

Computing Topological Field Theories

Lecture 1: Introduction to Lattice Field Theories

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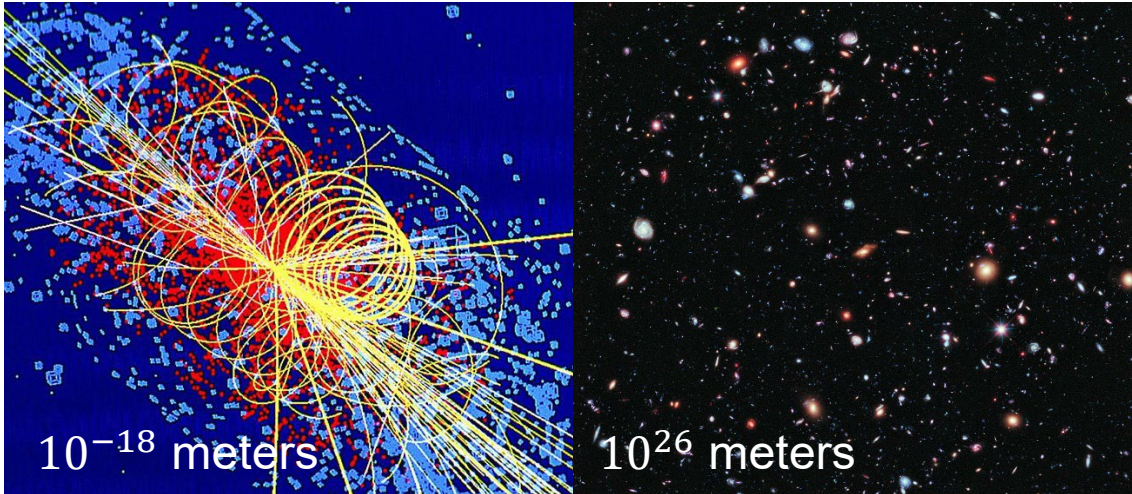
Motivation: open questions of particle physics

What we know...

Standard Model of particle physics

Content: all particles & forces (except for gravity)

Range:



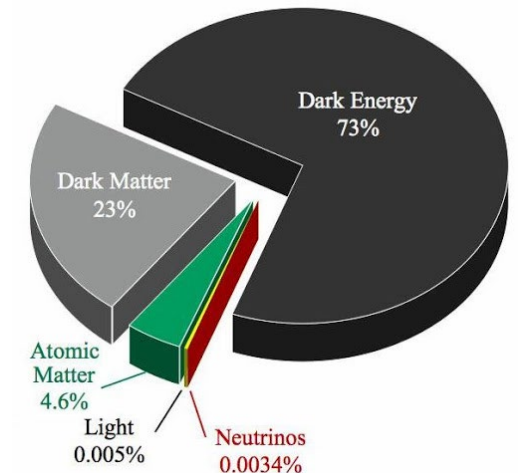
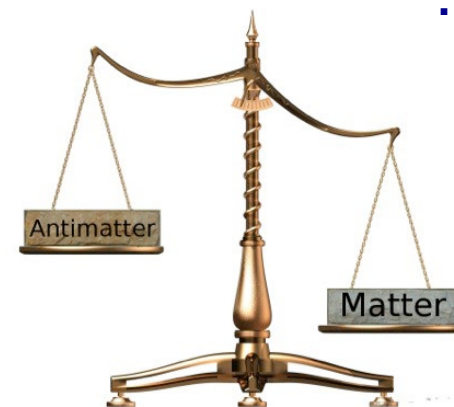
Precision: 0.0000000001 (electron g -factor)

... and what we don't know

Why is there more matter than antimatter in the universe?

Why doesn't the strong force distinguish between matter and antimatter?

What are dark matter and dark energy?



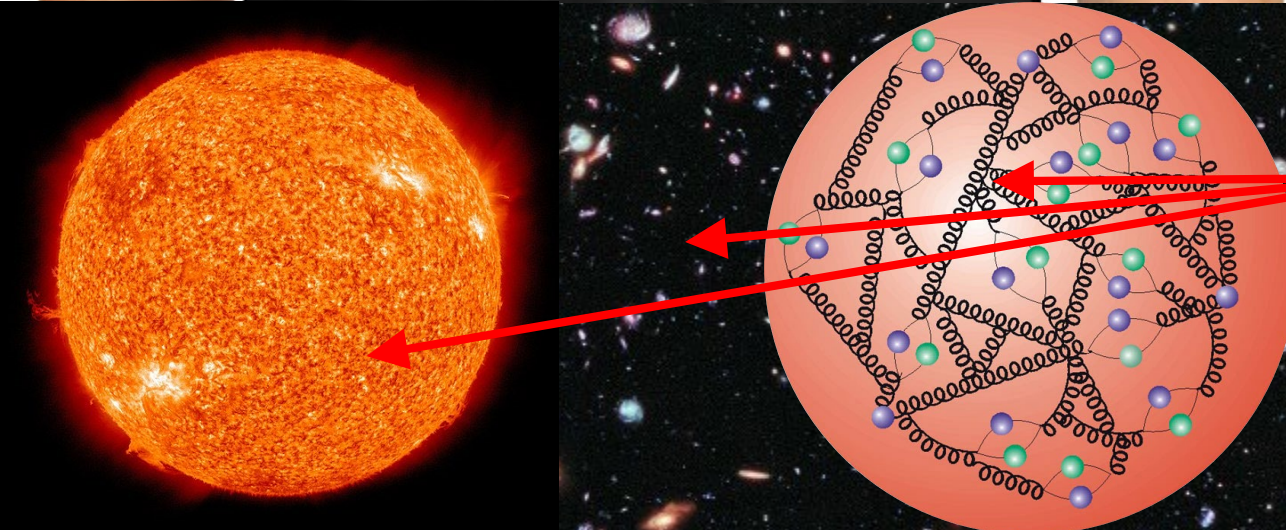
How can we answer these open questions?

$$\begin{aligned}\mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi)\end{aligned}$$

Simple equation

Beautiful but incomplete!

Need *new models* → lectures later today



Complex phenomena

Emergent structures!

Need *numerical computations* → this lecture

Overview: computing topological field theories

Numerical computations

Lecture 1: Monte Carlo method
High-precision lattice computations
Computational issues

Lecture 2: Machine learning
Efficient sampling,
thermodynamic observables...

Lecture 3: Tensor networks & quantum computing
Topological θ -terms,
chemical potentials...

Theoretical models

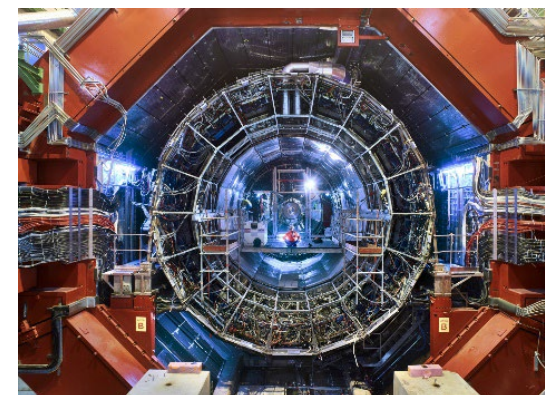
Standard Model
“Real world”
Quarks, gluons, Higgs...

1+1D ϕ^4 theory
Higgs toy model
Symmetry breaking...

1+1D Schwinger model
QCD toy model
 θ -term, confinement...

Experiments

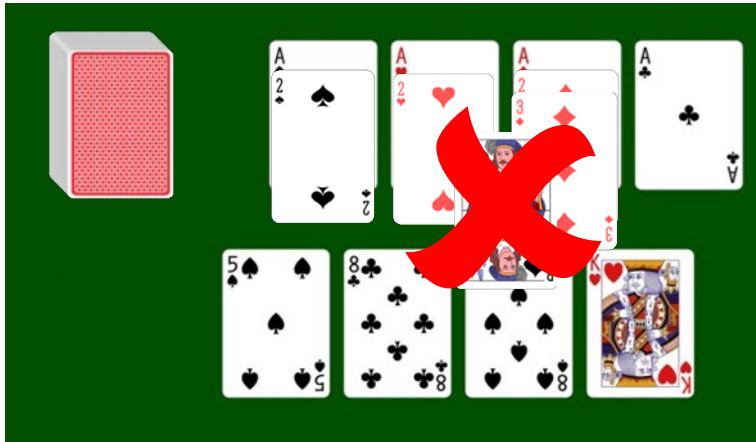
Observables
Spectrum, free energy,
entropy, pressure...
↓
LHC, cosmology, ...
Heavy-ion collisions,
Early-universe physics...



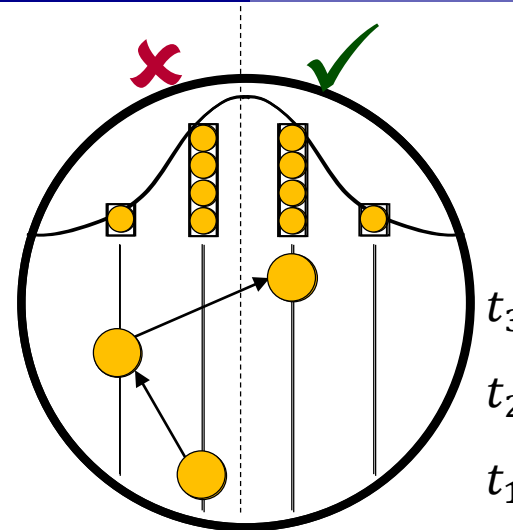
(Image credit: ALICE Collaboration / CERN)

The (solitaire) origin of the Monte Carlo method

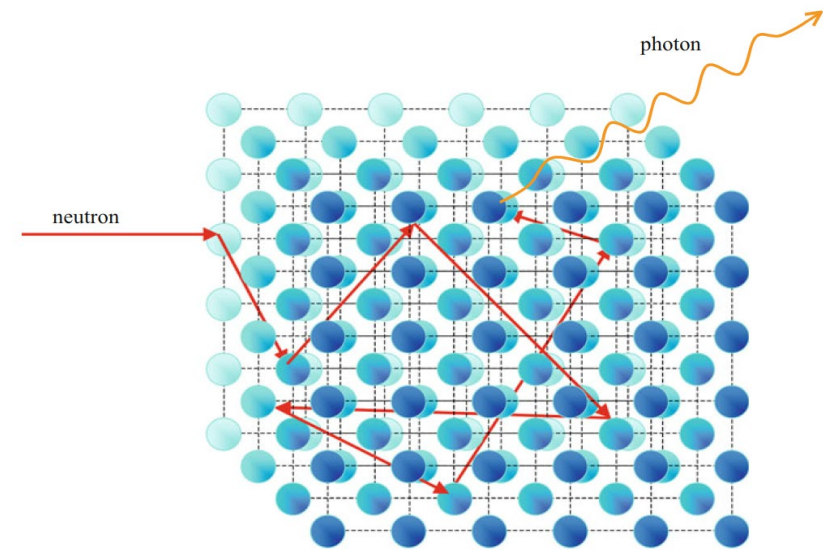
Solitaire



Neutron Diffusion



Monte Carlo method
(Markov chain \rightarrow MCMC)



Chance that a solitaire will come out successfully?

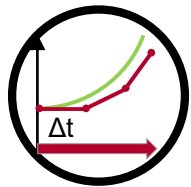
“I immediately thought of problems of neutron diffusion and other questions of mathematical physics”

Stanislaw Ulam, 1946

Monte Carlo and other methods drive science

1760s

Euler's method



1800s

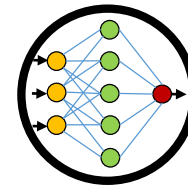
Fast Fourier Transformation

1950s

Fortran

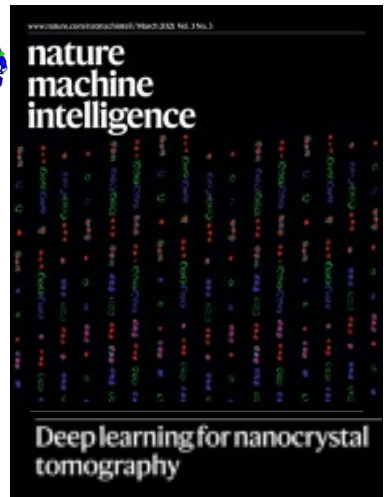
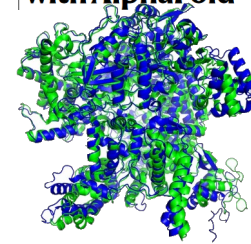
1980s

Deep Learning



Article

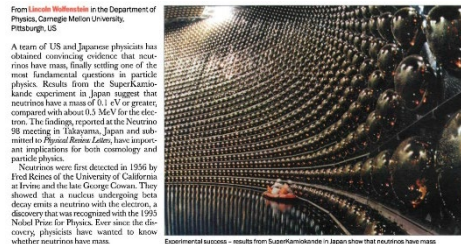
Highly accurate protein structure prediction with AlphaFold



nature

PHYSICS IN ACTION

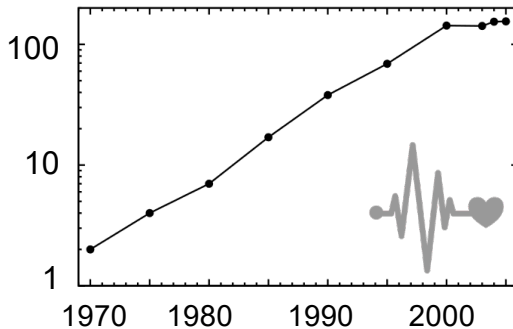
Neutrino mass discovered



Ann. Rev. Fluid Mech. 1978. 10: 11-31
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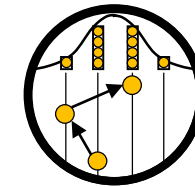
MONTE CARLO SIMULATION OF GAS FLOWS

Yearly papers with MC title in Phys Med Biol or Med Phys



Cosmological parameters from CMB and other data: A Monte Carlo approach

PHYSICAL REVIEW D 66, 103511 (2002)

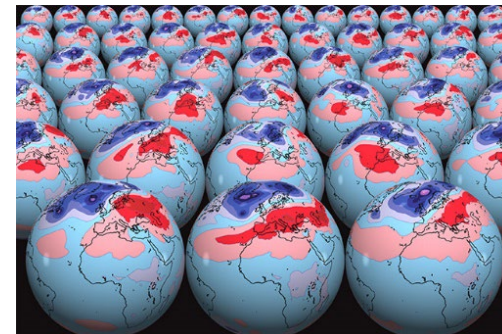


Ensemble methods for meteorological predictions

National Oceanic and Atmospheric Administration (NOAA)
National Weather Service

1940s

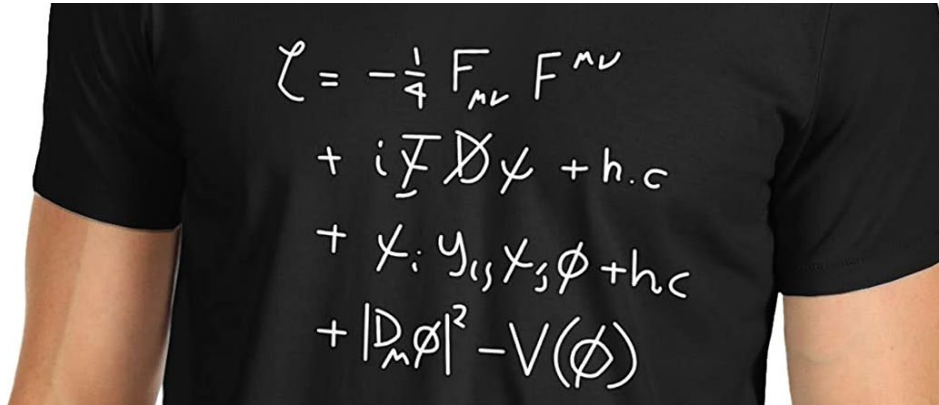
Monte Carlo simulations



Why do we need the Monte Carlo method in field theory?

\int

Integrate



$dF d\psi d\phi$

over forces (F), matter (ψ), Higgs field (ϕ)

Too complex:
no exact computation!



Way out:
approximation!

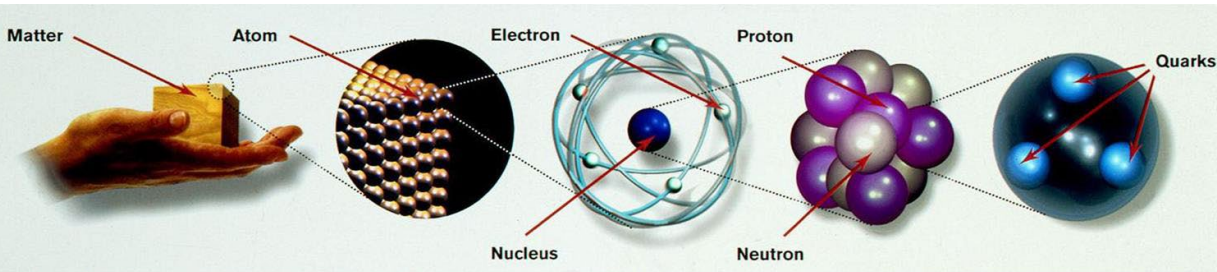


The most prominent example: “Lattice QCD”

What is Lattice QCD?

Quantum Chromodynamics (QCD)

Theory that describes how strong force (gluons) glues quarks into protons and neutrons



High energies

Perturbation theory: *small-coupling expansion*

Low energies

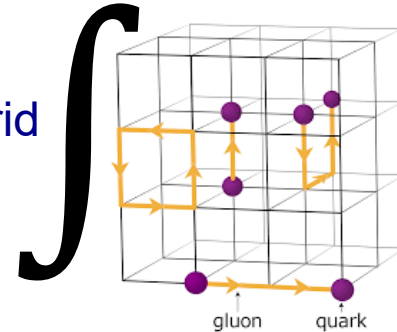
Non-perturbative regularization through *discretization*

→ “Lattice” QCD

Why do we need Monte Carlo?

Computational trick

Put quarks and gluons on spacetime grid and integrate over field configurations

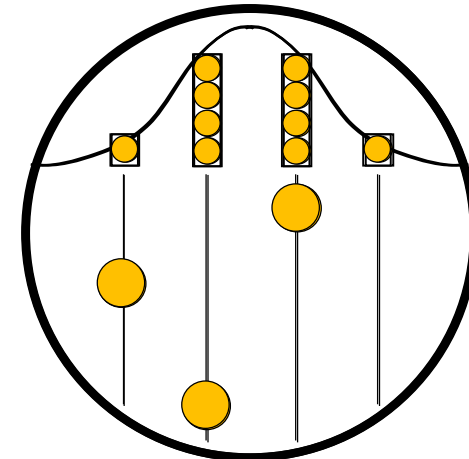


Size of spacetime lattice

Very large: up to $192 \times 96^3 \sim 10^8$ lattice points!

How to compute such integrals?

Monte Carlo: *sample* configurations



More details: let's start with the basics...

Quantum mechanics of point particle in 1+1D

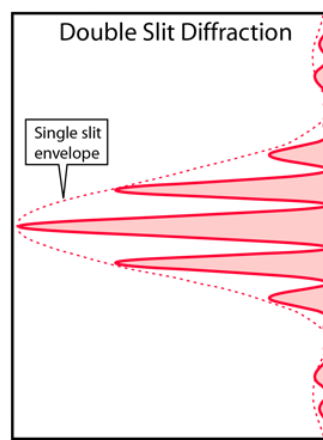
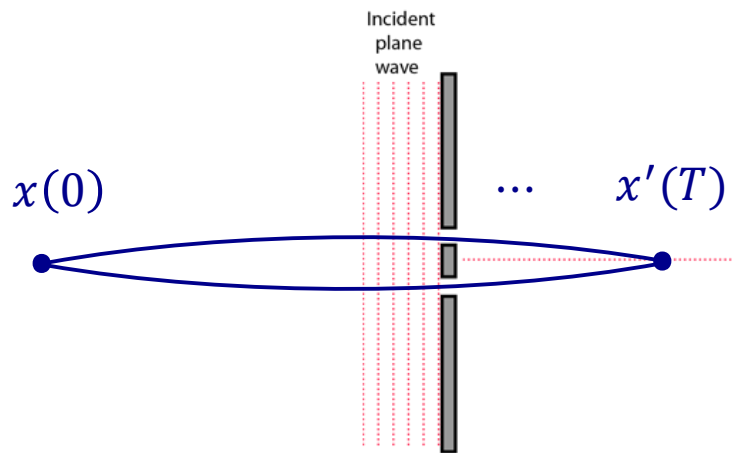
Transition amplitude

$$\langle x' | e^{-iHT} | x \rangle = \int_x^{x'} Dx e^{iS} = \int_x^{x'} Dx e^{i \int_0^T dt L(x, \dot{x})}$$

→ integral over all possible paths $x(t)$ from x to x'

→ weighted by classical action S evaluated along path

→ in 1+1D: $Dx = \prod_t dx(t)$, in 3+1D: $Dx = \prod_{t,i} dx_i(t)$



Scalar quantum field theory in 1+1D

Time evolution

$$\phi(\vec{x}, t) = e^{iHt} \phi(\vec{x}, t=0) e^{-iHt}, \text{ where } x \rightarrow \vec{x} = (\vec{x}, t)$$

Greens functions

$$\langle 0 | \phi(x_1) \cdots \phi(x_n) | 0 \rangle = \frac{1}{Z} \int \mathcal{D}\phi \phi(x_1) \cdots \phi(x_n) e^{iS}$$

→ VEVs of products of field operators, e.g. propagators: $\langle 0 | \phi(x) \phi(y) | 0 \rangle$ or 2 → 2 scattering: $\langle 0 | \phi(x_1) \cdots \phi(x_4) | 0 \rangle$

→ partition function: $Z = \int \mathcal{D}\phi e^{iS}$, where $t_1 > t_2 > \cdots > t_n$

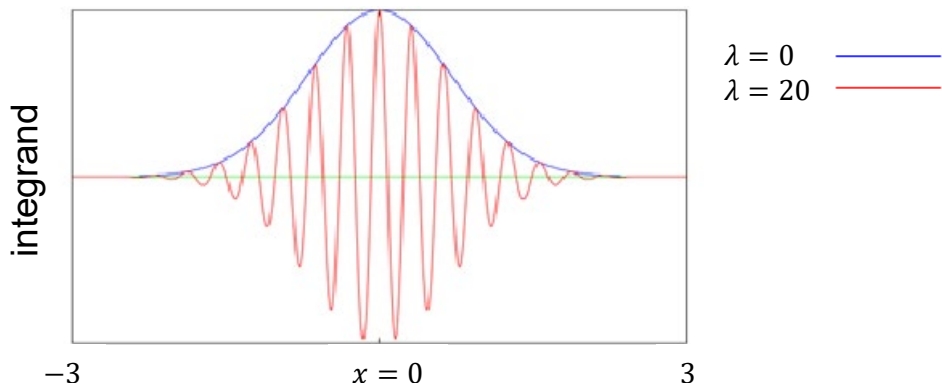
$$\begin{aligned} x_i(t) &\leftrightarrow \phi(\vec{x}, t) \\ i &\leftrightarrow \vec{x} \\ \prod_{t,i} dx_i(t) &\leftrightarrow \prod_{t,\vec{x}} d\phi(\vec{x}, t) \equiv \mathcal{D}\phi \\ S = \int dt L &\leftrightarrow S = \int dt d^3x \mathcal{L} \end{aligned}$$

Going from Minkowski to Euclidean spacetime

Minkowski spacetime

“Sign problem”

- Complex integrand $\propto \exp(iS[x(t)])$ is highly oscillatory
- Near-cancellation of positive & negative contributions
- MCMC requires *exponentially* large sample number



$$\int dx \exp(-x^2 + i\lambda x) \rightarrow \int dx \exp(-x^2) \cos(\lambda x)$$

Euclidean spacetime

No sign problem*

Wick rotation: $t \rightarrow i\tau$, path integral gets *real* weight factor

$$\text{Propagator: } \langle x' | U(\tau', \tau) | x \rangle = \int_x^{x'} [dx(\tau)] \exp\{-S_E[x(\tau)]\}$$

Euclidean spacetime = unphysical?

Can be advantageous, e.g. compute low-lying spectrum:

$$\begin{aligned} \langle 0 | A e^{-H\tau} A | 0 \rangle &= \frac{1}{Z} \int \mathcal{D}\phi e^{-S_E} A(\tau) A(0) \\ &= \sum_n \langle 0 | A | n \rangle e^{-E_n \tau} \langle n | A | 0 \rangle \\ &\xrightarrow{\tau \gg 0} |\langle 0 | A | 1 \rangle|^2 e^{-m_1 \tau} + \dots \end{aligned}$$

assuming $A(\tau) = \int d^3x \phi(\vec{x}, \tau)$, such that $\langle 0 | A | 1 \rangle \neq 0$ for one-particle state $|1\rangle$ with momentum $\vec{p} = 0$ and mass m_1

* actually, there can still be a sign problem (see later)

Going from continuous to discretized spacetime

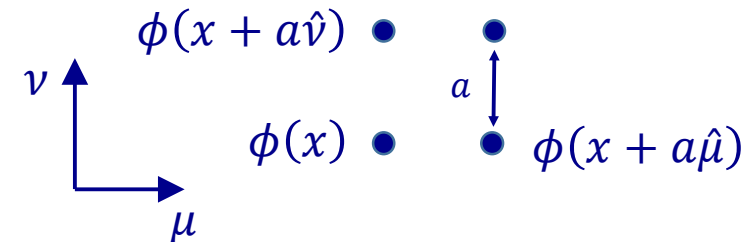
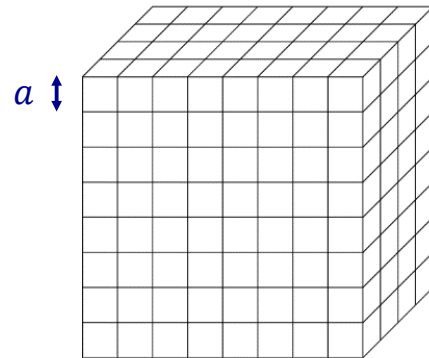
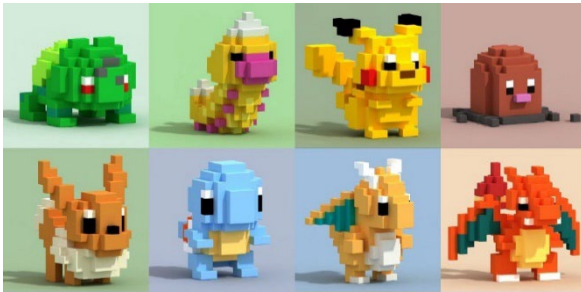
Infinite- vs. finite-dim. integration

Problem: infinite-dimensional integration

... over all field configurations: $\mathcal{D}\phi = \prod_x d\phi(x)$

Solution: space-time discretization

... on hypercubic lattice: $x_\mu = an_\mu, n_\mu \in \mathbb{Z}$



Example: lattice scalar field theory

Lattice scalar field

... is defined on lattice points only: $\phi(x), x \in \text{lattice}$

Partial derivatives

... become finite differences: $\partial_\mu \phi \equiv \frac{1}{a} [\phi(x + a\hat{\mu}) - \phi(x)]$

Space-time integrals

... are replaced by sums: $\int d^4x \rightarrow \sum_x a^4$

Action of lattice ϕ^4 -theory

... reads: $S = \sum_x a^4 \left\{ \frac{1}{2} \sum_\mu [\partial_\mu \phi(x)]^2 + \frac{m_0^2}{2} \phi(x)^2 + \frac{g_0}{4!} \phi(x)^4 \right\}$

Previously infinite-dimensional integrals

... now become finite \rightarrow discrete set of variables!

This looks familiar...

Fourier transforms

...

Fourier-transformed lattice field

$\tilde{\phi}(p) = \sum_x a^4 e^{-ipx} \phi(x)$ is periodic in momentum-space

Lattice momentum

$p_\mu \cong p_\mu + \frac{2\pi}{a}$ restricted to first Brillouin zone: $-\frac{\pi}{a} < p_\mu \leq \frac{\pi}{a}$

Inverse-Fourier-transformed lattice field

$\phi(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} e^{ipx} \tilde{\phi}(p)$, ultraviolet cutoff: $|p_\mu| \leq \frac{\pi}{a}$

Finite lattice volume

Hypercubic lattice with length $L_1 = L_2 = L_3 = L$ in spatial direction and length $L_4 = T$ in Euclidean time:

$$V = L^3 T, x_\mu = a n_\mu, n_\mu = 0, 1, 2, \dots, L_\mu - 1$$

Periodic boundary conditions

$$\phi(x) = \phi(x + a L_\mu \hat{\mu})$$

Discretized lattice momentum

$$p_\mu = \frac{2\pi}{a} \frac{l_\mu}{L_\mu} \text{ with } l_\mu = 0, 1, 2, \dots, L_\mu - 1$$

Momentum-space integration

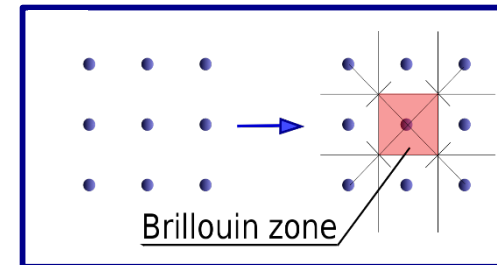
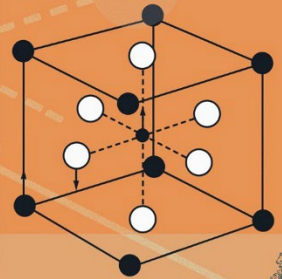
$$\int \frac{d^4 p}{(2\pi)^4} \rightarrow \frac{1}{a^4 L^3 T} \sum_{l_\mu}$$

Previously infinite integrals...

... are now regularized (finite a) and finite (finite V)

Recover “true” physics...

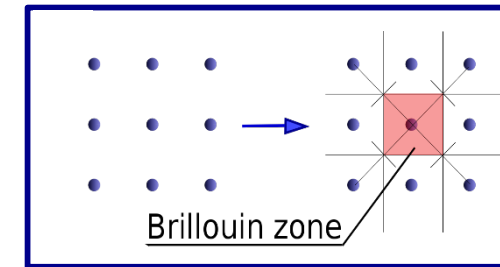
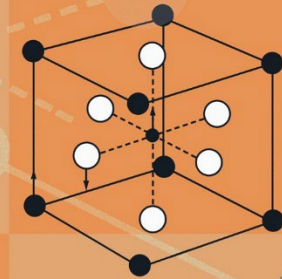
... by taking limits $L, T \rightarrow \infty$ and $a \rightarrow 0$



This looks familiar...

Fourier transforms

...



Fourier-transformed lattice field

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$p_\mu \cong p_\mu + \frac{2\pi}{a}$ restricted to first Brillouin zone: $-\frac{\pi}{a} < p_\mu \leq \frac{\pi}{a}$

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Discretized lattice momentum

$$p_\mu = \frac{2\pi}{a} \frac{l_\mu}{L_\mu} \text{ with } l_\mu = 0, 1, 2, \dots, L_\mu - 1$$

Momentum-space integration

$$\int \frac{d^4 p}{(2\pi)^4} \rightarrow \frac{1}{a^4 L^3 T} \sum_{l_\mu}$$

Previously infinite integrals...

... are now re

Recover "tr

... by taking

We can use similar computational methods (MCMC sampling, machine learning, tensor networks, quantum computing, ...) in particle *and* condensed matter physics!

Going beyond $\phi(x)$... How to deal with fermions?

Grassmann variables

Fermionic field operators

$$\{\psi_\alpha(x), \psi_\beta(x)\} = 0 \rightarrow \text{anti-commuting}$$

Grassmann variables

$$\text{Fulfil } \{\eta_i, \eta_j\} = \{\eta_i, \bar{\eta}_j\} = \{\bar{\eta}_i, \bar{\eta}_j\} = 0 \rightarrow \eta_i^2 = \bar{\eta}_i^2 = 0$$

Integral and derivative

$$\int d\eta_i (a + b\eta_i) = \frac{\partial}{\partial \eta_i} (a + b\eta_i) = b$$

Multiple integrals and derivatives

$$\int d\eta_j \int d\eta_i \eta_i \eta_j = \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_i} \eta_i \eta_j = 1$$

Derivation: $e^{\sum_{i,j} \bar{\eta}_i Q_{ij} \eta_j} = \prod_i e^{\bar{\eta}_i \sum_j Q_{ij} \eta_j} = \prod_i (1 + \bar{\eta}_i \sum_j Q_{ij} \eta_j)$
 then use integration rules and: $\det Q = \sum_\sigma (\text{sgn}(\sigma) \prod_i Q_{i,\sigma_i})$

Fermion determinant

Fermionic Greens function

$$\langle 0|A|0\rangle = \frac{1}{Z} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} A e^{-S_F}$$

Fermionic integration measure

$$\mathcal{D}\psi \mathcal{D}\bar{\psi} = \prod_x \prod_\alpha d\psi_\alpha(x) d\bar{\psi}_\alpha(x)$$

Fermionic action

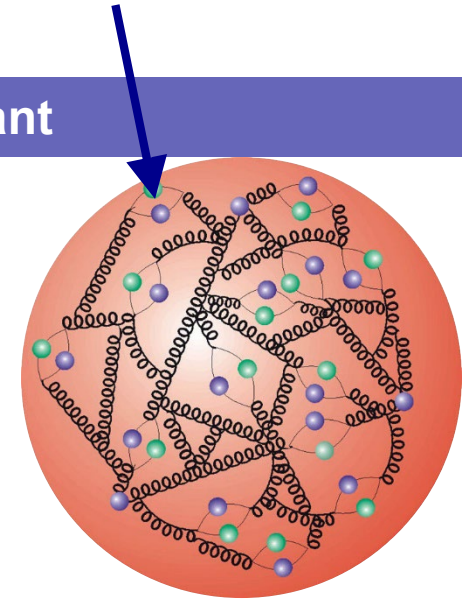
$$S_F = \int d^4x \bar{\psi}(x) (\gamma_\mu \partial_\mu + m) \psi(x)$$

Fermionic path integral

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\int d^4x \bar{\psi}(x) Q \psi(x)} = \det Q \rightarrow \text{huge matrix!}$$

Quenched approximation

Up to recently: neglected fermion dynamics ($\det Q = 1$)



Problems with (too many) fermions on the lattice

Naïve lattice fermions

Fermionic lattice action

$$S_F = \frac{1}{2} \sum_x \sum_\mu \bar{\psi}(x) (\gamma_\mu \partial_\mu + m) \psi(x) + \text{h. c.}$$

Resulting fermionic propagator...

$$\tilde{\Delta}(p) = \left[i \sum_\mu \gamma_\mu \frac{1}{a} \sin(p_\mu a) + m \right]^{-1}$$

... has too many poles

Expected pole at $p_\mu = (m, 0, 0, 0)$ but 15 additional poles at $p_\mu = (m, 0, 0, 0) + \pi^\mu/a$ (corners of Brillouin zone)!

Fermion “doubling” problem

S_F describes $2^d = 16$ instead of 1 particle flavors!

Nielsen-Ninomiya theorem

No *local, chiral* fermionic lattice actions without doublers

Wilson vs. staggered fermions

Wilson fermions (non-chiral)

$$\text{Add Wilson term: } S_F \rightarrow S_F^W = S_F - \frac{r}{2} a^2 \sum_x \bar{\psi}(x) \partial_\mu^2 \psi(x)$$

Modified propagator

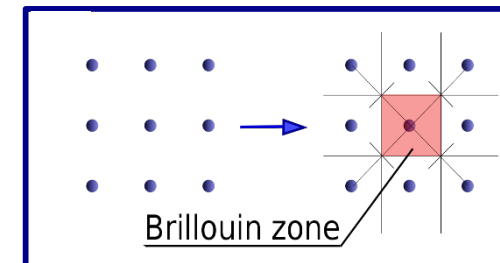
$$\tilde{\Delta}(p) = \left[i \sum_\mu \gamma_\mu \frac{1}{a} \sin(p_\mu a) + m + \sum_\mu \frac{2r}{a} \sin^2 \left(\frac{p_\mu a}{2} \right) \right]^{-1}$$

Doublers acquire masses $\propto r/a$ and decouple for $a \rightarrow 0$

Staggered fermions (non-local)

Distribute 4 components of ψ_α on different lattice points

→ reduction to 4 flavors → take 4th root of determinant



Going beyond fermions... How to deal with gauge fields?

Naïve lattice discretization

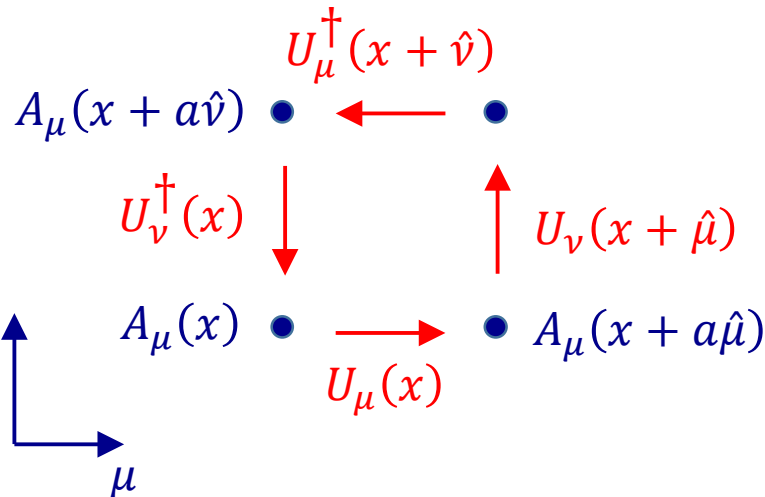
Naïve approach

Define vector gauge field $A_\mu(x)$ at each lattice point

Problem

Finite differences and sums of vector gauge fields don't preserve gauge symmetry: $F_{\mu\nu}(x) \rightarrow \underbrace{\Omega(x)}_{\text{position-dependent } SU(3) \text{ matrix}} F_{\mu\nu}(x) \Omega^\dagger(x)$

position-dependent $SU(3)$ matrix



Gauge-invariant discretization

Link variable

$$U_\mu(x) \equiv e^{iaA_\mu(x)} \in SU(3)$$

Gauge transformation

$$U_\mu(x) \rightarrow \Omega(x) U_\mu(x) \Omega^\dagger(x + a\hat{\mu})$$

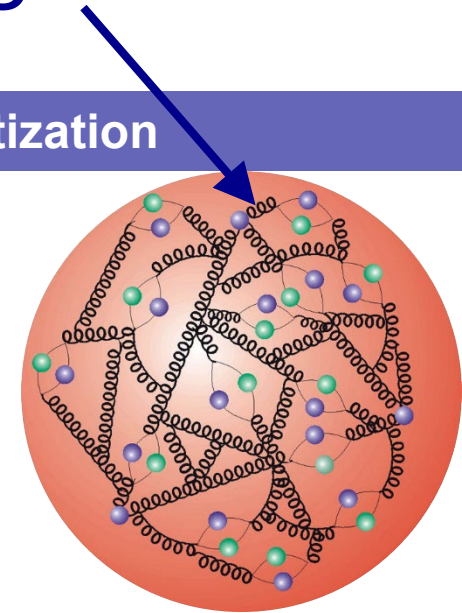
Simplest gauge invariant quantity

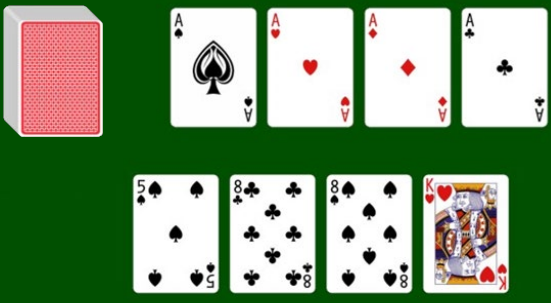
$$\begin{aligned} U_{\mu\nu}(x) &= U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + a\hat{\nu}) U_\nu^\dagger(x) \\ &= e^{ia^2 F_{\mu\nu}(x) + \mathcal{O}(a^3)} \Rightarrow \text{called "plaquette"} \end{aligned}$$

"Wilson" lattice gauge action

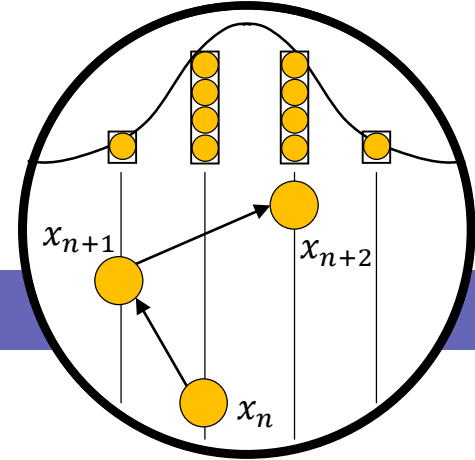
$$S_W = \frac{1}{g^2} \sum_{x, \mu > \nu} \text{Re Tr}[1 - U_{\mu\nu}(x)] + \mathcal{O}(a^2)$$

$$\rightarrow \frac{1}{2g^2} \int d^4x \text{Tr}[F_{\mu\nu}(x) F_{\mu\nu}(x)] \Rightarrow \text{gauge-invariant}$$





How to compute the integrals?



Monte Carlo method (MC)

Markov Chain ... method (MCMC)

Naïve approach

Randomly generate ensemble of “configurations” $\{x\}$

$$\rightarrow \langle x_f | U(\tau', \tau) | x_i \rangle = \frac{1}{N} \sum_{\{x\}} e^{-S(x)} = \underbrace{\langle e^{-S(x)} \rangle}$$

number of configurations
in ensemble

average value
within ensemble

Problem

Generate lots of irrelevant configurations → inefficient!

Solution

Generate configurations such that probability $P(x_n)$ of obtaining configuration x_n is $P(x) \propto \exp[-S(x)]$

→ configurations have high probability of being relevant!

Starting point

Initialization: Choose arbitrary starting point x_n

Proposal density: $g(x'|x_n)$ [e.g. Gaussian centered at x_n] suggests candidate x' for x_{n+1} , given previous value x_n

For each iteration n :

Generate x' and calculate $\alpha = \exp[-S(x')] / \exp[-S(x_n)]$

Accept or reject:

Generate uniform random number $u \in [0,1]$

If $u \leq \alpha$, accept candidate by setting $x_{n+1} = x'$

If $u \geq \alpha$, reject candidate and set $x_{n+1} = x_n$ instead

→ **Metropolis-Hastings algorithm**

Phenomenological results of lattice QCD

Computing the light QCD spectrum

QCD Lagrangian

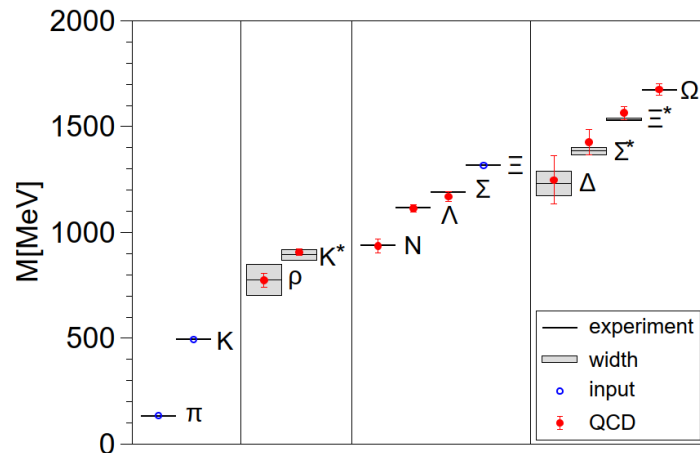
$$\mathcal{L} = \frac{1}{2g^2} \text{Tr} F_{\mu\nu} F^{\mu\nu} + \bar{\psi}_i [\gamma_\mu (\partial_\mu + A_\mu) + m_i] \psi_i$$

Input parameters of lattice calculation

Masses (e.g. assume $m_u = m_d \equiv m_{ud} \ll m_s$), coupling g

Input quantities from experiments

Precisely measured and computable: e.g. π , K , Ξ masses



BMW Collaboration,
Dürr et al. (2009)

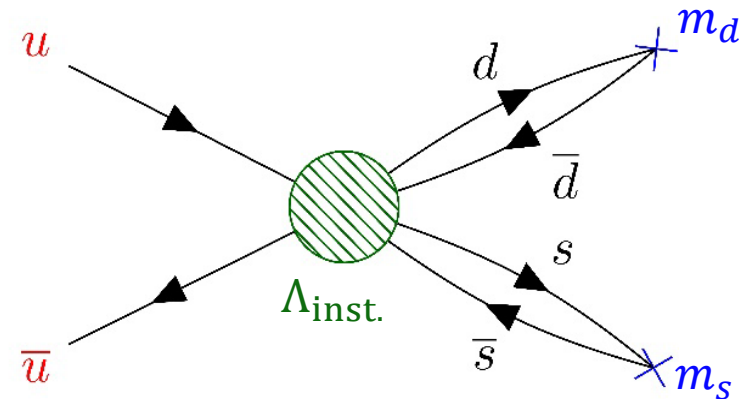
Computing topological phenomena

Axion mass at high temperatures

Temperature dependence of topological susceptibility

Topological mass contribution to up-quark

Compute $\frac{m_d m_s}{\Lambda_{\text{inst.}}}$, compare to $m_{u,\text{exp.}} = m_u + \frac{m_d m_s}{\Lambda_{\text{inst.}}} > 0$



How to probe BSM physics with lattice computations?

Example: strong CP problem

New physics beyond the Standard Model?

Theory

QCD vacuum: non-trivial topology $\rightarrow \theta$ -term

$$S_{\text{QCD}} \supset \frac{\theta}{16\pi^2} \int d^4x G\tilde{G} \rightarrow \text{violates CP symmetry}$$

Experiment

$G\tilde{G}$ yields mass: $m_{\eta'} \gg m_{\eta}$ ✓

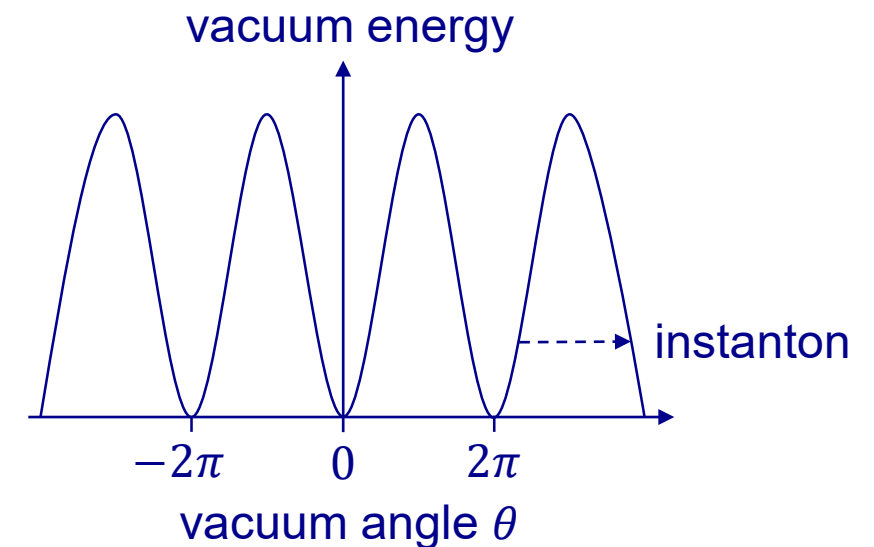
$\theta G\tilde{G}$ yields neutron electric dipole moment ✗

\rightarrow unobserved! $\theta < 10^{-10}$

BSM model building

Small number \rightarrow new symmetry \rightarrow new physics

(see lectures later today)



Possible solutions: (1) $m_u = 0$ or (2) axion

Theory

“Massless up-quark” solution

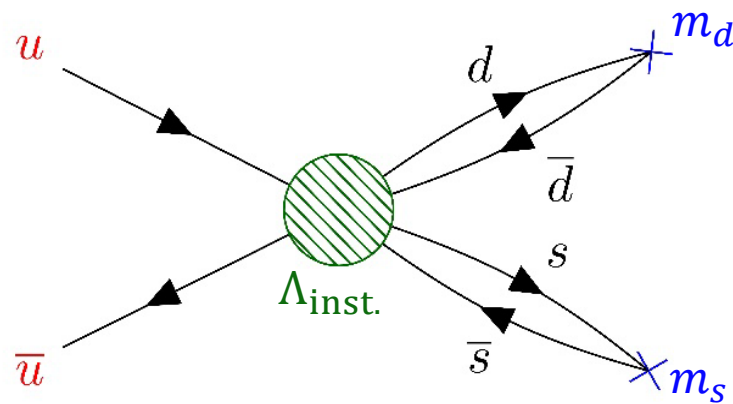
$m_u = 0$ eliminates $\theta \rightarrow \theta + \alpha$ with $U(1)_u$ rotation

Observed up-quark mass: $m_{u,\text{exp.}} = m_u + \frac{m_d m_s}{\Lambda_{\text{inst.}}} > 0$

“Axion” solution

Axion eliminates $\theta \rightarrow \theta + \frac{a}{f_a}$ with $U(1)_{\text{PQ}}$ rotation

Non-perturbative axion mass: $m_a = \frac{\Lambda_{\text{inst.}}}{f_a^2}$



Experimental tests

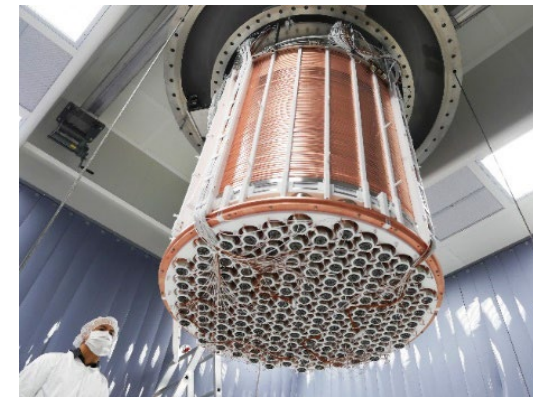
Massless up-quark solution

Lattice QCD: can compute both m_u and $\frac{m_d m_s}{\Lambda_{\text{inst.}}}$

Axion solution

Lattice QCD: can compute axion properties, e.g. $m_a(T)$

Dark matter experiments: search for axion(-like) particles



(Image credit: XENON Collaboration)

Testing $m_u = 0$ with lattice QCD

Computing both mass contributions

Two approaches

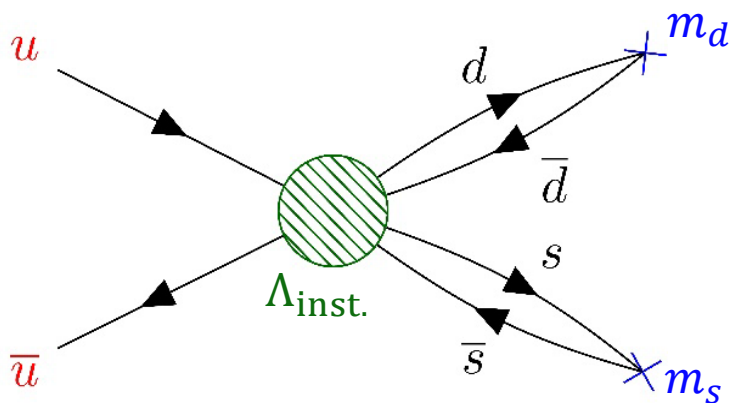
Computation of m_u yields $m_u(2 \text{ GeV}) \sim 2.130(41) \text{ MeV}$

Computation of topological mass contribution

Details of second approach

Compute $\frac{m_d m_s}{\Lambda_{\text{inst.}}}$, compare to $m_{u,\text{exp.}} = m_u + \frac{m_d m_s}{\Lambda_{\text{inst.}}} > 0$

→ if $m_{u,\text{exp.}} \gg \frac{m_d m_s}{\Lambda_{\text{inst.}}}$, we can rule out $m_u = 0$



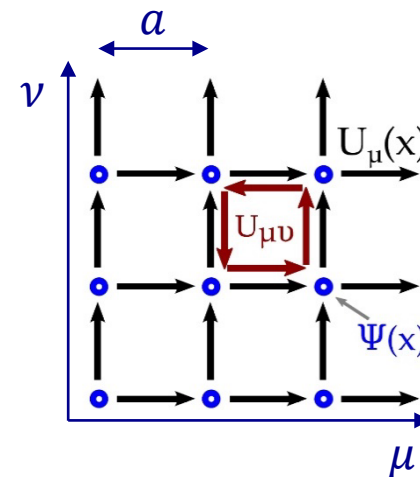
Details of method

Lattice QCD + refinements

Reduce lattice errors: Iwasaki improved gauge action

→ uses standard + *rectangular* plaquettes of size $2a \times a$

Twisted mass: $\psi(x) \rightarrow e^{-i\omega\gamma_5\tau^3/2} \psi(x)$, $m_\psi \rightarrow e^{i\omega\gamma_5\tau^3} m_\psi$



Alexandrou et al. (2020)

Lattice QCD results for topological mass contribution

Computing β_2/β_1

Procedure

Test how $m_{u,\text{exp.}} = m_u + \frac{m_d m_s}{\Lambda_{\text{inst.}}} > 0$ contributes to M_π^2

Compute $M_{\pi,i}^2 = \beta_1(m_u + m_d) + \beta_2 m_{s,i}(m_u + m_d) + \dots$

Results

$$\frac{\beta_2}{\beta_1} = \frac{M_{\pi,1}^2 - M_{\pi,2}^2}{m_{s,1}^2 M_{\pi,2}^2 - m_{s,2}^2 M_{\pi,1}^2} \Big|_{M_\pi^2 \rightarrow 0} = 0.63(39) \text{ GeV}^{-1}$$

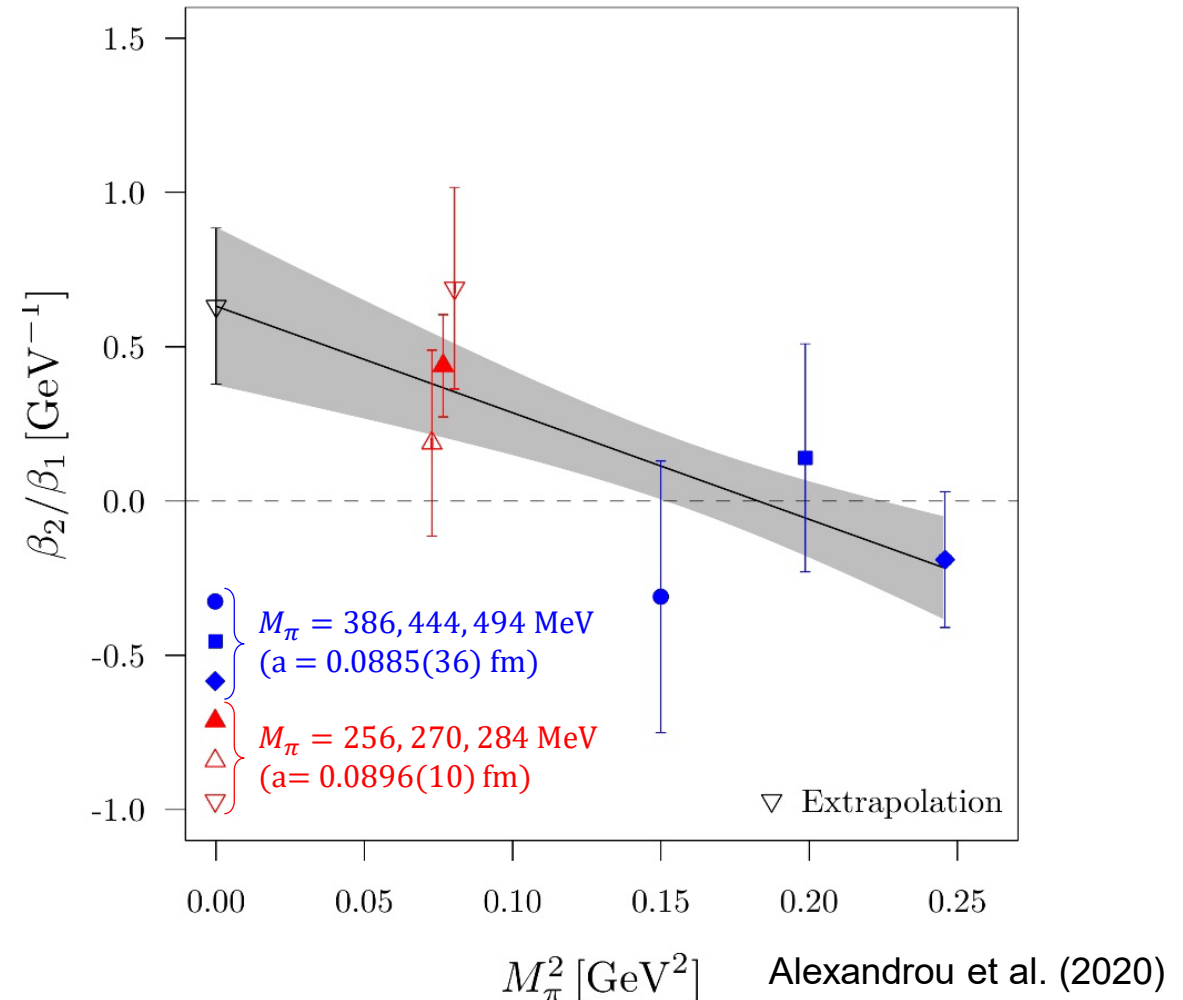
$$\frac{\beta_2}{\beta_1} \Big|_{M_\pi^2 \rightarrow 0} \approx 5 \text{ GeV}^{-1} \text{ required for } m_u = 0 \text{ solution}$$

Implication for strong CP problem

Implies $\frac{m_d m_s}{\Lambda_{\text{inst.}}} \ll m_{u,\text{exp.}}$ and rules out $m_u = 0$

Agrees with computation of $m_u(2 \text{ GeV}) \sim 2 \text{ MeV}$

Results



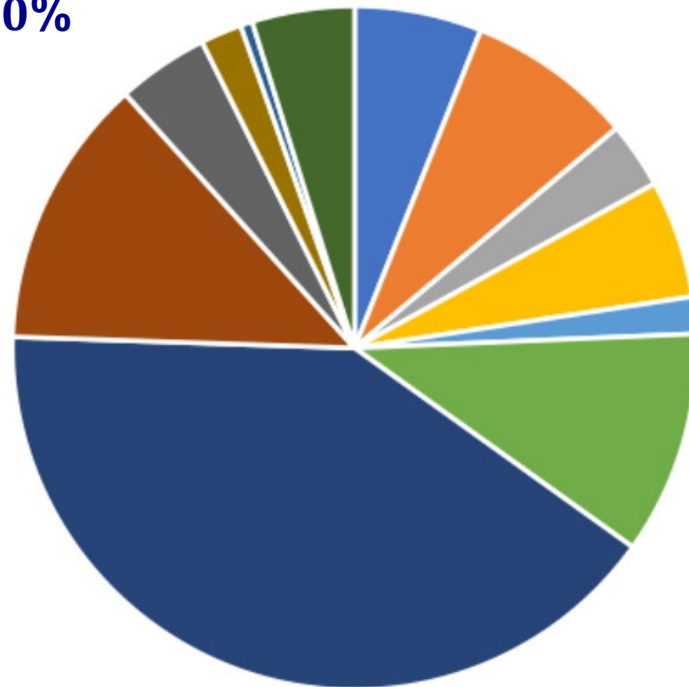
Outlook: MCMC is hungry & challenging

Computational costs of lattice field theory

Computational challenges of lattice field theory

Supercomputer usage for different fields (INCITE 2019)

→ **Lattice QCD: ~ 40%**



No direct computation of thermodynamic observables, ...

→ Machine learning (lecture tomorrow)

Baryon chemical potential, θ -term, real-time evolution, ...

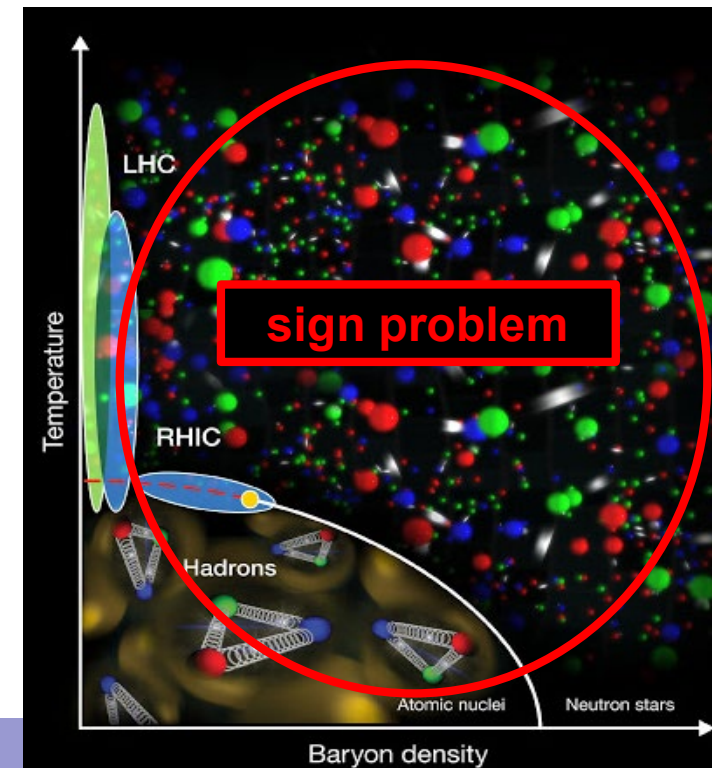
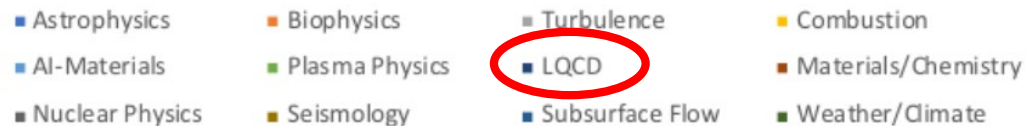


Figure credit:
Jack Wells,
Kate Clark



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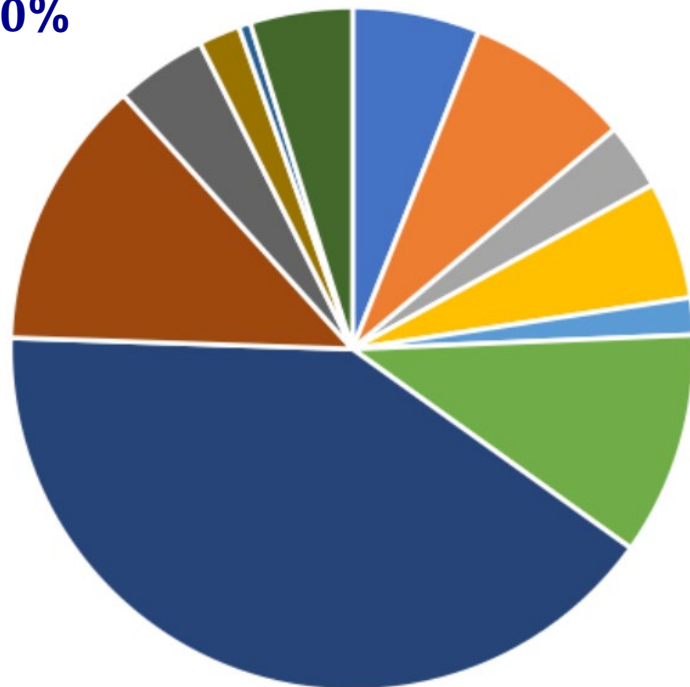
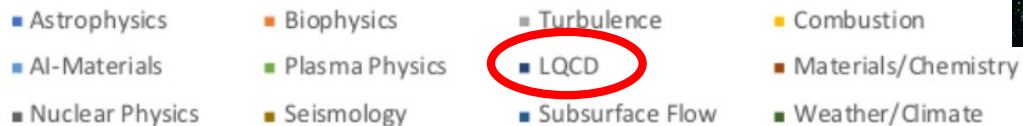


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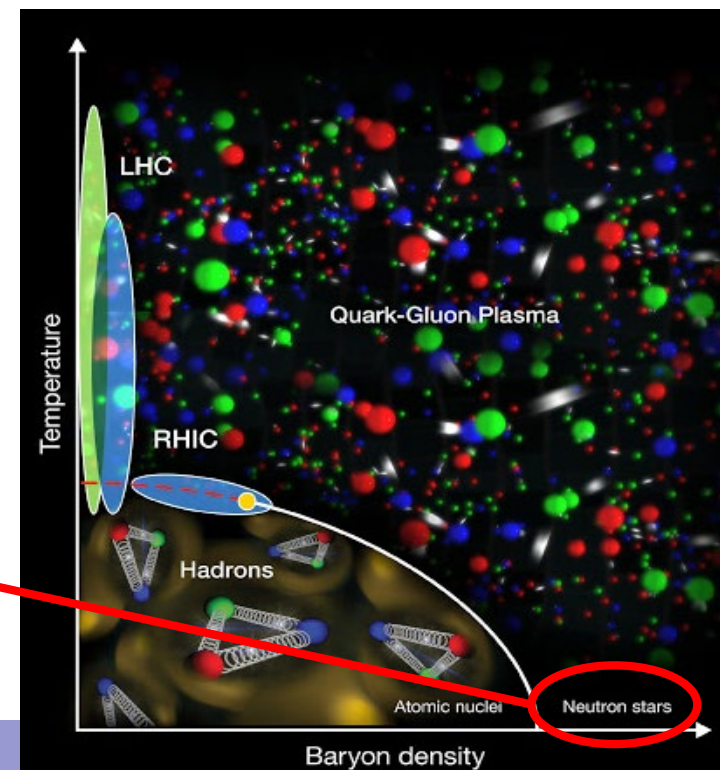


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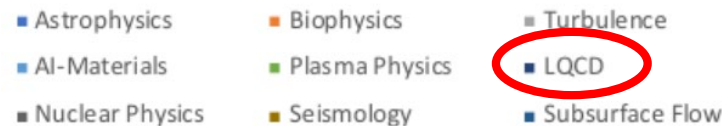
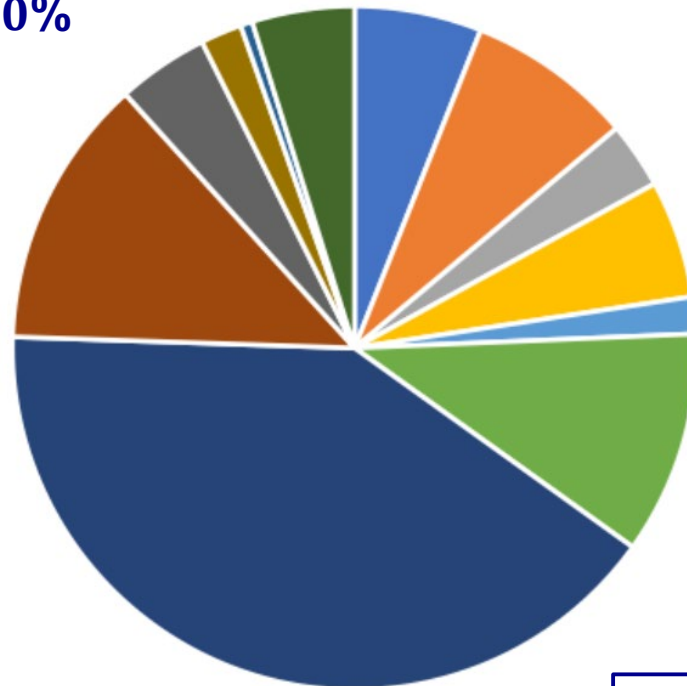
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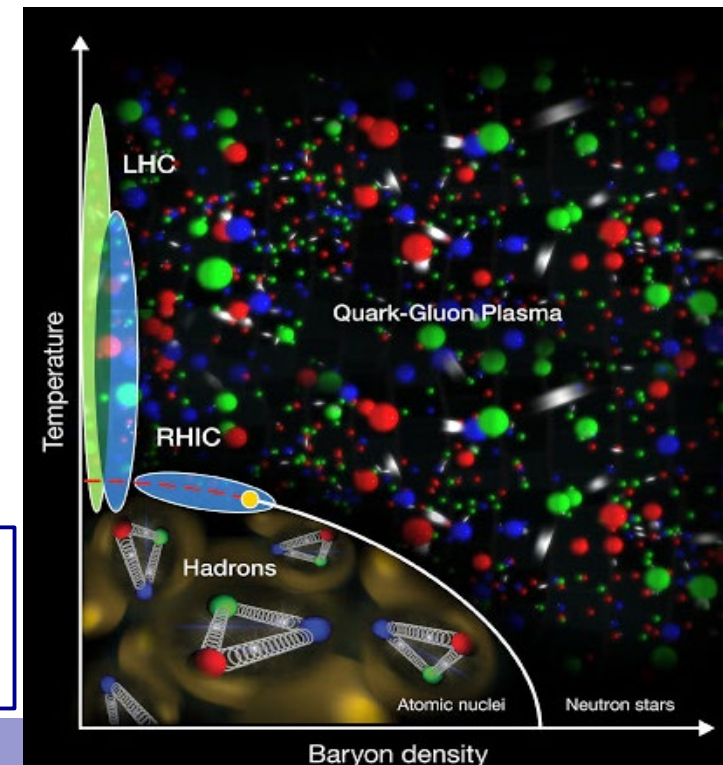
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Baryon chemical potential, θ -term, real-time evolution, ...

→ Tensor networks

→ Quantum computing

(lecture on Monday)



Thanks for listening!
Do you have any questions?

Figure credit:
Jack Wells,
Kate Clark