

LQCD I: Lattice Gauge Theories

Prof. Marina Krstic Marinkovic, ETH Zürich

4-10 August 2024, Lyceum Alpinum, Zuoz

PSI Particle Physics Summer School – From
Low to High: Particle Physics at the Frontier



Scientific trajectory

→ **2006** DESY Zeuthen (Th. Particle Phys.) / University of Oslo (Quantum Chemistry)



→ **2008 - 2009** MSc Thesis: DESY Zeuthen/Humboldt Universität zu Berlin, Germany



→ **2009 - 2013** PhD Thesis: HU Berlin, Germany



→ **2012 - 2014** Research Fellow: University of Southampton, UK



→ **2014 - 2017** CERN Fellow (Visiting Scientist since October 2017)



→ **2016 - 2019** Assistant Professor, Trinity College Dublin, Ireland



→ **2020 - 2021** Junior-professorship at LMU München (3+3y)



→ **2021 -** **Assistant Prof. in Computational Physics** (Tenure-track)

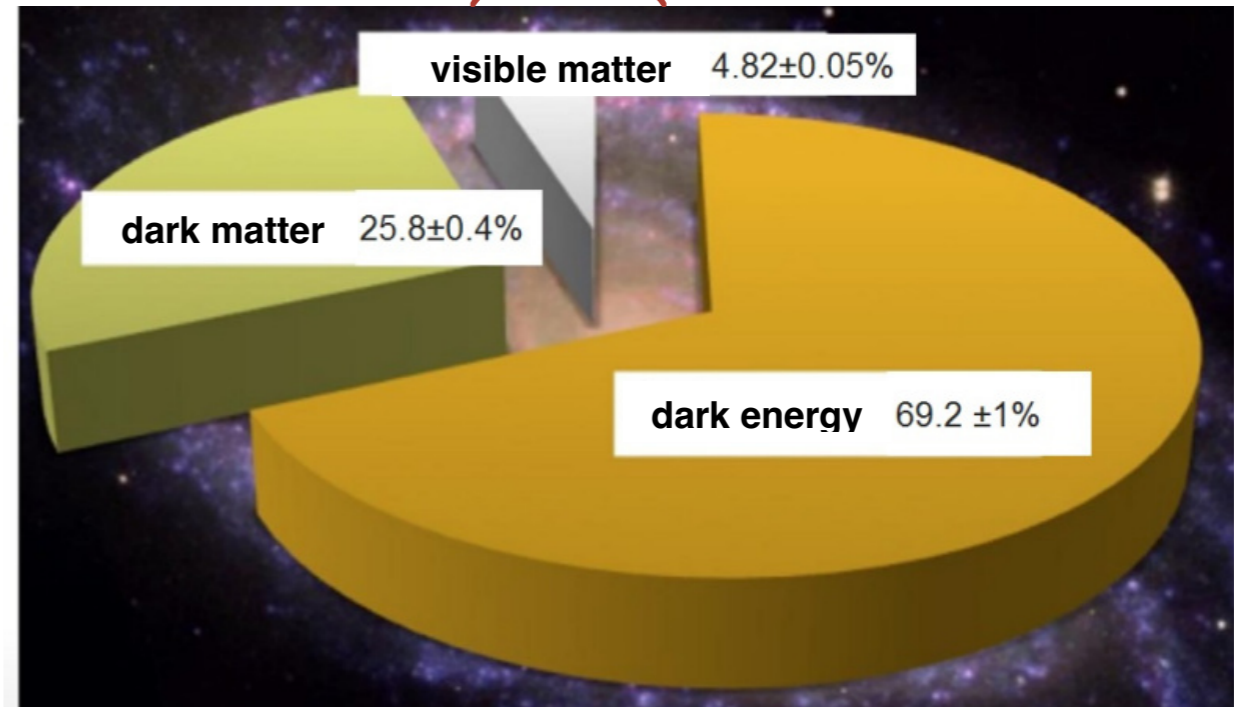
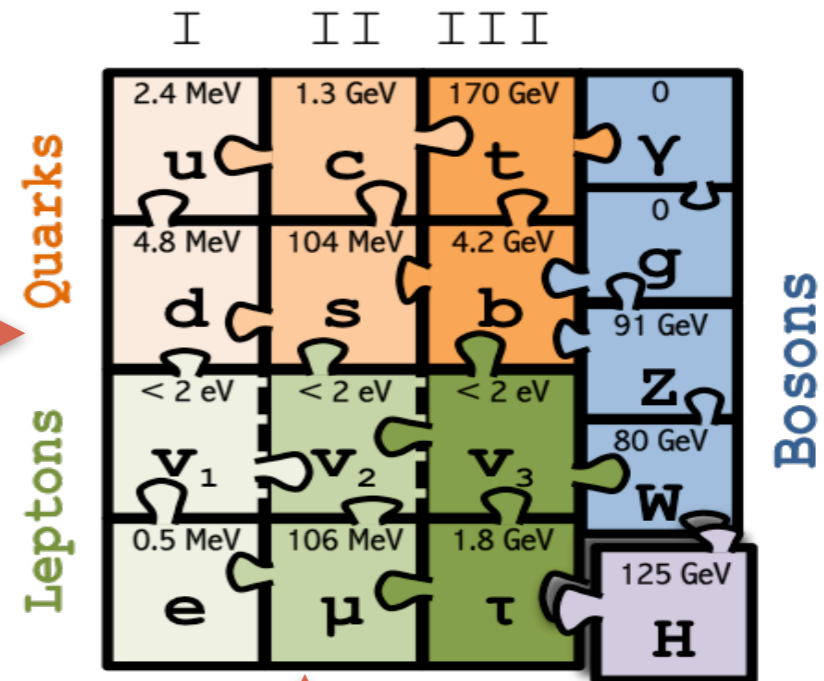


Building blocks of the universe

- **Four fundamental interactions:**

- Electromagnetism
- Weak
- Strong
- Gravity

Standard Model
of Particle Physics



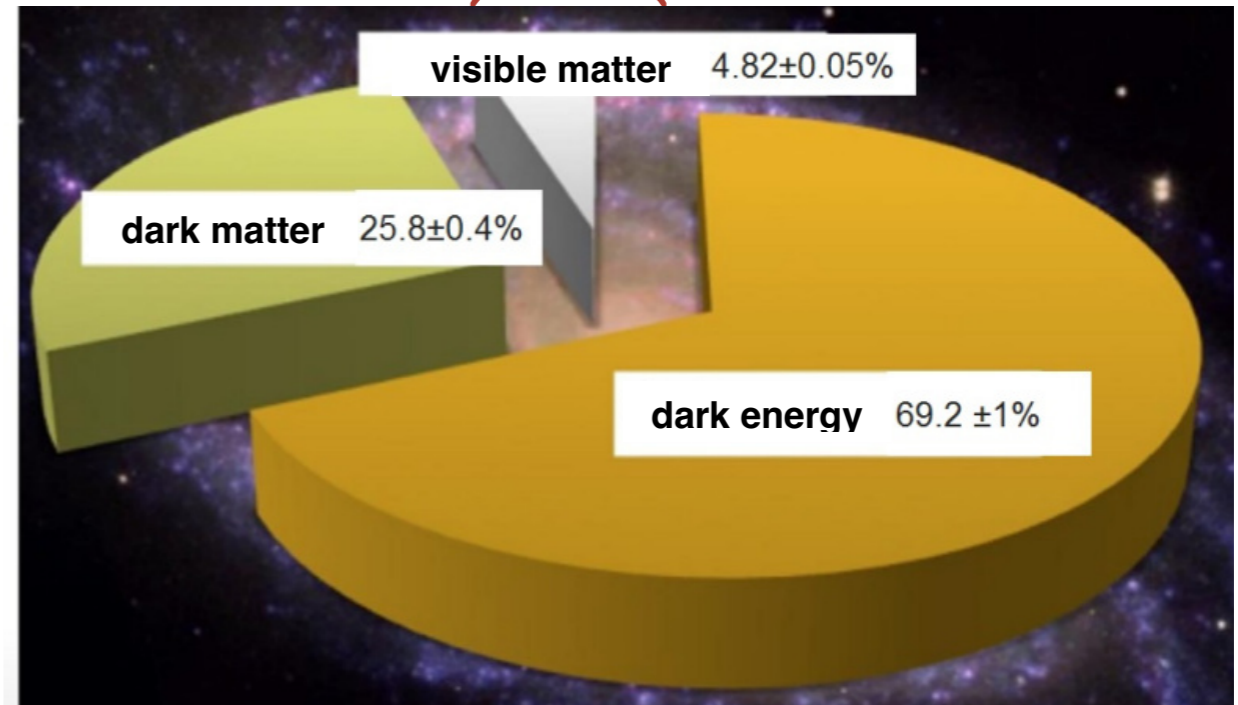
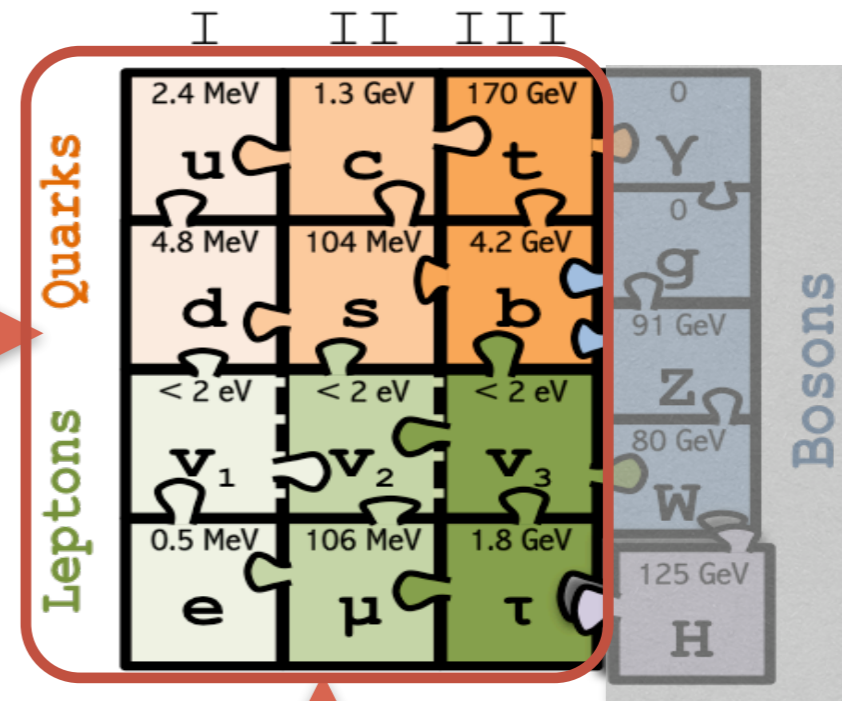
[Planck CMB Data (2013 and 2015)]
August 4 - 10, 2024

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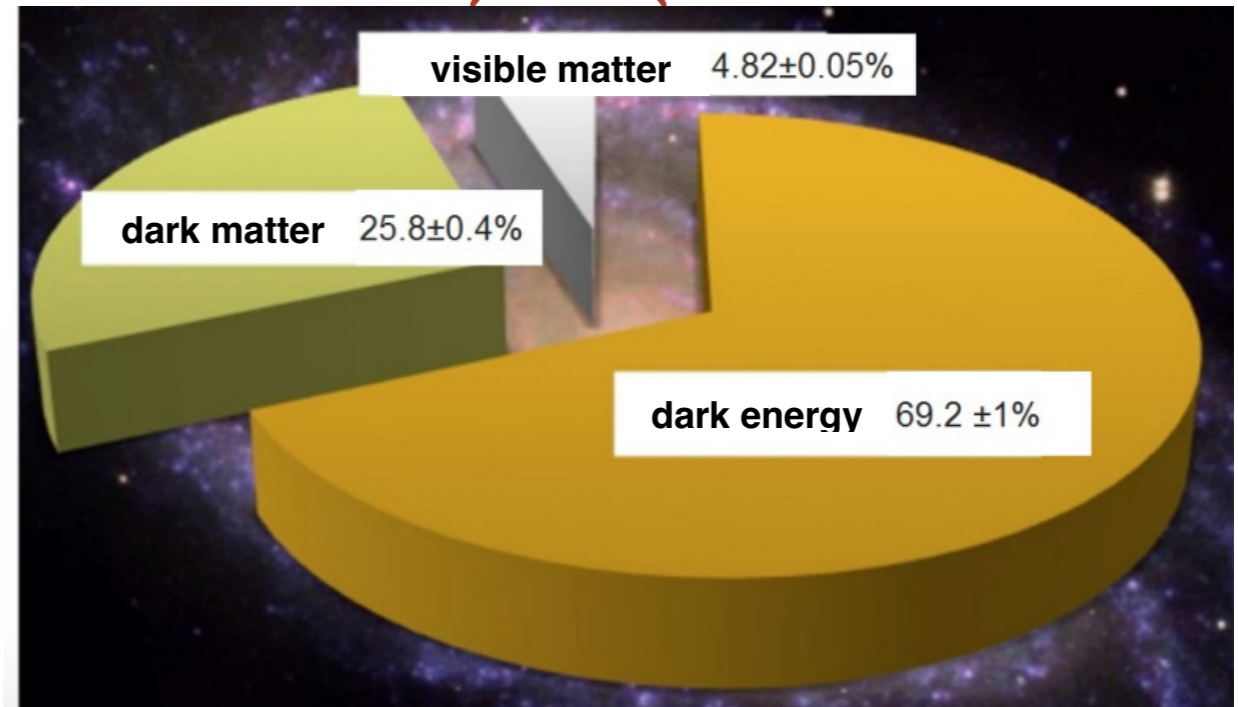
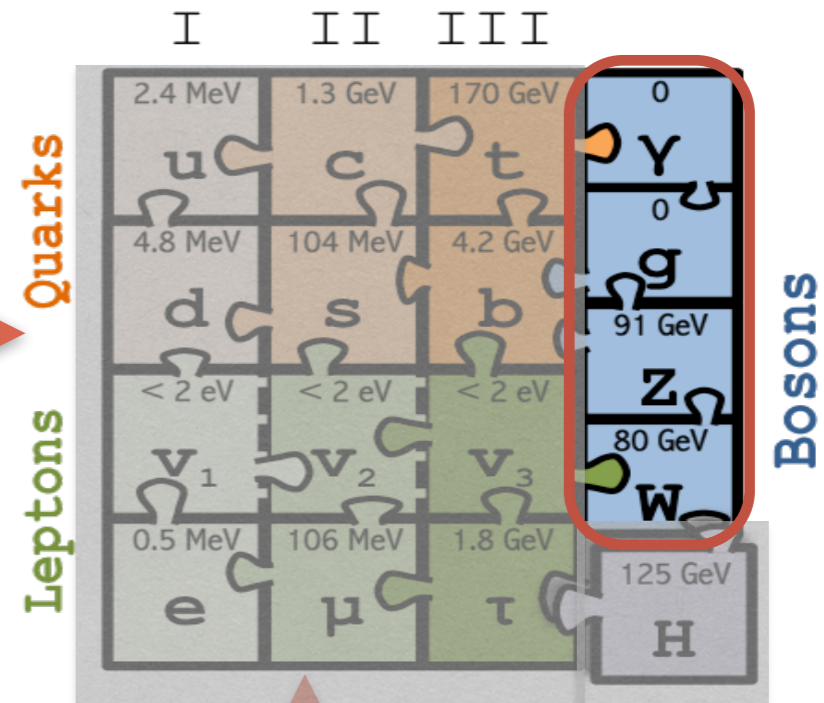
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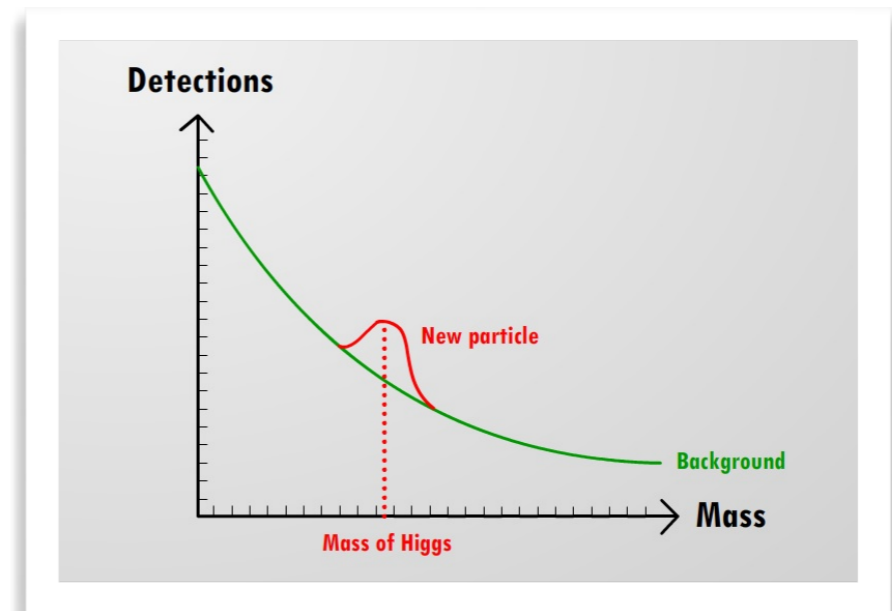
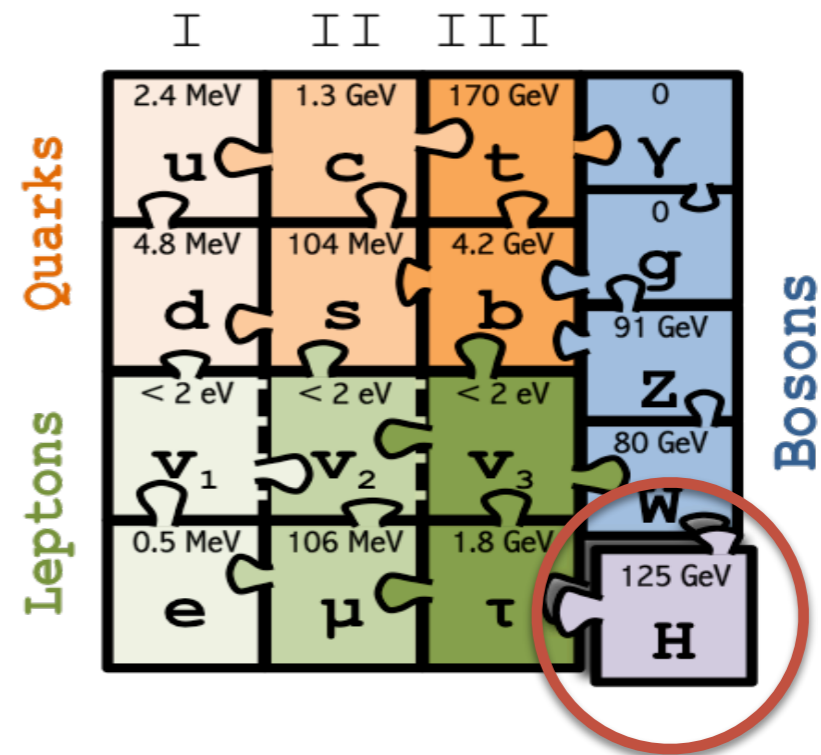


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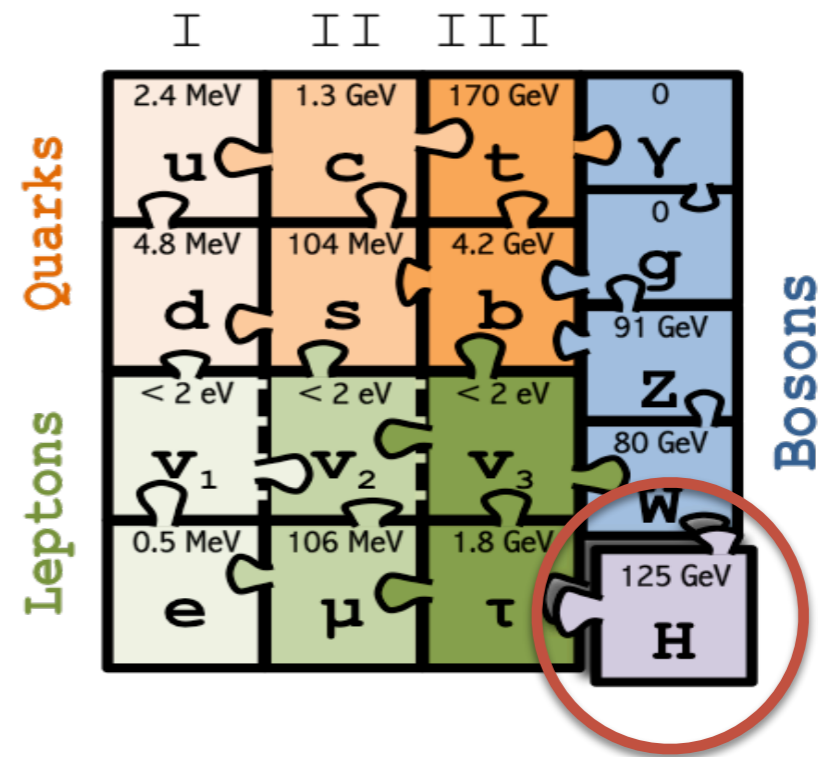


[<https://blog.higgshunters.org/>]

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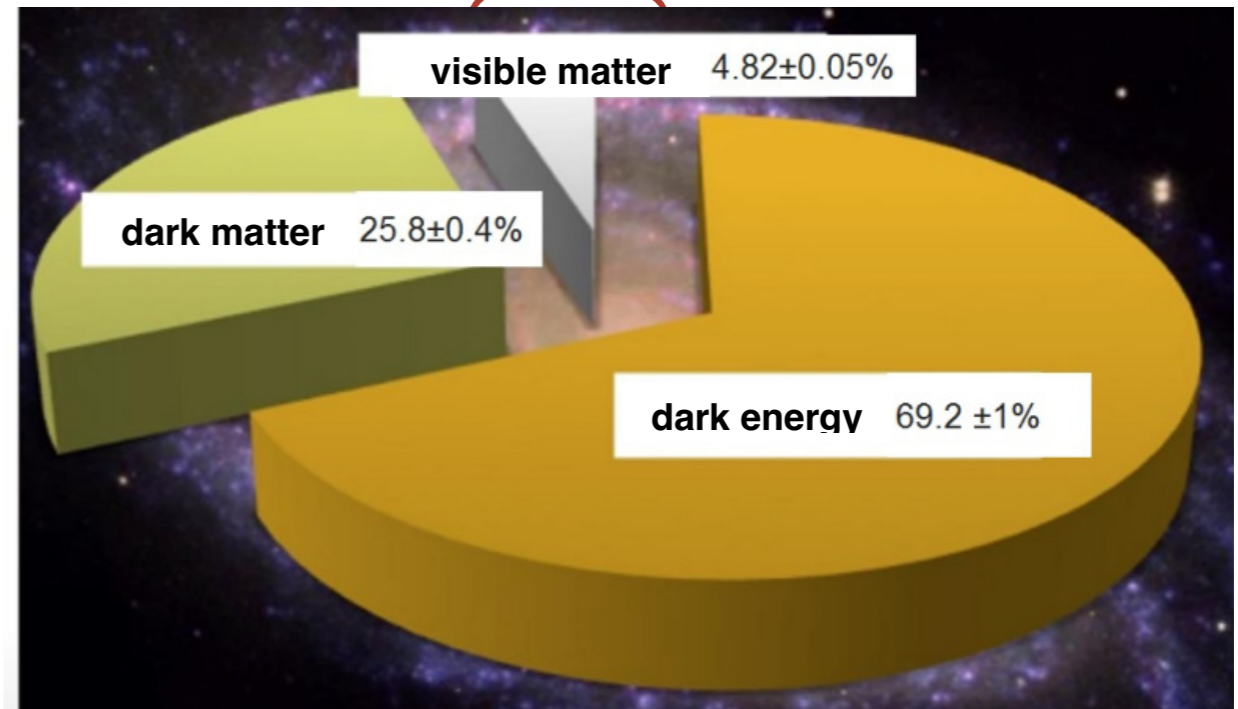
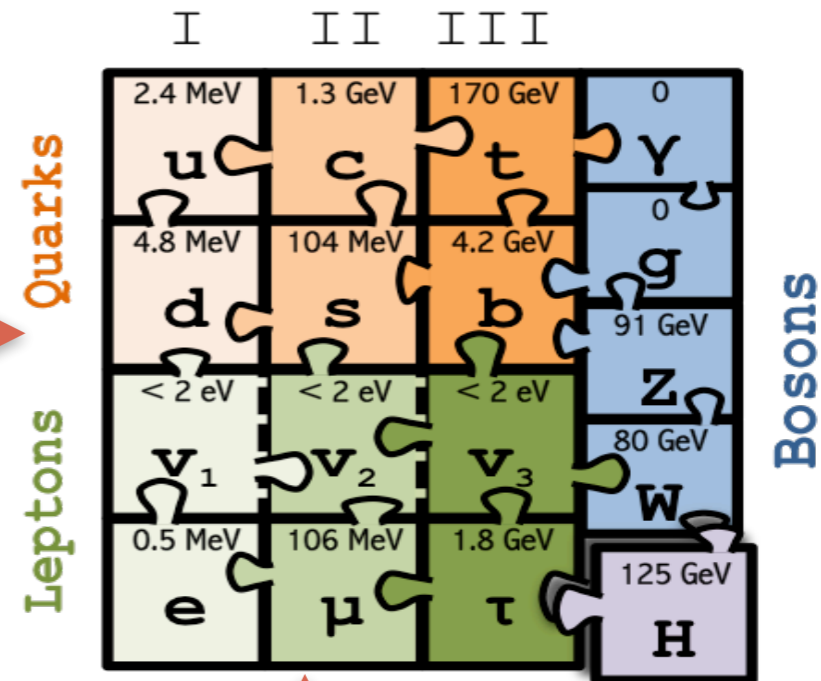
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See lectures in this school:

[R. Gonzalez Suarez; Wed., Fri.]

[P. F. Monni; Mon., Wed.]

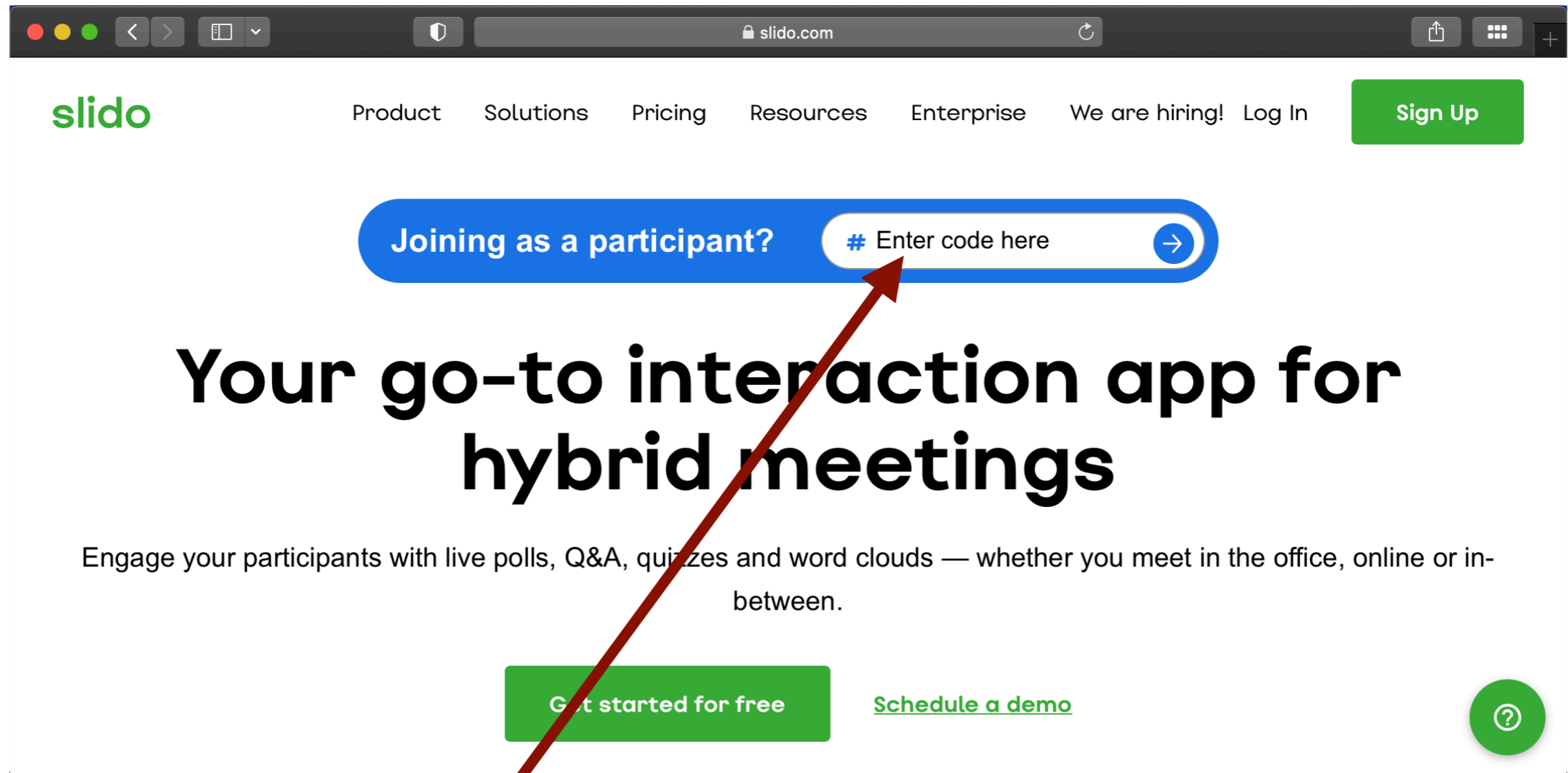
[V. Cirigliano; Tue., Thurs.]

[A. Soter; Mon., Tue.]

[Planck CMB Data (2013 and 2015)]

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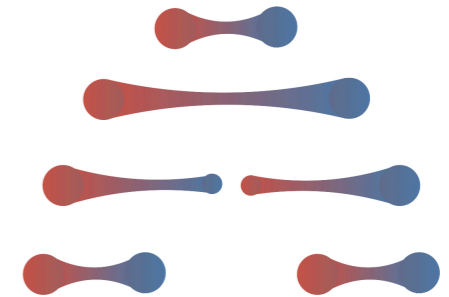


- Poll code: **#lattice1**

The strong interaction

- Commonly accepted theory of strong interaction is **Quantum Chromodynamics (QCD)**
- Fundamental parameters of **QCD**:
 - gauge coupling: g
 - quark masses: m_u, m_d, m_s, \dots

- **Two exciting properties of QCD**:
 - color confinement
 - asymptotic freedom



- Strong coupling “constant”:

$$\alpha_s(Q^2) = \frac{\bar{g}^2(Q^2)}{4\pi}$$

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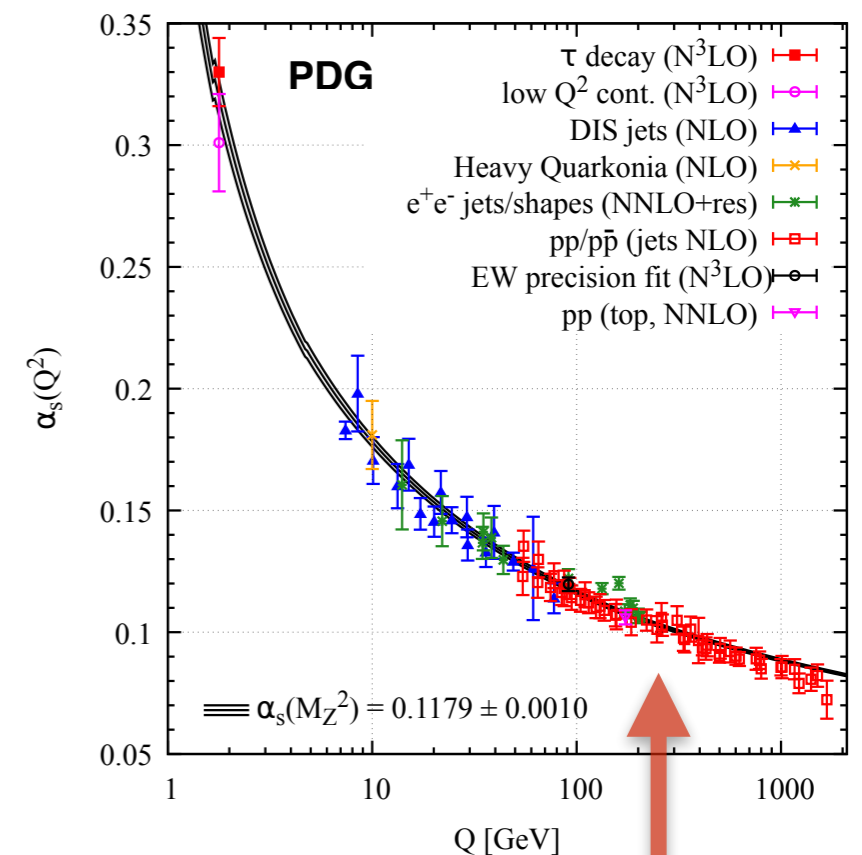
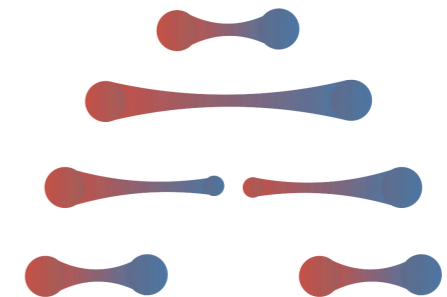
- color confinement
- asymptotic freedom

[D. Gross, F. Wilczek; D. Politzer (1973)]



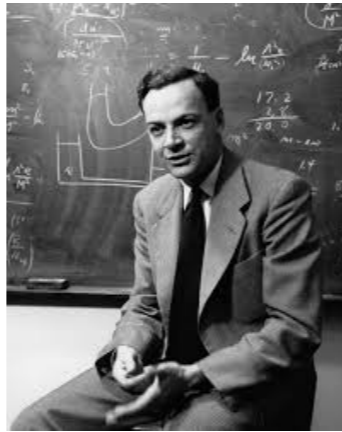
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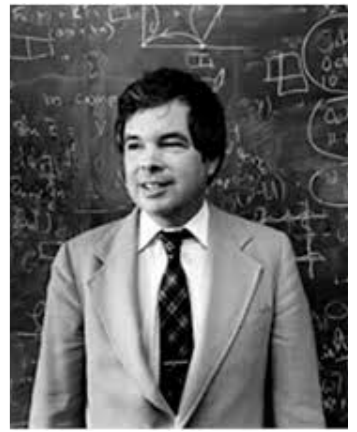


Non-perturbative treatment of QCD

[R. P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics" *Rev. Mod. Phys.* 20, 367 (1948)]

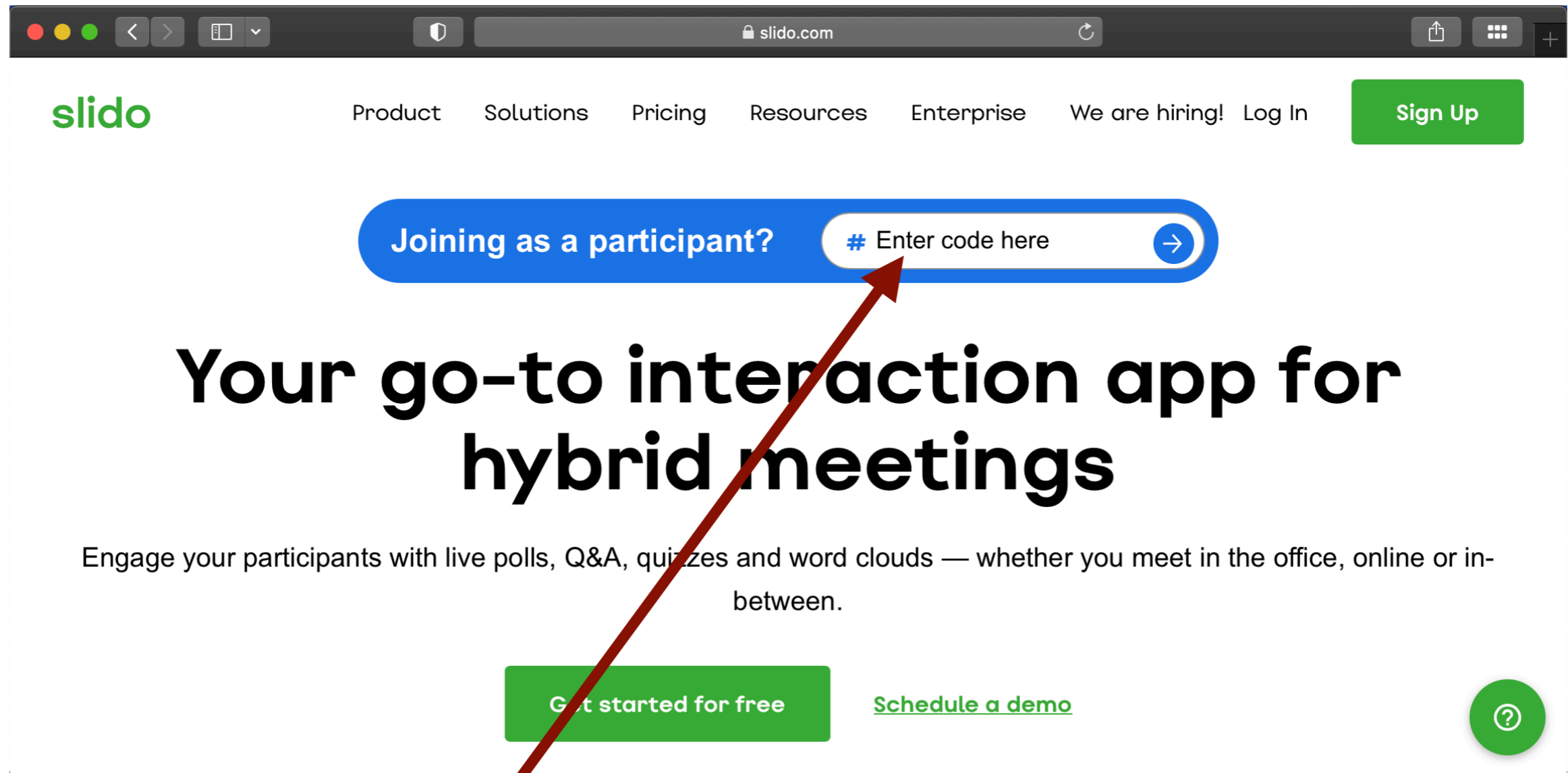


[K. Wilson, "Confinement of quarks" *Phys. Rev.D.* 10 (8): 2445–245 (1974)]



- (1) Path Integral quantization
- (2) Continuation to Euclidean time
- (3) Lattice regularization

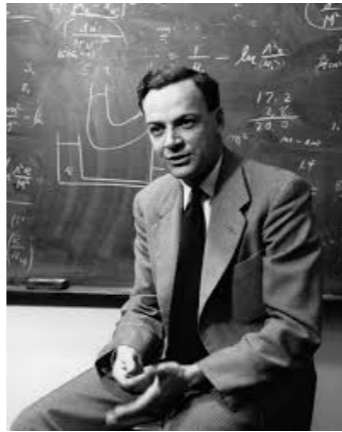
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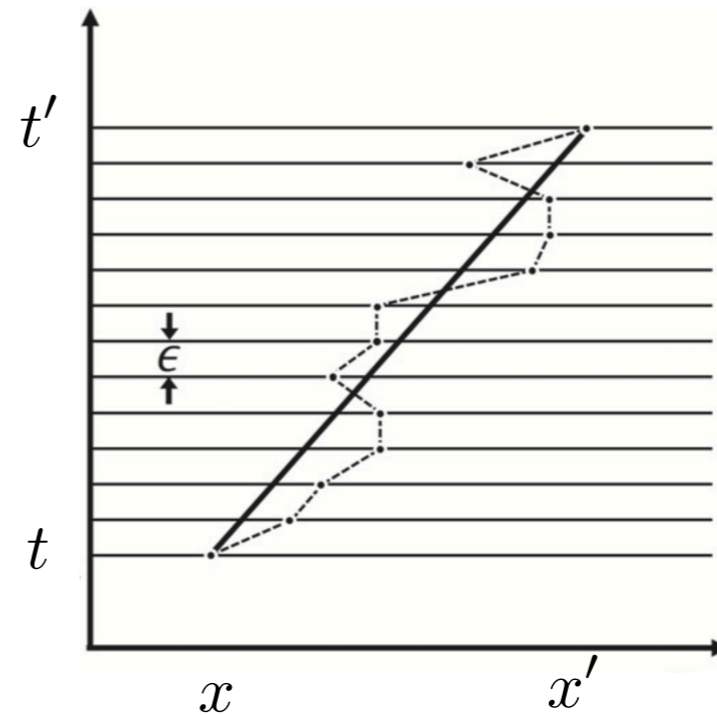


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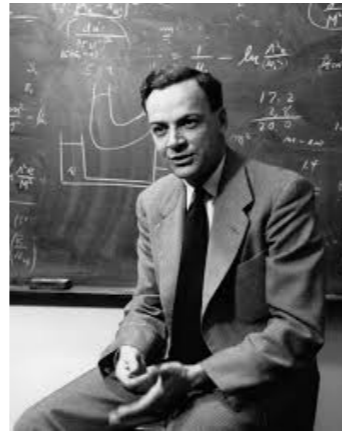
$$\langle x' | U(t', t) | x \rangle = \int dx_1 \langle x' | U(t', t_1) | x_1 \rangle \langle x_1 | U(t_1, t) | x \rangle$$



$$\langle x' | U(t', t) | x \rangle = \int \mathcal{D}x e^{\frac{i}{\hbar} S[x]}$$

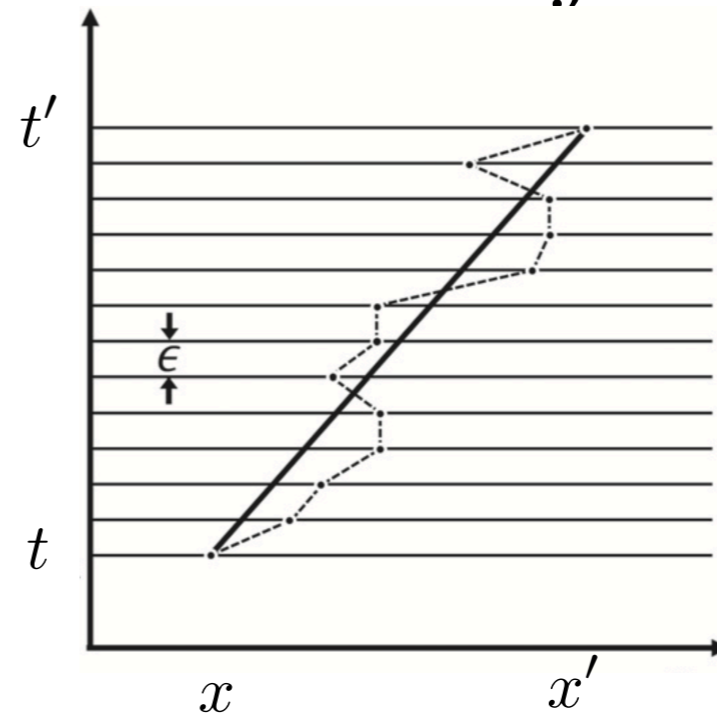
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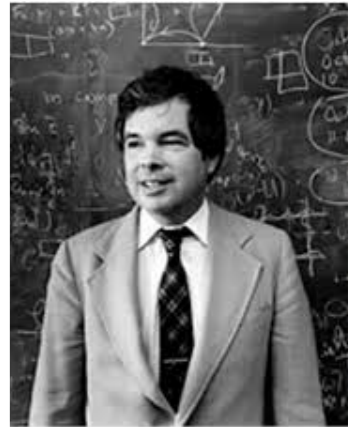
$$\epsilon \longrightarrow -i a$$

↓

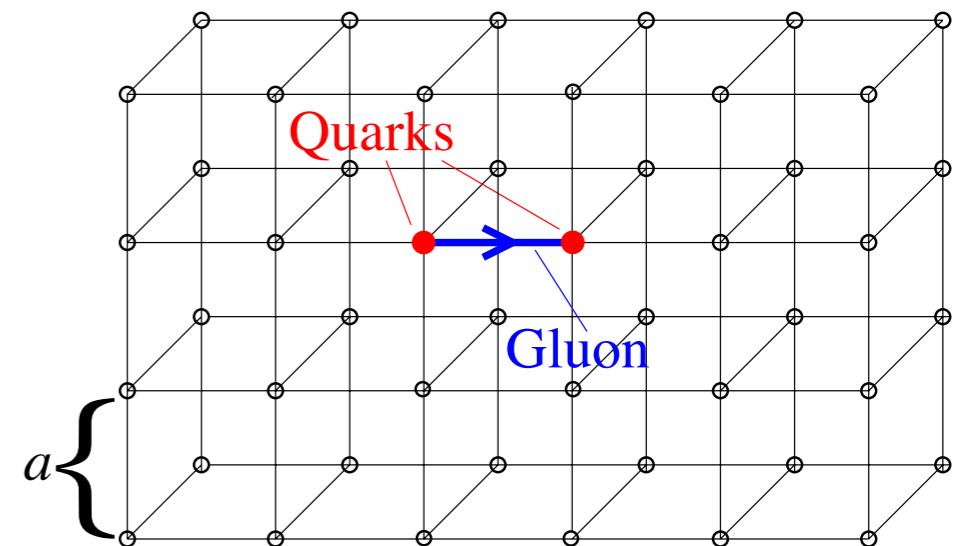
$$Z = \int \mathcal{D}x e^{-\frac{1}{\hbar} S_E[x]}$$

Non-perturbative treatment of QCD

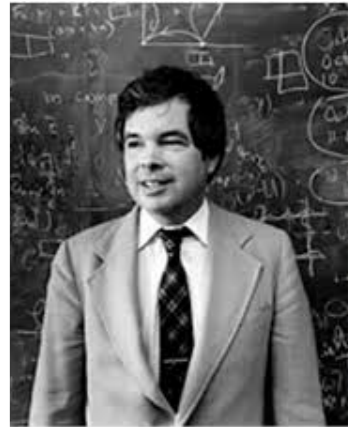
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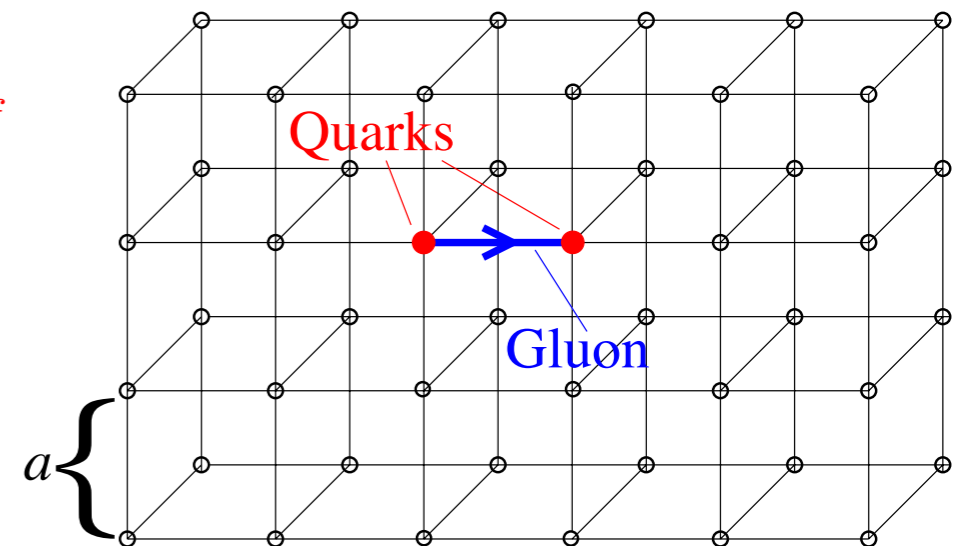


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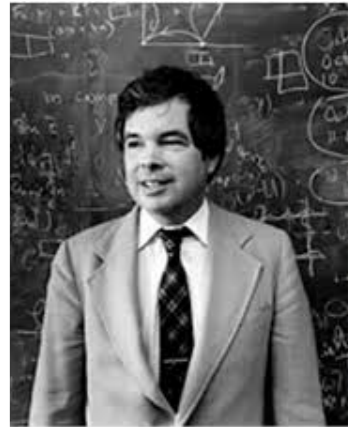
$$\mathcal{L}_{QCD}^E = \frac{1}{2g} F_{\mu\nu}^a F_{\mu\nu}^a + \sum_{f=u,d,s,\dots} \bar{\psi}_f \{ \gamma_\mu (\partial_\mu + iA_\mu^a T^a) + m_f \} \psi_f$$

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



Non-perturbative treatment of QCD

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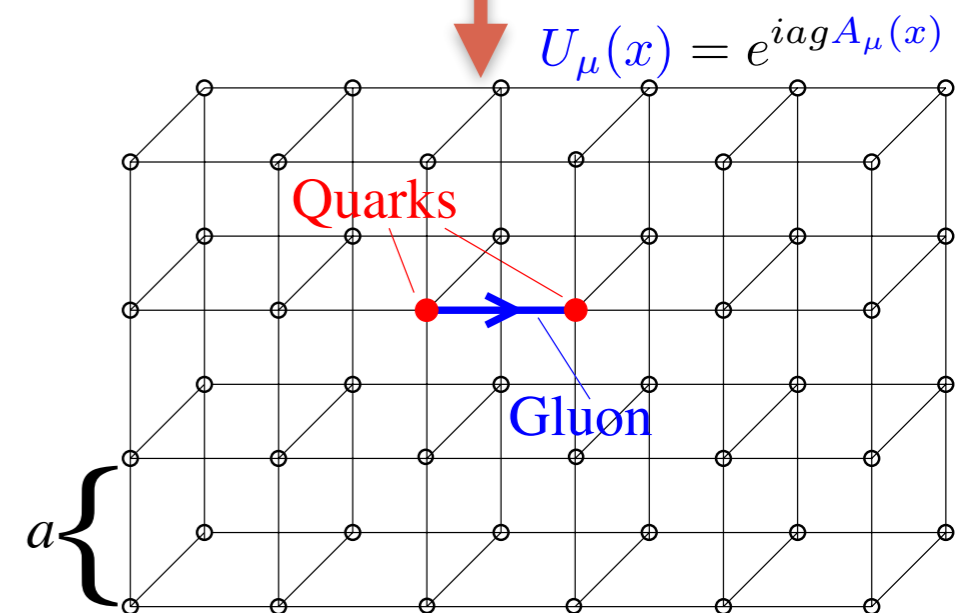


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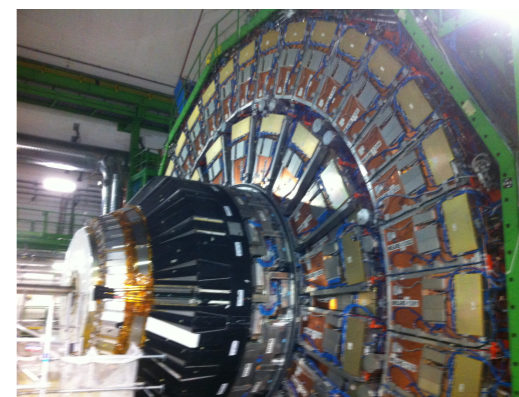
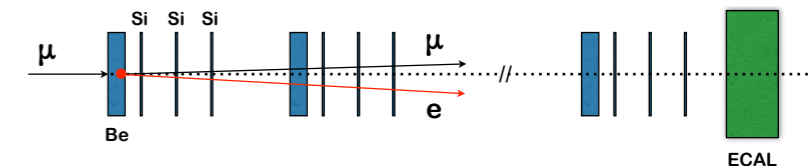
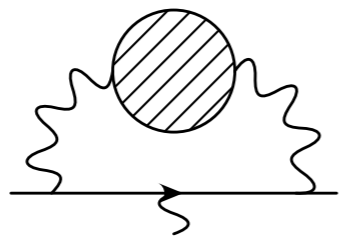


CLASSICAL STATISTICAL MECHANICS

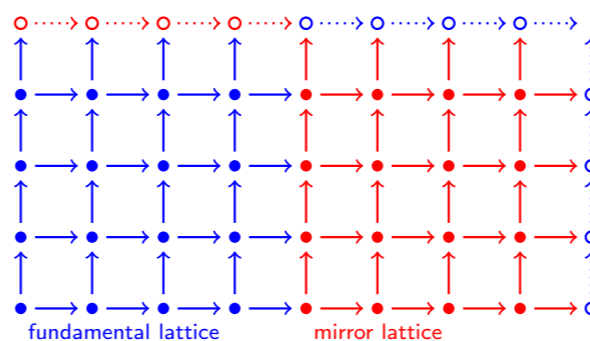
$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{QCD}^E}$$



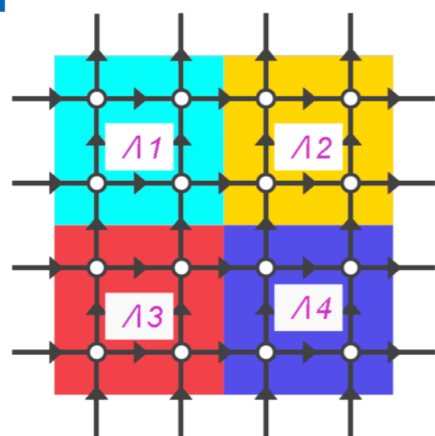
Physics (Theory&Experiment)



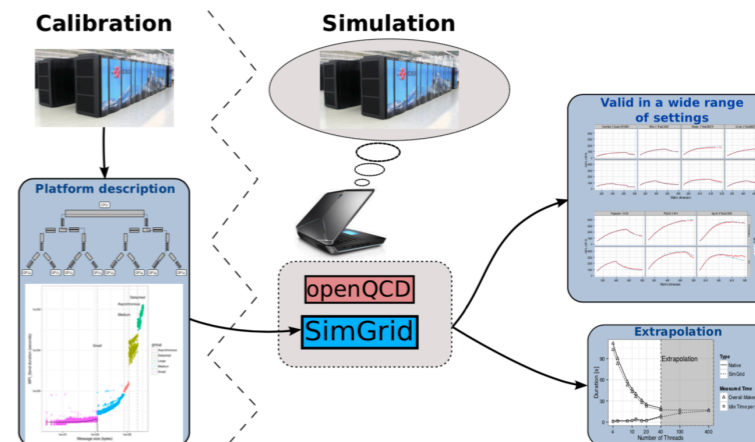
Lattice QCD



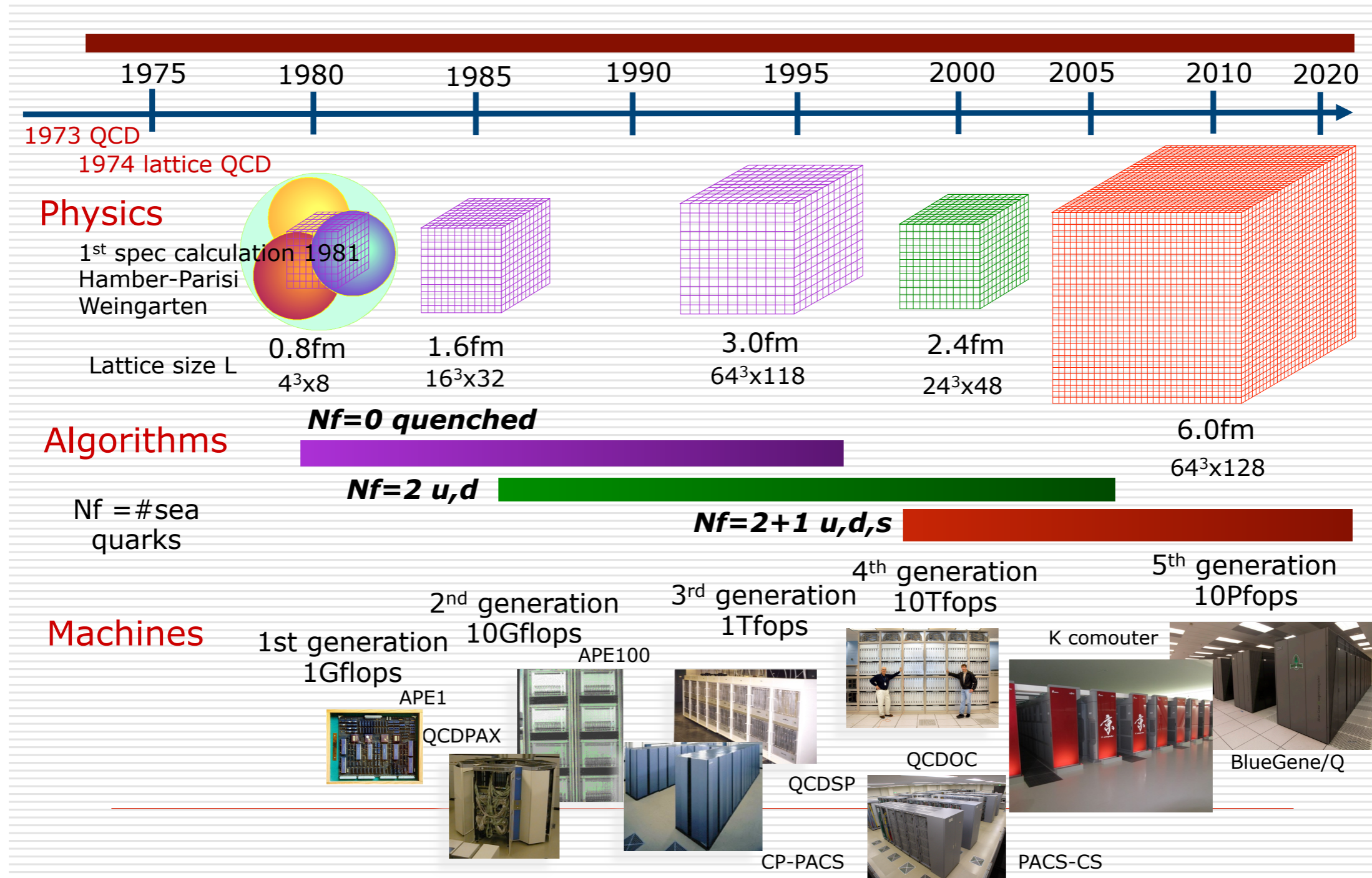
Computational Methods



Machines



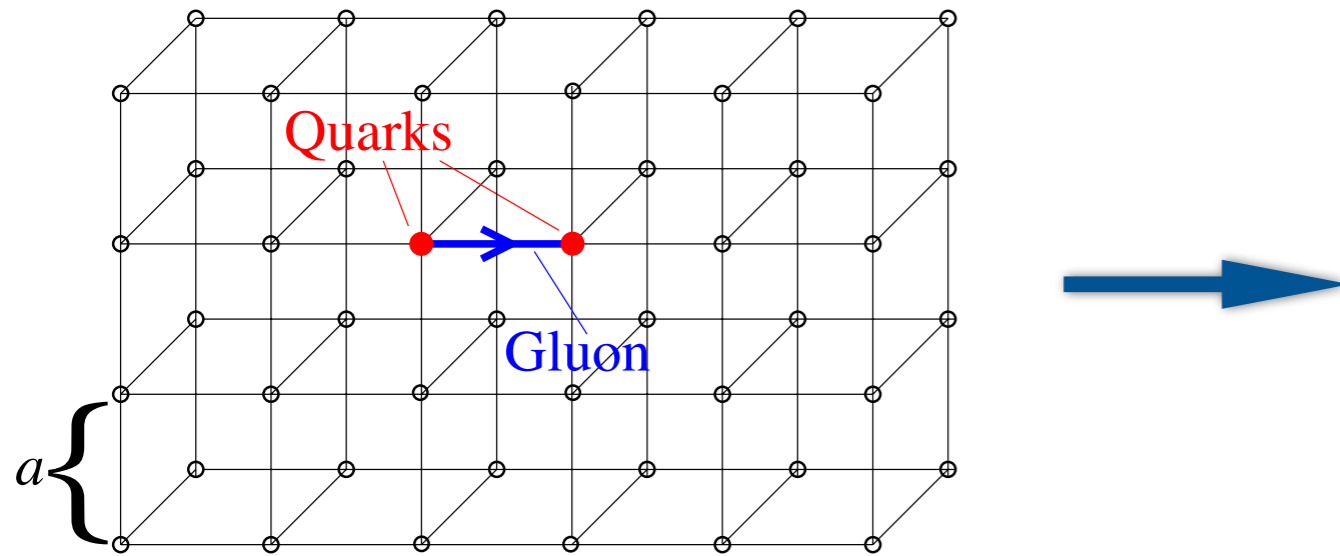
Development of Lattice QCD



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



Typical Lattice QCD Computation



<https://www.cscs.ch/publications/photo-gallery/>

- physical lattice size: $\sim 6\text{fm}$, spacing $0.05\text{-}0.1\text{fm}$
- $64^3 \times 128$ lattice $\rightarrow 34 \times 10^6$ points
- Operator dimensions: $10^7 \times 10^7$ matrices
- **Advanced computational methods** are needed
- **Large computer resources**: multiple TFlop years!



Altamira@IFCA, Santander



Wilson Cluster at Mainz U.

Backstage of LGT Calculations



[bbc tyne in pictures backstage at theatre royal; image by www.bbc.co.uk]

Plan of the Lectures:

- **Lecture 1: Path Integral Quantization and scalar fields on the lattice;** *Why do we need to consider discrete space/time?*
- **Lecture 2: QCD and QED on the lattice; Computational methods for lattice field theories;** *Why is LQCD so comp. expensive? What are the limitations? Where can we move the needle with Lattice QCD+QED?*

Part 1:
**Path Integral Quantization and
scalar fields on the lattice**

Outline

- ◉ **Point Mechanics vs. Classical Field Theory**
- ◉ **Path Integral in Quantum Mechanics (real and Euclidean time)**
- ◉ **Scalar Field Theory on the lattice**
- ◉ **Analogy with Statistical Mechanics and continuum limit**
- ◉ **Spectrum of the Scalar Theory on the lattice**

Classical Point Mechanics

- **Point Mechanics — 2nd Newton's law:**

$$m \frac{d^2 x}{dt^2} = m \partial_t^2 x = F(x) = - \frac{dV(x)}{dx}$$

m — mass of the classical non-relativistic point particle

$V(x)$ — external potential

- **The principle of least action:**

$$S[x] = \int dt \mathcal{L}(x, \partial_t x)$$

- **Lagrange function:**

$$\mathcal{L}(x, \partial_t x) = \frac{m}{2} (\partial_t x)^2 - V(x)$$

- **Euler-Lagrange equation:**

$$\partial_t \frac{\delta \mathcal{L}}{\delta(\partial_t x)} - \frac{\delta \mathcal{L}}{\delta x} = 0$$

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Classical Field Theory

- Generalization to systems with infinitely many d.o.f. (field values $\phi(\vec{x})$)

- Classical field e. o. m. for neutral scalars — Klein-Gordon eq.: $\partial_\mu \partial^\mu \phi = -\frac{dV(\phi)}{d\phi}$

- Again, the classical e. o. m obtained by minimizing the action:

$$S[\phi] = \int d^4x \mathcal{L}(\phi, \partial_\mu \phi)$$

$$\partial_\mu \frac{\delta \mathcal{L}}{\delta(\partial_\mu \phi)} - \frac{\delta \mathcal{L}}{\delta \phi} = 0$$

- A simple example of interacting scalar field theory (‘ ϕ^4 — theory’)

$$V(\phi) = \frac{m^2}{2} \phi^2 + \frac{\lambda}{4!} \phi^4$$

m — mass of the scalar field

λ — coupling strength of its self-interaction

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Point Mechanics vs. Classical Field Theory

Point Mechanics	Field Theory
time t	space-time $x = (t, \vec{x})$
particle coordinate x	field value ϕ
particle path $x(t)$	field configuration $\phi(x)$
action $S[x] = \int dt L(x, \partial_t x)$	action $S[\phi] = \int d^4x \mathcal{L}(\phi, \partial_\mu \phi)$
Lagrange function $L(x, \partial_t x) = \frac{m}{2}(\partial_t x)^2 - V(x)$	Lagrangian $\mathcal{L}(\phi, \partial_\mu \phi) = \frac{1}{2}\partial_\mu \phi \partial^\mu \phi - V(\phi)$
equation of motion $\partial_t \frac{\delta L}{\delta(\partial_t x)} - \frac{\delta L}{\delta x} = 0$	field equation $\partial_\mu \frac{\delta \mathcal{L}}{\delta(\partial_\mu \phi)} - \frac{\delta \mathcal{L}}{\delta \phi} = 0$
Newton's equation $\partial_t^2 x = -\frac{dV(x)}{dx}$	Klein-Gordon equation $\partial_\mu \partial^\mu \phi = -\frac{dV(\phi)}{d\phi}$
kinetic energy $\frac{m}{2}(\partial_t x)^2$	kinetic energy $\frac{1}{2}\partial_\mu \phi \partial^\mu \phi$
harmonic oscillator potential $\frac{m}{2}\omega^2 x^2$	mass term $\frac{m^2}{2}\phi^2$
anharmonic perturbation $\frac{\lambda}{4}x^4$	self-interaction term $\frac{\lambda}{4}\phi^4$

[Credit: U.-J. Wiese <https://inspirehep.net/literature/946884>]

● Point Mechanics vs. Classical Field Theory

Path Integral in Quantum Mechanics: real time (I)

- Time-dependent Schrödinger Eq.

$$i\hbar\partial_t |\Psi(t)\rangle = H |\Psi(t)\rangle$$

- Time evolution operator

$$U(t', t) = e^{-\frac{i}{\hbar}H(t'-t)}; \quad |\Psi(t')\rangle = U(t', t) |\Psi(t)\rangle$$

H – time independent Hamilton operator

- Transition amplitude of a non-relativistic point particle – a propagator:

$$\langle x' | U(t', t) | x \rangle$$

- Contains information about the energy spectrum of the theory.

Path Integral in Quantum Mechanics: real time (II)

- Propagator from x to x'

$$\langle x'|U(t',t)|x\rangle = \int dx_1 \langle x'|U(t',t_1)|x_1\rangle \langle x_1|U(t_1,t)|x\rangle$$

- Divide time interval into N elementary steps of size

$$[t',t]; \quad t' - t = N \epsilon$$

- Repeat previous procedure at all intermediate times

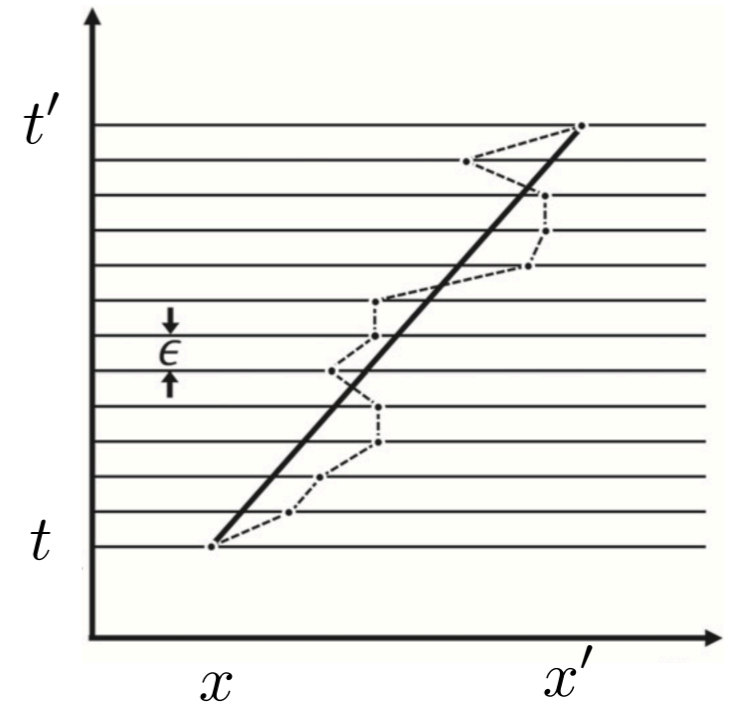
$$\langle x'|U(t',t)|x\rangle = \int dx_1 \int dx_2 \dots \int dx_{N-1} \langle x'|U(t',t_{N-1})|x_{N-1}\rangle \times \dots \times \langle x_2|U(t_2,t_1)|x_1\rangle \times \langle x_1|U(t_1,t)|x\rangle$$

- Take factor $\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle$; assume single non-relativistic point particle

$$H = \frac{p^2}{2m} + V(x)$$

- Insert complete set of states + BCH formula:

$$\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle = \frac{1}{2\pi} \int dp e^{-\frac{i\epsilon p^2}{2m\hbar}} e^{-\frac{i}{\hbar}p(x_{i+1}-x_i)} e^{-\frac{i\epsilon}{\hbar}V(x_i)}$$



Path Integral in Quantum Mechanics: real time (III)

$$\langle x_{i+1} | U(t_{i+1}, t_i) | x_i \rangle = \frac{1}{2\pi} \int dp e^{-\frac{i\epsilon p^2}{2m\hbar}} e^{-\frac{i}{\hbar} p(x_{i+1} - x_i)} e^{-\frac{i\epsilon}{\hbar} V(x_i)}$$

• $\int dp$ ill-defined: integrand rapidly oscillating f-on

• For it to be well-defined:

1. replace: $\epsilon \longrightarrow \epsilon - i a; \quad a \in \mathbb{R}$

2. evaluate $\int dp \dots$

3. take $a \rightarrow 0$ limit, one gets:

$$\langle x_{i+1} | U(t_{i+1}, t_i) | x_i \rangle = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} e^{\frac{i}{\hbar} \epsilon \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 - V(x_i) \right]}$$

• Insert into original propagator:

$$\langle x' | U(t', t) | x \rangle = \int \mathcal{D}x e^{\frac{i}{\hbar} S[x]}$$

$$\int \mathcal{D}x = \lim_{\epsilon \rightarrow 0} \sqrt{\frac{m}{2\pi i \hbar \epsilon}}^{N-1} \int dx_1 \int dx_2 \dots \int dx_{N-1}$$

Path Integral in Quantum Mechanics: real time (IV)

$$\langle x' | U(t', t) | x \rangle = \int \mathcal{D}x e^{\frac{i}{\hbar} S[x]}$$

$$\int \mathcal{D}x = \lim_{\epsilon \rightarrow 0} \sqrt{\frac{m}{2\pi i \hbar \epsilon}}^{N-1} \int dx_1 \int dx_2 \dots \int dx_{N-1}$$

- **The action is continuum limit of the discretised action:**

$$S[x] = \int dt \left[\frac{m}{2} (\partial_t x)^2 - V(x) \right] = \lim_{\epsilon \rightarrow 0} \sum_i \epsilon \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 - V(x_i) \right]$$

- **Summary:**

- (i) Integrate over all particle positions for each intermediate time t_i
- (ii) Amounts to integrating over all possible paths of a particle starting at x and ending at x'
- (iii) Each path weighted with oscillating phase
- (iv) Classical path: the smallest oscillations \Rightarrow largest contribution to the P.I. ($\hbar \rightarrow 0$ class. limit)

- **Note: definition of the path integral required an analytic continuation in time!**

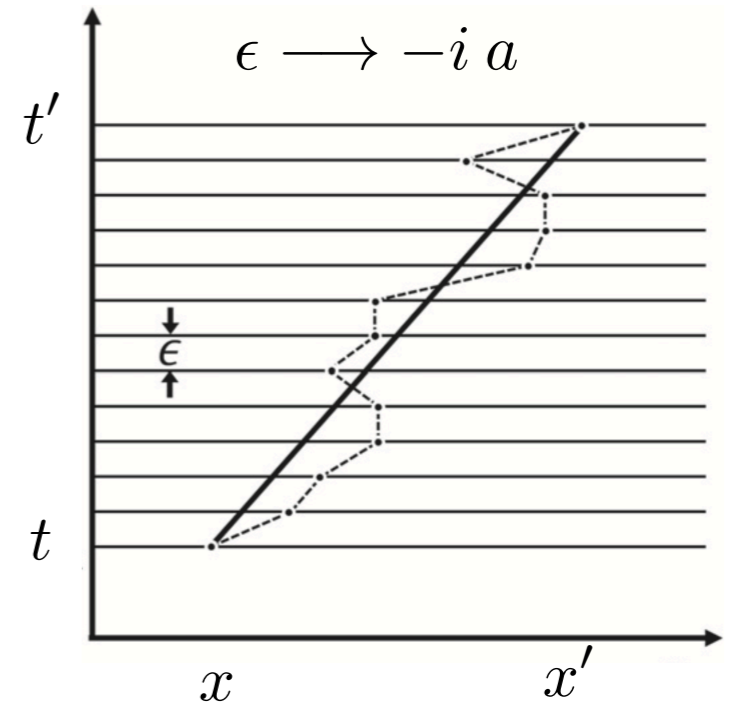
Euclidean Path Integral in Quantum Mechanics

- Statistical partition function: $Z = e^{-\beta H}; \quad \beta = \frac{1}{T}$
- $\beta = \frac{i}{\hbar}(t' - t) \implies e^{-\beta H} \Leftrightarrow U(t, t')$

System at finite temperature T



System propagating in purely imaginary time



- Repeat all the steps from the derivation in real time:

- (i) Divide Euclidean time interval into N time steps: $\beta = \frac{Na}{\hbar}$
- (ii) Insert complete set of position eigenstates

- The Euclidean Path Integral:

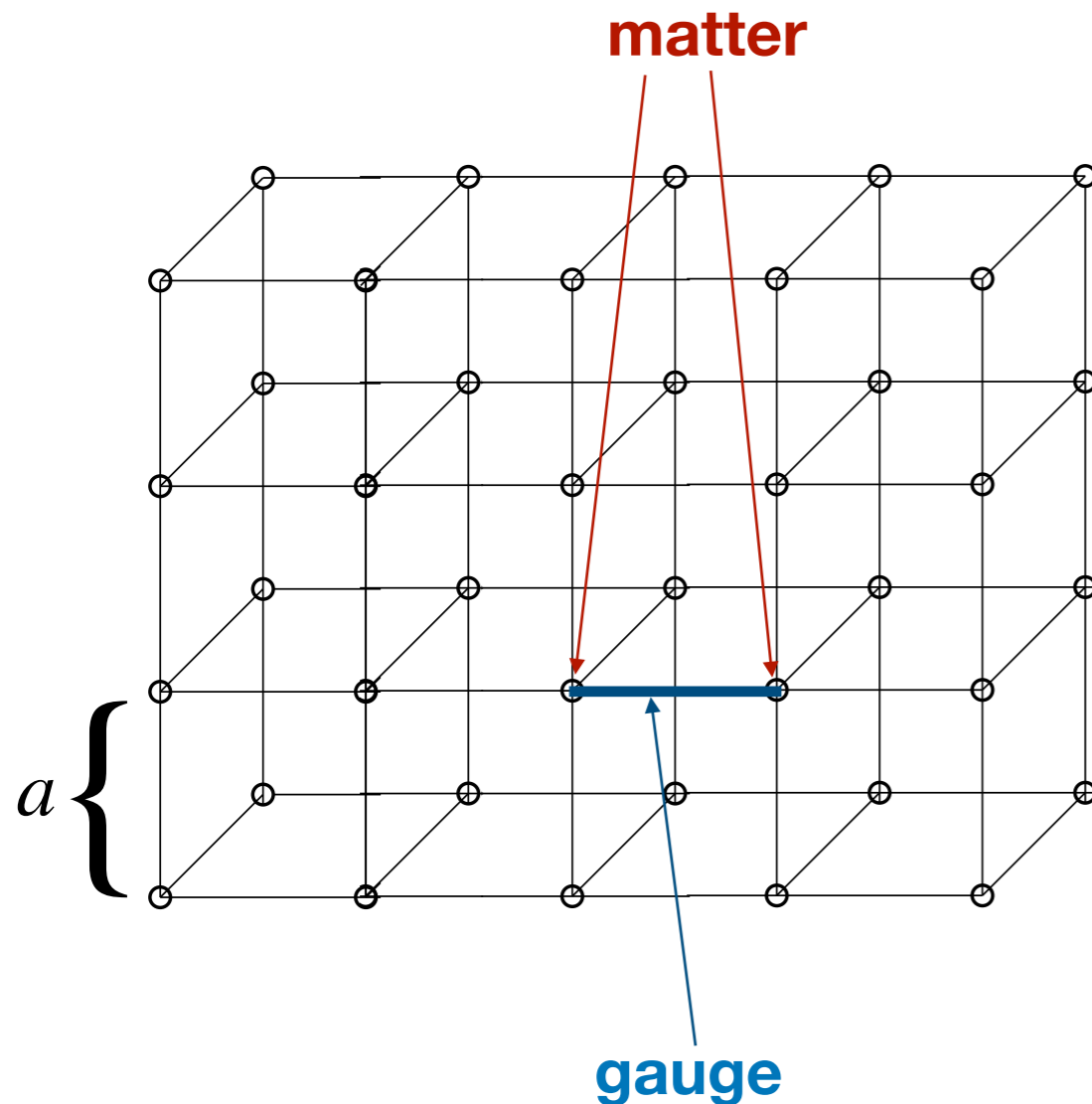
$$Z = \int \mathcal{D}x e^{-\frac{1}{\hbar} S_E[x]}$$

$$S_E[x] = \int dt \left[\frac{m}{2} (\partial_t x)^2 + V(x) \right] = \lim_{a \rightarrow 0} \sum_i a \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{a} \right)^2 + V(x_i) \right]$$

$$\int \mathcal{D}x = \lim_{a \rightarrow 0} \sqrt{\frac{m}{2\pi i \hbar a}}^N \int dx_1 \int dx_2 \dots \int dx_N$$

Scalar fields on the lattice

- Quantum field theories beyond tree level are plagued by UV divergencies
- Defining the theory on a lattice introduces a minimum length



- Lattice spacing acts as an UV cut-off: $\Lambda \sim \frac{1}{a}$

$$Z = \int \mathcal{D}\phi e^{-S_E[\phi]}$$

$$\int \mathcal{D}\phi = \prod_x \int d\phi(x)$$

$$S_E[\phi] = \int d^D x \left[\frac{1}{2} (\partial_\mu \phi)^2 + \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{4!} \phi^4 \right]$$

Scalar field theory

- **Discretize space-time and define matter fields on the sites of the lattice:**

$$x \longrightarrow an = (an_1, an_2, an_3, an_4); \quad n_\mu \in \mathbb{Z}$$
$$\phi(x) \longrightarrow \phi(an)$$

- **Momentum integrals are restricted to the first Brillouin zone:**

$$\int d^4x \longrightarrow a^4 \sum_{n_\mu} \equiv \sum_x$$
$$\int \frac{d^4k}{2\pi} \longrightarrow \int_{|k| < \frac{2\pi}{a}} \frac{d^4k}{2\pi} \equiv \int_k$$

- **Discretize the derivatives:**

$$\partial_\mu \phi(x) \longrightarrow \nabla_\mu \phi(x) = \frac{1}{a} [\phi(x + a\hat{\mu}) - \phi(x)]$$
$$\longrightarrow \nabla_\mu^* \phi(x) = \frac{1}{a} [\phi(x) - \phi(x - a\hat{\mu})]$$

Lattice action

- Discretized action (bare parameters)

$$S[\phi] = \sum_x \left[\frac{1}{2} \nabla_\mu \phi(x) \nabla_\mu \phi(x) + \frac{1}{2} m_0^2 \phi(x)^2 + \frac{\lambda_0}{4!} \phi(x)^4 \right]$$

- Scalar propagator

$$\begin{aligned} \Delta(k)^{-1} &= \sum_\mu \left[\frac{2}{a} \sin\left(\frac{k_\mu a}{2}\right) \right]^2 + m_0^2 \\ &= k^2 + m_0^2 + \mathcal{O}(a^2) \end{aligned}$$

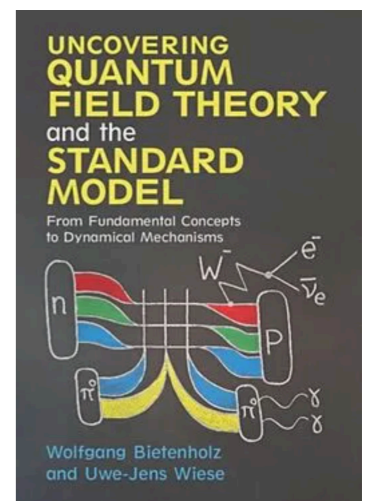
- Space time symmetry: $O(4) \longrightarrow H(4)$

- Rotation symmetry recovered in the continuum limit

From P.I. in Quantum Mech. to Statistical Stat. Mech.

Quantum mechanics	Classical statistical mechanics
Euclidean time lattice	d -dimensional spatial lattice
elementary time step a	crystal lattice spacing
particle position x	classical spin variable s
particle path $x(t)$	spin configuration s_x
path integral $\int \mathcal{D}x$	sum over configurations $\prod_x \sum_{s_x}$
Euclidean action $S_E[x]$	classical Hamilton function $\mathcal{H}[s]$
Planck's constant \hbar	temperature T
quantum fluctuations	thermal fluctuations
kinetic energy $\frac{1}{2}(\frac{x_{i+1}-x_i}{a})^2$	neighbor coupling $s_x s_{x+1}$
potential energy $V(x_i)$	external field energy $\mu B s_x$
weight of a path $\exp(-\frac{1}{\hbar} S_E[x])$	Boltzmann factor $\exp(-\mathcal{H}[s]/T)$
vacuum expectation value $\langle \mathcal{O}(x) \rangle$	magnetization $\langle s_x \rangle$
2-point function $\langle \mathcal{O}(x(0)) \mathcal{O}(x(t)) \rangle$	correlation function $\langle s_x s_y \rangle$
energy gap $E_1 - E_0$	inverse correlation length $1/\xi$
continuum limit $a \rightarrow 0$	critical behavior $\xi \rightarrow \infty$

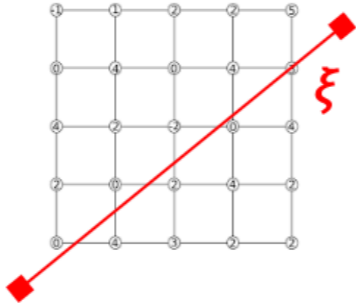
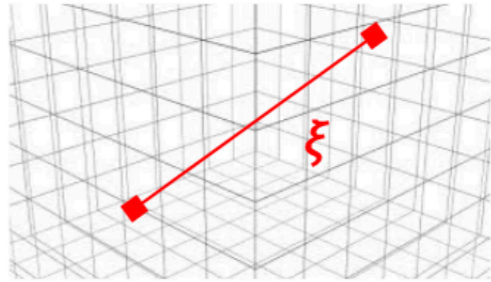
[See also:]



[Credit: U.-J. Wiese <https://inspirehep.net/literature/946884>]

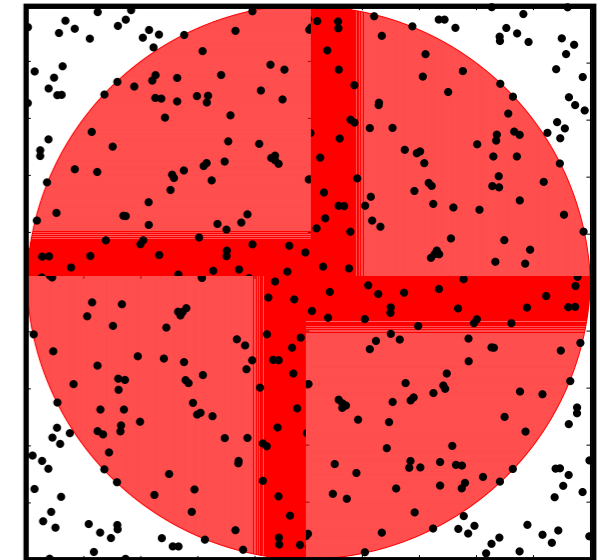
[To appear on 31 August 2024]

From Statistical Mech. to Quantum Field Theories

Classical Statistical Mechanics		Quantum Field Theories	
Partition function	$Z_\beta = \sum_\sigma e^{-\beta H(\sigma)}$	Feynman Path Integral	$Z = \int D[U] e^{[-1/g^2] S(U)}$
Inverse temperature	$\beta \sim 1/T$	Inverse gauge coupling	$\sim 1/g^2$
Correlation functions	$\langle \sigma(x) \sigma(y) \rangle \sim e^{- x-y /\xi}$	2-point functions	$\langle \text{Tr}(U(p)_x) \text{Tr}U(p)_y \rangle \sim e^{- x-y /r}$
Inverse correlation length	$1/\xi$	Particle mass: m	
2nd order phase transition $\xi/a \rightarrow \infty$ with a fixed		Continuum limit: $m a \rightarrow 0$ with m fixed	
2-d spatial lattice with physical lattice spacing a		4-d space-time lattice with unphysical cut-off a	

A tool for Lattice Simulations: *Monte Carlo* methods

- Monte Carlo: a numerical method for estimating high-dimensional integrals by random sampling



JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

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THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM

Los Alamos Laboratory

We shall present here the motivation and a general description of a method dealing with a class of problems in mathematical physics. The method is, essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences.



A tool for Lattice Simulations: Monte Carlo methods

- Ratio of the surface area of the circle and the square:

$$\rightarrow \frac{S_{circle}}{S_{square}} = \frac{\pi r^2}{4r^2}$$

- We can then express:

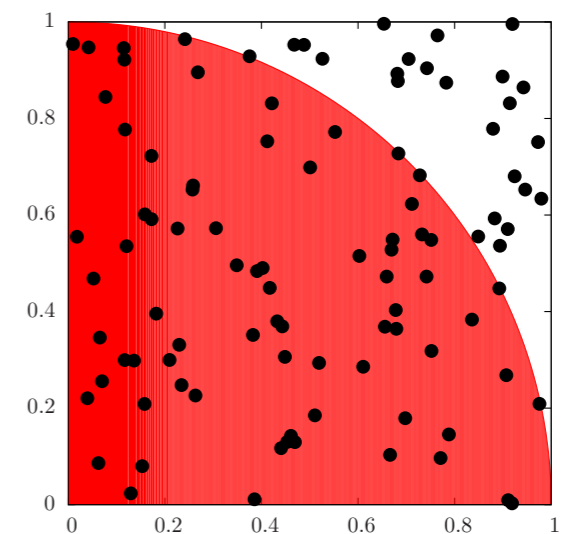
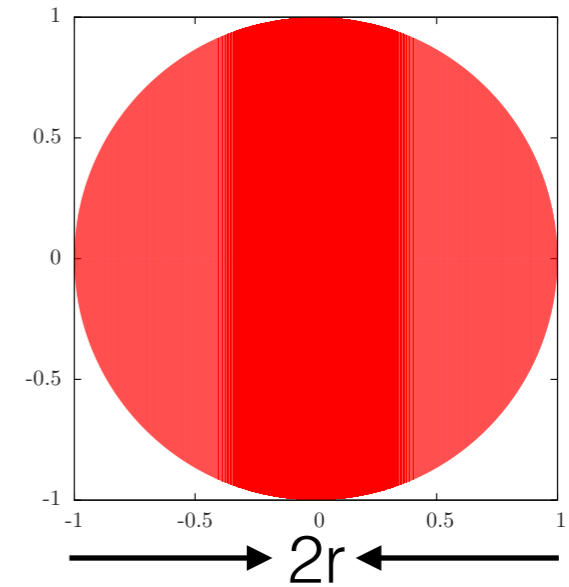
$$\rightarrow \pi = \frac{4S_{circle}}{S_{square}}$$

- If we know S_{circle}/S_{square} , we know the value of π

- Throw N random points on the surface of the square

$$\rightarrow \pi = \frac{4S_{circle}}{S_{square}} \approx \frac{N_{inside}}{N}$$

- For N - large, the value of π will be very well approximated



A tool for Lattice Simulations: Monte Carlo methods

- Calculating 1-dim integral:

$$\rightarrow I = \int_0^1 f(x) dx$$

- Again, throw N random points on the rectangular surface:
- Count those under the value of the function $f(x)$
- Then the value of the integral is obtained by:

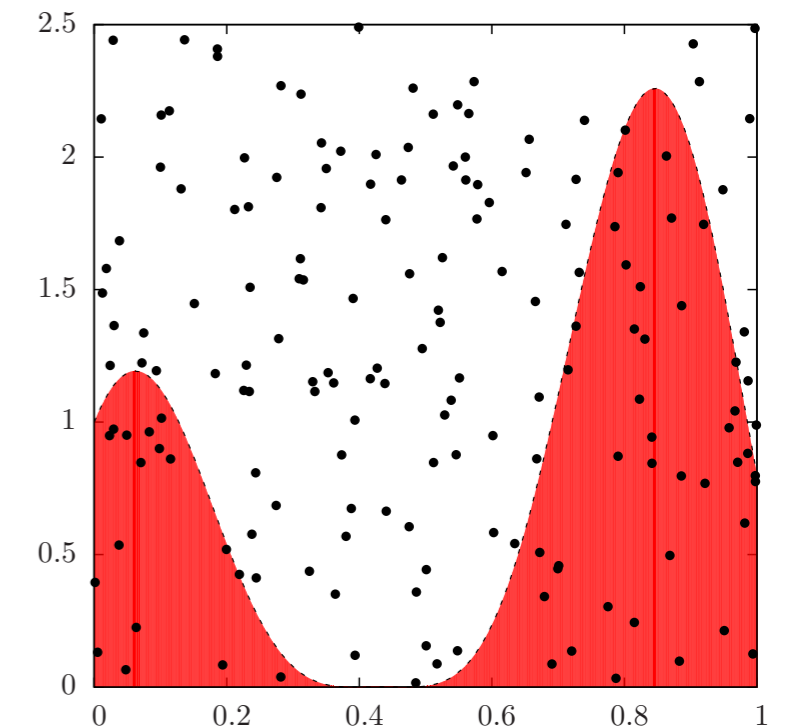
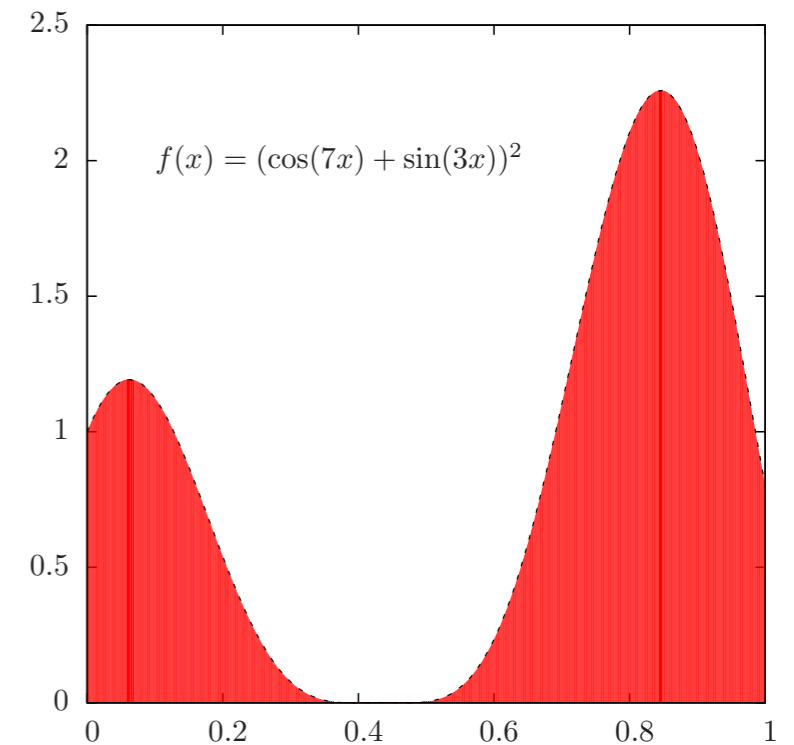
$$\rightarrow I \approx \langle I \rangle_N = 2.5 \times 1 \times \frac{N_{inside}}{N}$$

- For larger N, better and better approximation of the integral

- Monte Carlo error in d-dim: $\approx \frac{1}{\sqrt{N}}$

- Numerical integration error in d-dim: $\approx \frac{1}{N^{2/d}}$

- For $d > 4$, Monte Carlo is better than Numerical Integration!



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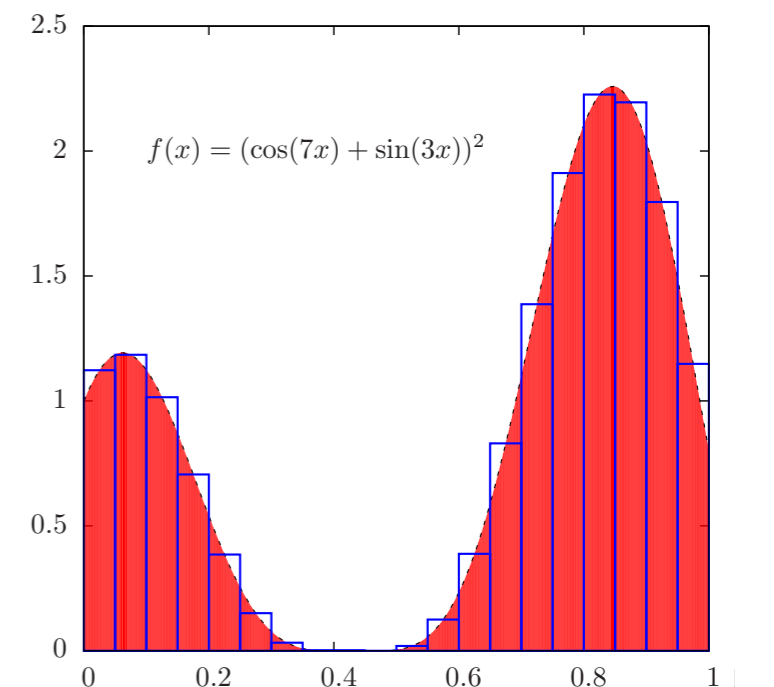
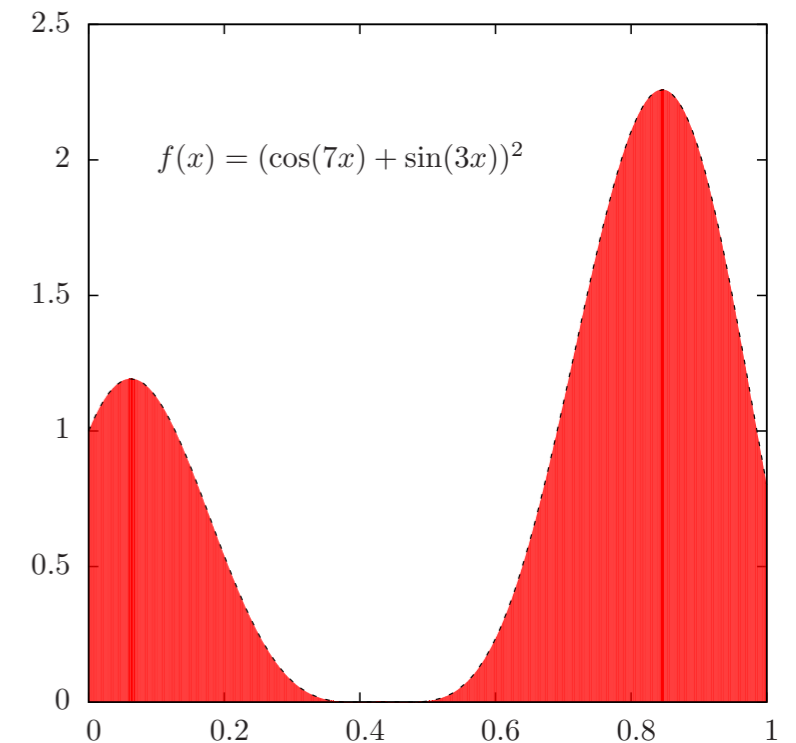
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Expectation values in Monte Carlo

- Ising model Hamiltonian (without external magnetic field):

$$H = -J \sum_{\langle x,y \rangle} s_x s_y; \quad \langle x,y \rangle \text{ — nearest neighbours}$$

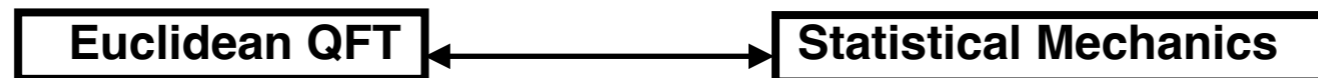
- Generate configurations of spins with probability $\sim e^{-\frac{H}{T}}$ (importance sampling)
- Expectation value of the observables as averages over ensemble of spin configurations

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

- How do we generate the ensemble $\{\bar{s}_k\}$?

Numerical Simulations

- Numerical approach exploits the analogy:



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

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

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

- Markov chains that converge exponentially to the equilibrium distr.
- The configurations $\{\phi_i\}$ are correlated by construction

$$Var[\bar{O}] = Var[O] \left(\frac{2\tau_O}{N_{cnfg}} \right)$$

– integrated autocorrelation time

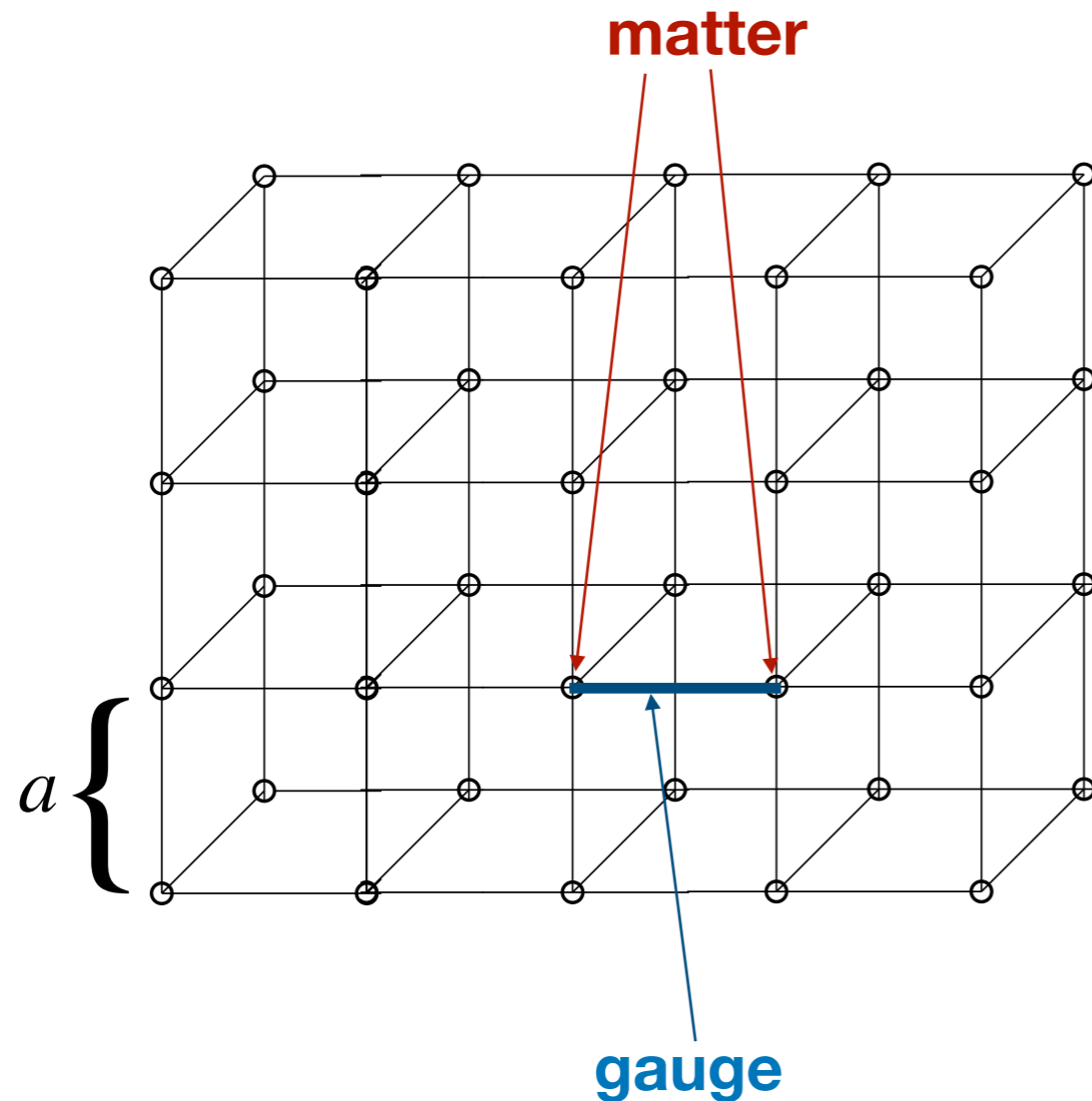
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$$Var[O] = \langle (O - \langle O \rangle)^2 \rangle$$

└─ property of QFT itself, should not depend of the Markov chain.

QFT on the lattice: symmetries

- **Translational Symmetry:**
Broken to discrete symmetry, but nicely restored in the continuum limit
- **Rotational Symmetry:**
Similar to translational symmetry. Finite number of irreducible representations (quantum numbers) instead of spin, but correct states are obtained in the continuum limit



In the first lecture:

- ◉ We have learned/reminded ourselves how to quantize:

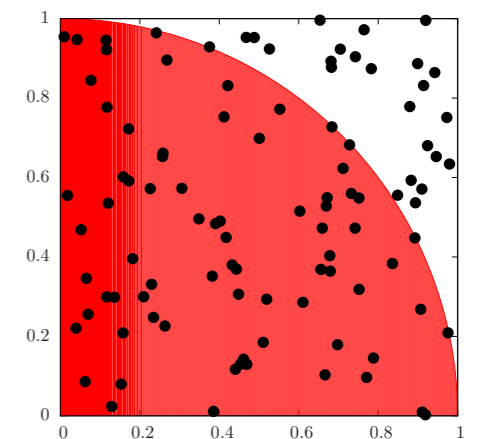
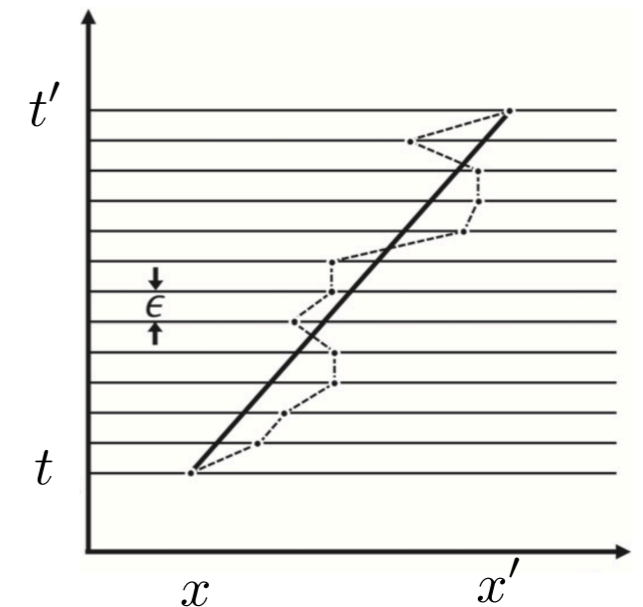
- Quantum Mechanics

- Scalar Field Theory

- ◉ Mapping to Classical Statistical Mechanics

- ◉ Monte Carlo Sampling of Spin Systems → Quantum Fields

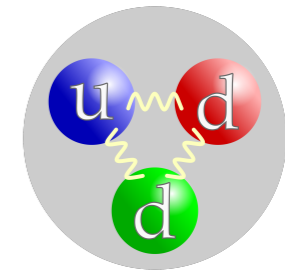
- ◉ Monte Carlo Errors, other sources of errors



In the lecture on Friday:

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

- We shall see how the numerical sampling is done in practice



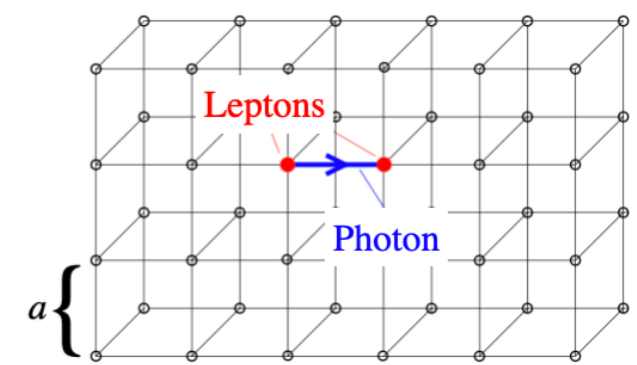
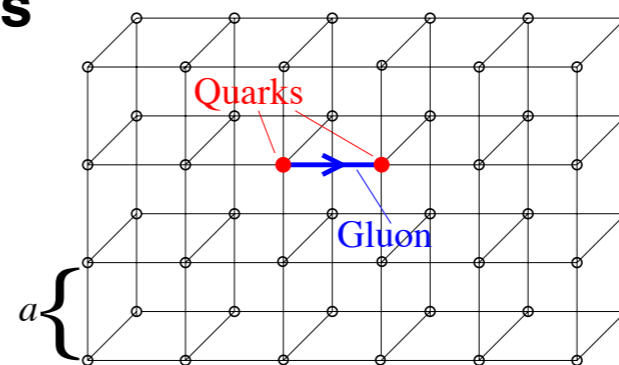
→ for scalar field theory

→ for QCD

- Why is QCD numerically so expensive?



- QED corrections to hadronic observables



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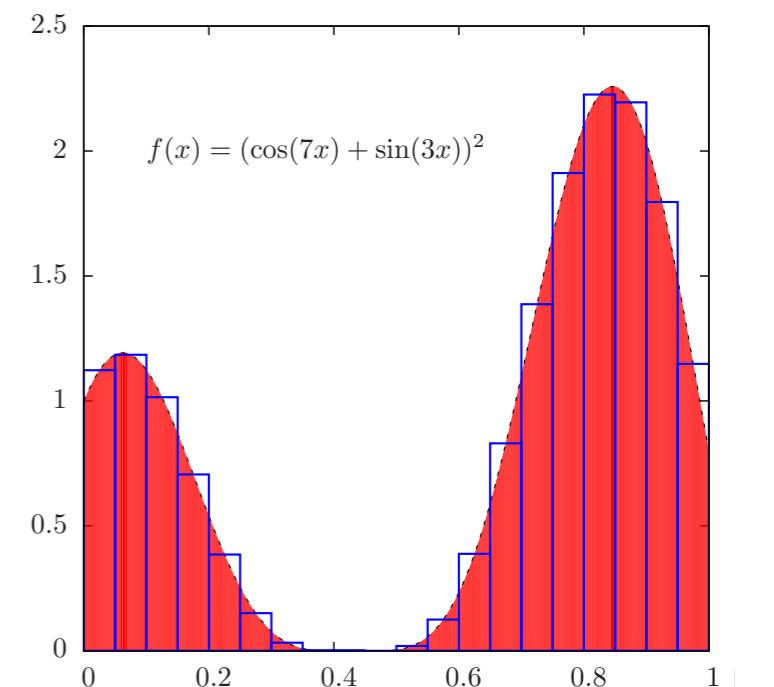
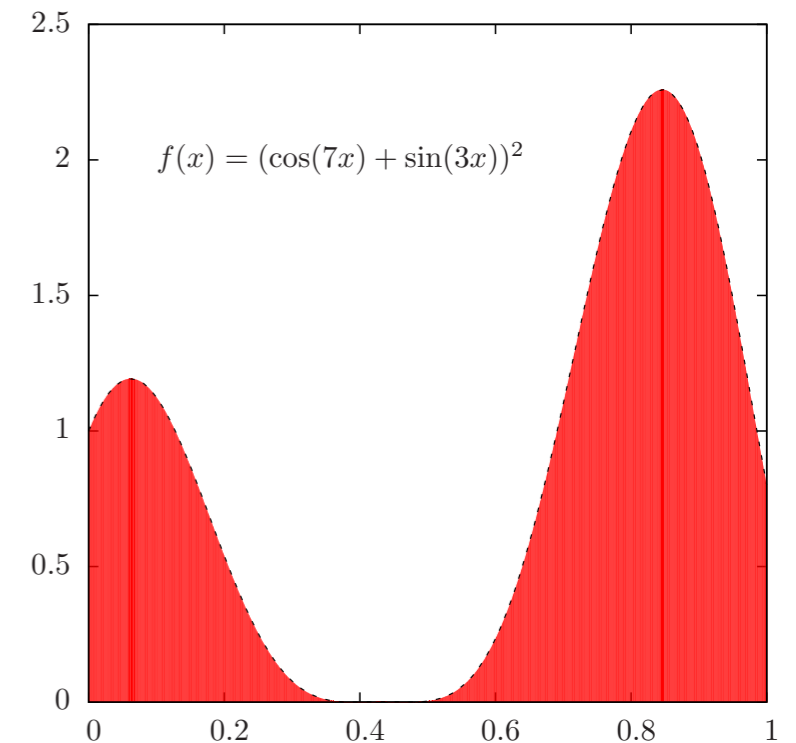
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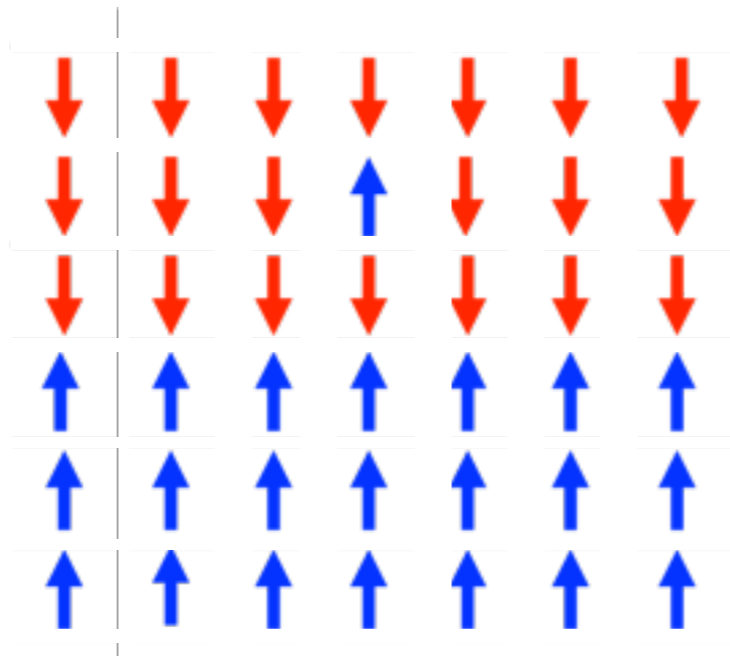
Classical statistical Mechanics: Ising Model

→ CLASSICAL HAMILTON FUNCTION:

$$\mathcal{H}[S] = -J \sum_{\langle xy \rangle} S_x S_y - \mu B \sum_x S_x$$

* $J > 0$; FERROMAGNETIC COUPLING CONST.

* μ COUPLING TO AN EXTERNAL MAG. FIELD B



Classical statistical Mechanics: Ising Model

- CLASSICAL PARTITION F-ON:

$$Z = \int \mathcal{D}s e^{-\mathcal{H}[s]/T}$$
$$= \prod_x \sum_{S_x = \pm 1} e^{-\frac{1}{T} \mathcal{H}[s]}$$

- THERMAL AVERAGES:

* MAGNETIZATION: $\langle S_x \rangle = \frac{1}{Z} \prod_x \sum_{S_x = \pm 1} S_x e^{-\frac{\mathcal{H}[s]}{T}}$

- * SPIN CORRELATION F-ON:

$$\langle S_x S_y \rangle = \frac{1}{Z} \prod_x \sum_{S_x = \pm 1} S_x S_y e^{-\frac{\mathcal{H}[s]}{T}}$$

Expectation values in the MC approach: spin systems

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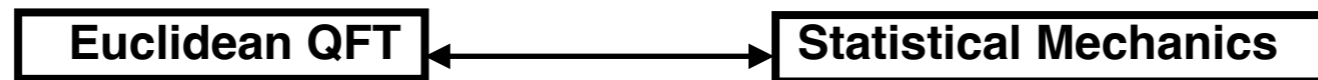
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└── property of QFT itself, should not depend of the Markov chain.

Detailed Balance

- Probability for a random transition $\phi \rightarrow \phi'$:

$$R(\phi' \leftarrow \phi)$$

- Sequence of probabilities in Markov chain, $P^{k+1}(\phi')$ depends only on $P^k(\phi)$

$$P^{k+1}(\phi') = \int [d\phi] P^k(\phi) R(\phi' \leftarrow \phi)$$

- Probabilities of ϕ' being initial or final configuration in a random update are equal

$$\sum_{\phi} R(\phi' \leftarrow \phi) P(\phi) = \sum_{\phi} R(\phi \leftarrow \phi') P(\phi')$$

- The above is known as a “balance equation”

Detailed Balance

- Calculate the sum using normalization of R

$$0 \leq R(\phi \leftarrow \phi') \leq 1, \quad \sum_{\phi} R(\phi \leftarrow \phi') = 1$$

- Obtain that equilibrium distribution $P(\phi')$ is a fixed point of the Markov Process

$$\sum_{\phi} R(\phi' \leftarrow \phi)P(\phi) = P(\phi')$$

- The solution of the balance equation can be obtained if ***detailed balance*** is fulfilled

$$R(\phi' \leftarrow \phi)P(\phi) = R(\phi \leftarrow \phi')P(\phi')$$

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.

$$p = \min\left(1, \frac{\pi(\phi')}{\pi(\phi)}\right)$$



The MR²T² algorithm

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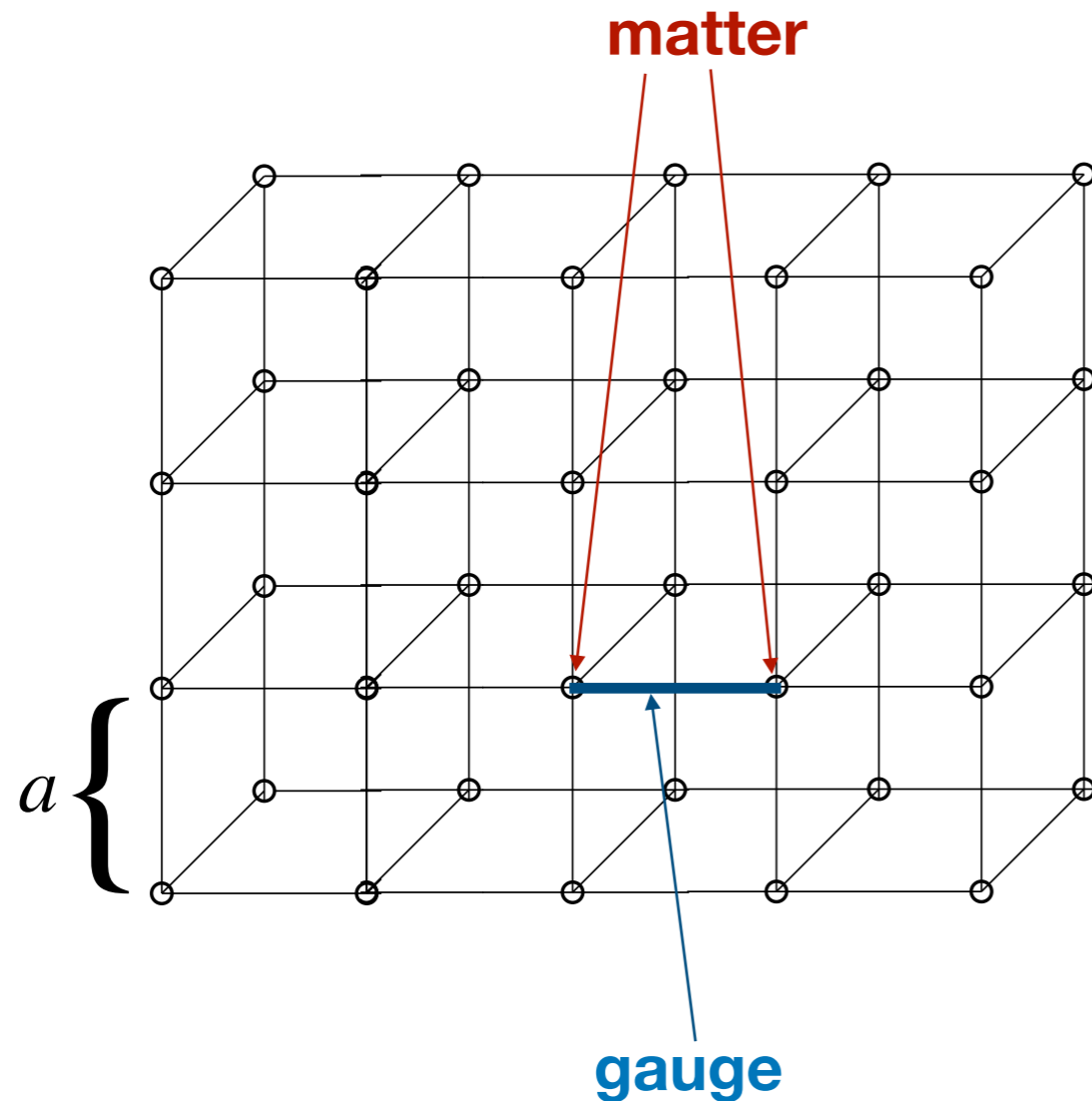
- The Metropolis Algorithm for Scalar F.T.:
- Given ϕ propose ϕ'
- Choose a random number $r \in [0,1]$
- If $S_E(\phi') < S_E(\phi)$, always accept, otherwise add ϕ' to the chain again if

$$e^{-\Delta S} > r;$$

$$\Delta S = S_E(\phi') - S_E(\phi)$$

QFT on the lattice: symmetries

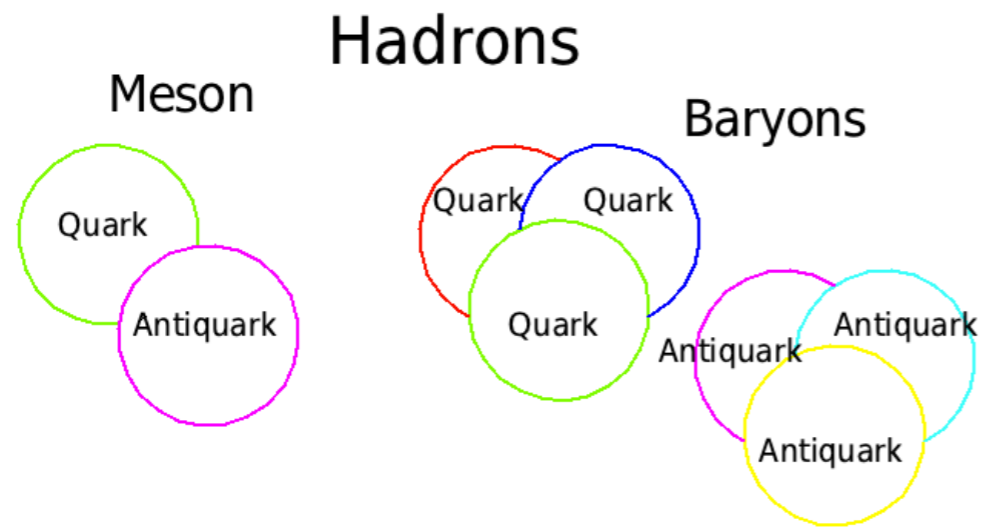
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Broken to discrete symmetry, but nicely restored in the continuum limit
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Similar to translational symmetry. Finite number of irreducible representations (quantum numbers) instead of spin, but correct states are obtained in the continuum limit



Strong interaction

→ quarks ($q_i = u, d, s, c, b, [t]$) elementary constituents of:

- mesons ($q\bar{q}$)
- baryons (qqq), ($\bar{q}\bar{q}\bar{q}$)



Quark / Antiquark	Symbol		Charge/e		Baryon number, B		Strangeness, S	
	q	\bar{q}						
up	u	\bar{u}	+2/3	-2/3	1/3	-1/3	0	0
down	d	\bar{d}	-1/3	+1/3	1/3	-1/3	0	0
charm	c	\bar{c}	+2/3	-2/3	1/3	-1/3	0	0
strange	s	\bar{s}	-1/3	+1/3	1/3	-1/3	-1	1
top	t	\bar{t}	+2/3	-2/3	1/3	-1/3	0	0
bottom	b	\bar{b}	-1/3	+1/3	1/3	-1/3	0	0

revisionworld

COLOUR: SU(3) symmetry

Quantum Chromodynamics

- QCD Lagrangian

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

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

- Covariant derivative: $D_\mu = \partial_\mu - ig_s A_\mu$

Quantum Chromodynamics

- QCD Lagrangian

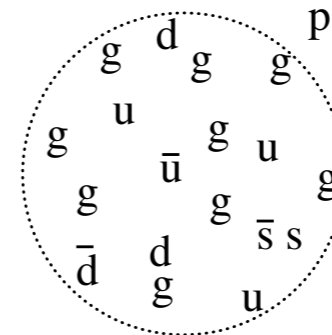
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- Covariant derivative: $D_\mu = \partial_\mu - ig_s A_\mu$

- Bare QCD parameters (N_f+1)

- gauge coupling g_s
- quark masses m_u, m_d, \dots

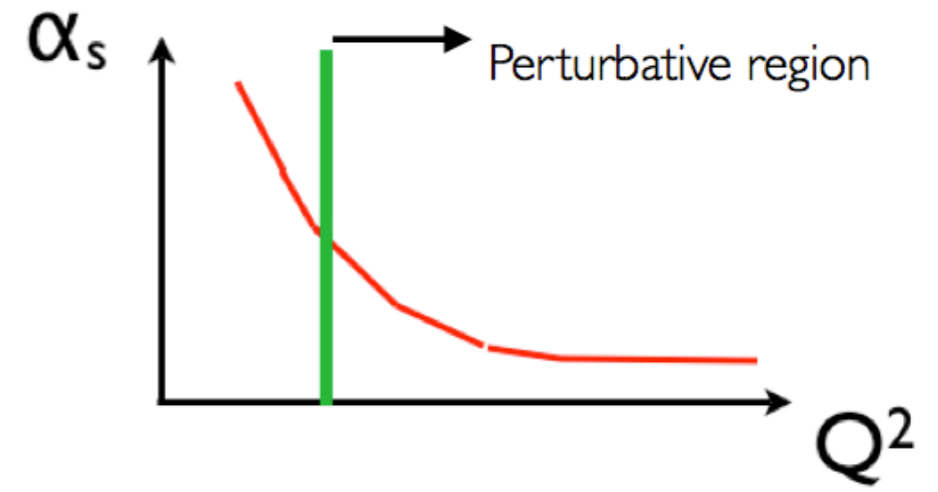


Quantum Chromodynamics

- QCD Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \sum_{f=u,d,s,\dots} \bar{\psi}_f \{ i\gamma_\mu (\partial_\mu - ig_s A_\mu^a T^a) - m_f \} \psi_f$$

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



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

$$\mathcal{L}_{QCD} = \frac{1}{2g^2} F_{\mu\nu}^a F_{\mu\nu}^a + \sum_{f=u,d,s,\dots} \bar{\psi}_f \{ \gamma_\mu (\partial_\mu + iA_\mu^a T^a) + m_f \} \psi_f$$

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

Path Integrals in Quantum Chromodynamics

- Each specific field configuration:

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

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

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

Lattice regularization of QCD

- Divergencies in continuum QCD → **regularization** is necessary!
- One possible regularization:
Introduce **momentum ultraviolet-cutoff** \Leftrightarrow minimum distance (FT)
- If required also: **local gauge symmetry** → **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

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

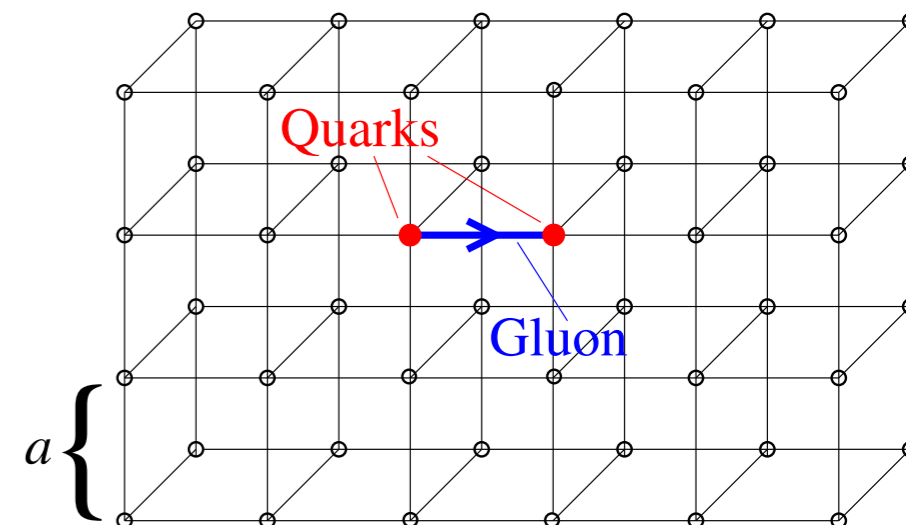
- Discretization prescription:

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

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

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

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



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:

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

- Let us examine gauge invariance \rightarrow

Gauge Invariance

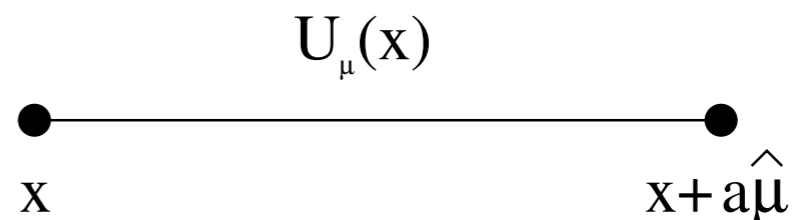
- $\Omega(n) \in SU(3)$:

$$\psi'(n) = \Omega(n)\psi(n)$$

$$\bar{\psi}'(n) = \bar{\psi}(n)\Omega(n)^\dagger$$

$$\bar{\psi}'(n)\psi'(n + \hat{\mu}) = \bar{\psi}(n)\Omega(n)^\dagger\Omega(n + \hat{\mu})\psi(n + \hat{\mu}) \quad (!)$$

- (!) not gauge invariant



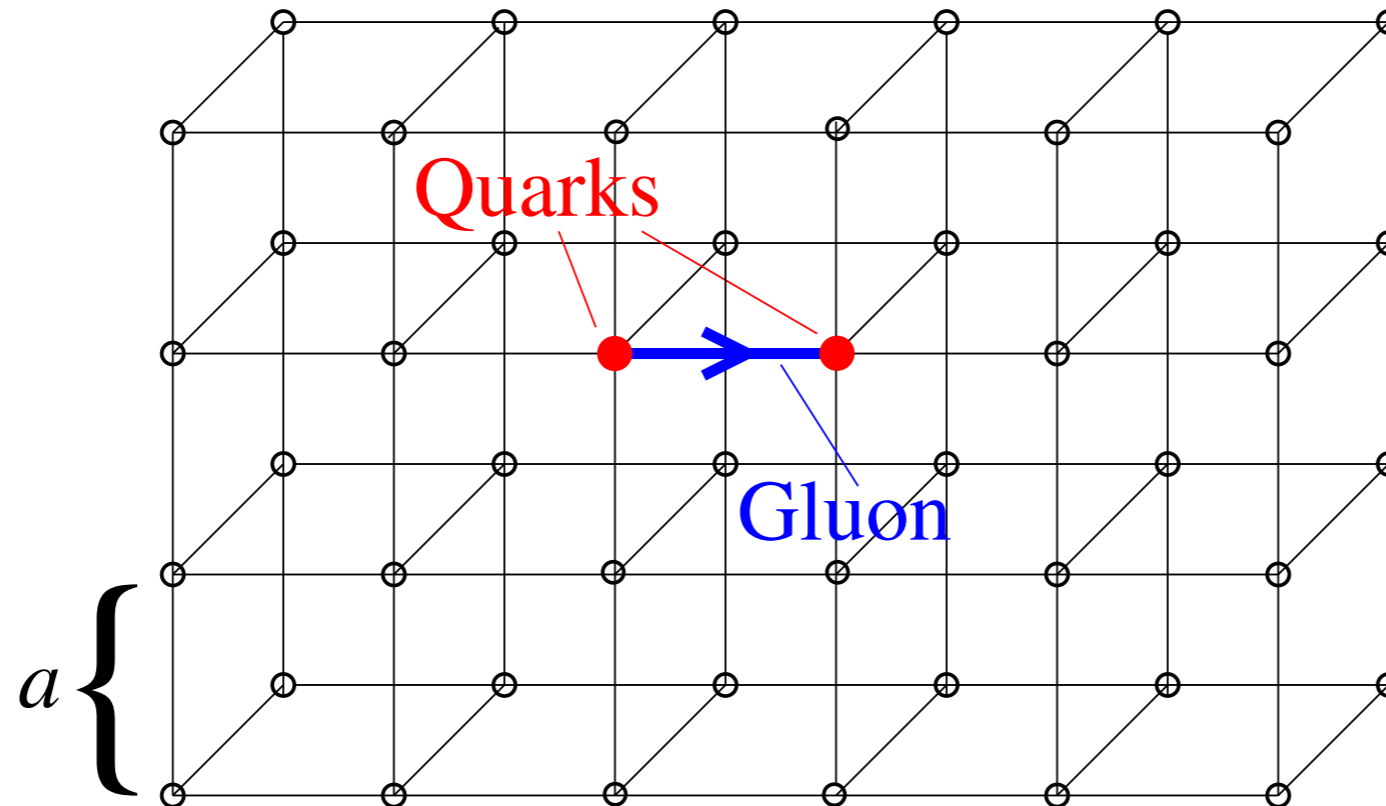
- Introduce **link variables** $U_\mu(n)$:

$$U'_\mu(n) = \Omega(n)U_\mu(n)\Omega(n + \hat{\mu})^\dagger$$

$$\bar{\psi}'(n)U'_\mu(n)\psi'(n + \hat{\mu}) = \bar{\psi}(n)U_\mu(n)\psi(n + \hat{\mu})$$

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

Quark and gluon fields on the lattice



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

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

Lattice fermion action (I)

- Fermionic action: $S_F = a^4 \sum_f \bar{\psi}(n) D(n, m) \psi(m)$
- 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**: obtained 16 instead of 1 fermionic particles!

Lattice fermion action (II)

- Wilson Dirac matrix D_W

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

- Wilson term: shifting the mass of the doublers to infinity, as $a \rightarrow 0$
- 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
 - $O(a), O(a^2), \dots$ discretization errors
 - different **rates** to approach continuum limit

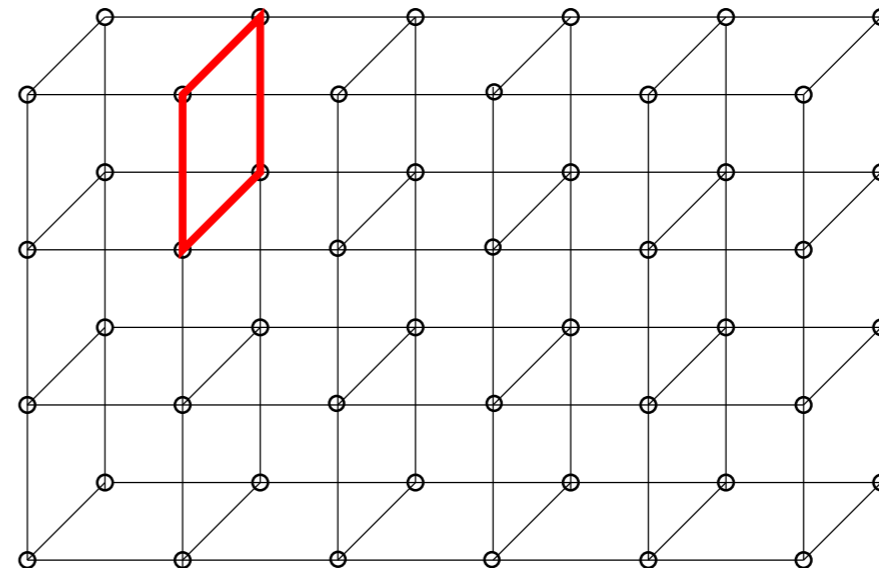
Lattice gauge action (I)

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

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

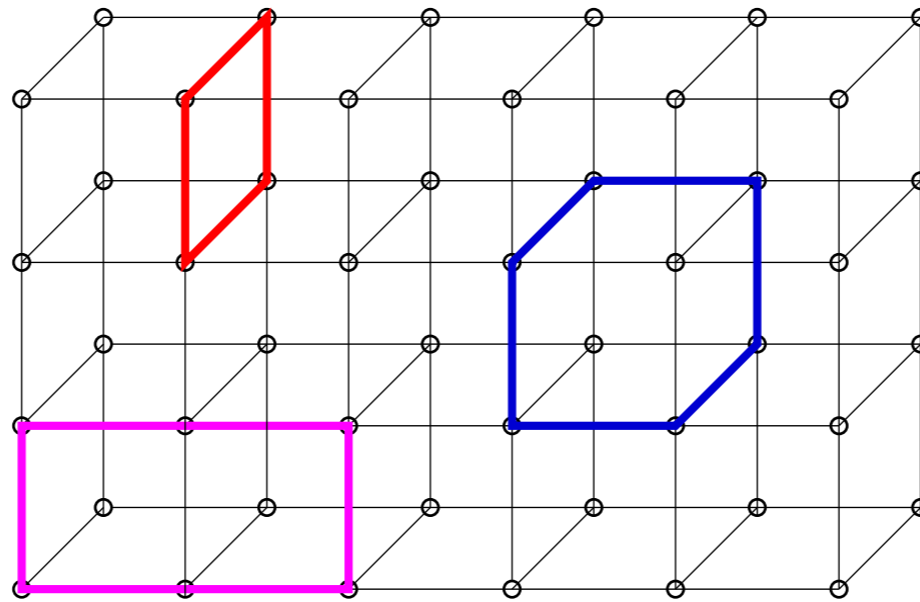
- **Wilson gauge action:**

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



Lattice gauge action (II)

- Improvement: taking into account larger Wilson loops



- All in the same universality class:
 - converge to $\text{tr} [F_{\mu\nu}(x)F_{\mu\nu}(x)]$ in the continuum limit
 - improvement reduces the discretization errors!
- Lattice artefacts in scaling behaviour:
 - Wilson gauge action: $O(a^2)$
 - 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

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

- 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: $\{U_0\} \longrightarrow \{U_1\} \longrightarrow \{U_2\} \longrightarrow \dots \longrightarrow \{U_i\} \longrightarrow \{U_{i+1}\} \longrightarrow \dots$

• The configurations are correlated by construction: $Var[\bar{O}] = Var[O] \left(\frac{2\tau_O}{N_{cnfg}}\right)$

The cost of dynamical fermions

$$S_{QCD}^E = S_G[U] + S_f[U, \psi, \bar{\psi}]$$

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

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

classical

- Fermions represented by Grassmann variables in P.I: expensive to manipulate on a 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

$$\langle O[\psi, \bar{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}U e^{-S_G[U]} \underbrace{[\det(\gamma_\mu D_\mu + m_q)]^{N_f}}_{\text{determinant}} O[\psi, \bar{\psi}, U]$$
$$\int \mathcal{D}\phi \mathcal{D}\phi^\dagger e^{-\phi^\dagger (D^\dagger(m_q)D(m_q))^{-1} \phi} \propto \underbrace{[\det(\gamma_\mu D_\mu + m_q)]^2}_{\text{determinant squared}}$$

- Determinant: non-local object on the lattice \rightarrow 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

$$\langle O[\psi, \bar{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\phi \mathcal{D}\phi^\dagger e^{-S_G[U] - \phi^\dagger (D^\dagger(m_q)D(m_q))^{-\frac{N_f}{2}} \phi} O[U, \phi, \phi^\dagger]$$
$$\int \mathcal{D}\phi \mathcal{D}\phi^\dagger e^{-\phi^\dagger (D^\dagger(m_q)D(m_q))^{-1} \phi} \propto [\det(\gamma_\mu D_\mu + m_q)]^2$$

- Determinant: non-local object on the lattice \rightarrow virtually impossible to compute exactly!

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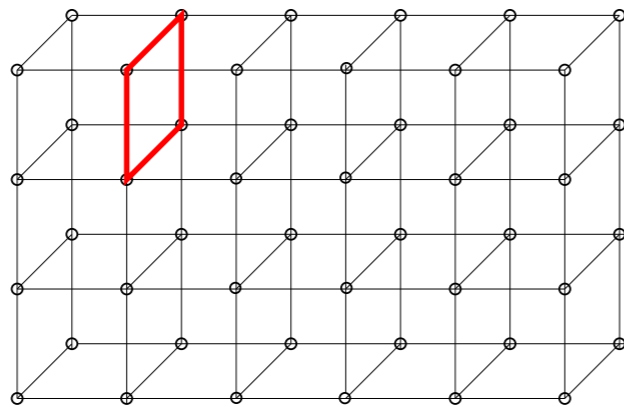
- $k = \text{cond}(M) \propto \frac{\lambda_{max}}{\lambda_{min}}$

The cost of dynamical fermions

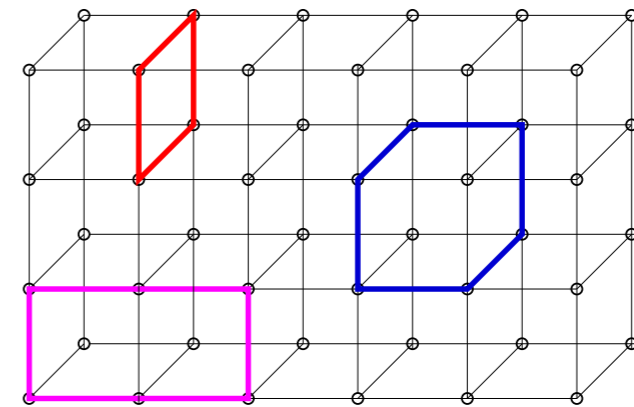
$$\langle O[\psi, \bar{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D} U e^{-S_G[U]} [\det (\gamma_\mu D_\mu + m_q)]^{N_f} O[\psi, \bar{\psi}, U]$$

S_G

Wilson



Luscher-Weisz

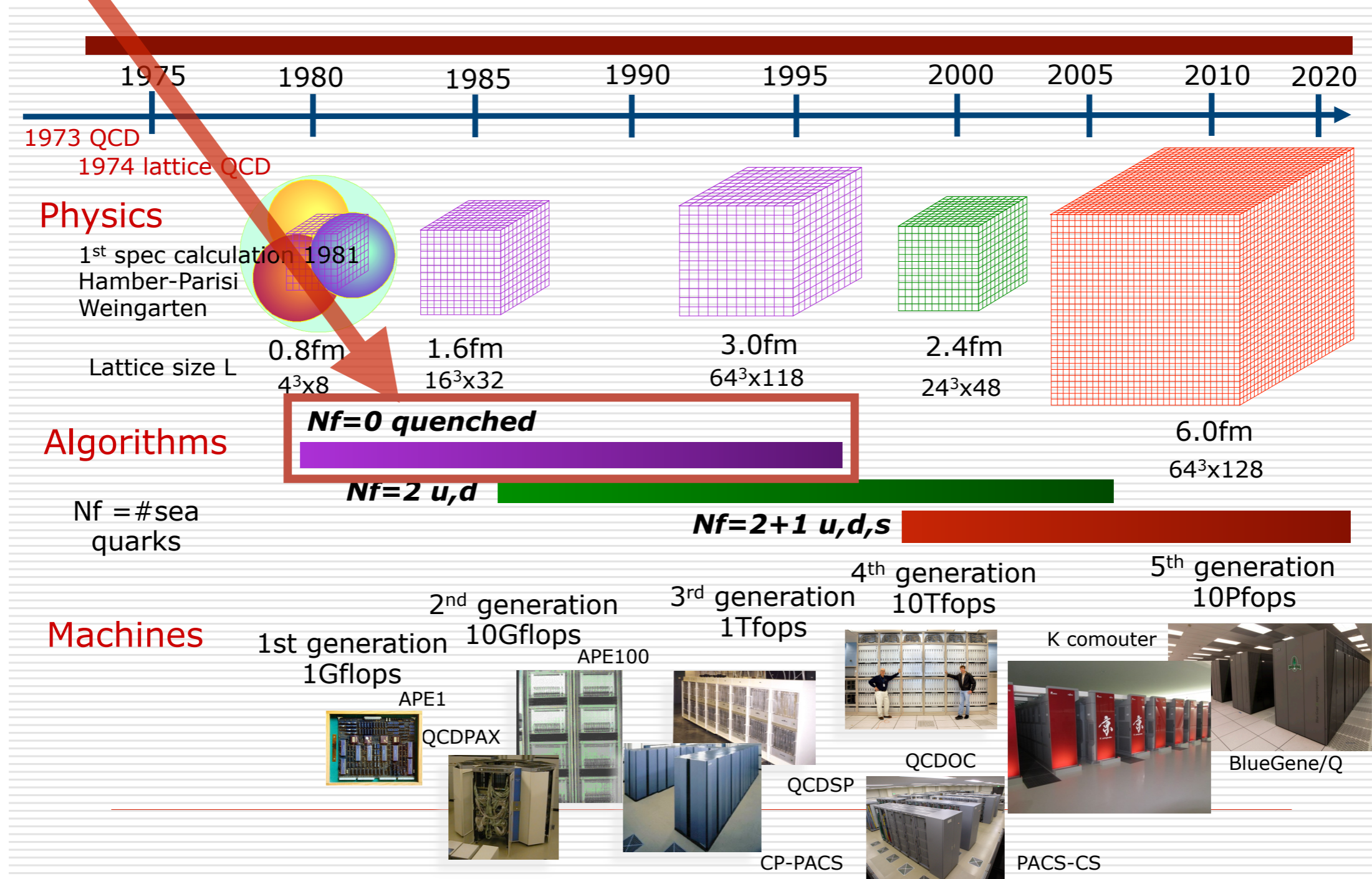


- Local objects: plaquettes, extended plaquettes (rectangles, chairs ...)
- Rate of convergence towards continuum limit: $O(a)$, $O(a^2)$, ...
- Monte Carlo algorithms with local updates sufficient in the approximation:

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

Development of Lattice QCD

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



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



The Metropolis algorithm

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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.

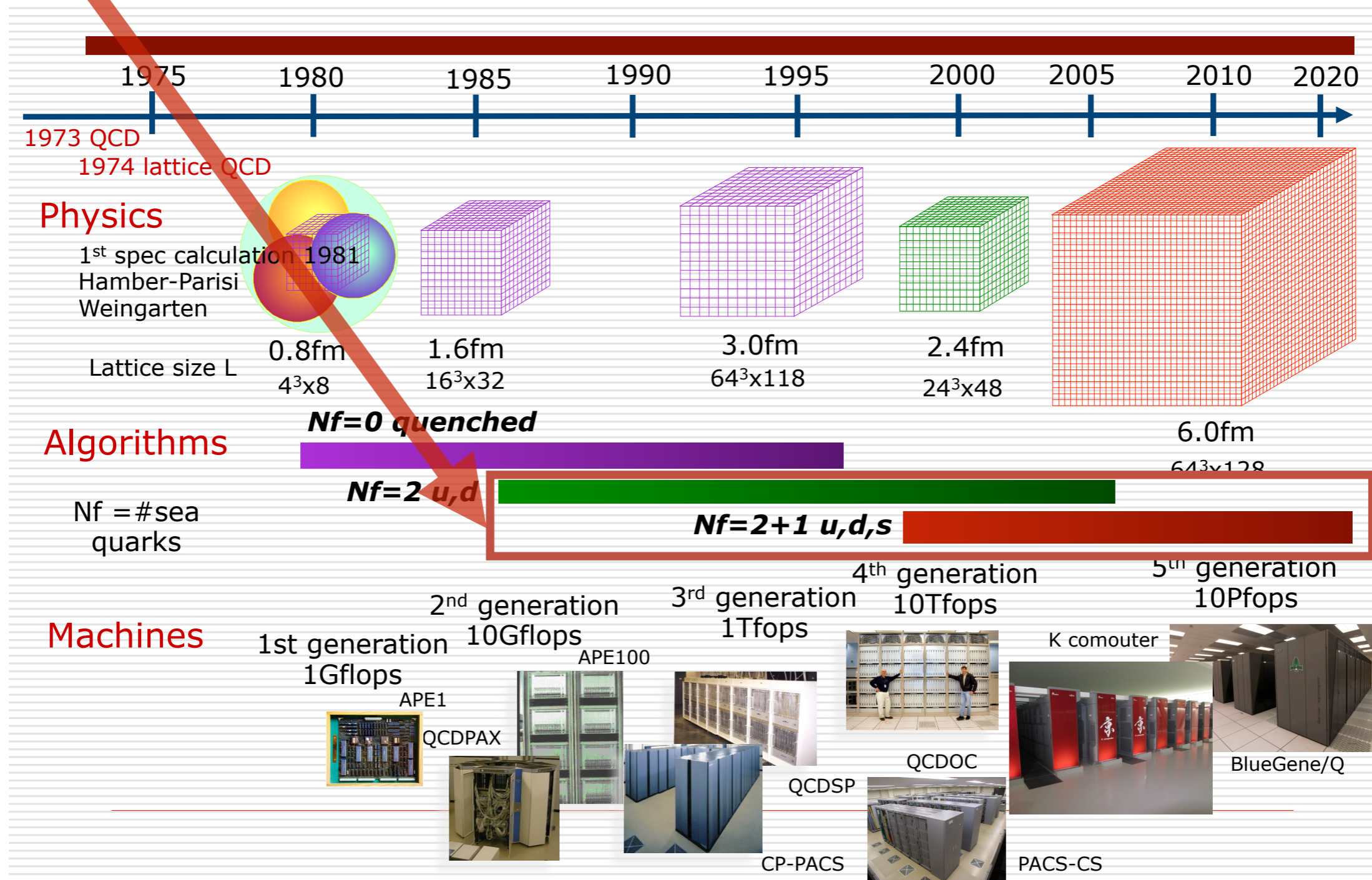
- The Metropolis Algorithm:
- Given $\{U\}$, **propose** $\{U'\}$ in a reversible, area-preserving way
- **Accept** the proposal as new entry with probability p , otherwise add $\{U\}$ to the chain again.

- $$p = \min\left(1, \frac{\pi(U')}{\pi(U)}\right)$$



Development of Lattice QCD

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



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

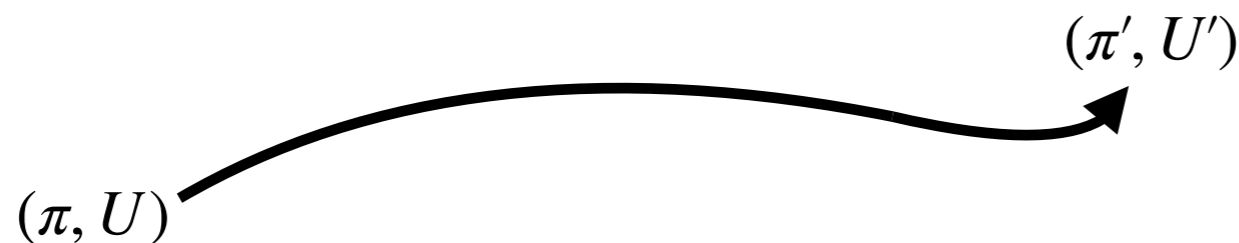


Hybrid Monte Carlo algorithm for QCD

- 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

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

- **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):

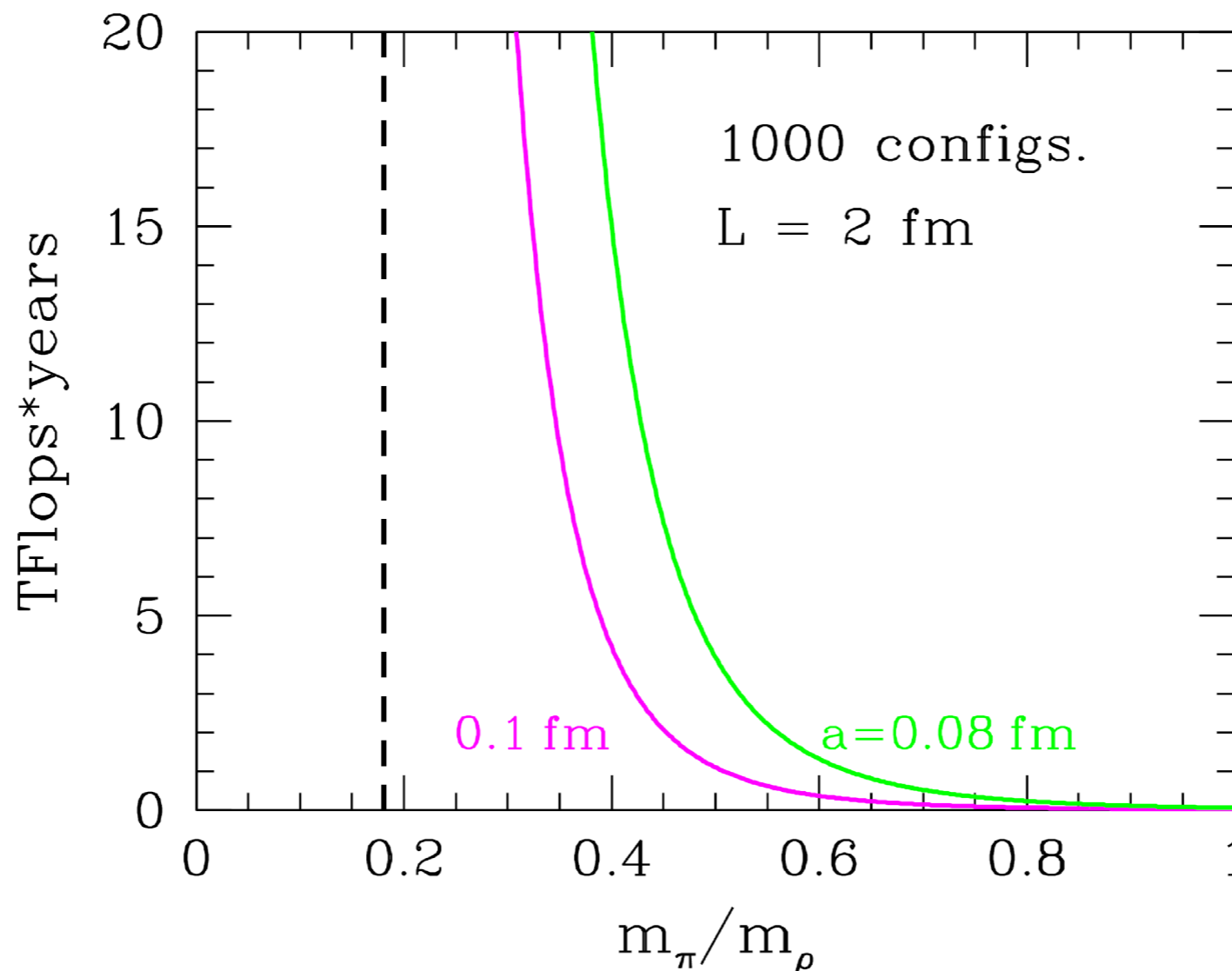


reversible, area-preserving scheme such as leap-frog, Omelyan...

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

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

“Berlin Wall”

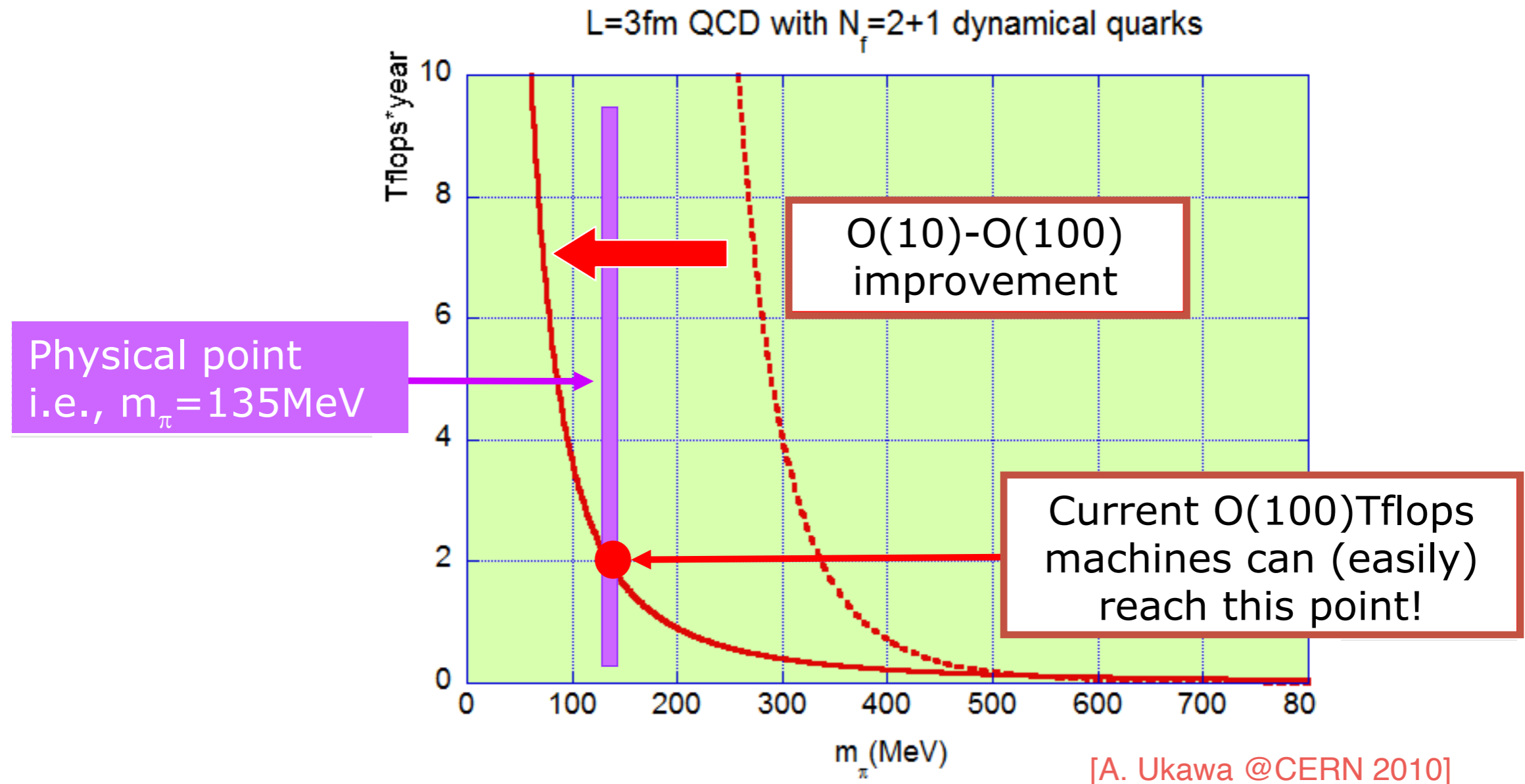


● Status in 2001: [A. Ukawa (2001)]

➔ quarks 16x heavier than in nature; coarse lattices $a \approx 0.1$ fm (typical length scale is 1fm)

➔ Cost of a simulation: $C \left[\frac{\#conf}{1000} \right] \left[\frac{m_q}{16m_{phys}} \right]^{-3} \left[\frac{L}{3fm} \right]^5 \left[\frac{a}{0.1fm} \right]^{-7}$; $C \approx 2.8$

Berlin Wall update



Simulating physical quark masses becomes reality!

In the second lecture:

- 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, QCD phase diagram etc.

Thank you!

