QCD on the lattice

Overview:
- Understanding lattice QCD
- Lattice QCD calculations: Spectroscopy
- Lattice QCD calculations: Matrix elements
- Open and unsolved problems in Lattice QCD
Why do I enjoy working in lattice QCD?
To understand the basic ingredients of lattice QCD calculations, we need to discuss:

- The path integral formulation of quantum mechanics
- Path integral quantum field theory
- Discretising fields and differential operators
- Regularisation / renormalisation
- The symmetries of QCD
- The Monte Carlo method
Lattice field theory uses Feynman’s path integral description of quantum mechanics.

Quantum mechanical amplitudes can be expressed as a “sum over histories”.

Consider a particle moving in one dimension. The wave-function a small time in the future can be expressed as

$$\psi(x_1, t+\epsilon) = \sqrt{\frac{im}{2\epsilon\hbar}} \int dx_0 \psi(x_0, t) e^{-\frac{i\epsilon}{\hbar} L(x_0, x_1)}$$

with $L$ the (classical) lagrange density.

We have already begun to discretise; we are defining the states of the system only on time-slices.
The path integral - reformulating quantum mechanics (2)

\[ \psi(x_1, t + \epsilon) = \sqrt{\frac{im}{2\epsilon \hbar}} \int dx_0 \, \psi(x_0, t) \, e^{-\frac{i\epsilon}{\hbar} \mathcal{L}(x_0, x_1)} \]

- The Lagrange density is \( \mathcal{L}(x, \dot{x}) = \frac{m}{2} \dot{x}^2 - V(x) \)
- For time-slices closely separated, define \( \dot{x} = \frac{x_1 - x_0}{\epsilon} \) then expanding for small \( \epsilon \) and introducing \( \eta = x_1 - x_0 \) gives

\[ \psi + \epsilon \frac{\partial}{\partial t} \psi = \sqrt{\frac{im}{2\epsilon \hbar}} \int d\eta \, e^{-\frac{im\eta^2}{2\hbar \epsilon}} (1 - i\frac{\epsilon}{\hbar} V)(\psi - \eta \frac{\partial}{\partial x} \psi + \frac{\eta^2}{2} \frac{\partial^2}{\partial x^2} \psi + \ldots) \]

- This used a saddle-point expansion around \( \epsilon = 0 \). Integrating \( \eta \) gives

\[ i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V\psi \]

\( \ldots \psi \) satisfies time-dependent Schrödinger’s equation

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Repeating this update many times will define an algorithm to solve the Schrödinger equation (given an initial wave-function).

For finite updates, the corresponding integral expression relating the final wave-function $\psi(x_f, t_f)$ to the initial wave-function $\psi(x_i, t_i)$ is

$$\psi(x_f, t_f) = \int dx_i \psi(x_i, t_i) Z(x_i, x_f)$$

with $Z$ the *path integral*

$$Z = \int \prod_{a=1}^{N-1} Dx_a \ e^{i \frac{\hbar}{\epsilon} S}$$

and $S$ is the classical action,

$$S = \sum_{a=1}^{N-1} \frac{m}{2\epsilon^2} (x_a - x_{a-1})^2 + V(x_a)$$
Minkowski, Wick and Euclid

- Some properties of theories in Minkowski space can be related by Wick rotation to corresponding theories in Euclidean space.
- Analytic continuation: $t \rightarrow i\tau$, $\frac{-i}{\hbar}S \rightarrow \frac{1}{\hbar}S$.

$$
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\rightarrow
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
$$
Correlation functions

- The path integral defines simple transition amplitudes like 
  \( \langle x_f, t_f | x_i, t_i \rangle \) but more complicated matrix elements also have representations

  \[
  \langle x_f, t_f | x(t_2) x(t_1) | x_i, t_i \rangle = \int \prod_{a=1}^{N-1} Dx_a x(t_2) x(t_1) e^{i \hbar S} \]

- In the Euclidean metric, the weight for field configurations is Wick rotated, so \( e^{i \hbar S} \rightarrow e^{-\frac{1}{\hbar} S} \)

- This gives correlation functions a useful property:

  \[
  \langle 0 | x(\tau_2) x(\tau_1) | 0 \rangle = \langle 0 | e^{H \tau_2} x e^{-H(\tau_2 - \tau_1)} x e^{-H \tau_1} | 0 \rangle = \sum_{n,m} \langle x | n \rangle \langle n | e^{-H(\tau_2 - \tau_1)} | m \rangle \langle m | x \rangle = \sum_n |\langle x | n \rangle|^2 e^{-E_n (\tau_2 - \tau_1)} \]
Correlation functions

Then with $\Delta \tau = \tau_2 - \tau_1$,

**Euclidean correlation functions**

$$\lim_{\Delta \tau \to \infty} \langle 0 | x(\tau_2) x(\tau_1) | 0 \rangle = Z e^{-E_1 \Delta \tau}$$

At large imaginary-time separations, $\Delta \tau \to \infty$ correlation functions fall exponentially with rate proportional to the energy of the lowest energy state that is excited.

We will see another (even more) crucial property of the Euclidean metric when we look at studying quantum field theories numerically.
Path integral quantum field theory

- QCD is a relativistic quantum field theory.
- Path integral quantisation extends to quantum field theory too:
  
<table>
<thead>
<tr>
<th>Theory</th>
<th>d.o.f</th>
<th>discretise</th>
<th>action</th>
<th>sum over all</th>
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<td>QM</td>
<td>$x(t)$</td>
<td>$t$</td>
<td>$S[x]$</td>
<td>paths</td>
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<tr>
<td>QFT</td>
<td>$\phi(x,t)$</td>
<td>$x, t$</td>
<td>$S[\phi]$</td>
<td>field configurations</td>
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- Discretise four-dimensional space-time on a 4d lattice: $x, t \rightarrow (a_{n_1}, a_{n_2}, a_{n_3}, a_{n_4}), n_\mu \in \mathbb{Z}$, $a$ is distance between sites.
- Matter fields (scalar bosons, quarks, ... ) are represented by integration variables at all lattice sites, $\phi_{n_1,n_2,n_3,n_4}$.
- The action is a function of all these variables and the path integral is the integral over these degrees of freedom.

QFT lattice path integral

\[ Z = \int \prod_{\mu, n_\mu} d\phi_{n_1,n_2,n_3,n_4} \, e^{-S(\phi)} \]
Comparing Minkowski and Euclid

<table>
<thead>
<tr>
<th></th>
<th>Minkowski</th>
<th>Euclidean</th>
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<tr>
<td>Weight of a field configuration</td>
<td>$e^{i\frac{S}{\hbar}}$</td>
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<td>Parameter</td>
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<td>temperature, $T$</td>
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<tr>
<td>Numerical approach?</td>
<td>Not easy!</td>
<td>Monte Carlo</td>
</tr>
</tbody>
</table>

- Statistical mechanical systems often exhibit interesting phase transitions.
- “Bare” lattice couplings in the action describe “theory space”.
- Correlation lengths of the lattice statistical mechanical system can diverge (in units of $a$) at certain points or sub-spaces of “theory space”.
- Continuum field theories can live at second-order phase transition points.
Regularising path integrals

- Path integrals have continuum representation too!

- When path integrals are expanded in the continuum in powers of the coupling constant (perturbation theory), we often encounter apparent divergences.

\[ q \approx \int d^4k \frac{1}{k^2} \frac{1}{(q - k)^2} \]

- These can usually be regulated by a (perturbative) renormalisation procedure.

- In a finite volume, lattice path integrals are certain to be (UV) finite - the divergences are cut-off automatically.

- The lattice provides a cut-off outside perturbation theory. This is a crucial property for QCD.
The action in Euclidean space for a (real) scalar field $\phi(x)$ is

$$S[\phi] = \int d^4x \, \phi(-\Box + m^2)\phi$$

with $\Box = \sum_{\mu=1}^{4} \frac{\partial^2}{\partial x_\mu^2}$.

$m$ is the (bare) boson mass.

This action is invariant under $SO(4)$ the Euclidean rotation group in four dimensions (the equivalent of Lorentz group), so theory is one of relativistic bosons.

A lattice version would define scalar fields that take values on lattice sites only.

Define $a$ to be the lattice spacing - the distance between adjacent sites.
To represent the differential operator \( \Box \), we can take linear combinations of the nearest neighbours of a site. A Taylor-series in \( a \) would give

\[
\phi(n_1 + a, n_2, n_3, n_4) = \phi(n_1, n_2, n_3, n_4) + a \frac{\partial}{\partial x_1} \phi(n_1, n_2, n_3, n_4) \\
+ \frac{a^2}{2} \frac{\partial^2}{\partial x_1^2} \phi(n_1, n_2, n_3, n_4) + \mathcal{O}(a^3)
\]

So the linear combination of nearest neighbours

\[
\frac{1}{a^2} \left( \phi(n_1 + a, n_2, n_3, n_4) + \phi(n_1 - a, n_2, n_3, n_4) - 2\phi(n_1, n_2, n_3, n_4) \right)
= \frac{\partial^2}{\partial x_1^2} \phi(n_1, n_2, n_3, n_4) + \mathcal{O}(a^2)
\]

gives a suitable representation of one term in \( \Box \).
The lattice action is then

\[
S[\phi] = \frac{a^4}{2} \sum_x \left\{ (m^2 + 8)\phi(x)^2 - \sum_{\mu=1}^{4} \phi(x)\phi(x + \hat{\mu}) \right\}
\]

The path integral is gaussian and it can be computed analytically. The propagator (in momentum space) for the theory is then

\[
\langle \phi(p')\phi(p) \rangle = \delta_{p,p'} \frac{1}{\sum_{\mu=1}^{4} \frac{2}{a} \sin^2(ap_\mu/2) + m^2}
\]

As \( a \to 0 \) the propagator for a scalar boson in the (Euclidean) continuum is recovered.

\[
\langle \phi(p')\phi(p) \rangle = \delta_{p,p'} \frac{1}{\sum_{\mu=1}^{4} p_{\mu}^2 + m^2}
\]
Local interactions can be added easily, for example define

\[ S[\phi] = S_0[\phi] + S_{\text{int}}[\phi] \]

with

\[ S_0[\phi] + S_{\text{int}}[\phi] = \lambda a^4 \sum_x \phi^4(x) \]

and we are simulating a Higgs field.

- For finite \( a \), the lattice theory differs from the continuum by terms proportional to \( a^2 \).
- These extra terms lead to *lattice artefacts*. Computing properties of the continuum theory will require extrapolation to \( a = 0 \).
- The lattice action is not unique: we could have used

\[
\frac{\alpha}{4} (\phi(x+2) + \phi(x-2)) + (1-\alpha)(\phi(x+1) + c_1 \phi(x-1)) - 2(1 - \frac{3}{4}\alpha)\phi(x)
\]

for any value of \( \alpha \).
- The influence of these artefacts can be reduced by *improvement*. 
Improvement

- The freedom to employ different representations of the lattice action with a common continuum limit is exploited to reduce discretisation artefacts.

- Classically, an improved version of the second-order derivative is

\[
\frac{\partial^2}{\partial x^2} \phi = \frac{4}{3a^2}(\phi_1 + \phi_{-1} - 2\phi_0) - \frac{1}{12a^2}(\phi_2 + \phi_{-2} - 2\phi_0) + \mathcal{O}(a^4)
\]

- The more complete procedure in a quantum field theory is the **Symanzik improvement programme**

- Symanzik improvement accounts for relative renormalisation of coefficients relating terms in the lattice action to their continuum counterparts.
Basic properties of QCD

To discretise a theory and write a useful lattice representation, it is important to do the best possible job of respecting the symmetries of the theory.

Symmetries define universality classes and ensure the correct approach to the continuum as we (try to) take $a \rightarrow 0$

Symmetries of QCD

- Poincaré invariance (Lorentz and translation invariance)
- Gauge invariance
- Discrete symmetries: parity, time-reversal, charge conjugation
- (Near) chiral symmetry (for massless quarks).
- (Near) flavour symmetry (for mass-degenerate quarks).

The QCD path integral is written in terms of the two fundamental fields, the quarks and the gluons.
Wilson’s big idea...

Wilson realised that ensuring *gauge invariance* means the gluon fields have to be given special treatment:

- **Quark fields on sites**
- **Gauge fields on links**
Starting from a path integral representation, we can formulate quantum field theory on a discretised version of space-time.

If we are interested in spectroscopy, the Euclidean metric is very useful. Correlation functions fall exponentially, with rate related to the energies of eigenstates.

The Euclidean metric also translates QFT into a statistical mechanics problem. There are then effective numerical techniques to attack these problems.

Symmetries define field theories - we will need to be careful what symmetries we keep or break when the field theory is put on a lattice.

An exact gauge symmetry on the lattice will be constructed by putting *quarks on sites, gluons on links*.
1. Show

\[ \frac{\partial^2}{\partial x^2} \phi = \frac{4}{3a^2} (\phi_1 + \phi_{-1} - 2\phi_0) - \frac{1}{12a^2} (\phi_2 + \phi_{-2} - 2\phi_0) + \mathcal{O}(a^4) \]

2. Compute an expression for the free scalar boson propagator:

\[ \langle \tilde{\phi}(p') \tilde{\phi}(p) \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, \tilde{\phi}(p') \tilde{\phi}(p) \, e^{-S} \]

where

\[ \tilde{\phi}(p) = \sum_x \phi(x) e^{ipx} \]

and

\[ S[\phi] = \frac{a^4}{2} \sum_x \left\{ (m^2 + 8)\phi(x)^2 - \sum_{\mu=1}^{4} \phi(x)\phi(x + \hat{\mu}) \right\} \]