Introduction to Lattice QCD

C. Alexandrou
University of Cyprus, The Cyprus Institute and DESY-Zeuthen

Bibliography

1. J. W. Negele, *QCD and Hadrons on a lattice*, NATO ASI Series B: Physics vol. 228, 369, eds. D. Vautherin, F. Lenz and J.W. Negele.
2. M. Lüscher, *Advanced Lattice QCD*, Les Houches Summer School in Theoretical Physics, Session 68: Probing the Standard Model of Particle Interactions, Les Houches 1997, 229, hep-lat/9802029.
3. R. Gupta, *Introduction to Lattice QCD*, hep-lat/9807028.
4. P. Lepage, *Lattice for Novices*, hep-lat/0506036.
5. H. Wittig, Lecture week, SFB/TR16, 3-7 Aug. 2009, Bonn.
6. H. J. Rothe, *Quantum Gauge Theories: An introduction*, World Scientific, 1997.
7. I. Montvay and G. Münster, *Quantum Fields on a Lattice*, Cambridge University Press, 1994.
8. C.Gattringer and C. B. Lange, *Quantum Chromodynamics on the Lattice - An Introductory Presentation*, Springer, 2009.

Outline

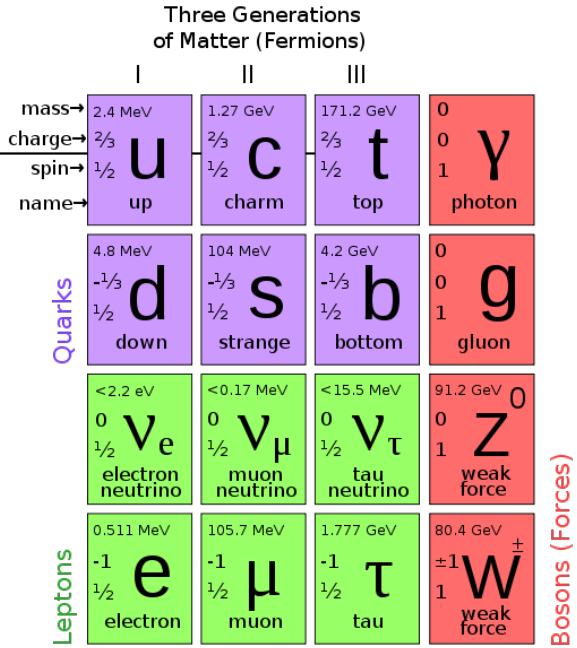
Standard model

The Standard Model (SM) is a synthesis of three of the four forces of nature described by gauge theories with coupling constants:

- Strong Interactions: $\alpha_s \sim 1$
- Electromagnetic interactions: $\alpha_{em} \approx 1/137$
- Weak interactions: $G_F \approx 10^{-5}\ GeV^{-2}$.

Basic constituents of matter:

- Six quarks, $u,\ d,\ s,\ c,\ b,\ t$, each in 3 colors, and six leptons $e,\ \nu_e,\ \mu,\ \nu_\mu,\ \tau,\ \nu_\tau$
- The quarks and leptons are classified into 3 generations of families.
- The interactions between the particles are mediated by vector bosons: the 8 gluons mediate strong interactions, the $W^\pm$ and Z mediate weak interactions, and the electromagnetic interactions are carried by the photon γ.
- The weak bosons acquire a mass through the Higgs mechanism.
- The SM is a local gauge field theory with the gauge group $SU(3) \times SU(2) \times U(1)$ specifying the interactions among these constituents.



Masses in the Standard Model

Parameters	Number	Comments
Masses of quarks	6	$u,\ d,\ s$ light $c,\ b$ heavy $t = 175 \pm 6\ GeV$
Masses of leptons	6	$e,\ \mu,\ \tau$ $M_{\nu_e,\ \nu_\mu,\ \nu_\tau}$ non-zero
Mass of $W^\pm$	1	80.3 GeV
Mass of Z	1	91.2 GeV
Mass of gluons, γ		0 (Gauge symmetry)
Mass of Higgs	1	$125.03^{+0.26}_{-0.27}\ (\text{stat})^{+0.13}_{-0.15}\ (\text{sys})$ GeV discovered at LHC, 2012

QCD – Gauge theory of the strong interaction

- Lagrangian: formulated in terms of quarks and gluons

$$\mathcal{L}_{\rm QCD} = -\tfrac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} + \sum_f \overline{\psi}_f \left(i\gamma^\mu D_\mu - m_f\right) \psi_f, \quad f = u, d, s, c, b, t$$

$$D_\mu = \partial_\mu - ig(\tfrac{1}{2}\lambda^a) A^a_\mu$$

Harald Fritzsch

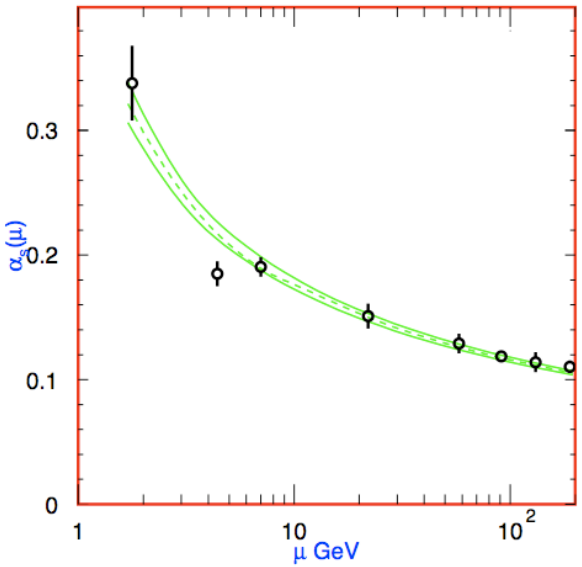
Murray Gell-Mann

Heinrich Leutwyler

Phys.Lett. B47 (1973) 365

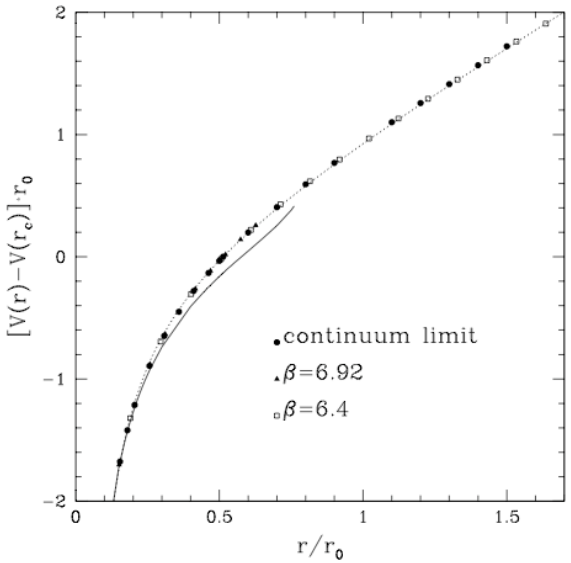
Properties of QCD

Asymptotic freedom: $g(\mu)$



[Yao et al., PDG 2006]

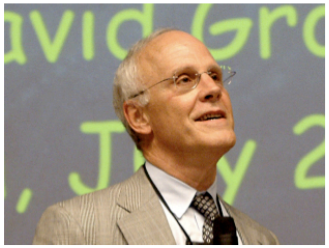
Confinement



[Necco & Sommer, Nucl Phys B622 (2002) 328]

Nobel Prize in Physics 2004

"...for the discovery of asymptotic freedom in the theory of the strong interaction"



David Gross

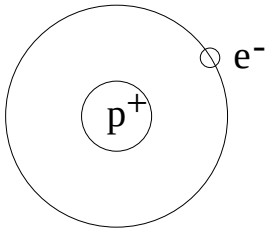
Frank Wilczek

David Politzer

QCD versus QED

- QCD is the theory of strong interactions formulated in terms of quarks and gluons as the basic degrees of freedom of hadronic matter.
- Conventional perturbative approach cannot be applied for hadronic process at scales $\lesssim 1$ GeV since the strong coupling constant $\alpha_s \sim 1$
  $\Longrightarrow$ we cannot calculate the masses of mesons and baryons from QCD even if we are given α_s and the masses of quarks.
- Bound state in QCD very different from QED e.g. the binding energy of a hydrogen atom is to a good approximation the sum of it constituent masses. Similarly for nuclei the binding energy is $\mathcal{O}(\mathrm{MeV})$. For the proton almost all the mass is attributed to the strong non-linear interactions of the gluons.

QED



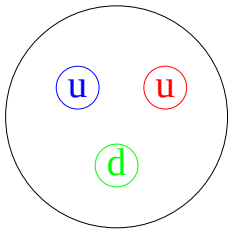
$M_e = 0.5$ MeV

$M_p = 938$ MeV

$E_{binding} = 13.6$ eV

Hydrogen Atom (EM force)

QCD



$M_u \sim 3$ MeV

$M_d \sim 6$ MeV

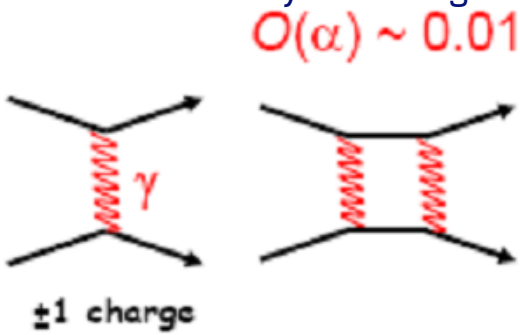
$M_p = 938$ MeV

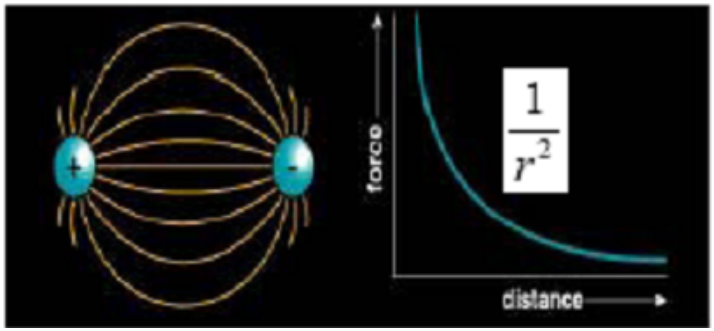
Proton (Strong force)

QCD versus QED

Quantum Electrodynamics (QED): The interaction is due to the exchange of photons. Every time there is an exchange of a photon there is a correction in the interaction of the order of 0.01.

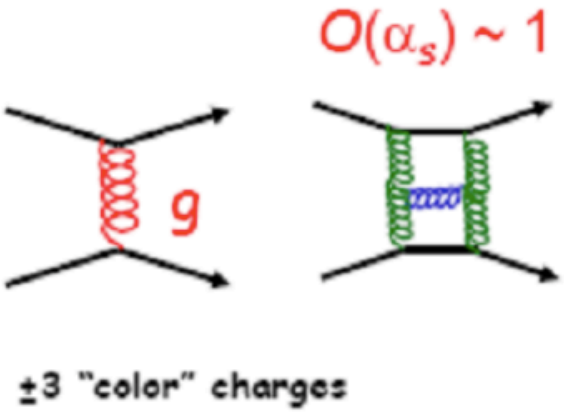
→ we can apply perturbation theory reaching whatever accuracy we like

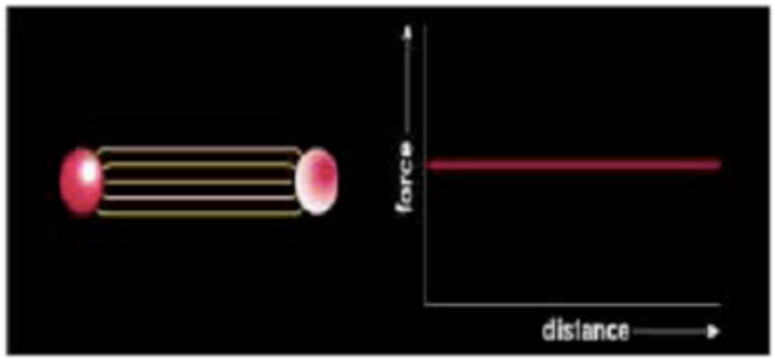




QCD: Interaction due to exchange of gluons. In the energy range of ~ 1GeV the coupling constant is ~1

→ We can no longer use perturbation theory





QCD on the lattice

Why Lattice QCD?

- Discrete space-time lattice acts as a non-perturbative regularization scheme with the lattice spacing a providing an ultraviolet cutoff at $\pi/a \rightarrow$ no infinities. Furthermore, renormalized physical quantities have a finite well behaved limit as $a \rightarrow 0$.
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems. These simulations allow us to calculate correlation functions of hadronic operators and matrix elements of any operator between hadronic states in terms of the fundamental quark and gluon degrees of freedom.

Like continuum QCD lattice QCD has as unknown input parameters the coupling constant α_s and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).
$\Longrightarrow$Lattice QCD provides a well-defined approach to calculate observables non-perturbative starting directly from the QCD Langragian.

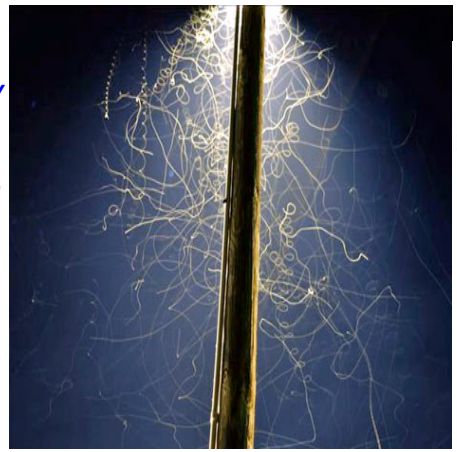
QCD on the lattice

Why Lattice QCD?

- Discrete space-time lattice acts as a non-perturbative regularization scheme with the lattice spacing a providing an ultraviolet cutoff at $\pi/a \rightarrow$ no infinities. Furthermore, renormalized physical quantities have a finite well behaved limit as $a \rightarrow 0$.
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems. These simulations allow us to calculate correlation functions of hadronic operators and matrix elements of any operator between hadronic states in terms of the fundamental quark and gluon degrees of freedom.

Like continuum QCD lattice QCD has as unknown input parameters the coupling constant α_s and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).
$\Longrightarrow$Lattice QCD provides a well-defined approach to calculate observables non-perturbative starting directly from the QCD Langragian.

Walking down the street one night, someone found Nasruddin crawling on his hands and knees under a lamp post near his own front door..
Nasruddin, what's wrong? What are you doing here?
Looking for my house key. I can't get in until I find it..
Oh? Let me help you.
The friend joined Nasruddin in the search, and together they combed all the area under the lamp, but could find nothing.
That's strange, Nasruddin. It's just not here. Are you sure this is where you dropped it?
Here? No, of course not. I dropped the key over there in the shadows by the door.
But - Nasruddin, if you lost the key there, why are you looking here under the lamp?
Well, it's very simple. Over there it's so dark I can't see a thing, and here it's as bright as day!



Path Integrals-An overview

Path integrals in one-dimensional quantum mechanics

Time evolution of a quantum mechanical system:

$$|\psi(t_f)\rangle = e^{-iH(t_f-t_i)}\,|\psi(t_i)\rangle \text{ , where } H \text{ is the Hamiltonian and } \hbar \text{ is set to one.}$$

Evolution of a quantum position eigenstate $|x_i\rangle$ from time t_i to time t_f:

$$\langle x_f, t_f |\, x_i, t_i\rangle = \langle x_f |\, e^{-iH(t_f-t_i)}\,|x_i\rangle$$

Break $t \equiv t_f - t_i$ into a large number N of time slices separated by $\Delta t = (t_f - t_i)/N$:

$$e^{-iHt} = e^{-iH\Delta t}\int dx_{N-1}\,|x_{N-1}\rangle\langle x_{N-1}|\,e^{-iH\Delta t}\int dx_{N-2}\,|x_{N-2}\rangle\langle x_{N-2}|\cdots e^{-iH\Delta t}$$

$$\langle x_{k+1}|\,e^{-i\Delta t\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}\,|x_k\rangle \overset{\Delta t\to 0}{\sim} \int\frac{dp}{2\pi}\langle x_{k+1}|\,p\rangle e^{-i\Delta t\frac{p^2}{2m}}e^{-i\Delta t V(x_k)}\langle p\,|x_k\rangle$$

$$\sim \int\frac{dp}{2\pi}e^{ip(x_{k+1}-x_k)-i\Delta t\,\frac{p^2}{2m}-i\Delta t\,V(x_k)} = \sqrt{\frac{2m\pi}{\Delta t}}\,e^{i\Delta t\left[\frac{m}{2}\left(\frac{(x_{k+1}-x_k)}{\Delta t}\right)^2-V(x_k)\right]}+\mathcal{O}(\Delta t^2)$$

$$\langle x_f|\,e^{-iH(t_f-t_i)}\,|x_i\rangle = \int\mathcal{D}(x_1,\cdots,x_{N-1})e^{i\Delta t\sum_k\left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2-V(x_k)\right]}$$

$$\to \int_{x(0)=x_i}^{x(t)=x_f}\mathcal{D}[x(t)]e^{iS_{\text{classical}}[x(t)]}$$

i.e. the evolution operator is the sum over all paths weighted by the exponential of the classical action.

Path integrals in one-dimensional quantum mechanics

Time evolution of a quantum mechanical system:

$$|\psi(t_f)\rangle = e^{-iH(t_f-t_i)}\,|\psi(t_i)\rangle \text{ , where } H \text{ is the Hamiltonian and } \hbar \text{ is set to one.}$$

Evolution of a quantum position eigenstate $|x_i\rangle$ from time t_i to time t_f:

$$\langle x_f, t_f | x_i, t_i\rangle = \langle x_f | e^{-iH(t_f-t_i)} | x_i\rangle$$

Break $t \equiv t_f - t_i$ into a large number N of time slices separated by $\Delta t = (t_f - t_i)/N$:

$$e^{-iHt} = e^{-iH\Delta t}\int dx_{N-1}\,|x_{N-1}\rangle\langle x_{N-1}|\,e^{-iH\Delta t}\int dx_{N-2}\,|x_{N-2}\rangle\langle x_{N-2}|\cdots e^{-iH\Delta t}$$

$$\langle x_{k+1}|\,e^{-i\Delta t\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}\,|x_k\rangle \overset{\Delta t\to 0}{\sim} \int\frac{dp}{2\pi}\,\langle x_{k+1}|\,p\rangle e^{-i\Delta t\frac{p^2}{2m}}e^{-i\Delta t V(x_k)}\langle p\,|x_k\rangle$$

$$\sim \int\frac{dp}{2\pi}e^{ip(x_{k+1}-x_k)-i\Delta t\,\frac{p^2}{2m}-i\Delta t\,V(x_k)} = \sqrt{\frac{2m\pi}{\Delta t}}\,e^{i\Delta t\left[\frac{m}{2}\left(\frac{(x_{k+1}-x_k)}{\Delta t}\right)^2-V(x_k)\right]}+\mathcal{O}(\Delta t^2)$$

$$\begin{aligned}\langle x_f|\,e^{-iH(t_f-t_i)}\,|x_i\rangle &= \int\mathcal{D}(x_1,\cdots,x_{N-1})e^{i\Delta t\sum_k\left[\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2-V(x_k)\right]}\\ &\to \int_{x(0)=x_i}^{x(t)=x_f}\mathcal{D}[x(t)]e^{iS_{\text{classical}}[x(t)]}\end{aligned}$$

i.e. the evolution operator is the sum over all paths weighted by the exponential of the classical action.

Many degrees of freedom:

$$\left\langle x_f^1, \cdots, x_f^N \right| e^{-iH(t_f - t_i)} \left| x_i^1, \cdots, x_i^N \right\rangle \int_{x^1(0)=x_i^1, \cdots, x^N(0)=x_i^N}^{x^1(t)=x_f^1, \cdots, x^N(t)=x_f^N} \mathcal{D}[x^1(t), \cdots, x^N(t)] e^{iS_{\text{classical}}[x^1(t), \cdots, x^N(t)]}$$

Time-ordered product

$$\begin{aligned} \hat{T}\mathcal{O}(t_1)\mathcal{O}(t_2)e^{-iHt} &= e^{-iH(t_f - t_2)}\mathcal{O}(t_2)e^{-iH(t_2 - t_1)}\mathcal{O}(t_1)e^{-iH(t_1 - t_i)} \\ &\to \int \mathcal{D}[x(t)]\, O(x(t_1))\, O(x(t_2))\, e^{iS_{cl}[x(t)]} \end{aligned}$$

i.e. we automatically get the time-ordered product.

Classical limit

Include $\hbar$ in the expressions and consider $\hbar \to 0$

$$\int \mathcal{D}[x(t)]\, e^{iS_{\text{cl}}[x(t)]/\hbar} \overset{\text{SPA}}{\to} e^{iS_{cl}[x_{cl}(t)]/\hbar} \left(det \left(m\frac{d^2}{dt^2} + V''(x) \right) \right)^{-1/2} + \mathcal{O}(\hbar)$$

i.e. the leading correction are quadratic fluctuations around the classical path.

Many degrees of freedom:

$$\left\langle x_f^1, \cdots, x_f^N \right| e^{-iH(t_f - t_i)} \left| x_i^1, \cdots, x_i^N \right\rangle \int_{x^1(0)=x_i^1, \cdots, x^N(0)=x_i^N}^{x^1(t)=x_f^1, \cdots, x^N(t)=x_f^N} \mathcal{D}[x^1(t), \cdots, x^N(t)] e^{iS_{\text{classical}}[x^1(t), \cdots, x^N(t)]}$$

Time-ordered product

$$\begin{aligned} \hat{T}\mathcal{O}(t_1)\mathcal{O}(t_2)e^{-iHt} &= e^{-iH(t_f - t_2)}\mathcal{O}(t_2)e^{-iH(t_2 - t_1)}\mathcal{O}(t_1)e^{-iH(t_1 - t_i)} \\ &\to \int \mathcal{D}[x(t)]\, O(x(t_1))\, O(x(t_2))\, e^{iS_{cl}[x(t)]} \end{aligned}$$

i.e. we automatically get the time-ordered product.

Classical limit
Include $\hbar$ in the expressions and consider $\hbar \to 0$

$$\int \mathcal{D}[x(t)]\, e^{iS_{\text{cl}}[x(t)]/\hbar} \overset{\text{SPA}}{\to} e^{iS_{cl}[x_{cl}(t)]/\hbar} \left(det \left(m\frac{d^2}{dt^2} + V''(x) \right) \right)^{-1/2} + \mathcal{O}(\hbar)$$

i.e. the leading correction are quadratic fluctuations around the classical path.

Rotation to Euclidean time

Under Wick rotation

$$\begin{aligned} x_0 &\equiv t \to -ix_4 \equiv -i\tau \,, \\ p_0 &\equiv E \to ip_4 \,. \end{aligned}$$

The Euclidean convention is

$$\begin{aligned} x_E^2 &= \sum_{i=1}^{4} x_i^2 = \vec{x}^{\,2} - t^2 = -x_M^2 \,, \\ p_E^2 &= \sum_{i=1}^{4} p_i^2 = \vec{p}^{\,2} - E^2 = -p_M^2 \,. \end{aligned}$$

$$e^{-\tau H} \to \int \mathcal{D}[x_1, \cdots, x_{N-1}] e^{-\Delta\tau \sum_k \left[\frac{m}{2} \left(\frac{x_k - x_{k-1}}{\Delta\tau} \right)^2 + V(x_{k-1}) \right]}$$

i.e. the Lagrangian is effectively replaced by the Hamiltonian in the exponent

- Euclidean path purely real
- Similar to statistical mechanics: $Z = Tre^{-\tau H} = \int dx \, \langle x | \, e^{-H\tau} \, | x \rangle = \int \mathcal{D}(x_1, \cdots, x_N) e^{-S(x_1, \cdots, x_N)}$

$$S[x] \equiv \int_{\tau_i}^{\tau_f} d\tau \, L(x, \dot{x}) \equiv \int_{\tau_i}^{\tau_f} dt \, \left[\frac{m \, \dot{x}(\tau)^2}{2} + V(x(\tau)) \right] ,$$

$\Longrightarrow$ forms the basis of numerical simulations

Low lying spectrum

Setting

$$x_{\rm i} = x_{\rm f} \equiv x \qquad\qquad t_{\rm f} - t_{\rm i} \equiv t = \tau$$

the propagator is written as

$$\langle x|\, {\rm e}^{-Ht}\, |x\rangle = \sum_n \langle x|\ \psi_n\rangle\, {\rm e}^{-E_n t}\, \langle \psi_n|\ x\rangle$$

where $|\psi_n\rangle$ is the energy eigenstate with eigenvalue E_n. The sum is dominated by the lowest-energy states when T is large, because of the exponentials, and in the limit of very large T only the groundstate, $|\psi_0\rangle$, contributes:

$$\langle x|\, {\rm e}^{-Ht}\, |x\rangle \ \stackrel{t\to\infty}{\longrightarrow}\ {\rm e}^{-E_0 t}\ |\langle x|\ \psi_0\rangle|^2\ .$$

We extract the groundstate energy E_0 by integrating over x,

$$\int dx\ \langle x|\, {\rm e}^{-Ht}\, |x\rangle \ \stackrel{t\to\infty}{\longrightarrow}\ {\rm e}^{-E_0 t},$$

and then, going back to the previous equation, we determine the groundstate wave-function $\psi_{E_0}(x) \equiv \langle x|\ E_0\rangle$.

Numerical evaluation

Develop a numerical procedure for evaluating the propagator using a path integral in its discrete version

$$t_j = t_i + j\,\Delta t \qquad \text{for } j = 0, 1 \ldots N\,\Delta t = t$$

$\rightarrow x = \{x(t_0), x(t_1) \ldots x(t_N)\}$: refer to such a path as a "configuration".
Integral over all paths becomes an ordinary integral over all possible values for each of the $x(t_j)$'s:

$$\int \mathcal{D}x(t) \rightarrow A \int_{-\infty}^{\infty} dx_1\, dx_2 \ldots dx_{N-1}, \quad x_j \equiv x(t_j)\,, \quad A = \left(\frac{2\pi m}{\Delta t}\right)^{N/2}$$

We don't integrate over the endpoints since they are held fixed; for example, in the Tre^{-tH} the boundary conditions are: $x_0 = x_N = x$.
$\Longrightarrow$ we have reduce Quantum Mechanics to a problem in numerical integration.
Comment: $\frac{(x_j - x_{j-1})}{\Delta t}$ can be arbitrarily large in our path integral; i.e. paths can be arbitrarily rough. While not so important for our one-dimensional problem, this becomes a crucial issue for four-dimensional field theories. It is dealt with using renormalization theory.

Evaluation of excited states

To analyze excited states using path integrals, we interrupt the propagation of the groundstate by introducing new operators at intermediate times. Consider, for example,

$$\langle x(t_2)x(t_1)\rangle \equiv \frac{1}{Z}\mathrm{Tr}\hat{x}(t_2)\hat{x}(t_1)\, e^{-H(t_f-t_i)} = \frac{\int \mathcal{D}x(t)\, x(t_2)x(t_1)\, \mathrm{e}^{-S[x]}}{\int \mathcal{D}x(t)\, \mathrm{e}^{-S[x]}}\,, \quad t_2 > t_1$$

with $x_\mathrm{i} = x_\mathrm{f} = x$.
The numerator on the right-hand side equals

$$\int dx\ \langle x|\, \mathrm{e}^{-H(t_\mathrm{f}-t_2)}\, \hat{x}\, \mathrm{e}^{-H(t_2-t_1)}\, \hat{x}\, \mathrm{e}^{-H(t_1-t_\mathrm{i})}\, |x\rangle\,.$$

Setting $T = t_\mathrm{f} - t_\mathrm{i}$ and $t = t_2 - t_1$ we can rewrite the full expression as

$$\langle \hat{x}(t_2)\hat{x}(t_1)\rangle = \frac{1}{Z}\sum_n \langle\psi_n|\, e^{Ht_2}\hat{x}e^{-Ht_2}\, e^{Ht_1}\hat{x}e^{-Ht_1}\, e^{-HT}\, |\psi_n\rangle = \frac{\sum_n \mathrm{e}^{-E_nT}\, \langle\psi_n|\, \hat{x}\, \mathrm{e}^{-(H-E_n)t}\, \hat{x}\, |\psi_n\rangle}{\sum \mathrm{e}^{-E_nT}}.$$

If $T \gg t$ and large, then the groundstate $|\psi_0\rangle$ dominates:

$$G(t) \equiv \langle x(t_2)x(t_1)\rangle \to \sum_m \langle\psi_0|\, \hat{x}\, |\psi_m\rangle\, \langle\psi_m|\, \mathrm{e}^{-(H-E_0)t}\, \hat{x}\, |\psi_0\rangle\,.$$

In our harmonic oscillator example, the state propagating between the two x's cannot be $|\psi_0\rangle$ since x switches the parity of the state. Thus if we now make t large (but still $\ll T$)

$$G(t) \overset{t\ \text{large}}{\longrightarrow} |\langle\psi_0|\, x\, |\psi_1\rangle|^2\ \mathrm{e}^{-(E_1-E_0)t}$$

where $|\psi_1\rangle$ is the first excited state. Consequently we can extract the first excitation energy from the large-t dependence of $G(t)$,

$$\log\left(\frac{G(t)}{G(t+a)}\right) \to (E_1 - E_0)a,$$

and then, going back to $G(t)$, we can determine the quantum mechanical transition matrix element $\langle\psi_0|\, x\, |\psi_1\rangle$.

Monte Carlo averages

Here we focus on the zero-temperature limit of large T.
For an arbitrary functional $\Gamma[x]$ employ a Monte Carlo procedure:

$$\langle \Gamma[x] \rangle = \frac{\int \mathcal{D}x(t)\, \Gamma[x]\, \mathrm{e}^{-S[x]}}{\int \mathcal{D}x(t)\, \mathrm{e}^{-S[x]}},$$

is a weighted average over paths with weight $\exp(-S[x])$. We generate a large number, N_{cf}, of random paths or configurations,

$$x^{(\alpha)} \equiv \{x_0^{(\alpha)} x_1^{(\alpha)} \ldots x_{N-1}^{(\alpha)}\} \qquad \alpha = 1, 2 \ldots, N_{cf},$$

on our grid in such a way that the probability $P[x^{(\alpha)}]$ for obtaining any particular path $x^{(\alpha)}$ is

$$P[x^{(\alpha)}] \propto \mathrm{e}^{-S[x^{(\alpha)}]}.$$

Then an unweighted average of $\Gamma[x]$ over this set of paths approximates the weighted average over uniformly distributed paths:

$$\langle \Gamma[x] \rangle \approx \overline{\Gamma} \equiv \frac{1}{N_{cf}} \sum_{\alpha=1}^{N_{cf}} \Gamma[x^{(\alpha)}].$$

$\overline{\Gamma}$ is our "Monte Carlo estimator" for $\langle \Gamma[x] \rangle$ on our lattice.
The Monte Carlo uncertainty $\sigma_{\overline{\Gamma}}$ in our estimate is a potential source of error; it is estimated in the usual fashion:

$$\sigma^2_{\overline{\Gamma}} \approx \frac{1}{N_{cf}} \left\{ \frac{1}{N_{cf}} \sum_{\alpha=1}^{N_{cf}} \Gamma^2[x^{(\alpha)}] - \overline{\Gamma}^2 \right\}.$$

This becomes

$$\sigma^2_{\overline{\Gamma}} = \frac{\langle \Gamma^2 \rangle - \langle \Gamma \rangle^2}{N_{cf}} \text{ for large } N_{cf}.$$

The statistical uncertainties vanish as $1/\sqrt{N_{cf}}$ when N_{cf} increases.

Metropolis Algorithm

We need an algorithm to to create our set of random paths $x^{(\alpha)}$ with probability $\frac{e^{-S[x]}}{Z}$, where $Z = \int \mathcal{D}[x(t)] e^{-S[x]}$.
$\Longrightarrow$ a simple procedure, though not always the best, is the Metropolis Algorithm:

- Start with an arbitrary path $x^{(0)}$
- Modify by visiting each of the sites on the lattice, and randomizing the x_j's at those sites, one at a time, in a particular fashion as described below $\rightarrow$ generate a new random path from the old one: $x^{(0)} \rightarrow x^{(1)}$. This is called "updating" the path.
- Apply to $x^{(1)}$ to generate path $x^{(2)}$, and so on until we have N_{cf} random paths.

The algorithm for randomizing x_j at the j^{th} site is:

- Generate a random number $-\epsilon < \zeta \leq \epsilon$, with uniform probability;
- Let $x_j \rightarrow x_j + \zeta$ and compute the change ΔS in the action;
- If $\Delta S < 0$ retain the new value for x_j, and proceed to the next site;
- If $\Delta S > 0$ accept change with probability $\exp(-\Delta S)$ i.e. generate a random number η uniformly distributed between 0 and 1; retain the new value for x_j if $\exp(-\Delta S) > \eta$, otherwise restore the old value; proceed to the next site.

Comments:

- Choice of ϵ: should be tuned so that 40%–60% of the x_j's are changed on each pass (or "sweep") through the lattice. Then ϵ is of order the typical quantum fluctuations expected in the theory. Whatever the ϵ, successive paths are going to be quite similar and so contain rather similar information about the theory. Thus when we accumulate random paths $x^{(\alpha)}$ for our Monte Carlo estimates we should keep only every N_{cor}-th path; the intervening sweeps erase correlations, giving us configurations that are statistically independent. The optimal value for N_{cor} depends upon the theory, and can be found by experimentation. It also depends on the lattice spacing a.
- Initial configuration: Guess the first configuration $\rightarrow$ discard some number of configurations at the beginning, before starting to collect $x^{(\alpha)}$'s. This is called "thermalizing the lattice."

Metropolis Algorithm

We need an algorithm to to create our set of random paths $x^{(\alpha)}$ with probability $\frac{e^{-S[x]}}{Z}$, where $Z = \int \mathcal{D}[x(t)] e^{-S[x]}$.
$\Longrightarrow$ a simple procedure, though not always the best, is the Metropolis Algorithm:

- Start with an arbitrary path $x^{(0)}$
- Modify by visiting each of the sites on the lattice, and randomizing the x_j's at those sites, one at a time, in a particular fashion as described below $\rightarrow$ generate a new random path from the old one: $x^{(0)} \rightarrow x^{(1)}$. This is called "updating" the path.
- Apply to $x^{(1)}$ to generate path $x^{(2)}$, and so on until we have N_{cf} random paths.

The algorithm for randomizing x_j at the j^{th} site is:

- Generate a random number $-\epsilon < \zeta \leq \epsilon$, with uniform probability;
- Let $x_j \rightarrow x_j + \zeta$ and compute the change ΔS in the action;
- If $\Delta S < 0$ retain the new value for x_j, and proceed to the next site;
- If $\Delta S > 0$ accept change with probability $\exp(-\Delta S)$ i.e. generate a random number η uniformly distributed between 0 and 1; retain the new value for x_j if $\exp(-\Delta S) > \eta$, otherwise restore the old value; proceed to the next site.

Comments:

- Choice of ϵ: should be tuned so that 40%–60% of the x_j's are changed on each pass (or "sweep") through the lattice. Then ϵ is of order the typical quantum fluctuations expected in the theory. Whatever the ϵ, successive paths are going to be quite similar and so contain rather similar information about the theory. Thus when we accumulate random paths $x^{(\alpha)}$ for our Monte Carlo estimates we should keep only every N_{cor}-th path; the intervening sweeps erase correlations, giving us configurations that are statistically independent. The optimal value for N_{cor} depends upon the theory, and can be found by experimentation. It also depends on the lattice spacing a.
- Initial configuration: Guess the first configuration $\rightarrow$ discard some number of configurations at the beginning, before starting to collect $x^{(\alpha)}$'s. This is called "thermalizing the lattice."

Statistical errors

An important part of any Monte Carlo analysis is the estimate of the statistical errors.

- **The "statistical bootstrap," method:**
  The bootstrap procedure provides new, almost *zero-cost* random ensembles of measurements by synthesizing them from the original ensemble of N_{cf} measurements.

  Consider an ensemble $\{G^{(\alpha)}, \alpha = 1 \ldots N_{cf}\}$ of Monte Carlo measurements
  - Construct a "bootstrap copy" of that ensemble by selecting $G^{(\alpha)}$'s at random from the original ensemble, taking N_{cf} in all while allowing duplications and omissions
    $\rightarrow$ resulting ensemble of G's may have two or three copies of some $G^{(\alpha)}$'s, and no copies of others
  - Use new ensemble to obtain a new estimate of some the quantity of interest.
  - Repeat this procedure to generated as many bootstrap copies of the original ensemble as one wishes, and from each we can generate a new estimate.

  The distribution of these estimates approximates the distribution of the quantity that would have been obtained from the original Monte Carlo, and so can be used to estimate the statistical error in our original estimate.
- **The "Jackknife" method:** Similar to boostrap but remove a set of measurements at a time from the sample set. In general easier to use than boostrap.
- **The "binning" method:**
  At the end of a simulation we have set of configurations $x^{(\alpha)}$, and for each a set of measurements like $G^{(\alpha)}$, our propagator. We partially average or bin the measurements: For example, instead of storing each of

  $$G^{(1)} \quad G^{(2)} \quad G^{(3)} \quad G^{(4)} \quad G^{(5)} \ldots$$

  we might instead store

  $$\overline{G}^{(1)} \equiv \frac{G^{(1)} + G^{(2)} + G^{(3)} + G^{(4)}}{4} \qquad \overline{G}^{(2)} \equiv \frac{G^{(5)} + G^{(6)} + G^{(7)} + G^{(8)}}{4} \qquad \ldots$$

  Binning reduces or can even remove the effects of correlations between different configurations.

Statistical errors

An important part of any Monte Carlo analysis is the estimate of the statistical errors.

- **The "statistical bootstrap," method:**
  The bootstrap procedure provides new, almost *zero-cost* random ensembles of measurements by synthesizing them from the original ensemble of N_{cf} measurements.

  Consider an ensemble $\{G^{(\alpha)}, \alpha = 1 \ldots N_{cf}\}$ of Monte Carlo measurements
  - Construct a "bootstrap copy" of that ensemble by selecting $G^{(\alpha)}$'s at random from the original ensemble, taking N_{cf} in all while allowing duplications and omissions
    $\rightarrow$ resulting ensemble of G's may have two or three copies of some $G^{(\alpha)}$'s, and no copies of others
  - Use new ensemble to obtain a new estimate of some the quantity of interest.
  - Repeat this procedure to generated as many bootstrap copies of the original ensemble as one wishes, and from each we can generate a new estimate.

  The distribution of these estimates approximates the distribution of the quantity that would have been obtained from the original Monte Carlo, and so can be used to estimate the statistical error in our original estimate.
- **The "Jackknife" method:** Similar to boostrap but remove a set of measurements at a time from the sample set. In general easier to use than boostrap.
- **The "binning" method:**
  At the end of a simulation we have set of configurations $x^{(\alpha)}$, and for each a set of measurements like $G^{(\alpha)}$, our propagator. We partially average or bin the measurements: For example, instead of storing each of

  $$G^{(1)} \quad G^{(2)} \quad G^{(3)} \quad G^{(4)} \quad G^{(5)} \ldots$$

  we might instead store

  $$\overline{G}^{(1)} \equiv \frac{G^{(1)} + G^{(2)} + G^{(3)} + G^{(4)}}{4} \qquad \overline{G}^{(2)} \equiv \frac{G^{(5)} + G^{(6)} + G^{(7)} + G^{(8)}}{4} \qquad \ldots$$

  Binning reduces or can even remove the effects of correlations between different configurations.

Scalar field theory

Let the continuum $\vec{r}$ be defined on lattice points i.e. $\vec{r} \to \vec{n} \equiv (n_1, n_2, n_3)a$ where a is the lattice spacing.
$\Longrightarrow$ equivalent to many-body problem where:

$$\hat{x}_i, \hat{p}_i \to \hat{\phi}(\vec{n}), \hat{\pi}(\vec{n}) \qquad \hat{x}_i \, |x\rangle = x_i \, |x\rangle \to \hat{\phi}(\vec{n}) = \phi(\vec{n}) \, |\phi\rangle \, .$$

We then have

$$\int d^3r \left\{ \frac{1}{2}\pi^2(\vec{r}) + \frac{1}{2}|\vec{\nabla}\phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\} \to \sum_{\vec{n}} a^3 \left\{ \frac{1}{2}\pi^2(\vec{n}) + \frac{1}{2a^2}\sum_{i=1}^{3} |\phi(\vec{n}+a\mu_i) - \phi(\vec{n})|^2 + V(\phi(\vec{n})) \right\}$$

where μ_i denotes a displacement by one lattice site in the i^{th} direction.
The evolution operator in Euclidean time:

$$e^{-t\sum_{\vec{n}} a^3 \left\{ \frac{1}{2}\pi^2(\vec{n}) + F(\phi(\vec{n})) \right\}} = \int \mathcal{D}[\phi(\vec{n})] e^{-\Delta t a^3 \sum_{\vec{n},k} \left[\frac{1}{2\Delta t^2} \left(\phi_{k+1}(\vec{n}) - \phi_k(\vec{n})\right)^2 + F(\phi_k(\vec{n})) \right]}$$

Take isotropic lattice i.e. $\Delta t = a$
$\Longrightarrow$ time slicing replaces $\hat{\pi}^2(\vec{n})$ by $\frac{1}{\Delta t}(\phi_{k+1}(\vec{n}) - \phi_k(\vec{n}))^2 \equiv \frac{1}{\Delta t}(\phi(n + a\mu_0) - \phi(n))^2$ which has the same structure as the discrete spatial derivative and where $n = (n_0, n_1, n_2, n_3)a$.

$$\Longrightarrow \mathcal{O}(\phi) e^{-t\int d^3r \left\{ \frac{1}{2}\pi^2(\vec{r}) + \frac{1}{2}|\vec{\nabla}\phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\}} \to \int \mathcal{D}[\phi(n)] O(\phi) e^{-S_{\text{cl}}[\phi]}$$

where $S_{\text{cl}}[\phi] = \sum_n a^4 \left\{ \sum_{i=0}^{3} \frac{\left(\phi(n+a\mu_i) - \phi(n)\right)^2}{a^2} + V(\phi(n)) \right\}$.
Note that S_{cl} is completely symmetric in time and space $\to$ if we choose periodic b.c. then the shortest dimension acts as a finite temperature.

Coherent States for bosons

Goal: generalize the scalar field example for second quantized boson and fermion fields.

For the Feynman path integral of our 1-d QM example we needed:

- Eigenstates of $\hat{x}$, $\hat{x}\,|x\rangle = x\,|x\rangle$ and
- Unity: $\int dx\,|x\rangle\,\langle x| = 1$

The analogs for creation and annihilation operators are provided by boson coherent states.

Consider a creation operator $a^\dagger$ then

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \qquad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \qquad |n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n |0\rangle$$

Define the coherent state $|z\rangle$ by

$$|z\rangle \equiv e^{z a^\dagger}\,|0\rangle = \sum_n \frac{z^n}{n!}\left(\hat{a}^\dagger\right)^n |0\rangle = \sum_n \frac{z^n}{\sqrt{n!}}\,|n\rangle$$

Properties:

$$\begin{aligned}
\hat{a}\,|z\rangle &= \sum_n \frac{z^n}{\sqrt{n!}}\hat{a}\,|n\rangle = z\sum_n \frac{z^{n-1}}{\sqrt{(n-1)!}}\,|n-1\rangle = z\,|z\rangle \\
\langle z|\,z'\rangle &= \sum_{mn}\langle m|\,\frac{z^{*m}}{\sqrt{m!}}\frac{z'^n}{\sqrt{n!}}\,|n\rangle = e^{z^* z'} \\
\langle z| : A(\hat{a}^\dagger\hat{a}) : |z\rangle' &= e^{z^* z'} A(z^*, z') \qquad (1) \\
1 &= \int \frac{dz dz^*}{2\pi i} e^{-z^* z'}\,|z\rangle\,\langle z|
\end{aligned}$$

Coherent States for bosons

Goal: generalize the scalar field example for second quantized boson and fermion fields.
For the Feynman path integral of our 1-d QM example we needed:

- Eigenstates of $\hat{x}$, $\hat{x}\,|x\rangle = x\,|x\rangle$ and
- Unity: $\int dx\,|x\rangle\,\langle x| = 1$

The analogs for creation and annihilation operators are provided by boson coherent states.
Consider a creation operator $a^\dagger$ then

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \qquad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \qquad |n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n |0\rangle$$

Define the coherent state $|z\rangle$ by

$$|z\rangle \equiv e^{za^\dagger}\,|0\rangle = \sum_n \frac{z^n}{n!}\left(\hat{a}^\dagger\right)^n |0\rangle = \sum_n \frac{z^n}{\sqrt{n!}}\,|n\rangle$$

Generalize for a set of creation operators $\hat{a}^\dagger_\alpha$

$$\begin{aligned}
|z\rangle &= e^{\sum_\alpha z_\alpha \hat{a}^\dagger_\alpha}\,|0\rangle \\
\hat{a_\alpha}\,|z\rangle &= z_\alpha\,|z\rangle \\
\langle z| : A(\hat{a}^\dagger \hat{a}) : |z\rangle' &= e^{\sum_\alpha z_\alpha z'_\alpha}\,A(z^*, z') \\
1 &= \int \prod_\alpha \frac{dz_\alpha z^*_\alpha}{2\pi i} e^{-z^*_\alpha z'_\alpha}\,|z\rangle\,\langle z| \equiv \int d\mu(z)\,|z\rangle\,\langle z|
\end{aligned}$$

Path integral using coherent states

Time slicing the evolution operator:

$$\langle z_f|\, e^{-tH}\, |z_i\rangle = \langle z_f|\, e^{-\Delta t H} \int d\mu(z_{N-1})\, |z_{N-1}\rangle\, \langle z_{N-1}|\, e^{-\Delta t H} \int d\mu(z_{N-2}) \cdots e^{-\Delta t H}\, |z_i\rangle$$

The matrix element of the infinitesimal evolution operator is

$$d\mu(z_k)\, \langle z_k|\, e^{-tH}\, |z_{k-1}\rangle = \prod_\alpha \frac{dz^*_{k,\alpha} dz_{k,\alpha}}{2i\pi}\, e^{-\sum_\alpha z^*_{k,\alpha}(z_{k,\alpha}-z_{k-1,\alpha}) - \Delta t H(z^*_{k,\alpha}, z_{k-1,\alpha})}$$

resulting in

$$\langle z_f|\, e^{-tH}\, |z_i\rangle = \int \mathcal{D}[z^*_{k,\alpha}, z_{k,\alpha}] e^{-S(z^*_{k,\alpha}, z_{k,\alpha})}$$

$$S(z^*, z) = \sum_k \Delta t \left\{ \sum_\alpha z^*_{k,\alpha} \left(\frac{z_{k,\alpha} - z_{k-1,\alpha}}{\Delta t} \right) + H(z^*_{k,\alpha}, z_{k-1,\alpha}) \right\}$$

Coherent states for fermions

Fermions are represented by anti-commuting creation and annihilation operators $c_\alpha^\dagger$ and $c_\alpha \rightarrow$ need to introduce anti-commuting Grassmann variables ξ such that

$$\hat{c}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle \qquad \hat{c}_\alpha \hat{c}_\beta |\xi\rangle = \xi_\alpha \xi_\beta |\xi\rangle = -\xi_\beta \xi_\alpha |\xi\rangle = -\hat{c}_\beta \hat{c}_\alpha |\xi\rangle$$

Since $\xi_\alpha^2 = 0$ (Pauli principle) the only functions allowed are monomials.
The rules for integration over a Grassmann variable ξ and ξ^* are

$$\int d\xi_\alpha = \int d\xi_\alpha^* = 0, \int d\xi_\alpha \xi_\alpha = \int d\xi_\alpha^* \xi_\alpha^* = 1$$

A fermion coherent state is defined by

$$|\xi\rangle \equiv e^{-\sum_\alpha \xi_\alpha c_\alpha^\dagger} |0\rangle$$

with similar properties to bosons. The path integral have similar form to that for bosons with some minus signs that distinguish between bosons and fermions.

Integration over fermions

For numerical evaluation we can not have the path integrals in terms of Grassmann variables. Fortunately for normalizable field theories we can integrate analytically over the fermionic degrees of freedom
Recall Gaussian integral

$$\int \prod_i \frac{dz_i^* dz_i}{2i\pi} e^{-z_i^* H_{ij} z_j + J_i^* z_i + z_i^* J_i} = [detH]^{-1} e^{J_i^* H_{ij}^{-1} J_j}$$

An analogous result is obtained for Grassmann "Gaussian": For one pair of Grassmann variables we have

$$\int d\xi^* d\xi \, e^{-\xi^* a \xi} = \int d\xi^* d\xi (1 - \xi^* a \xi) = a$$

This generalizes to

$$\int \prod_i d\xi_i^* d\xi_i \, e^{-\xi_i^* H_{ij} \xi_j + \eta_i^* \xi_i + \xi_i^* \eta_i} = [detH] \, e^{\eta_i^* H_{ij}^{-1} \eta_j}$$

i.e. the only difference is that $detH$ appears in the numerator $\rightarrow$ accounts for the minus sign of fermion loops.
If our action is of the form $S(\xi^*, \xi, \phi) = \xi_i^* M(\phi)_{ij} \xi_j + S_B(\phi)$ then

$$\int d\xi^* d\xi d\phi \, e^{\xi_i^* M(\phi)_{ij} \xi_j + S_B(\phi)} = \int d\phi \, detM(\phi) \, e^{S_B(\phi)}$$

i.e. $S_{\text{eff}}(\phi) = \ln detM(\phi) + S_B(\phi)$

Fermion propagators

Consider the time ordered product of field creation and annihilation operators at space-time points $j = (x_j, t_j)$ and $i = (x_i, t_i)$ respectively:

$$\langle \hat{T}\psi_i\bar{\psi}_j\rangle = Tr\,\hat{T}\psi_i\bar{\psi}_j\, e^{-\bar{\psi}M(\phi)\psi+S_B(\phi)} = \int \mathcal{D}[\phi]\mathcal{D}[\bar{\xi}\xi]\xi_i\bar{\xi}_j\, e^{-\bar{\xi}M(\phi)\xi+S_B(\phi)} = \int \mathcal{D}[\phi]\, M^{-1}_{ij}(\phi)\, e^{S_{\rm eff}(\phi)}$$

In general for n pairs of creation and annihilation operators

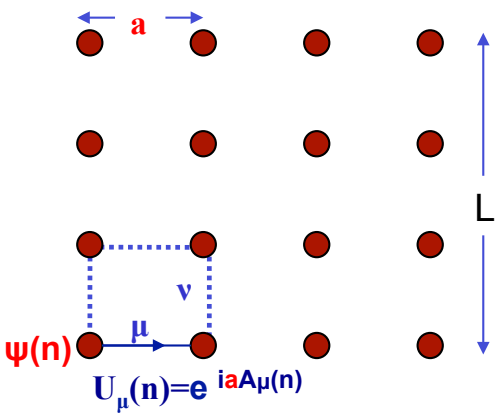
$$\begin{aligned}
& \int \mathcal{D}(\xi^*,\xi)\,\xi_{i_1}\cdots\xi_{i_n}\xi^*_{j_n}\cdots\xi_{j_1}\, e^{-\xi^* M\xi} \\
= \quad & \frac{\delta^{2n}}{\delta\eta^*_{i_1}\cdots\delta\eta^*_{i_n}\delta\eta_{j_n}\cdots\delta\eta_{j_1}} \int \mathcal{D}(\xi^*,\xi)\, e^{-\xi^*_i M_{ij}\xi_j+\eta^*_i\xi_i+\xi^*_i\eta_i}\,|^{\eta=\eta^*=0} \\
= \quad & \frac{\delta^{2n}}{\delta\eta^*_{i_1}\cdots\delta\eta^*_{i_n}\delta_{j_n}\cdots\delta\eta_{j_1}}\, detM\, e^{\eta^*_i M^{-1}_{ij}\eta_j}\,|^{\eta=\eta^*=0} \\
= \quad & \sum_P (-1)^P M^{-1}_{i_{P_n}j_n}\cdots M^{-1}_{i_{P_1}j_1}\; e^{\ln detM}
\end{aligned}$$

where P denotes a permutation of the indices. This is nothing else but Wick's theorem.
$\Longrightarrow$ fermions can be integrated out and we are left only with an effective action with the bosonic degrees of freedom.
Boundary conditions:

$$Tre^{-tH} = \int dz^*_0\, dz_0\, e^{-z^*_0 z_0}\,\langle \pm z_0|\, e^{-tH}\,|z_0\rangle = \int dz^*_0\, dz_0\, e^{-z^*_0 z_0}\int d\mathcal{D}[z^*,z]\, e^{-S(z^*,z)}$$

where the plus is for bosons and minus for fermions and
$S(z^*,z) = \pm z^*_0(\pm z_0 - z_{N-1}) + H_{0.N-1} + z^*_{N-1}(z_{N-1}-z_{N-2}) + H_{N-1,N-2} + \cdots + z^*_1(z_1-z_0)H_{1,0}$.

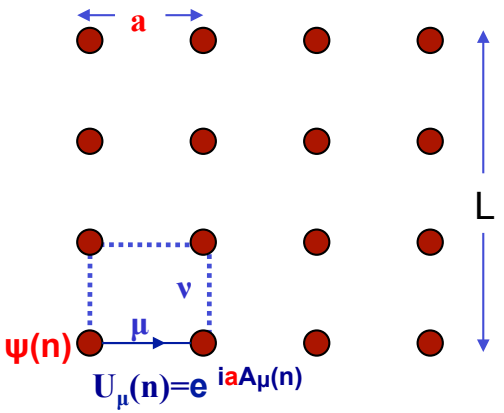
QCD on the lattice



Lattice QCD: K. Wilson, 1974 provided the formulation; M. Creutz, 1980 performed the first numerical simulation

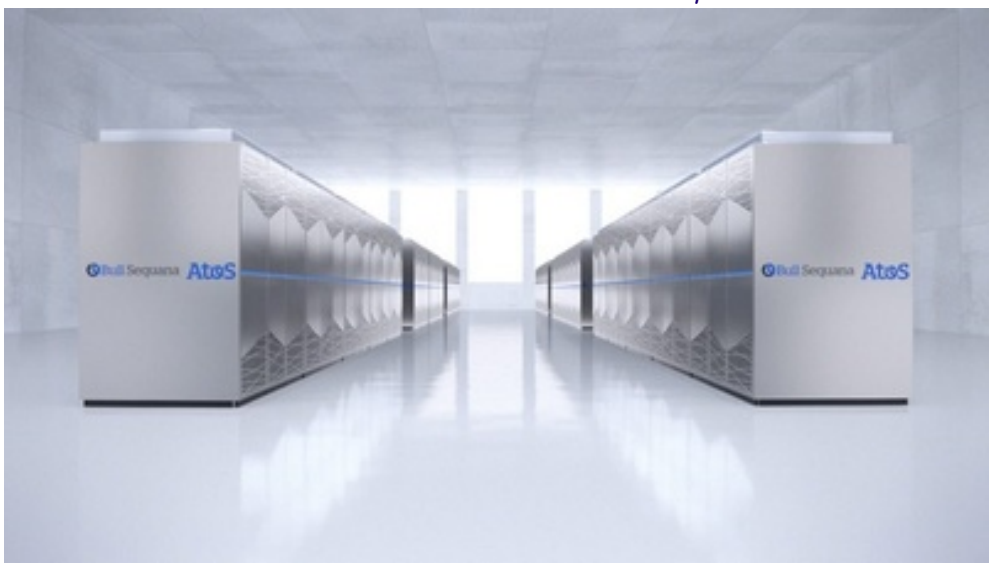
- Discretization of space-time with lattice spacing a and implement gauge invariance
  - quark fields $\psi(x)$ and $\bar{\psi}(x)$ on lattice sites
  - Introduce parallel transporter connecting point x and $x + a\hat{\mu}$: $U_\mu(x) = e^{iaA_\mu(x)}$ i.e. gauge field $U_\mu(x)$ is defined on links
- Finite a provides an ultraviolet cutoff at $\pi/a \rightarrow$ non-perturbative regularization; Finite $L \rightarrow$ discrete momenta in units of $2\pi/L$ if periodic b.c.
- Construct an appropriate action S and rotate into imaginary time: $S = S_G + S_F$ where $S_F = \sum_x \bar{\psi}(x) D \psi(x)$ i.e. quadratic in the fermions
  $\longrightarrow$ can be integrated out
- Path integral over gauge fields:
  $Z \sim \int \mathcal{D}U_\mu(x) \prod_f det(D_f[U])\, e^{-S_G[U]}$
  $\rightarrow$ Monte Carlo simulation to produce a representative ensemble of $\{U_\mu(x)\}$ using the largest supercomputers $\rightarrow$
  Observables: $\langle \mathcal{O} \rangle = \sum_{\{U_\mu\}} O(D^{-1}, U_\mu)$

QCD on the lattice



Lattice QCD: K. Wilson, 1974 provided the formulation; M. Creutz, 1980 performed the first numerical simulation

- Discretization of space-time with lattice spacing a and implement gauge invariance
- Finite a provides an ultraviolet cutoff at $\pi/a \rightarrow$ non-perturbative regularization; Finite $L \rightarrow$ discrete momenta in units of $2\pi/L$ if periodic b.c.
- Path integral over gauge fields:
  $Z \sim \int \mathcal{D}U_\mu(x) \prod_f det(D_f[U])\, e^{-S_G[U]}$
  $\rightarrow$ Monte Carlo simulation to produce a representative ensemble of $\{U_\mu(x)\}$ using the largest supercomputers $\rightarrow$
  Observables: $\langle \mathcal{O} \rangle = \sum_{\{U_\mu\}} O(D^{-1}, U_\mu)$



JUWELS (Jülich Wizard for European Leadership Science): 12 Pflop/s, one of the biggest in Europe
EU to build two exascale machines in the next 3 years

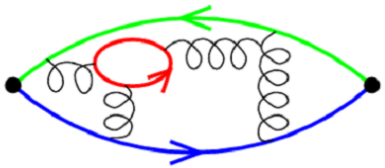
Hadron mass

First goal: reproduce the low-lying masses

- Use Euclidean correlation functions:

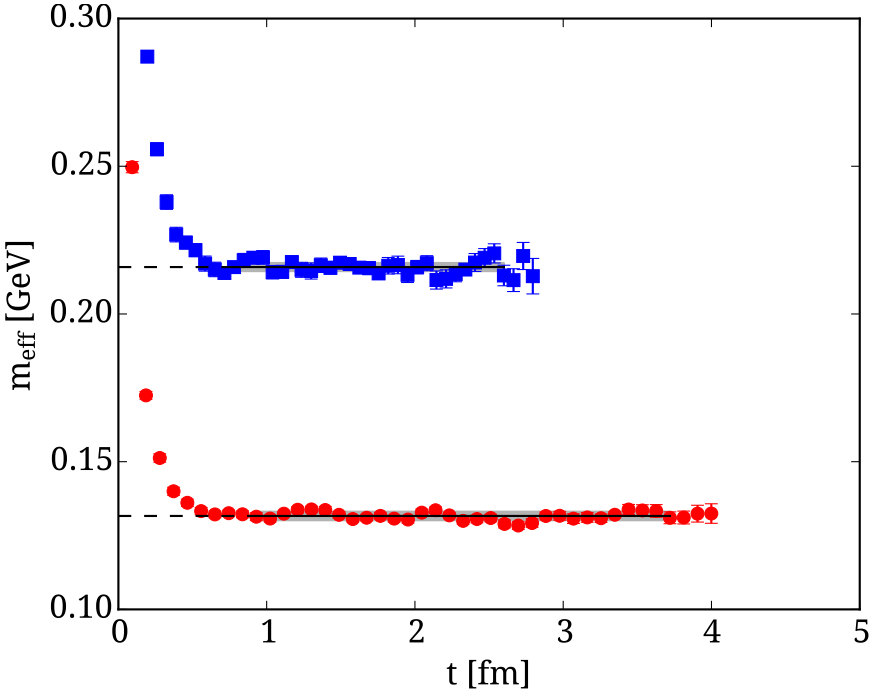
$$G(\vec{q}, t_s) = \sum_{\vec{x}_s} e^{-i\vec{x}_s\cdot\vec{q}} \langle J(\vec{x}_s, t_s) J^\dagger(0)\rangle$$

$$= \sum_{n=0,\cdots,\infty} A_n e^{-E_n(\vec{q})t_s} \overset{t_s\to\infty}{\longrightarrow} A_0 e^{-E_0(\vec{q})t_s}$$



Interpolating field with the quantum numbers of π^+: $J(x) = \bar{d}(x)\gamma_5 u(x)$

- Large Euclidean time evolution gives ground state for given quantum numbers $\Longrightarrow$ enables determination of low-lying hadron properties
- $aE_{\rm eff}(\vec{q}, t_s) = \ln\left[G(\vec{q}, t_s)/G(\vec{q}, t_s + a)\right]$
  $= aE_0(\vec{q}) + \text{excited states}$
  $\to aE_0(\vec{q}) \overset{\vec{q}=0}{\to} am$



$N_f = 2+1+1$ TM fermions at $m_\pi = 210$ MeV
$N_f = 2$ TM plus clover fermions at physical pion mass

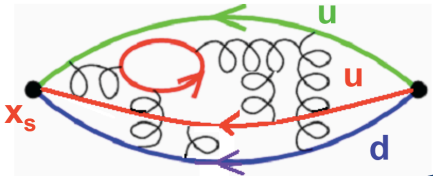
Hadron mass

First goal: reproduce the low-lying masses

- Use Euclidean correlation functions:

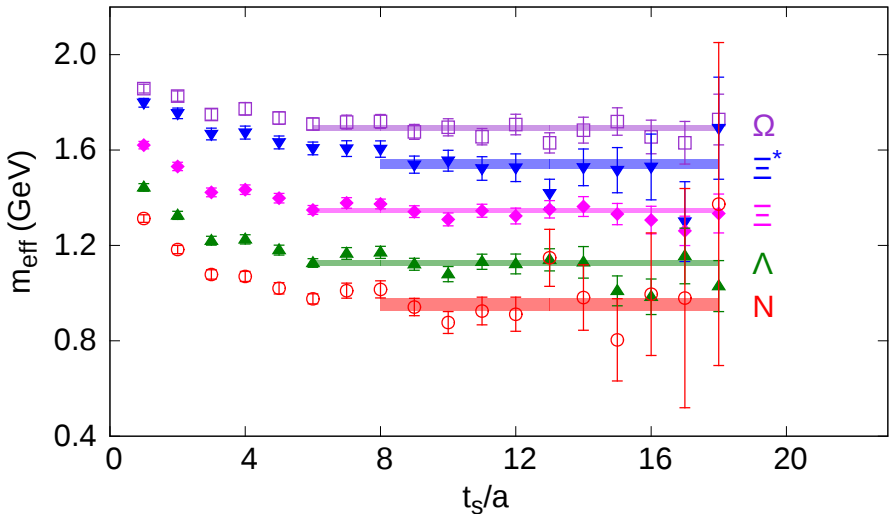
$$G(\vec{q}, t_s) = \sum_{\vec{x}_s} e^{-i\vec{x}_s\cdot\vec{q}} \langle J(\vec{x}_s, t_s) J^\dagger(0)\rangle$$

$$= \sum_{n=0,\cdots,\infty} A_n e^{-E_n(\vec{q})t_s} \overset{t_s\to\infty}{\longrightarrow} A_0 e^{-E_0(\vec{q})t_s}$$



Interpolating field with the quantum numbers of p: $J(x) = \epsilon^{abc}\left(u^{a\top}(x) C\gamma_5 d^b(x)\right) u^c(x)$

- Large Euclidean time evolution gives ground state for given quantum numbers $\Longrightarrow$ enables determination of low-lying hadron properties
- $aE_{\rm eff}(\vec{q}, t_s) = \ln\left[G(\vec{q}, t_s)/G(\vec{q}, t_s + a)\right]$
  $= aE_0(\vec{q}) + \text{excited states}$
  $\rightarrow aE_0(\vec{q}) \overset{\vec{q}=0}{\rightarrow} am$



$N_f = 2$ TM plus clover fermions at physical pion mass

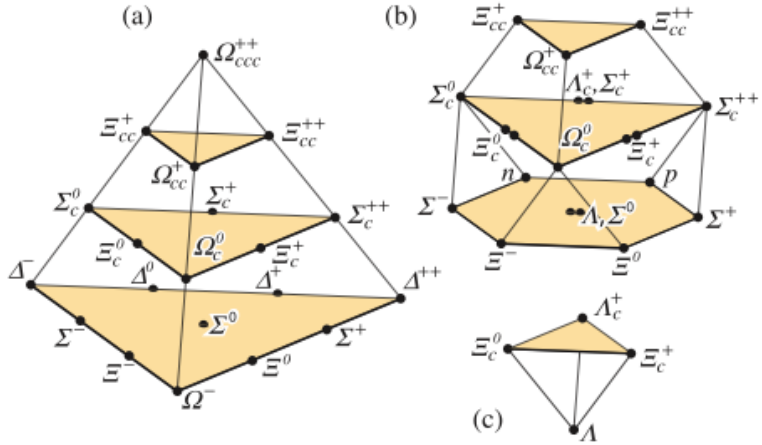
Noise to signal increases with t_s:$\sim e^{(m_h - \frac{3}{2}m_\pi)t_s}$

Hyperons and Charmed baryons

SU(4) representations:

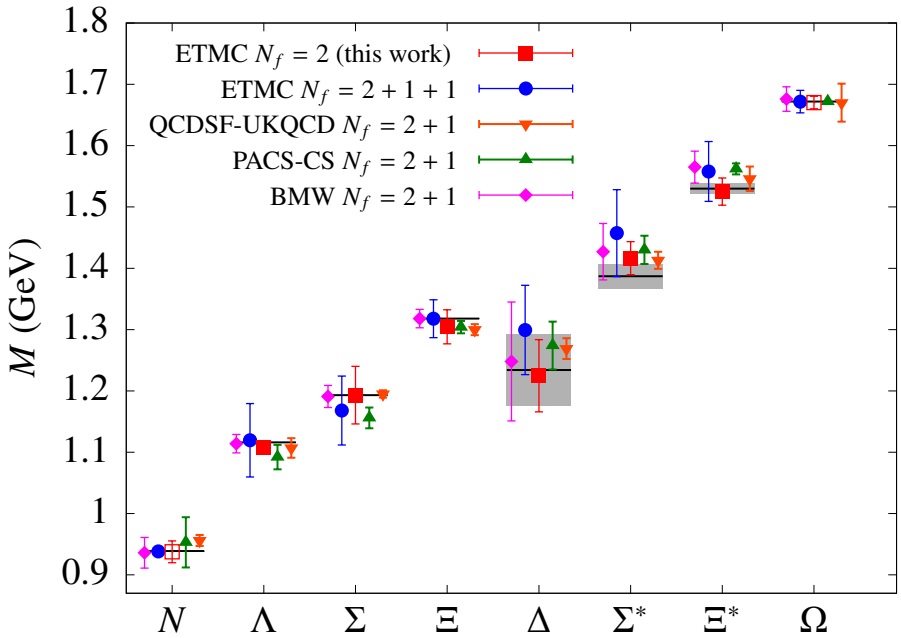
$$4 \otimes 4 \otimes 4 = 20 \oplus 20 \oplus 20 \oplus \overline{4}$$

$$\square \otimes \square \otimes \square = \square\square\square \oplus \begin{array}{|c|c|}\hline \\ \hline\end{array} \oplus \begin{array}{|c|}\hline \\ \hline\end{array} \oplus \begin{array}{|c|}\hline \\ \hline \\ \hline\end{array}$$



Spectrum using $N_f = 2$ simulations with physical pion mass

- We still need continuum extrapolation
- Volume dependence
- But NO chiral extrapolation, which was the biggest systematic error



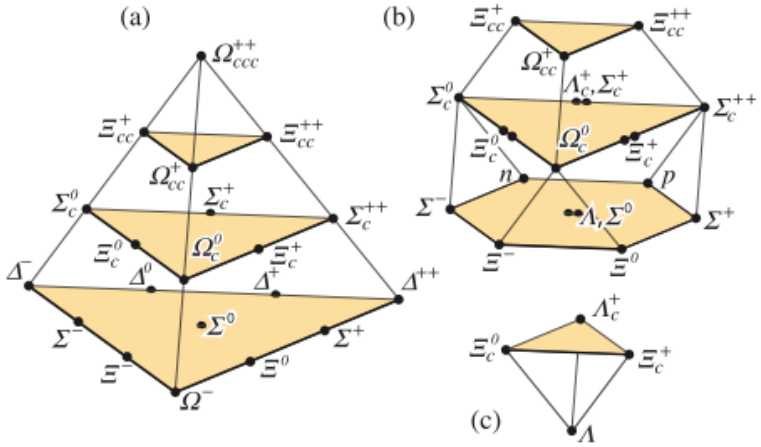
C.A., Ch. Kallidonis arXiv:1704.02647

Hyperons and Charmed baryons

SU(4) representations:

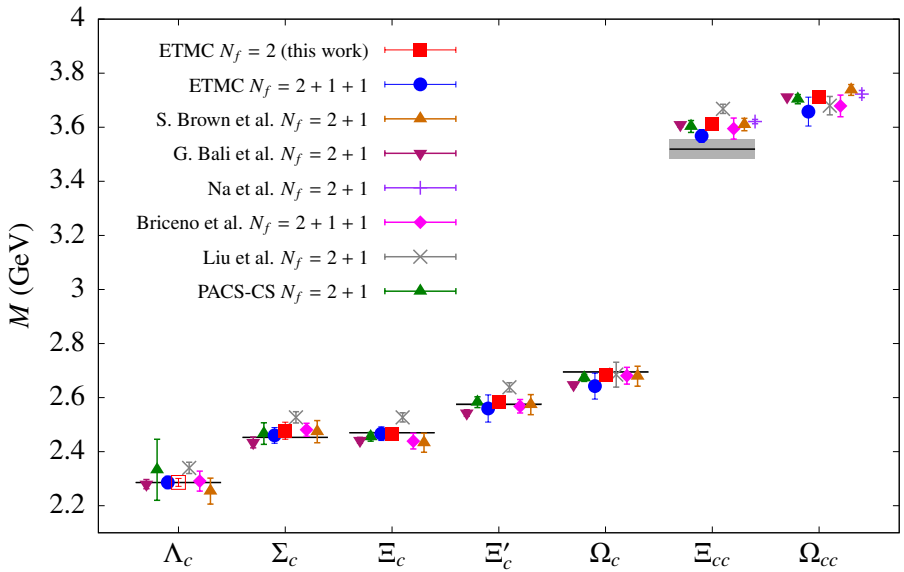
$$4 \otimes 4 \otimes 4 = 20 \oplus 20 \oplus 20 \oplus \overline{4}$$

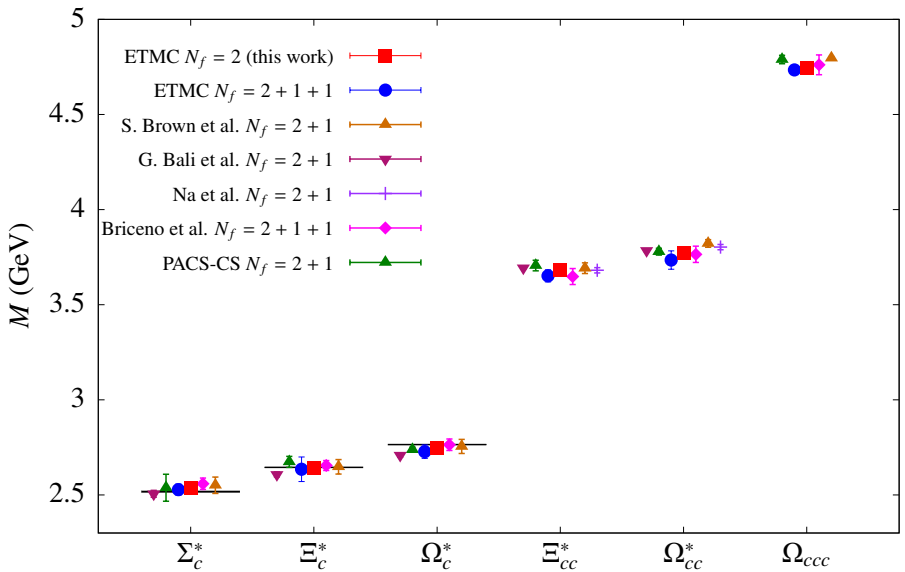
$$\square \otimes \square \otimes \square = \square\square\square \oplus \begin{array}{ll}\square & \square \\ \square & \end{array} \oplus \begin{array}{ll}\square & \square \\ \square & \end{array} \oplus \begin{array}{l}\square \\ \square \\ \square\end{array}$$



Spectrum using $N_f = 2$ simulations with physical pion mass

- We still need continuum extrapolation
- Volume dependence
- But NO chiral extrapolation, which was the biggest systematic error



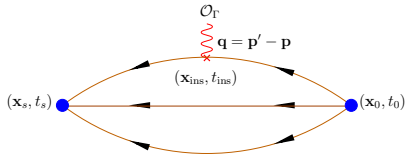


C.A., Ch. Kallidonis arXiv:1704.02647

Nucleon form factors

Evaluation of three-point functions:

$$G^{\mu\nu}(\Gamma, \vec{q}, t_s, t_{\rm ins}) = \sum_{\vec{x}_s, \vec{x}_{\rm ins}} e^{i\vec{x}_{\rm ins}\cdot\vec{q}}\, \Gamma_{\beta\alpha}\, \langle J_\alpha(\vec{x}_s, t_s)\mathcal{O}^{\mu\nu}(\vec{x}_{\rm ins}, t_{\rm ins})\overline{J}_\beta(\vec{x}_0, t_0)\rangle$$



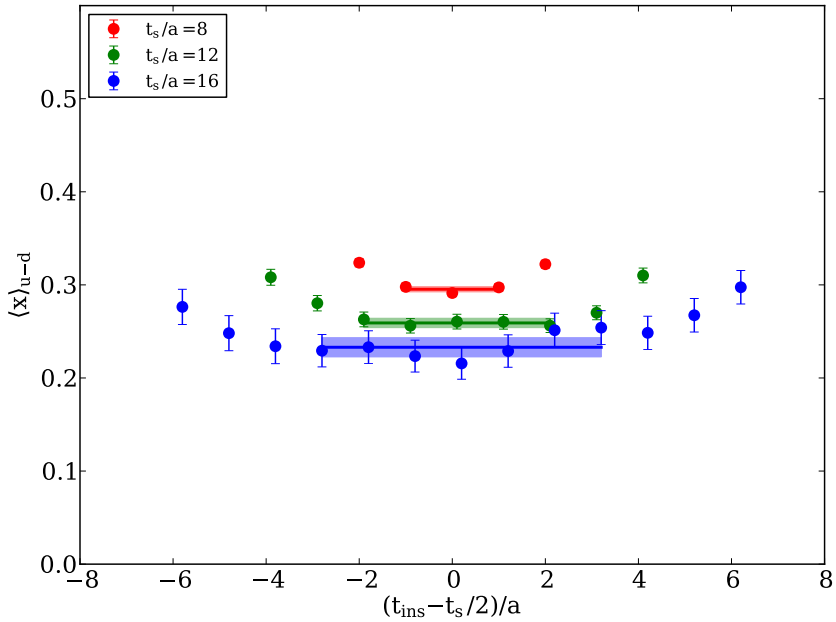
connected contribution

Form ratio by dividing the three-point correlator by an appropriate combination of two-point functions:

$$R(t_s, t_{\rm ins}, t_0) \xrightarrow[(t_s - t_{\rm ins})\Delta \gg 1]{(t_{\rm ins} - t_0)\Delta \gg 1} \mathcal{M}[1 + \ldots e^{-\Delta(\mathbf{p})(t_{\rm ins} - t_0)} + \ldots e^{-\Delta(\mathbf{p}')(t_s - t_{\rm ins})}]$$

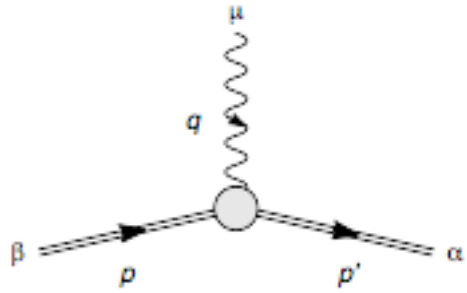
- $\mathcal{M}$ the desired matrix element
- $t_s, t_{\rm ins}, t_0$ the sink, insertion and source time-slice
- $\Delta(\mathbf{p})$ the energy gap with the first excited state

Connect lattice results to measurements:
$\mathcal{O}_{\overline{\rm MS}}(\mu) = Z(\mu, a)\mathcal{O}_{\rm latt}(a)$
$\Longrightarrow$ evaluate $Z(\mu, a)$ non-perturbatively



Proton radius puzzle

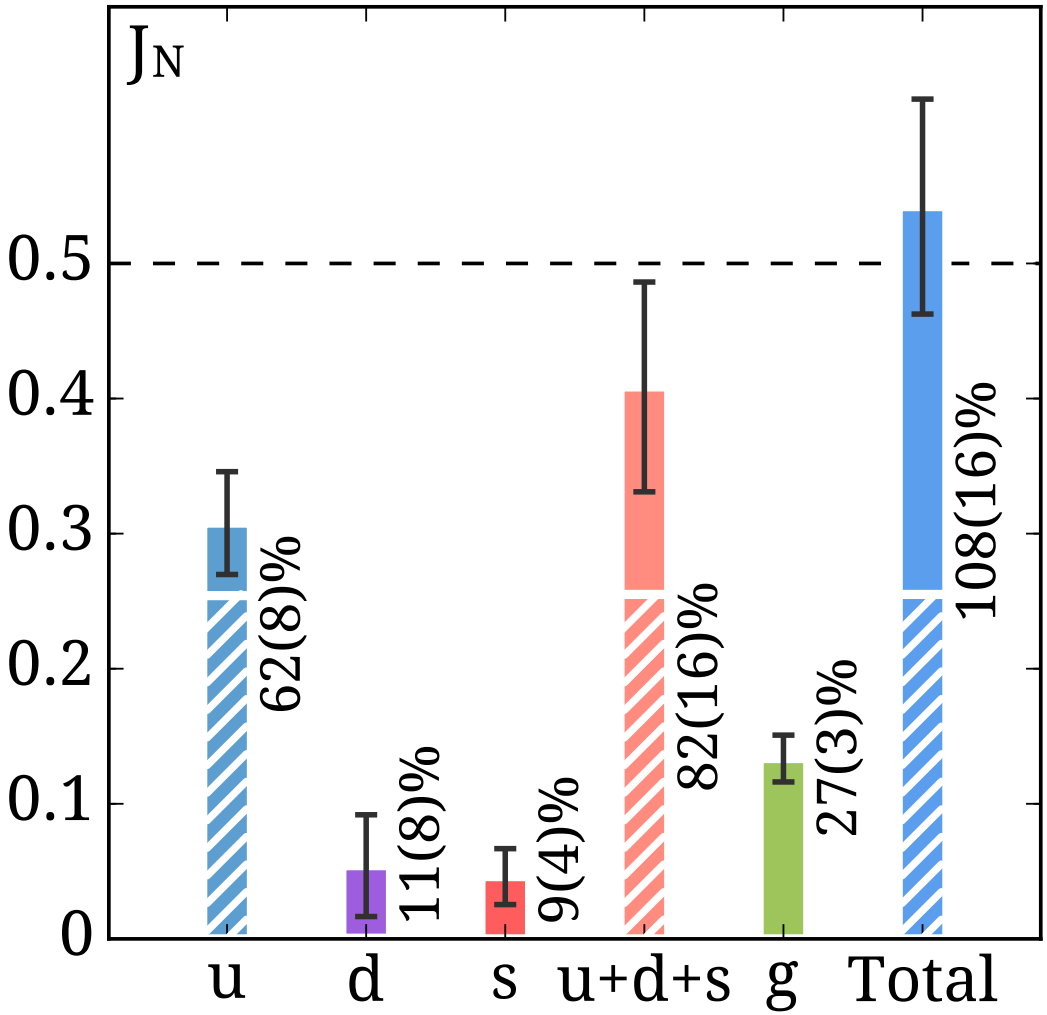
$$\langle N(p',s')|j^{\mu}(0)|N(p,s)\rangle = \bar{u}_N(p',s')\left[\gamma^{\mu}F_1(q^2) + \frac{i\sigma^{\mu\nu}q_{\nu}}{2m}F_2(q^2)\right]u_N(p,s)$$



- Proton radius extracted from muonic hydrogen is 7.7 σ different from the one extracted from electron scattering, R. Pohl *et al.*, Nature 466 (2010) 213
- Muonic measurement is ten times more accurate

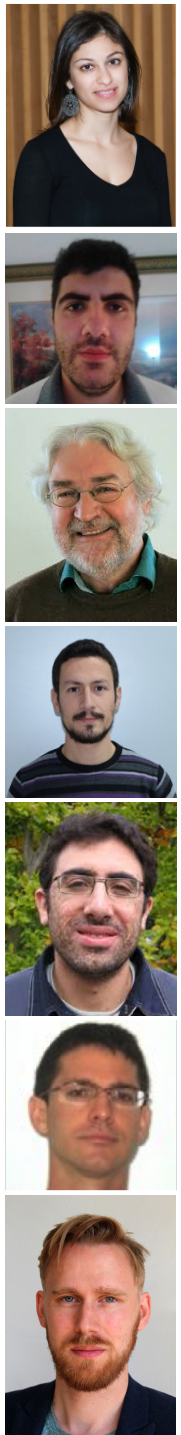
The proton spin puzzle

1987: the European Muon Collaboration showed that only a fraction of the proton spin is carried by the quarks $\Longrightarrow$ ETMC has now provided the solution



Recent results from lattice QCD at the physical point

C.A. *et al.*, arXiv:1706.02973



Conclusions

- Lattice QCD is a successful framework for non-perturbative calculations $\rightarrow$ simulations of the full theory at the physical point are now possible
- After getting agreement with experiment it enables predictions of new quantities
- New ideas and techniques are needed for the study of e.g. resonances, multi-quark states, decays, etc
- Can be used to study models beyond the SM

Acknowledgments

European Twisted Mass Collaboration (ETMC)

Cyprus (Univ. of Cyprus, Cyprus Inst.), France (Orsay, Grenoble), Germany (Berlin/Zeuthen, Bonn, Frankfurt, Hamburg, Münster), Italy (Rome I, II, III, Trento), Netherlands (Groningen), Poland (Poznan), Spain (Valencia), Switzerland (Bern), USA (Temple)

As simulations at the physical pion mass and more computer resources are becoming available we expect many physical results on key hadron observables that will impact both experiments and phenomenology

New ideas and approaches are needed and welcome

Please join and contribute