



Lattice QCD for hadron and nuclear physics: introduction and basics

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HOUSEKEEPING

- Web page for these lectures at <http://www.maths.tcd.ie/~ryan/MIT2016>
- lectures, homework problems and data as well as references will all be there

LECTURE PLAN

● Lecture 1:

- Theory and experiment motivation for hadron and nuclear physics.
- QCD overview.
- Why consider lattice calculations.
- Introduction to lattice framework including the path integral and discretisation.

● Lecture 2:

- Convergence through universality - how well to lattice calculations do?
- Fitting data - tricks and pitfalls
- Some aspects of discretisation to consider.
- Strategies for precision calculations

● Lecture 3:

- New ideas enabling precision physics
- Recent results - the state-of-the-art.

● Lecture 4:

- New frontiers - scattering and resonances in a lattice calculation.
- Open challenges in hadronic and nuclear physics.
- The exascale era.

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Aim: a pedagogic introduction to lattice QCD - to understand methods, the difficulties and the results and errors in a calculation.

INTRODUCTION

There are many interesting questions in hadronic and nuclear physics that we would like to answer from first principles:

- What is the nature of the X,Y,Z states in charmonium and bottomonium?
- What is the dynamics and structure of exotic and hybrid states?
- How sensitive are “fine-tuned” quantities like $M_n - M_p$ to the values of fundamental parameters?
- What is the equation of state of dense nuclear matter in neutron stars?
- Can we test/break the Standard Model at low energies
 - relevant since SM complete with Higgs
 - no significant BSM physics observed other than $g - 2$ and proton radius.
 - Can we determine reliable inputs for Dark Matter searches?

Not an exhaustive list of course!

An overview of QCD

QCD

Quantum theory of the strong interaction, built from fundamental variables - gauge and fermion fields.

$$\mathcal{L} = \frac{1}{4g^2} G_{\mu\nu}^a G_{\mu\nu}^a + \sum_j \bar{q}_j (i\gamma^\mu D_\mu + m_j) q_j$$

where $G_{\mu\nu}^a \equiv \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + if_{abc} A_\mu^b A_\nu^c$

and $D_\mu \equiv \partial_\mu + it^a A_\mu^a$

That's it!

from F.A. Wilczek

- This doesn't look too bad - a bit like QED which we have a well-developed toolkit to deal with.

CONTINUUM QCD

In fact **QCD** is very different to QED. Strong interactions are

- asymptotically free
- **confining**
- **chirally broken**



- **A Non-perturbative theory:** Observables are not analytic in the QCD coupling.
- Perturbation theory will fail - a non-perturbative regulator needed to study physics at hadronic scales in terms of fundamental fields.

a good regulator will

- make the integral tractable
- regulate the momentum integrals

A lattice discretisation does both!

A CLOSER LOOK AT CONTINUUM QCD

The Lagrangian is given by

$$\mathcal{L} = \bar{\psi}(i\gamma_{\mu}D_{\mu} - m) - \frac{1}{4}F_{\mu\nu}^a F_b^{\mu\nu}$$

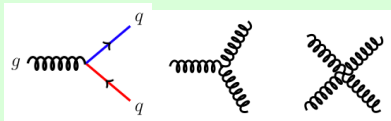
where the gluon field strength is $F_{\mu\nu}^a = \partial_{\mu}A_{\nu}^a - \partial_{\nu}A_{\mu}^a + gf^{abc}A_{\mu}^b A_{\nu}^c$ and the covariant derivatives are $D_{\mu} = \partial_{\mu} - igA_{\mu}^a t^a$.

Quark fields ψ have colour, flavour and spin

$$\psi_{i,f,\alpha} \begin{cases} i & \in \{\text{red, blue, green}\} \\ f & \in \{\text{u, d, s, c, b, t}\} \\ \alpha & 1/2 \end{cases}$$

The gluon fields, A_{μ} live in the adjoint rep of SU(3) colour

There are 8 gluons that also carry colour, selfinteracting



A CLOSER LOOK AT CONTINUUM QCD

$$\mathcal{L} = \bar{\psi} (i\gamma_{\mu} D_{\mu} - m) \psi - \frac{1}{4} F_{\mu\nu}^a F_b^{\mu\nu}$$

Symmetries of the theory include

- SU(3) local gauge symmetry is preserved at each point in spacetime.
- Lorentz, C, P and T, and global flavour
- $\psi \rightarrow e^{i\alpha} \psi$ and in the $m = 0$ limit $\psi \rightarrow e^{i\gamma_5 \alpha} \psi$

Preserve as much of this structure as possible in the lattice theory.

Free parameters in the theory are

- the coupling g between quarks and gluons - dimensionless.
- the quark mass(es) m_q - dimensionful.

If we can solve the theory, everything else is a prediction including hadronic masses e.g. the proton mass, form factors, He binding energy, equations of state (e.g. for a neutron star) ...

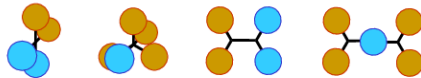
OBJECTS OF INTEREST

● Quark ● AntiQuark

Mesons/Baryons



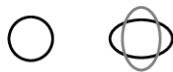
Molecules/Multiquarks



Hybrids



Glueballs



+ Effects due to the complicated QCD vacuum

A CONSTITUENT MODEL

- QCD has fundamental objects: **quarks** (in 6 flavours) and **gluons**
- Fields of the lagrangian are combined in colorless combinations: the mesons and baryons. **Confinement**.

quark model object	structure
meson	$3 \otimes \bar{3} = 1 \oplus 8$
baryon	$3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10$
hybrid	$\bar{3} \otimes 8 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 8 \oplus 10 \oplus 10$
glueball	$8 \otimes 8 = 1 \oplus 8 \oplus 8 \oplus 10 \oplus 10$
⋮	⋮

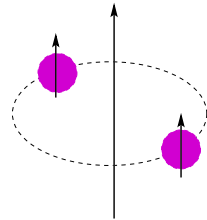
- **This is a model.** QCD does not always respect this constituent picture! There can be strong mixing.

CLASSIFYING STATES: MESONS

- Recall that continuum states are classified by J^{PC} multiplets (representations of the Poincaré symmetry):
 - Recall the naming scheme: $n^{2S+1}L_J$ with $S = \{0, 1\}$ and $L = \{0, 1, \dots\}$
 - J , hadron angular momentum, $|L - S| \leq J \leq |L + S|$
 - $P = (-1)^{(L+1)}$, parity
 - $C = (-1)^{(L+S)}$, charge conjugation. Only for $q\bar{q}$ states of same quark and antiquark flavour. So, not a good quantum number for eg heavy-light mesons ($D_{(s)}$, $B_{(s)}$).

MESONS

- two spin-half fermions $^{2S+1}L_J$
- $S = 0$ for antiparallel quark spins and $S = 1$ for parallel quark spins;



- States in the **natural spin-parity** series have $P = (-1)^J$ then $S = 1$ and $CP = +1$:
 - $J^{PC} = 0^{-+}, 0^{++}, 1^{--}, 1^{+-}, 2^{--}, 2^{-+}, \dots$ allowed
- States with $P = (-1)^J$ but $CP = -1$ forbidden in $q\bar{q}$ model of mesons:
 - $J^{PC} = 0^{+-}, 0^{--}, 1^{-+}, 2^{+-}, 3^{-+}, \dots$ forbidden (by quark model rules)
 - These are **EXOTIC** states: not just a $q\bar{q}$ pair ...

BARYONS

Baryon number $B = 1$: three quarks in colourless combination

- J is half-integer, C not a good quantum number: states classified by J^P
- **spin-statistics**: a baryon wavefunction must be antisymmetric under exchange of any 2 quarks.
- totally antisymmetric combinations of the colour indices of 3 quarks
- the remaining labels: flavour, spin and spatial structure must be in totally symmetric combinations

$$|qqq\rangle_A = |\text{color}\rangle_A \times |\text{space, spin, flavour}\rangle_S$$

With three flavours, the decomposition in flavour is

$$3 \otimes 3 \otimes 3 = 10_S \oplus 8_M \oplus 8_M \oplus 1_A$$

WHY LATTICE QCD ?

- A systematically-improvable non-perturbative formulation of QCD
 - Well-defined theory with the lattice a UV regulator
- Arbitrary precision is in principle possible
 - of course algorithmic and field-theoretic “wrinkles” can make this challenging!
- Starts from first principles - i.e. from the QCD Lagrangian
 - inputs are quark mass(es) and the coupling - can explore mass dependence and coupling dependence but getting to physical values can be hard!
 - in principle can calculate inputs for nuclear many-body calculations with better accuracy than experimental measurements. Starting from nucleon-nucleon phase shifts and on to hyperon-nucleon (YN) etc.

A typical road map

- Develop methods and verify calculations through precision comparison with lattice and with experiment.
- Make predictions - subsequently verified experimentally.
- Make robust, precise calculations of quantities beyond the reach of experiment.

A POTTED HISTORY

- **1974** Lattice QCD formulated by K.G. Wilson
- **1980** Numerical Monte Carlo calculations by M. Creutz
- **1989** “and extraordinary increase in computing power (10^8 is I think not enough) and equally powerful algorithmic advances will be necessary before a full interaction with experiment takes place.” Wilson @ Lattice Conference in Capri.
- **Now** at *100TFlops – 1PFlop*
- Lattice QCD contributes to development of computing **QCDSPP - QCDOC - BlueGene**.

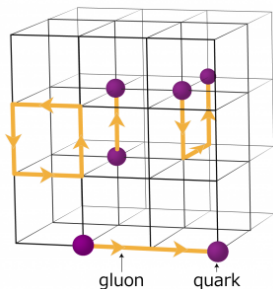


Learning from history ...

better computers help but better ideas are crucial!
that's what we will focus on ...

LIFE ON A LATTICE

- Quark fields $\psi(x)$ live on sites and carry colour, flavour and Dirac indices as in continuum
- Gauge fields are $SU(3)$ matrices: $U_\mu(x)$, $\mu = 0, \dots, 3$.
- Under gauge transformation: $\psi(x) \rightarrow \Lambda(x)\psi(x)$ and $U_\mu(x) \rightarrow \Lambda(x)U_\mu(x)\Lambda(x+a\hat{\mu})^{-1}$



- lattice spacing a a dimensionful parameter, not a parameter of the discrete theory - emerges from the dynamics.

- Continuum and lattice gauge fields:

$A_\mu(x) \rightarrow U(x, \mu) = e^{-iagA_\mu^b(x)t^b}$ and make derivatives gauge invariant e.g

$$\nabla_\mu^{\text{fwd}} \psi(x) = \frac{1}{a} [U_\mu(x)\psi(x+a\hat{\mu}) - \psi(x)]$$

- Gauge invariant quantities are closed loops $\prod_{\mathcal{P}} U_\mu(x)$ and $\bar{\psi}(x)\gamma_\mu U_\mu(x)\psi(x+a\hat{\mu})$

A SIMPLER THEORY

For a first look at discretisation consider $\phi^4(x)$ scalar theory:

$$Z = \int \mathcal{D}\phi e^{-S[\phi]} \quad \text{and} \quad S^{\text{continuum}}[\phi] = \int d^d x \left(\frac{1}{2} (\partial_\mu \phi(x))^2 + \frac{1}{2} m^2 \phi(x)^2 + \frac{\lambda}{4!} \phi(x)^4 \right)$$

Discretising on a regular lattice with spacing a - the scalar fields live on the lattice sites.

- fields: $\phi(x) \rightarrow \phi_n, x = na$
- integrals: $\int dx_i \rightarrow a \sum_{n_i} \int \mathcal{D}\phi \rightarrow \prod_n d\phi_n$
- derivatives: $\partial_\mu \phi(x) \rightarrow \Delta_\mu \phi_n = \frac{1}{a} (\phi_{n+\hat{\mu}} - \phi_n)$ and $\Delta^* \phi_n = \frac{1}{a} (\phi_n - \phi_{n-\hat{\mu}})$

So that

$$S^{\text{lattice}}[\phi] = a^4 \sum_n \left(\frac{1}{2} (\Delta_\mu \phi_n)^2 + \frac{1}{2} m^2 \phi_n^2 + \frac{\lambda}{4!} \phi_n^4 \right) = a^4 \sum_n \left(-\frac{1}{2} \phi_n (\Delta^* \Delta_\mu) \phi_n + \frac{1}{2} m^2 \phi_n^2 + \frac{\lambda}{4!} \phi_n^4 \right)$$

In the functional integral the measure $\mathcal{D}\phi$ involves only lattice points \Rightarrow a discrete set of integration points. If the lattice is finite \Rightarrow finite dimensional integrals.

HOMEWORK EXERCISE

- Derive the expression for the discretised scalar action, checking you get the correct powers of a and coefficients.
- Repeat the steps for a complex scalar field and for a 2-component complex scalar field ie $\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$. This is relevant as a model for the SM Higgs.
- Consider the limit $\lambda \rightarrow \infty$ and show that the scalar action reduces to the Ising model

$$-S = -K \sum_{n,\mu} \phi_n \phi_{n+\mu} \text{ - with } \phi_n = \pm 1.$$

DISCRETISATION - CONSEQUENCES

A field theory defined on a space-time lattice with non-zero lattice spacing has a cut-off in momentum space.

Consider a fourier transformation of (discrete) ϕ using standard definitions

$$\tilde{\phi}(p) = a^4 \sum_x e^{-ipx} \phi(x) \quad \text{and} \quad \phi(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} e^{ipx} \tilde{\phi}(p)$$

Transformed fields are periodic in momentum space and restrict to the first Brillouin zone: $\phi(p) = \phi(p + \frac{2\pi}{a} n_\mu)$, $n_\mu \in \mathbb{Z}$ or $|p_\mu| \leq \pi/a = \Lambda_{\text{cutoff}}$ a UV cutoff.

Field theories regularised in a natural way.

On a finite lattice with $L_{\text{spatial}} = L$ and $L_{\text{temporal}} = T$ the volume is $V = LT$

Then momenta are discretised $p_\mu = \frac{2\pi}{a} \frac{n_\mu}{L}$ and

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

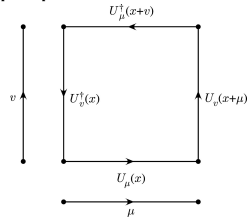
To recover the continuum theory take $L, T \rightarrow \infty$ and $a \rightarrow 0$.

BACK TO QCD: THE DISCRETE GAUGE \mathcal{G} FERMION ACTIONS

Gauge Actions

Recall that $U_\mu(x) = e^{iagA_\mu^b(x)t^b} \in SU(3)$ on the link $(x \rightarrow x + \hat{\mu})$. A parallel transporter of $SU(3)$ colour on links. Then the field strength is represented by “plaquettes”

$$U_{\mu\nu}(x) = U_\nu^\dagger(x) U_\mu^\dagger(x + \hat{\nu}) U_\nu(x + \hat{\mu}) U_\mu(x) = e^{-a^2 F_{\mu\nu}(x)}$$



The simplest (Wilson) gauge action is built from 1×1 plaquettes

$$S_g = \sum_x \sum_{1 \leq \mu < \nu \leq 4} \beta \left\{ 1 - \frac{1}{3} \text{ReTr}(U_{\mu\nu}(x)) \right\} = -\frac{\beta}{12} \sum_{x\mu\nu} a^4 \text{Tr} F_{\mu\nu}(x) F_{\mu\nu}(x) + \mathcal{O}(a^5)$$

where $\beta = 6/g^2$. The $1/3$ comes from assuming $N_c = 3$ and can be generalised.

Exercises

- Check this reproduces the continuum limit ($a \rightarrow 0$)
- Try to write down an action including 1×2 planar loops

DISCRETE FERMION ACTIONS

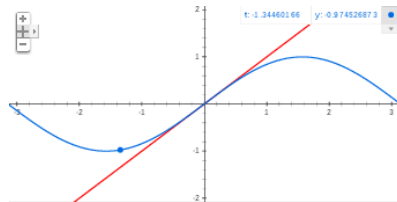
The “naive” fermion action is

$$S_f = a^4 \sum_{x,\mu} \left(\bar{\psi}(x) \gamma_\mu \left(\nabla_\mu^* + \nabla_\mu \right) \psi(x) + m \bar{\psi}(x) \psi(x) \right) = a^4 \int_p \bar{\psi}(-p) \left[\frac{i}{a} \sin(p_\mu a) \gamma_\mu + m \right] \psi(p)$$

Where discretisation replaces $p_\mu \rightarrow \sin(p_\mu a)/a$.

Why is it naive?

- Very different at edges of the Brillouin zone!
- Naive fermions - tried to describe 1 particle but got 16.
- Now what?



FERMION DOUBLING AND A NO-GO THEOREM

Nilsen-Ninomiya no-go

Cannot construct a lattice fermion action that

- has the correct continuum limit
- is ultra-local
- is undoubled
- is chirally symmetric

Note that there is no unique (or even “best”) choice for discretisation. Choose the scheme that preserves the physics of interest or has important properties e.g. discretisation errors or that you can afford!

CHOOSE YOUR POISON AKA NO FREE LUNCH THEOREM!

ACTION

improved Wilson

twisted mass

staggered

domain wall

overlap

ADVANTAGES

computationally fast

computationally fast
automatic improvement

computationally fast

improved chiral symmetry

exact chiral symmetry

DISADVANTAGES

breaks chiral symmetry
needs operator improvement

breaks chiral symmetry
violations of isospin

fourth root

complicated contractions

computationally demanding

needs tuning

computationally expensive

All actions should be $\mathcal{O}(a)$ -improved $\Rightarrow \langle O_{\text{phys}}^{\text{latt}} \rangle = \langle O_{\text{cont}}^{\text{latt}} \rangle + \mathcal{O}(a^2)$

Path integrals and correlation functions

SOLVING QCD

Recall we want to calculate properties of physical observables from \mathcal{L} .

In continuum QCD the Feynman Path Integral is

$$\mathcal{Z} = \int DA_\mu D\psi D\bar{\psi} e^{iS_{\text{QCD}}}, \quad S_{\text{QCD}} = \int d^4x \mathcal{L}_{\text{QCD}}$$

Observables \mathcal{O} , determined from

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int DA_\mu D\psi D\bar{\psi} \mathcal{O} e^{iS_{\text{QCD}}}$$

In discrete (finite-size lattice) theory do this integral numerically. **How?**

First idea: quadrature. A $32^3 \times 64$ lattice means $4 \times 32^3 \times 64 \times 8 = 67, 108, 864$ variables!

Better idea: statistical methods. Importance Sampling is a crucial idea - motivates the last step in our set up - Wick rotation.

$$\mathcal{Z} = \int DA_\mu D\psi D\bar{\psi} e^{iS_{\text{QCD}}} \xrightarrow{t \rightarrow i\tau} \mathcal{Z}_E = \int DA_\mu D\psi D\bar{\psi} e^{-S_{\text{QCD}}}$$

FIELD THEORY ON A EUCLIDEAN LATTICE



- Monte Carlo simulations are only practical using **importance sampling**
- Need a non-negative weight for each field configuration on the lattice

Minkowski → Euclidean

- **Benefit:** can isolate lightest states in the spectrum (as we will see!).
- **Problem:** direct information on scattering is lost and must be inferred indirectly.
- To access radial and orbital excitations and resonances need a **variational method**.

CORRELATORS IN A LATTICE EUCLIDEAN FIELD THEORY (EFT) I

- In lattice EFT physical observables \mathcal{O} is determined from

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\Psi \mathcal{D}\bar{\Psi} \mathcal{O} e^{-S_{QCD}}$$

- Analytically integrate Grassman fields $(\Psi, \bar{\Psi}) \rightarrow$ factors of $\det M$ the fermion mx.

$$\langle \mathcal{O} \rangle \stackrel{N_f=2}{=} \frac{1}{Z} \int \mathcal{D}U \det M^2 \mathcal{O} e^{-S_G}$$

The expectation value is calculated by importance sampling of gauge fields and averaging over ensembles.

- Simulate N_{cfg} samples of the field configuration, then

$$\langle \mathcal{O} \rangle = \lim_{N_{cfg} \rightarrow \infty} \frac{1}{N_{cfg}} \sum_{i=1}^{N_{cfg}} \mathcal{O}_i[U_i]$$

- At N_{cfg} finite correlation functions have a (improvable!) statistical uncertainty $\sim 1/\sqrt{N_{cfg}}$.
- Calculating $\det M$ for M a large, sparse matrix with small eigenvalues takes $> 80\%$ of compute cycles in configuration generation. $\det M = 1$ is the quenched approximation.

CORRELATORS IN LATTICE EFT II

- We are interested in **two-point correlation functions** built from **interpolating operators** (functions of Ψ):
 - Eg the local meson operator $\mathcal{O}(x) = \bar{\Psi}_a(x)\Gamma\Psi_b(x)$
 - Γ an element of the Dirac algebra with possible displacements; a and b flavour indices
- The two-point function is then

$$C(t) = \langle \mathcal{O}(x)\mathcal{O}^\dagger(0) \rangle = \langle \bar{\Psi}_a(x)\Gamma\Psi_b(x)\bar{\Psi}_b(0)\Gamma^\dagger\Psi_a(0) \rangle$$

where $x \equiv (t, \mathbf{x}); t \geq 0$

- Using **Wick's theorem** to contract quark fields replaces fields \rightarrow quark propagators

$$C(t, \mathbf{x}) = -\langle \text{Tr}(M_a^{-1}(0, x)\Gamma M_b^{-1}(x, 0)\Gamma^\dagger) \rangle + \delta_{ab}\langle \text{Tr}(\Gamma M_a^{-1}(x, x))\text{Tr}(\Gamma^\dagger M_a^{-1}(0, 0)) \rangle$$

where the trace is over spin and colour.

- For **flavour non-singlets** ($a \neq b$) this leads to

$$C(t, \mathbf{x}) = \langle \text{Tr}(\gamma_5 M_a^{-1}(x, 0)^\dagger \gamma_5 \Gamma M_b^{-1}(x, 0)\Gamma^\dagger) \rangle$$

- We consider the correlation function in momentum space at zero momentum

$$C(\vec{p}, t) = \int d^3x e^{i\vec{p}\cdot\vec{x}} C(\vec{x}, t, 0, 0) \text{ and } C(0, t) = C(t) \sim \sum_{\vec{x}} C(\vec{x}, t, 0, 0)$$

ASIDE ON WICK'S THEOREM

We used Wick's theorem to contract quark fields and replace with propagators ...



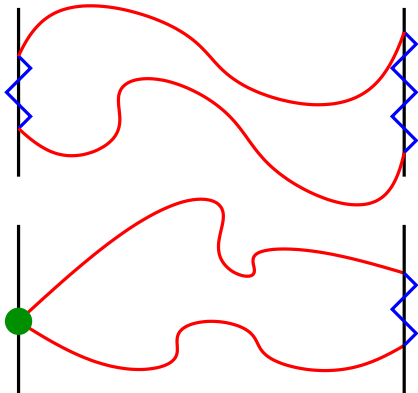
- Example — four field insertions: $\langle \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \rangle$
- the pairwise contraction can be done in two ways:
 $\psi_i \bar{\psi}_j \psi_k \bar{\psi}_l$ and $\psi_i \bar{\psi}_j \psi_k \bar{\psi}_l$
- giving the propagator combination
 $M_{ij}^{-1} M_{kl}^{-1} - M_{jk}^{-1} M_{il}^{-1}$
- minus-sign from the anti-commutation in second term.
- More fields means more combinations. Important in (eg.) isoscalar meson spectroscopy. **We will see this again later**

NOTES

- Fermions in lagrangian → **fermion determinant**
- Fermions in measurement → **propagators**
- The integral over gauge fields is done using **importance sampling**.
- γ_5 hermiticity: $M^{-1}(x, y) = \gamma_5 M^{-1}(y, x)^\dagger \gamma_5$ allows us to rewrite the correlator in terms of propagators from origin to all sites. **Point (to-all) propagators**
- practically: $M(x, 0 : U)^{-1}$ compute a single column (in space-time indices) with linear solvers
- for flavour singlets $a = b$ terms like $M^{-1}(x, x)$ - requires the inverse of the **full** fermion M on each config. **More on this later**

Come back later to the costs in a lattice calculation

PROPAGATOR CARTOON

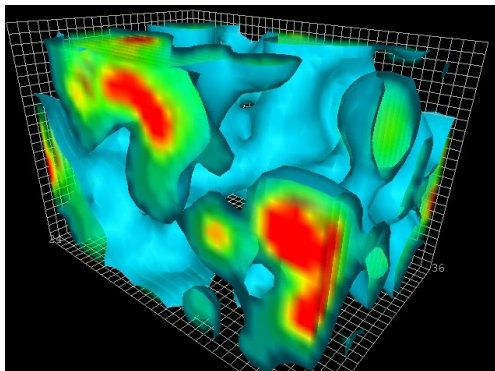


The most general operator.

A restricted correlation function accessible to one point-to-all computation.

Saves compute time but doesn't use all information in the correlator. Precludes disconnected contributions ie flavour singlets.

TYPICALLY SIZE OF A LATTICE CALCULATION



[from D.Leinweber]

There are 2 compute intensive steps:

1. Generating Configurations - snapshots of the QCD vacuum

Volume: $32^3 \times 256$ (sites) $U_\mu(x)$ defined by $4 \times 8 \times 32^3 \times 256$ real numbers

2. Quark Propagation

Volume: $32^3 \times 256$ (sites) $\rightarrow M$ is a 100 million x 100 million sparse matrix with complex entries.

Solving QCD requires supercomputing resources worldwide.



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