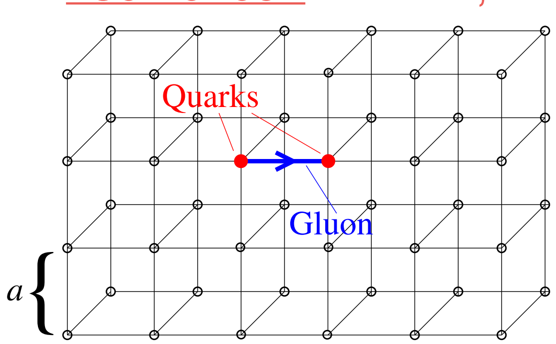
➡ expand about isosymmetric theory

QCD TREATED NON-PERTURBATIVELY,
α_{em} "SMALL"

[R123: 1303.4896, PRD87(2013)11]

HVP: { [RBC/UKQCD: JHEP09 (2017) 153, PRL121(2018)022003]
[BMW: Borsanyi et al. Nature 593 (2021)7857]
[Mainz: PRD106(2022)11] }

… [decay rates, see e.g. N. Tantalo 2301.02097 LATT22, M.Di Carlo LATT23]

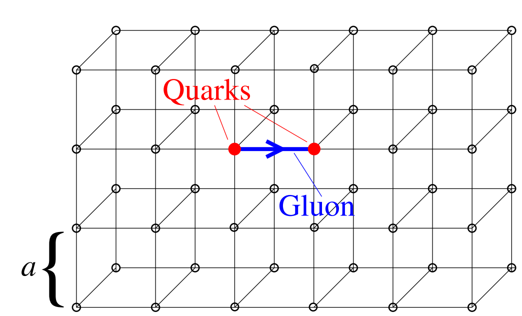


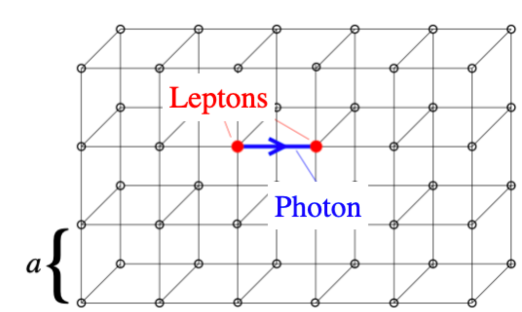
$O(\alpha_{em}), O(m_u - m_d)$

➡ simulate QED+QCD

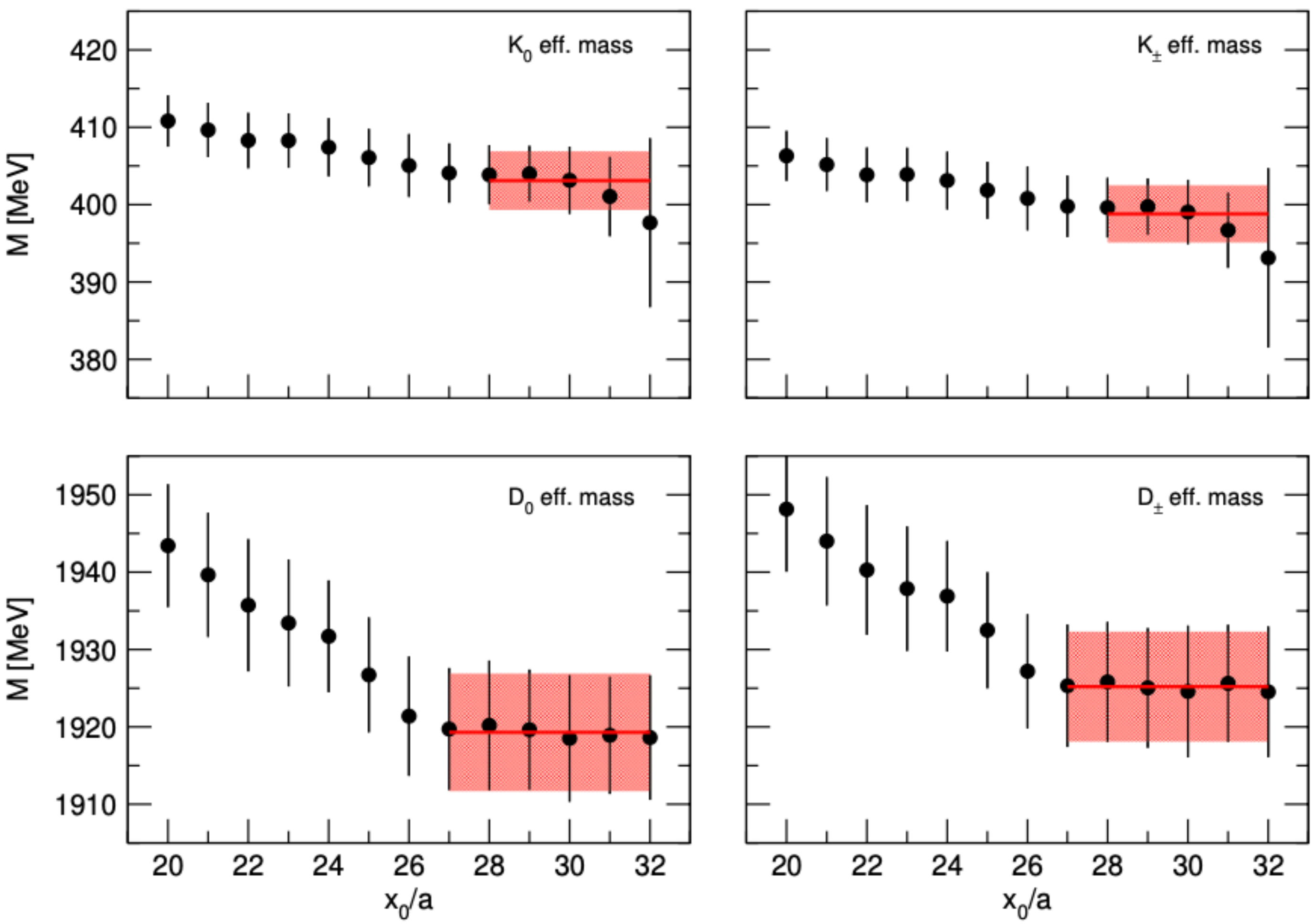
QCD AND QED TREATED
NON-PERTURBATIVELY,

[Duncan,Eichten, hep-lat/9602005, PRL76(1996),
Blum et al. 0708.0484 *PRD* 76 (2007)114508, …]
[BMW: 1406.4088 Science 347 (2015),
QCDSF: 1509.00799, *JHEP* 04(2016) 093,
RCstar: 2209.13183 JHEP 03(2023)012, …]

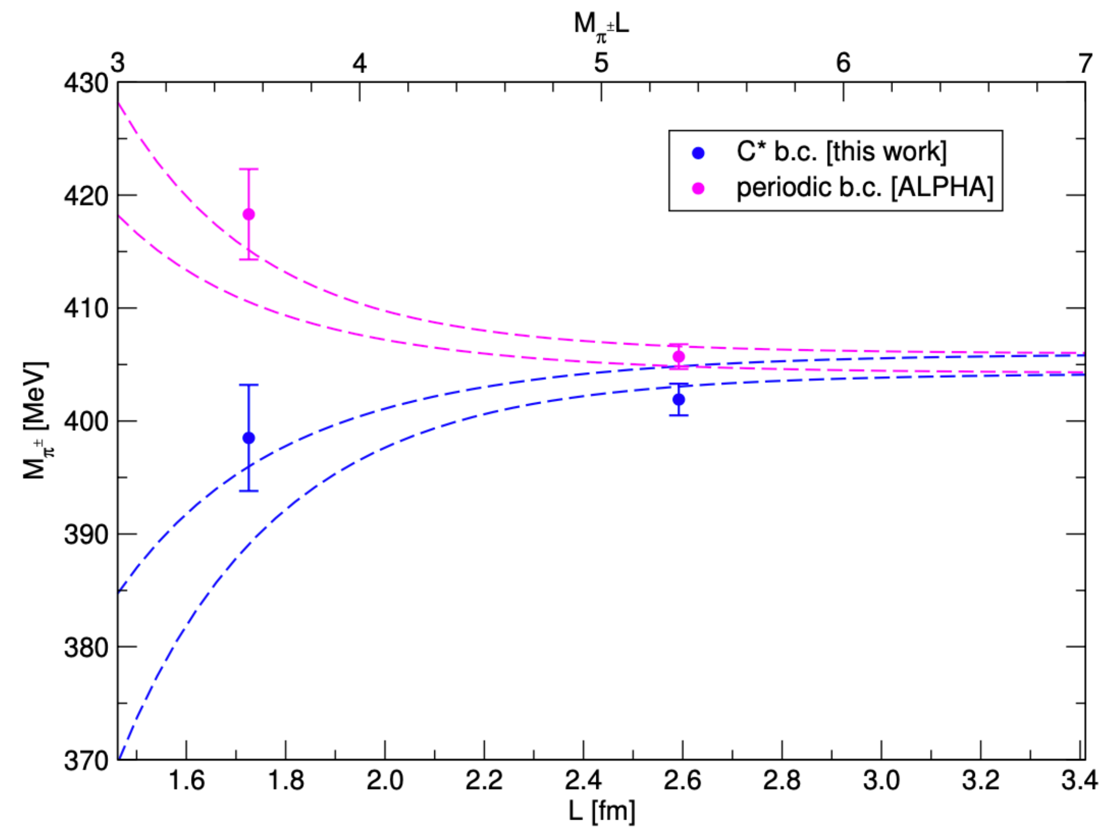




Dynamical QCD+QED with C-parity b.c.'s



[Bushnaq et al. JHEP03(2023)012]



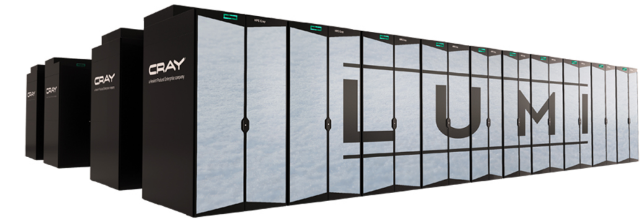
[Campos et al. Eur.Phys.J.C 80 (2020) 3, Bushnaq et al. JHEP03(2023)012]

Dynamical QCD+QED with C-parity b.c.'s

[openQ*D: https://gitlab.com/rcstar/openQxD]
[Campos, Fritzsch, Hansen, MKM, Patella, Ramos, Tantalo EPJC 80 (2020) 3]

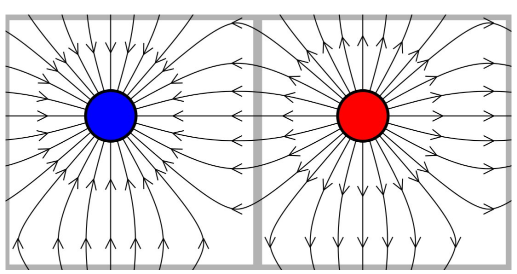
[R. Gruber, Kozhevnikov MKM, Schulthess, Solca arXiv:2202.07388,]

[Illustration: cscs.ch]



[Illustration of the HPE Cray EX cabinets. Copyright: Hewlett Packard Enterprise]

- Signature: C boundary conditions
- QCD+QED dynamical simulations



RC*

[Lucini et al., JHEP '15]
[MKM @ LAT'17]
[A. Patella @ LAT'17]
[M. Hansen @ LAT'17]
[Hansen et al., PRD '18]
[Campos et al., EPJC '20]
[Jens Lücke @ APLAT'20]
[Jens Lücke @ LATT'21]
[Madeline Dale @ LATT'21]
[Lucius Bushnaq @ LATT'21]
[Roman Gruber @ LATT'21]
ETH zürich CSCS
[Jens Lücke @ LATT'21]
[Alessandro Cotellucci @ LATT'22]
[Paola Tavella @ LATT'22]
[Anian Altherr @ LATT'22]
[Roman Gruber @ LATT'22]
[Letizia Parato @ LATT'24]
[Roman Gruber @ LATT'24]
[Alessandro Cotellucci @ LATT'24]

ensemble	lattice	β	α
A400a00b324	64×32^3	3.24	0
B400a00b324	80×48^3	3.24	0
A450a07b324	64×32^3	3.24	0.007299
A380a07b324	64×32^3	3.24	0.007299
A500a50b324	64×32^3	3.24	0.05
A360a50b324	64×32^3	3.24	0.05
C380a50b324	96×48^3	3.24	0.05

- configuration generation, reweighting
- a first look at the baryon spectrum
- noise reduction techniques
- implementation on new hardware

[L. Bushnaq et al. arXiv:2209.13183 JHEP 03(2023)012]

Clover-Wilson fermions $N_f = 1 + 2 + 1$