Introduction to lattice quantum chromodynamics

CFNS Summer School 2022 on the physics of the electron ion collider

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William & Mary

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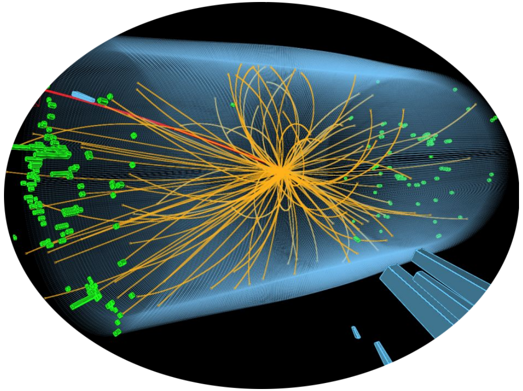
Strong nuclear force

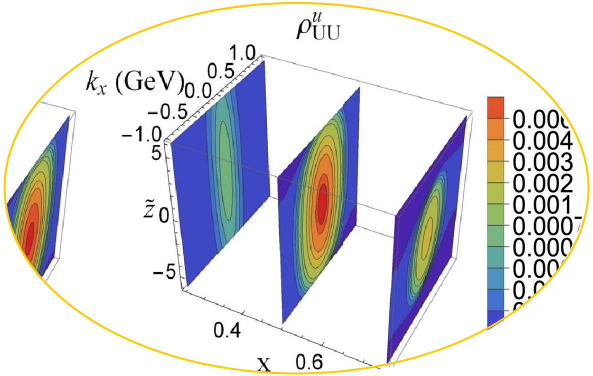


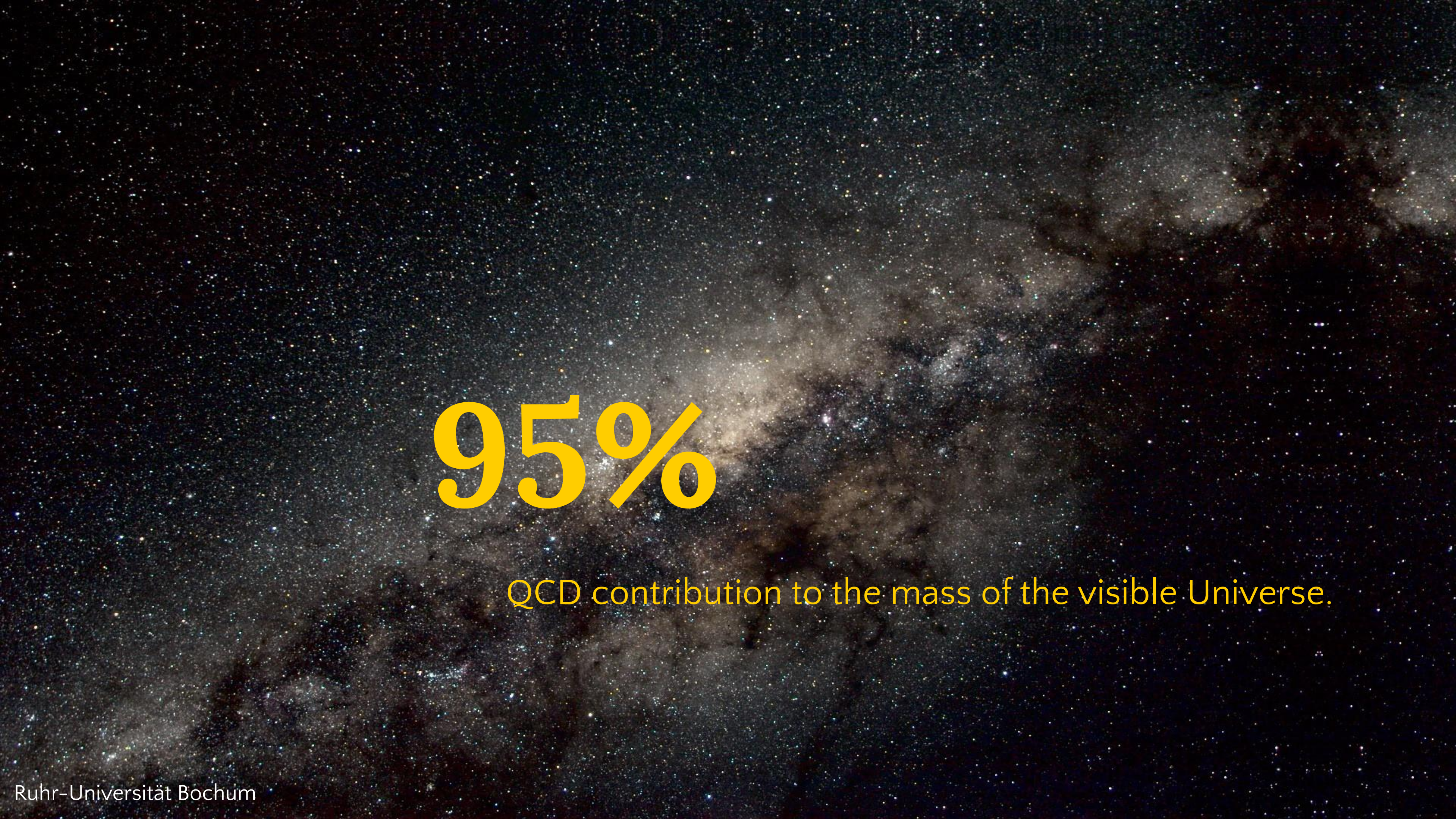
How do we get this?

... from this?

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) + \sum_f \overline{\psi}_f(x)\left[\gamma_\mu D^\mu + m_f \mathbb{I}\right]\psi_f(x)$$

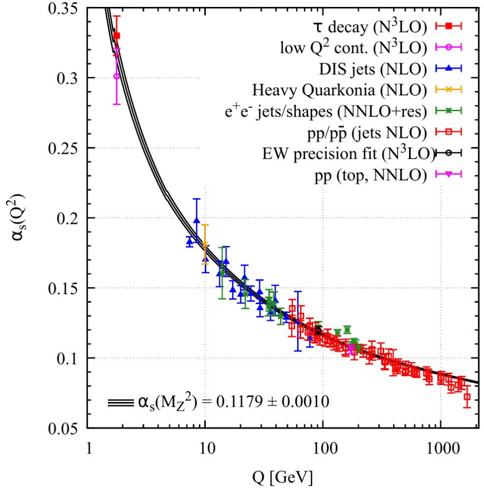
Or this?



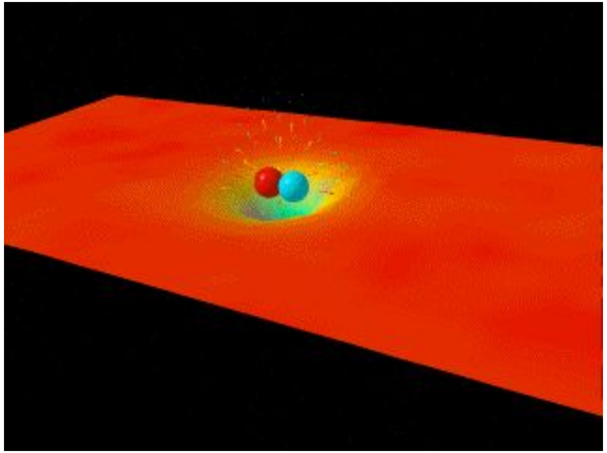

95%
QCD contribution to the mass of the visible Universe.
Ruhr-Universität Bochum

Properties of quantum chromodynamics

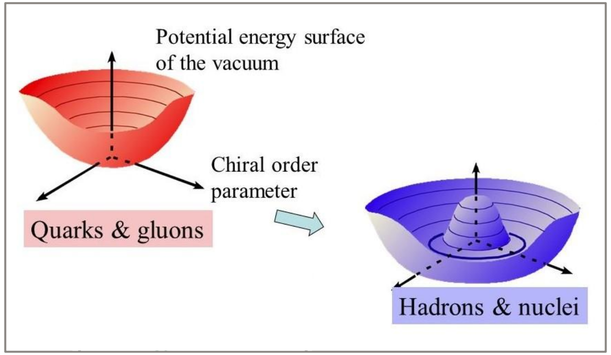
Asymptotic freedom



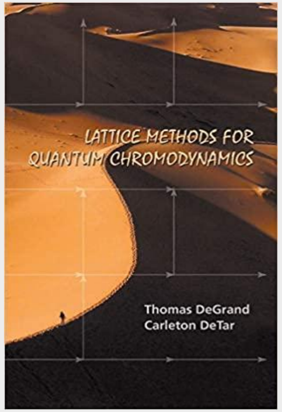
Confinement



Chiral symmetry breaking



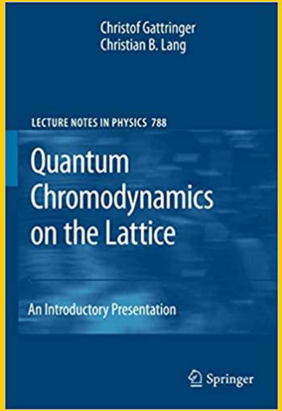
Some references



DeGrand and DeTar

Lattice methods for quantum chromodynamics

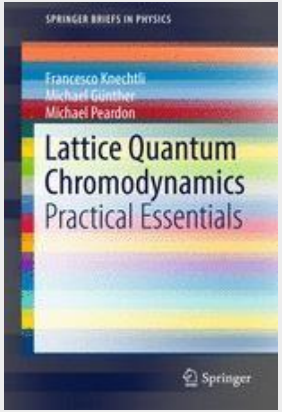
World Scientific 2006



Gattringer and Lang

Quantum chromodynamics on the lattice

Springer 2010



Knechtli, Günther & Peardon

Lattice quantum chromodynamics: practical essentials

Springer 2017

Lecture outline

Lecture 1

- Path integrals and lattice field theory
- Quantum chromodynamics

Lecture 2

- Spin models
- Numerical integration
- Monte Carlo methods

Lecture 3

- Gauge field Monte Carlo
- Correlation functions

1.1

Path integrals and lattice field theory

From Lagrangians to the lattice

Field theory: a reminder

Quantum field theory (QFT) brings together quantum mechanics and special relativity

- Describes all known fundamental particles and their interactions
- Describes many condensed matter systems

QFT typically formulated in the Lagrangian approach

$$\mathcal{L} = \boxed{\frac{1}{2}\partial_\mu \hat{\phi}(x) \partial^\mu \hat{\phi}(x)} - \boxed{\frac{1}{2} m^2 \hat{\phi}(x)^2} - \boxed{\frac{1}{4}\lambda\, \hat{\phi}(x)^4}$$

kinetic term   mass term   interaction

$\mathcal{S} = \int \mathrm{d}^4x\, \mathcal{L}(x)$ is the action

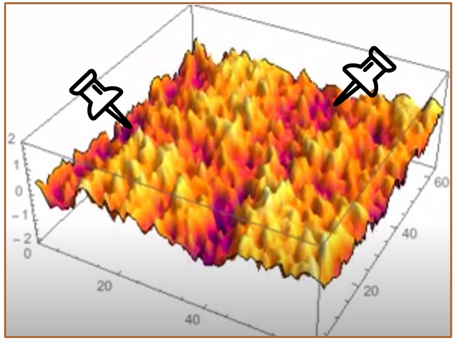
Magnets?
"No one understands magnets", but QFT at least gives you some pretty good predictions

Correlation functions

Many-body systems described by **correlation functions**

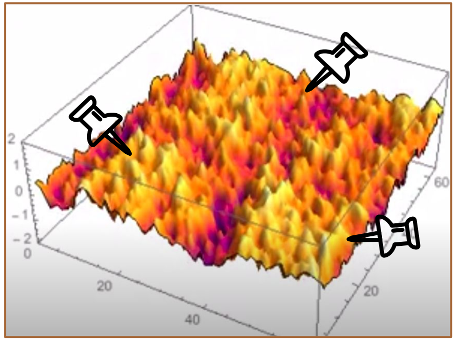
- Two-point function

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle$$



- Three-point function

$$\langle 0|\hat{\phi}(\mathbf{x}_3, t_3)\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle$$



Path integrals in quantum mechanics

Path integrals provide one **representation** of correlation functions

Example: the propagator

Describes the probability of finding a free particle at point x_2 at time t_2, given that it started at point x_1 at some earlier time t_1

Path integrals in quantum mechanics

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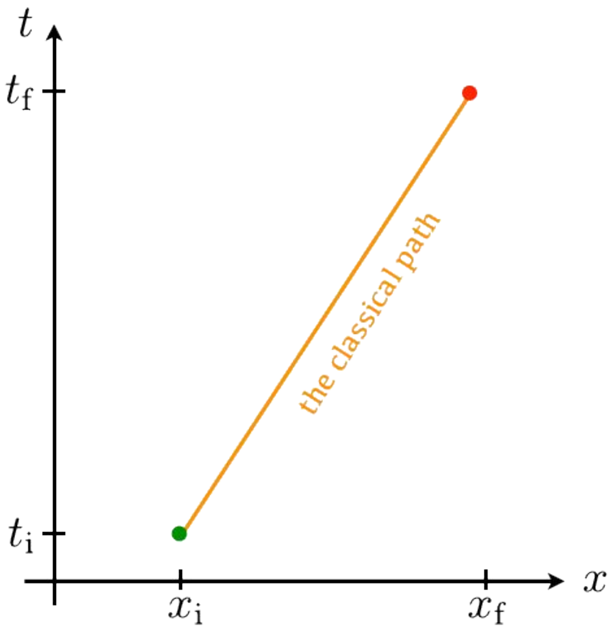

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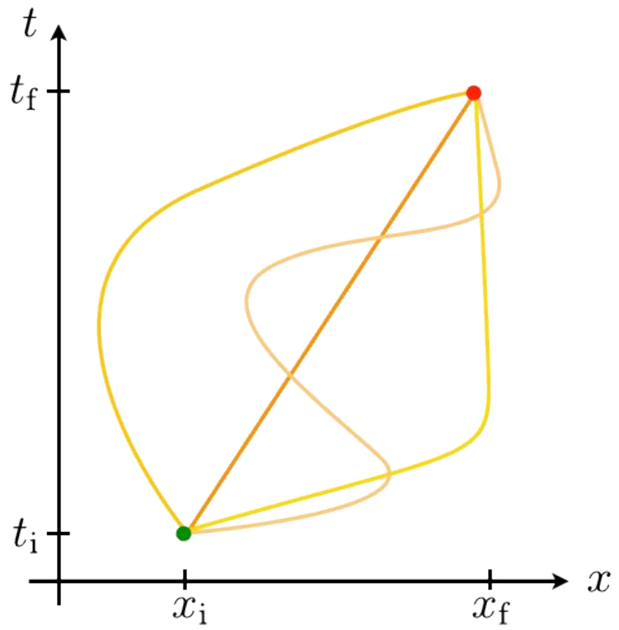


Dudek, Lattice QCD and the hadron spectrum

Example: the propagator

Describes the probability of finding a free particle at point x_2 at time t_2, given that it started at point x_1 at some earlier time t_1

Path integral prescription tells us to **sum over all paths**

$$\langle \mathbf{x}_f, t_f | \mathbf{x}_i, t_i \rangle = \int \mathcal{D}x \, e^{-iS(x)}$$

Each path is weighted by the corresponding **action**

Path integrals in quantum field theory

Path integrals in field theory sum over all possible **field configurations**

Correlation functions can be calculated from the path integral

Remember: these are what we want – they describe our system!

- Two-point function

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_2, t_2)\phi(\mathbf{x}_1, t_1)\, e^{-iS[\phi(x)]}$$

- Three-point function

$$\langle 0|\hat{\phi}(\mathbf{x}_3, t_3)\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_3, t_3)\phi(\mathbf{x}_2, t_2)\phi(\mathbf{x}_1, t_1)\, e^{-iS[\phi(x)]}$$

Our job – calculating these path integrals

Calculating path integrals I

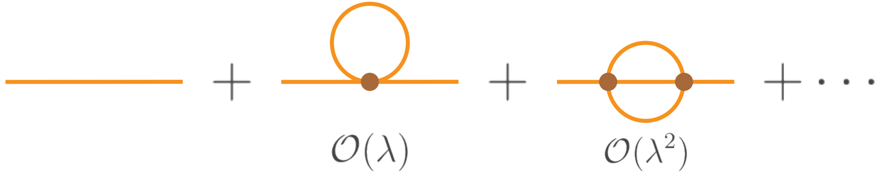
Free theories can be solved exactly, but they are not very interesting

Unfortunately, interacting quantum field theories generally cannot be solved exactly

Weakly coupled theories can be well-approximated by **perturbation theory**

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_2, t_2)\phi(\mathbf{x}_1, t_1)\left[1 + \frac{i}{4}\lambda\, \phi(x)^4 + \dots\right]$$

which we represent by Feynman diagrams



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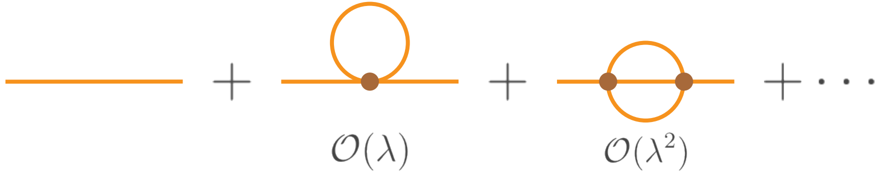


But what happens for strongly-coupled theories, where the expansion breaks down?

Like QCD at low energies

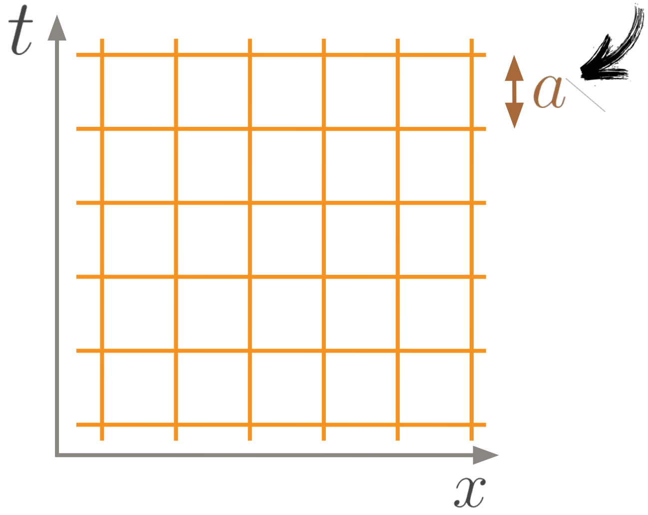
Calculating path integrals II: the lattice

Rigorous definition of our **sum over all field configurations** provided by discretising spacetime

Our path integral is now a product of integrals

$$\int \mathcal{D}\phi(x) := \prod_x \int_{-\infty}^{\infty} \mathrm{d}\phi_x$$

Prescription: do a single real-valued integral at each discrete spacetime point



Each of these integrals runs over field values at each lattice site

Seems like progress: unfortunately we have now replaced an unknown path integral object with an infinite number of divergent integrals. Not ideal.

Calculating path integrals II: Euclidean path integrals

To overcome this, we can **Wick rotate** – or analytically continue to imaginary time

$$t \to -it_{\mathrm{E}} \qquad \mathcal{S} = \int \mathrm{d}^3\mathbf{x}\,\mathrm{d}t\,\mathcal{L} \to -i\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}\tau\,\mathcal{L} := -i\mathcal{S}_{\mathrm{E}}$$

Geometrically, this corresponds to moving from **Minkowski** to **Euclidean** spacetime

$$\eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \to \delta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This leads us to a Euclidean path integral

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\,\phi(\mathbf{x}_2, \tau_2)\phi(\mathbf{x}_1, \tau_1)\,e^{-\mathcal{S}_{\mathrm{E}}[\phi(x)]}$$

Complex Gaussian integrals do not converge

$$\int_{-\infty}^{\infty} \mathrm{d}u\, e^{i\alpha u^2}$$

Solved by analytic continuation

$$u \to u(1 - i\epsilon)$$

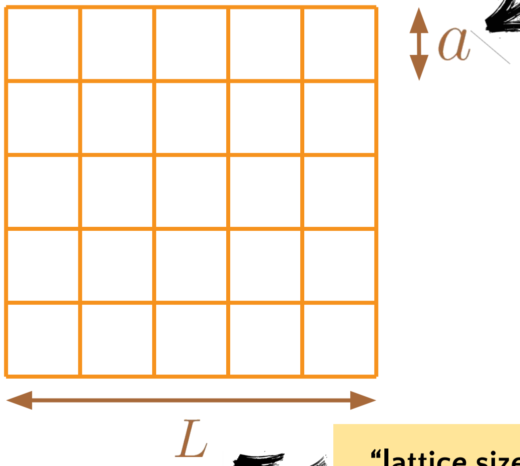
Calculating path integrals II: the lattice

We have not quite removed all infinities yet – we are still integrating over an infinite volume

Work in a **finite volume**, **discretised**, **Euclidean spacetime lattice**

“lattice spacing”

This is *the lattice*



“lattice size”

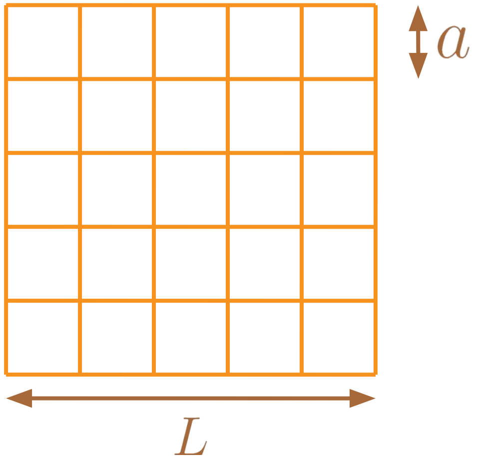
In principle, we now have everything we need to calculate our (finite) path integrals

- Lattice spacing provides an **ultraviolet cutoff** (**regulator**) –> integral at each spacetime point is finite
- Lattice volume provides an **infrared cutoff** –> finite number of (finite) integrals

Calculating path integrals II: the lattice

We have not quite removed all infinities yet – we are still integrating over an infinite volume

Work in a **finite volume**, **discretised**, **Euclidean spacetime lattice**



In principle, we now have everything we need to calculate our (finite) path integrals

- Lattice spacing provides an **ultraviolet cutoff** (**regulator**)
- Lattice volume provides an **infrared cutoff**

In practice, exactly solving even these these integrals is not feasible

A 16x16x16x16 lattice gives a 65536-dim integral

Euclidean path integrals: looking ahead

Our solution to these integrals will be numerical: **Markov chain Monte Carlo** estimation

Next lecture

Interpret the path integral weight as a **Boltzmann probability**

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_2, \tau_2)\phi(\mathbf{x}_1, \tau_1)\, e^{-\mathcal{S}_{\mathrm{E}}[\phi(x)]}$$

Allows us to estimate the integral stochastically

Recall from statistical mechanics: probability of finding system in state with energy *E* is *exp(–E/*k_B*T)*.

Euclidean path integrals: looking ahead

Our solution to these integrals will be numerical: **Markov chain Monte Carlo** estimation

Next lecture

Interpret the path integral weight as a Boltzmann probability

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_2, \tau_2)\phi(\mathbf{x}_1, \tau_1)\, e^{-\mathcal{S}_{\mathrm{E}}[\phi(x)]}$$

Allows us to estimate the integral stochastically

Recall from statistical mechanics: probability of finding system in state with energy *E* is *exp(–E/k_BT)*.

When people refer to "lattice QCD" they often mean the numerical evaluation of the path integral . But the lattice part (the **discrete Euclidean spacetime grid**) is separate from the numerical part (the **Markov chain Monte Carlo** integration)!

If we could do these integrals analytically, we would never need the numerical integration part, and it would still be "lattice QCD".

Summary: lecture 1.1

- Path integral representation of quantum mechanics: sum over all possible “paths”
- Path integral representation of quantum field theories: sum over all possible field values
- Correlation functions capture all the information we need about our field theory
- Path integration can be defined rigorously by introducing a finite spacetime lattice
- Resulting integrals can be carried out numerically by “Wick rotating” to Euclidean spacetime

1.2

Quantum chromodynamics

From quarks and gluons to hadrons

The strong nuclear force

Quark model: mesons formed from a quark and antiquark, **baryons** formed from three quarks.

Exotic states have quantum numbers that cannot be described by the quark model (**tetraquarks**, **pentaquarks**, **glueballs** …). Understanding these states is a high priority for nuclear physics and the EIC.

Quantum chromodynamics (**QCD**) is the mathematical theory of the strong nuclear force

- binds **quarks** and **gluons** together to form **hadrons**
- binds **protons** and **neutrons** (**nucleons**) into **nuclei**

Defined by a Lagrangian that includes quark fields, gluon fields, and their interactions

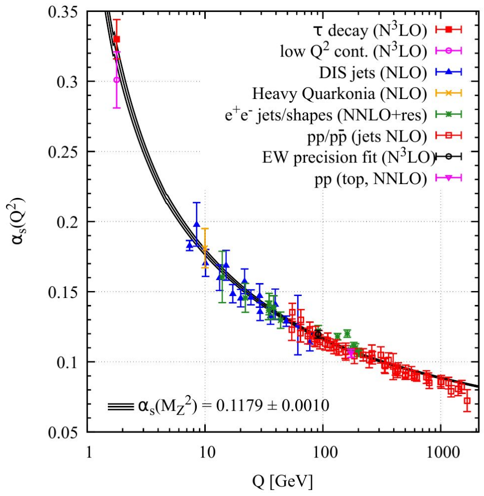
Key challenge: predicting the properties of hadrons and nuclei from first principles

This means: starting from the QCD Lagrangian and without assuming any particular behaviour or model.

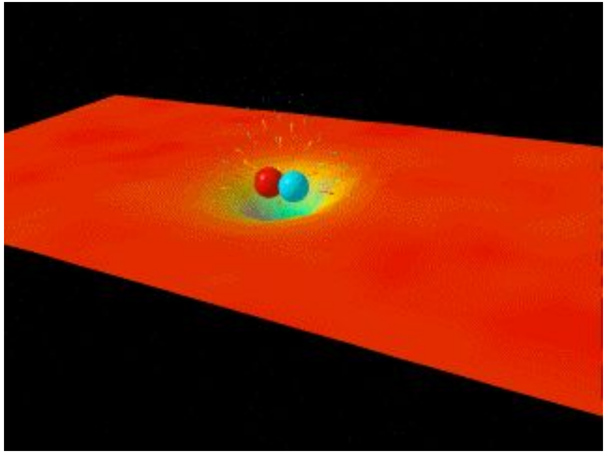
AKA: why first principles predictions are hard

Properties of quantum chromodynamics

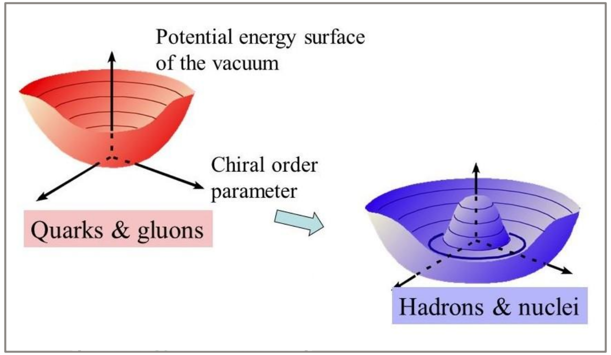
Asymptotic freedom



Confinement



Chiral symmetry breaking



QCD fields

QCD fields (the “fundamental degrees of freedom”)

Quark fields

$$\psi^{i}_{f\,\alpha}(x)$$

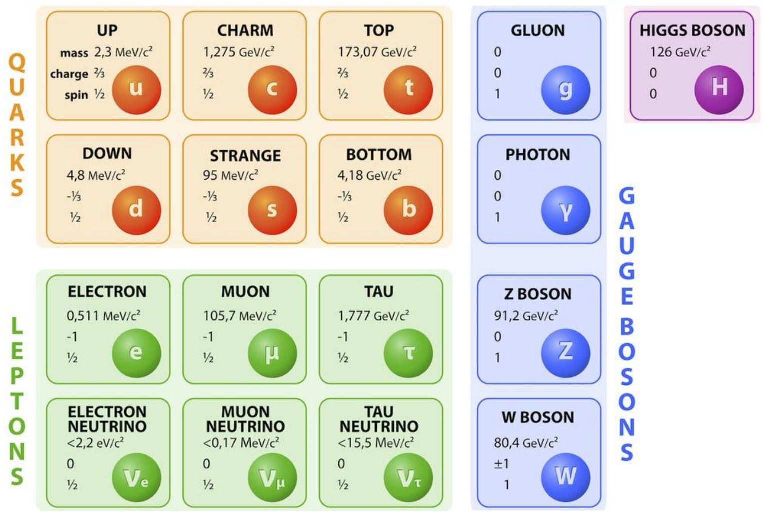
- Four component spinor (α runs from 1 to 4)
- Six flavours of quark (*f* runs from 1 to 6)
- Three colours (*i* runs from 1 to 3)

Gluon fields

$$A^{ij}_{\mu}(x) = \sum_{a=1}^{8} A^{a}_{\mu}(x) t^{a}_{ij}$$

- Four component vector (μ runs from 1 to 4)
- 3x3 matrices (*i, j* run from 1 to 3)

Standard model of particle physics



The t^{a}_{ij} are generators of the *SU(3)* gauge group in the adjoint representation

QCD Lagrangian

From now on: assume Euclidean metric

QCD Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4} F_{\mu\nu}(x) F^{\mu\nu}(x) + \sum_f \overline{\psi}_f(x) \left[\gamma_\mu D^\mu + m_f \mathbb{I}\right] \psi_f(x)$$

QCD Lagrangian

QCD Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) + \sum_f \overline{\psi}_f(x)\left[\gamma_\mu D^\mu + m_f\mathbb{I}\right]\psi_f(x)$$

gauge sector — fermion sector

Free massive quark $\overline{\psi}_f\left[\gamma_\mu\partial^\mu + m_f\mathbb{I}\right]\psi_f$

Gluon–quark interaction $-igA^a_\mu\left(\overline{\psi}_f\gamma^\mu t^a\psi\right)$

Field strength tensor $F_{\mu\nu} = \frac{i}{g}[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu - ig[A_\mu, A_\nu]$

kinetic term — self-interaction

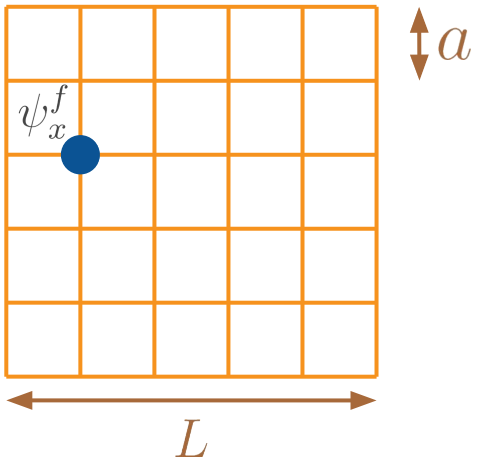
Gauge covariant derivative $D_\mu = \partial_\mu - igA_\mu$

Quarks on the lattice

We now need to put QCD on the lattice (or **discretise** the theory)

Fermions live on the lattice sites (or nodes)

We have a number of ways to discretise the derivative



Example: the nearest-neighbour difference operator

Simplest option

$$\partial_\mu \psi(x) \rightarrow \nabla_\mu \psi_x = \frac{1}{a}\left(\psi_{x+a\hat{\mu}} - \psi_x\right)$$

Errors are $O(a^2)$, which can be removed by adding **improvement terms**

Quarks on the lattice

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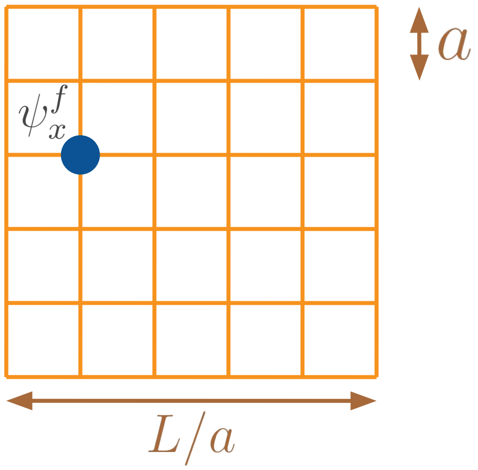


Fermions live on the lattice sites (or nodes)

We have a number of ways to discretise the derivative

Free fermion part of the Lagrangian becomes

$$\sum_f \overline{\psi}_f \left[\gamma_\mu \partial^\mu + m_f \mathbb{I}\right] \psi_f \to \sum_f \overline{\psi}^f_x \left[\gamma_\mu \nabla^\mu + a m_f \mathbb{I}\right] \psi^f_x$$

which we can represent more abstractly as

$$\sum_f \overline{\psi}^f_y D_{yx} \psi^f_x$$

“lattice Dirac operator”

A note on units: computers don’t like dimensionful quantities – all quantities are expressed in dimensionless **lattice units**.

In other words, physical quantities are expressed in terms of the number of lattice spacings they occupy.

Fermion doubling

These extra poles correspond to extra particles, called **fermion doublers**. These doublers are unphysical fermions, which don't exist in continuum QCD.

Free fermion propagator obtained by solving

$$D_{yx}\psi^f_x = 0$$

Solution is the free fermion lattice propagator

Solutions to the fermion doubling problem give rise to the many different **lattice fermion actions** (the origin of a lot of jargon you might hear).

Examples: Wilson fermions, domain-wall fermions, overlap fermions, staggered fermions, twisted mass fermions…

Example: the "naive" lattice Dirac operator

Choice of Dirac operator is

$$D_{yx} = \gamma_\mu \delta_{y,x-a\hat{\mu}} - \gamma_\mu \delta_{y,x+a\hat{\mu}} + am\delta_{y,x}$$

leads to the fermion propagator

$$S^{ab}_x = \delta^{ab}\, a \frac{-i\sum_\mu \gamma_\mu \sin(ak_\mu) + am}{\sum_\mu \sin^2(ak_\mu) + a^2m^2}$$

The **Nielsen-Ninomiya theorem** states that you cannot avoid fermion doublers if you want chiral fermions on the lattice.

In fact, this generalises to any regulator.

Propagator has **extra poles** – propagator describes multiple fermions with the same mass!

Gluons on the lattice

Consider the **quark bilinear** in the continuum

$$\overline{\psi}^j_f(y)\,\delta_{ji}\,\psi^i_f(x)$$

This combination is not gauge-invariant

To make this gauge invariant, we need the combination

$$\overline{\psi}^j_f(y)\,\left[e^{ig\int_x^y \mathrm{d}z_\mu \cdot A^\mu(z)}\right]_{ji}\,\psi^i_f(x)$$

Extra **Wilson line** (or **parallel transporter**) “transports” the color from one fermion to another

On the lattice the shortest possible path is a **gauge link**

$$\overline{\psi}^j_{x+a\hat{\mu}}\,\left[e^{iagA^\mu_x}\right]_{ji}\,\psi^i_x := \overline{\psi}_{x+a\hat{\mu}}\,U^\mu_x\,\psi_x$$

SU(3) matrix

Gluons on the lattice

Like our fermion derivatives, the errors are *O(a ˆ2)* and can be removed (**improved**) by adding different closed loops. Different choices of **Improvement terms** lead to more jargon: Iwasaki action, Lüscher–Weisz action…

Gluon action must be gauge invariant – build action from **closed loops**

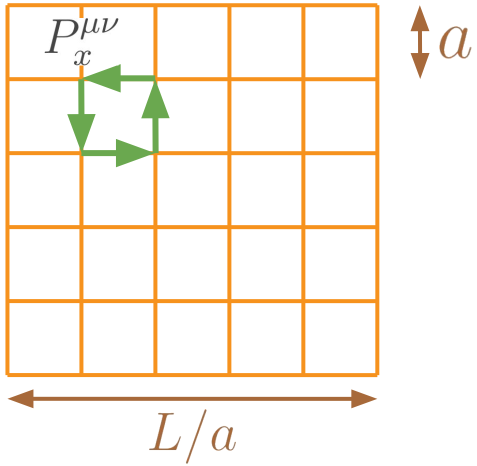
Example: the Wilson action

Smallest closed loop is a 1x1 loop (a **plaquette**)

$$P_x^{\mu\nu} = U_x^\mu \, U_{x+a\hat{\mu}}^\nu \, U_{x+a\hat{\nu}}^{\mu\dagger} \, U_x^{\nu\dagger}$$

Wilson action is a sum over all possible plaquettes

$$\mathcal{L}_{\text{Wilson}} = \frac{2}{g^2} \sum_{\mu<\nu} \text{Re}\,\text{Tr}\left(1 - P_x^{\mu\nu}\right)$$



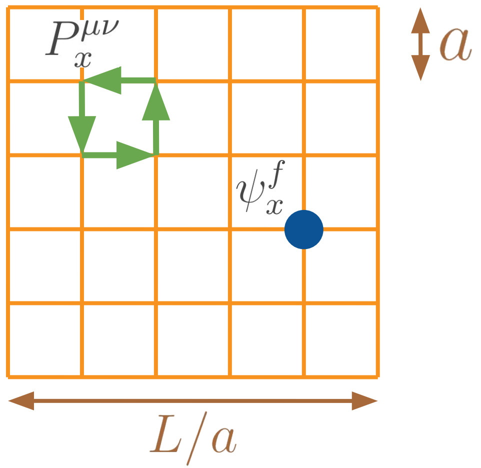
QCD on the lattice

Reminder: QCD in the continuum

$$\mathcal{L}_{\rm QCD} = -\frac{1}{4} F_{\mu\nu}(x) F^{\mu\nu}(x) + \sum_f \overline{\psi}_f(x) \left[\gamma_\mu D^\mu + m_f \mathbb{I}\right] \psi_f(x)$$

QCD on the lattice

$$\mathcal{L}_{\rm LQCD} = \mathcal{L}_g(U_x) + \sum_f \overline{\psi}\,{}^f_y D_{yx}(U)\, \psi^f_x$$



Different discretisations are possible, provided they agree in the **continuum limit** (a -> 0)

Fermions and Grassmann numbers

For path integrals involving scalar fields, commuting operators are replaced by (ordinary) numbers

$$\langle 0|\hat{\phi}(\mathbf{x}_2, t_2)\hat{\phi}(\mathbf{x}_1, t_1)|0\rangle = \int \mathcal{D}\phi(x)\, \phi(\mathbf{x}_2, \tau_2)\phi(\mathbf{x}_1, \tau_1)\, e^{-\mathcal{S}_{\mathrm{E}}[\phi(x)]}$$

Fermion operators anticommute and must be replaced by **anticommuting numbers** (**Grassmann numbers**)

$$\theta_A\theta_B = -\theta_B\theta_A$$

Computers don't like anticommuting numbers; use

$$\int \mathcal{D}\overline{\psi}\mathcal{D}\psi\, \exp\left[-\overline{\psi}D(U)\psi\right] = \det D(U)$$

Gaussian integral

Determinant becomes part of the Boltzmann probability factor in our Markov chain Monte Carlo

$$\langle 0|\overline{\psi}\psi|0\rangle = \int \mathcal{D}U\, \overline{\psi}\psi\, \boxed{\det D(U)\, e^{-\mathcal{S}_{\mathrm{LQCD}}[\overline{\psi},\psi,U]}}$$

Fermions and Grassmann numbers

Fermion determinant computationally expensive to calculate and cost increases as quark mass decreases.
Old calculations (pre 2005) neglected the fermion determinant completely (the **quenched approximation**). These days, many calculations still use **unphysically heavy quark masses** and require a **chiral extrapolation**.

For path integrals involving scalar fields, commuting operators are replaced by (ordinary) numbers

$$\langle 0|\hat{\phi}(\mathbf{x}_2,t_2)\hat{\phi}(\mathbf{x}_1,t_1)|0\rangle = \int \mathcal{D}\phi(x)\,\phi(\mathbf{x}_2,\tau_2)\phi(\mathbf{x}_1,\tau_1)\,e^{-S_{\mathrm{E}}[\phi(x)]}$$

Fermion operators anticommute and must be replaced by **anticommuting numbers** (**Grassmann numbers**)

$$\theta_A\theta_B = -\theta_B\theta_A$$

Computers don't like anticommuting numbers; use

$$\int \mathcal{D}\overline{\psi}\mathcal{D}\psi\ \exp\left[-\overline{\psi}D(U)\psi\right] = \det D(U)$$

Determinant becomes part of the Boltzmann probability factor in our Markov chain Monte Carlo

$$\langle 0|\overline{\psi}\psi|0\rangle = \int \mathcal{D}U\,\overline{\psi}\psi\,\boxed{\det D(U)\,e^{-S_{\mathrm{LQCD}}[\overline{\psi},\psi,U]}}$$

Summary: lecture 1.2

- QCD describes fundamental interactions of the strong nuclear force in terms of quarks and gluons
- Lattice QCD formulated with quarks on the lattice sites and $SU(3)$ link variables representing gluons
- Gluon action built from closed loops of link variables, such as plaquettes
- Fermions on the lattice suffer from fermion doubling; intimately connected to existence of chiral fermions in a regulated theory
- Different discretisations possible, but any choice should lead to QCD in the continuum limit of vanishing lattice spacing

Looking ahead: lecture 2

- Spin models ubiquitous in condensed matter and QFT applications
- Statistical field theory and QFT closely connected through path integral formalism
- Correlation functions evaluated through high-dimensional integrals
- Direct numerical evaluation not feasible – **Monte Carlo** methods necessary
- **Markov chain Monte Carlo** used to create probability distributions
- Provides statistical estimate of path integrals

Thank you

Questions?

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Gauge theory example: electromagnetism

Transformations of the **gauge potential** leave **Maxwell's equations** invariant

$$\mathbf{A} \to \widetilde{\mathbf{A}} = \mathbf{A} + \nabla\Lambda \qquad V \to \widetilde{V} - \frac{\partial \Lambda}{\partial t}$$

$$\nabla \times \mathbf{A} = \mathbf{B} \qquad \nabla V = \frac{\partial \mathbf{A}}{\partial t} - \mathbf{E}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

In four-vector notation

$$A^\mu \to \widetilde{A}^\mu = A^\mu - \partial^\mu \Lambda \qquad F^{\mu\nu} = \partial^\mu A^\nu - \partial^\mu A^\nu \to \widetilde{F}^{\mu\nu} = \partial^\mu \widetilde{A}^\nu - \partial^\mu \widetilde{A}^\nu = F^{\mu\nu}$$

This leads to charge conservation (by Noether's theorem)

$$J^\mu = (\rho, \mathbf{J}) = \partial_\nu F^{\mu\nu} \qquad \partial_\mu J^\mu = 0$$

Strictly speaking, this is a **global**, not a **local**, gauge symmetry – but it is a more familiar example than most local gauge symmetries.

A more familiar group: SU(2)

Lie algebras of *SU(2)* and *SO(3)* are **isomorphic**
SU(2) is the **double cover** of *SO(3)*

Angular momentum operators

- satisfy commutation relations that define the **Lie algebra** of the group *SO(3)*

  $$[L_i, L_j] = i\epsilon_{ijk}L_k$$

- exponentiating gives elements of 3D rotation group (*SO(3)*)

  $$R(\hat{n}, \phi) = \exp\left[-i\phi L_{\hat{n}}\right]$$

- generate spatial rotations

Pauli spin matrices

- satisfy commutation relations

  $$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

- exponentiating gives elements of *SU(2)* group
- generate quantum mechanical spin