Talent 2013 Wednesday, July 10^{th}

Lattice QCD for nuclear physics

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outline:

- Direct lattice QCD output?
- physical observables of interest?
  - connection to lattice data?
  - A no-go theorem and Luscher's solution
- Derivation of Luscher formula
  - S-wave two-particle interactions
  - Higher partial waves?
- Bound state from finite volume (FV) formalism?
  - Deuteron?
- Some recent results from NPLQCD collaboration:
  - $\pi\pi$ scattering phase shift
  - Nucleon-nucleon scattering parameters
  - multi-nucleon systems
  - Hyperon - nucleon scattering

- Lattice QCD output:

1) Create the state with a given $\underbrace{\text{quantum number}}_{\text{number of particles, spin, isospin, ...}}$

using a suitable interpolating operator: "source"

at time zero.

2) Annihilate the state with the corresponding interpolating

operator at some later time t: "Sink"

3) Take the vaccum expectation value of the sink-source operator : "correlator" by "importance sampling"

- averaging over many number of guage configurations

→ The higher the number of configuration : The lower the statistical uncertainty of the calculation.

5) obtain the time evolution of your correlator using an "effective mass plot" (EMP). Identify the plateau in the EMP and therefore read off the ground state energy of the state.

Example : Two-pion energy eigenvalues

$$C_{\pi^+\pi^+}(t,\vec{x},\vec{y}) = \langle 0 | \pi^-(t,\vec{x}) \, \pi^-(t,\vec{y}) \, \pi^+(0,\vec{0}) \, \pi^+(0,\vec{0}) | 0 \rangle$$

with $\pi^+(x,t) = \bar{u}(\vec{x},t)\, \gamma_5 \, d(\vec{x},t)$

project into a two-pion state with total momentum $\vec{P}$ and relative momentum $\vec{q}$:

Fourier transform of $C_{\pi^+\pi^+}(t,\vec{x},\vec{y})$: $C_{\pi^+\pi^+}(\vec{q},t) = \sum_{\vec{x},\vec{y}} e^{i\vec{q}\cdot(\vec{x}-\vec{y})} \langle 0 | \pi^-(t,\vec{x}) \pi^-(t,\vec{y}) \pi^+(t,\vec{0}) \pi^+(t,\vec{0}) | 0 \rangle$

for zero total momentum $\vec{P} = 0$.

Now insert a complete set of energy eigenstates → the large time behavior of $C_{\pi^+\pi^+}$ is given by : $A_2 \, e^{-E^0_{\pi^+\pi^+} t}$

On the other hand the large time behavior of one pion correlator is given by: $A_1 e^{-E^0_{\pi^+} t}$

Take the ratio: $G_{\pi^+\pi^+}(\vec{q}, t) = \dfrac{C_{\pi^+\pi^+}(\vec{q}, t)}{C_{\pi^+}(t)\, C_{\pi^+}(t)} \xrightarrow{\text{large time}} B_0 e^{-\Delta E_0 t}$

Define: $am_{eff} = -\log\left[\dfrac{G_{\pi^+\pi^+}(\vec{q}, t)}{G_{\pi^+\pi^+}(\vec{q}, t-1)}\right] \quad (= \Delta E_0)$

T : total number of time slices

This procedure seems pretty straightforward, but why are LQCD calculations complicated and costly?

- Gauge configuration production – Monte Carlo sampling
  need sufficient statistics
  many measurements required
- Wick contractions become more complicated when more and more hadrons are added.

Wick contractions? Example: single pion correlator

$$C_{\pi^+}(\vec{p}, t) = \sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \langle 0 |\, \underbrace{\bar{d}(x)\gamma_5 u(x)}_{\pi^+(x)}\ \underbrace{\bar{u}(0)\gamma_5 d(0)}_{(\pi^+(x))^+} \,| 0 \rangle$$

d, u carry spin and color indices as well

$$= -\sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \langle 0 | \mathrm{Tr}\left[D_d^{-1}(0, x)\gamma_5 D_u^{-1}(x, 0)\gamma_5 \right] | 0 \rangle$$

point to all propagator → easier to compute

D^{-1} denotes the inverse of the Dirac operator or simply fermion propagator.

Note that this is not the only place where fermions appear. There are fermionic terms in QCD action as well. It is then easy to see that in taking vacuum expectation value, one can replace them with : $[\det D]^{N_f}$ → number of flavors

Explicitly : $\langle 0 | \mathrm{Tr}\, [D_d^{-1}(0,x)\gamma_5 D_u^{-1}(x,0)\gamma_5] | 0 \rangle$

$$= \frac{\int \mathcal{D}U\, [\det D]^{N_f}\, e^{-S_{gauge}}\, \mathrm{Tr}[D_d^{-1}(0,x)\gamma_5 D_u^{-1}(x,0)\gamma_5]}{\int \mathcal{D}U\, [\det D]^{N_f}\, e^{-S_{gauge}}}$$

- The Dirac operator matrix is a big matrix → Inverting it is quite costly. Its determinant also needs to be evaluated when preparing gauge configurations that are needed to make measurements.

- Signal to noise issue for nucleonic systems.

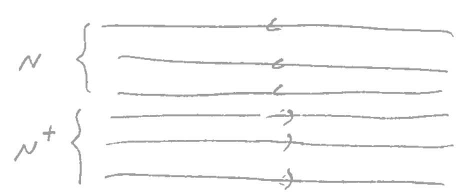
  Lepage argument for why the signal in LQCD calculations of nucleonic correlators degrade quickly?

  Single nucleon : Remember that : $\sigma^2(C) = \langle CC^\dagger \rangle - |\langle C \rangle|^2$

  variance → a measure of stat uncertainty

  $\langle CC^\dagger \rangle \sim \langle NN^\dagger\, NN^\dagger \rangle \xrightarrow{t\to\infty}$?

  pictorially :

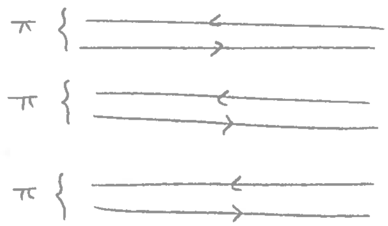


→ $e^{-2m_n t}$

But this is not the only possible scenario! In fact this correlation function at large time will approach its ground state which is 3π's and not $2N$! Note that: $m_{3\pi} = 3 \times m_\pi \simeq 3 \times 140 = 420$ MeV

$m_{2N} = 2 \times m_n \simeq 2 \times 980 = 1960$ MeV !

pictorially:



$\to e^{-3m_\pi t}$ Therefore: $\frac{\text{Signal}}{\text{noise}} \sim e^{-(m_n - \frac{3}{2} m_\pi) t}$

□ Question? what is the signal to noise ratio for a LQCD calculation of the mass of a nucleus with A number of nuclei?

□ Question? It is often said that LQCD calculations at lighter pion masses are quite challanging. Can you explain why this is the case based on the signal/noise issue?

NPLQCD 2012 calculation: $m_\pi \simeq 800$ MeV, $m_n \simeq 1.8$ GeV. Comment on signal/noise in this calculation

Given these difficulties, is there any hope to get spectral info on multi-nucleon systems from LQCD?

NPLQCD recent progress:
- Much algorithm development: Contractions are now available up to ^{28}Si!
- There is a golden window of plateau just before the signal/noise issue becomes severe.

That's because the overlap factors on mult-N States are big enough to compensate for the signal degradation due to noise.

→ Slides : NPL QCD calculation of spectrum at SU(3) flavor symmetric point with $m_\pi \simeq 800$ MeV + Demonstration of plateaus and golden window

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• Nucleon-nucleon, interactions from LQCD :

LQCD is performed on Euclidean space-time → only spectral info + matrix elements

How about interactions? Can we obtain for example NN or YN phase shifts directly from LQCD? How about three-body force parameters?

we saw on monday's lecture that there is an approach by HAL QCD collaboration that aims to calculate the potentials out of NBS wavefunctions calculated with LQCD. Since this potentials are scheme dependent and the specification of errors is not possible in this approach, the phase shift predictions based on this method can be arbitrarily wrong and is not a direct prediction of QCD. Today we want to learn a method based on Luscher's finite volume formalism.

One might ask why can't we evaluate the element's of S-matrix from

LQCD in Euclidean space-time and analytically continue the result back to Minkowski space with $\tau \to it$? The answer is in fact No. As stated by Maiani-Testa's no-go theorem, one can not obtain the elements of S-matrix from Euclidean Lattice Green's functions in infinite volume except at kinematic threshold. Since we are not interested in only kinematic threshold, we should think of a way to get around this no-go theorem. This leads us to the luscher formalism.

Statement of luscher formula:

The energy shift of two interacting scalar particles in a finite cubic volume with periodic BC is related to the S-wave scattering phase shift of infinite volume via:

$$q \cot \delta(q) = \frac{1}{\pi L} S\left(\frac{L^2 q^2}{4\pi^2}\right)$$

$$E_{NR} = E - 2m = \frac{q^2}{m}$$

phase shift

$$S(x) \equiv \sum_{\vec{j}}^{\Lambda_{\vec{j}}} \frac{1}{|\vec{j}|^2 - x^2} - 4\pi\Lambda_{\vec{j}}$$

non-relativistic interacting energies

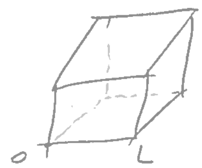
integer valued vectors

Derivation of luscher formula:

There are many derivations presented for luscher formula. Here we follow the derivation given by Beane, et. al. in 0312.004

But before getting into the details of derivation, let's discuss some preliminary points:

→ periodic boundary condition:



$$\psi(\vec{x}) = \psi(\vec{x} + \vec{n} L), \quad n_i \in \mathbb{Z}$$

$$\xrightarrow{\text{fourier transform}} \vec{P} = \frac{2\pi \vec{n}}{L}, \quad n_i \in \mathbb{Z}$$

→ As a result the energy spectrum of the system is discretized.

□ Discussion point: How does the energy spectrum of two interacting particle looks like in infinite volume? Discuss both bound-state and scattering states.

In FV the non-interacting case is trivial: Two-plain waves with

energy: $E_{NR} = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} = \frac{\vec{P}^{\,2}}{4m} + \frac{\vec{q}^{\,2}}{m}$ with: $\begin{cases} \vec{P} = \vec{P}_1 + \vec{P}_2 \\ \vec{q} = \frac{\vec{P}_1 - \vec{P}_2}{2} \end{cases}$

$\vec{P}_1$ $\vec{P}_2$

$\vec{P}_1$ and $\vec{P}_2$ are both integer multiplets of $\frac{2\pi}{L}$:

Ground State: $\vec{P}_1 = 0$, $\vec{P}_2 = 0 \Rightarrow E_{NR}^{(0)} = 0$

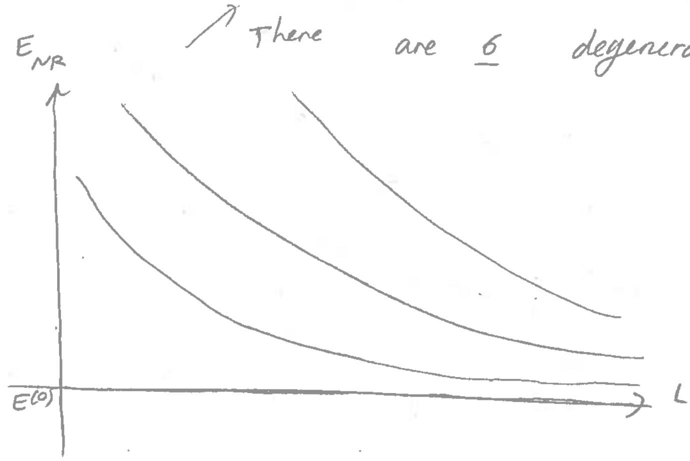
Constraining to $\vec{P} = 0$

First excited state: $\vec{P}_1 = \frac{2\pi}{L}(1,0,0)$, $\vec{P}_2 = \frac{2\pi}{L}(-1,0,0) \Rightarrow E_{NR}^{(1)} = \frac{4\pi^2}{m L^2}$

There are <u>6</u> degenerate States

As a function of volume:

They all approach zero at infinite volume.



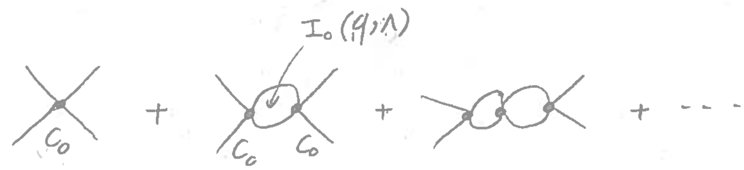
What happens if you turn on the interactions? The levels will be shifted, but one expects that the volume dependence of scattering states remains power-law. How about bound-states? we get back to this question when we discuss the Luscher formula in more detail.

Derivation: So the goal is to find the energy shift the two-particle state experinces when the interactions are present.

The claim is that this energy shift can be related to the scattering phase shift of infinite valume (and in general the elements of S-matrix).

Let's evaluate the scattering amplitude of a two nucleon system in S-wave using the pionless EFT that we've become familiar with in the previous lectures:

$$iT = \frac{4\pi}{m_n}\frac{1}{q\cot\delta_s - iq} =$$



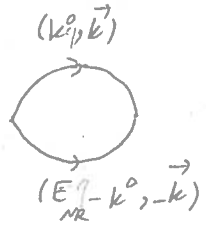
$$= C_0 + C_0 I_0(q,\Lambda) C_0 + \cdots = C_0\left(1 + I_0(q,\Lambda)C_0 + \cdots\right)$$

$$= \frac{C_0}{1 - I_0(q,\Lambda)C_0} = T$$

Inverting this gives:

$$C_0 = \frac{T}{1 + I_0(q,\Lambda)T}$$

How about finite volume? Note that the loop that we calculated before is an integral over the momentum running in the loop. Since in FV all momenta are discretized, the integral over continuous momenta is replaced with sum over discrete momenta. Explicitly: $\int \frac{d^3k}{(2\pi)^3} \longrightarrow \frac{1}{L^3}\sum_{\vec{k}}$

$I_0^V =$ 

$= \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{E_{NR} - \frac{\vec{k}^2}{m_n}}$ while: $I_0 = \int \frac{d^3k}{(2\pi)^3} \frac{1}{E_{NR} - \frac{\vec{k}^2}{m_n}}$

Note that as $|\vec{k}| \to \infty$, this sum diverges the same way as I_0 diverges and therefore one can choose a momentum cut-off just as in infinite volume to regularize this. But as we will see, the final result only depends on the difference between I_0 and I_0^V and the cutoff dependent parts of sum cancel. Now finite volume version of scattering amplitud is:

$$T^V = C_0 + C_0 I_0^V(q,\Lambda) C_0 + \cdots = \frac{C_0}{1 - I_0^V(q,\Lambda) C_0}$$

replacing C_0 in terms of $I_0(q,\Lambda)$ and T gives:

$$T^V = \frac{\frac{T}{1 + I_0(q,\Lambda) T}}{1 - \frac{T}{1 + I_0(q,\Lambda)} I_0^V(q,\Lambda)} = \frac{T}{1 - \delta I_0^V(q) T} \quad \text{with } \delta I_0^V(q) = I_0^V(q,\Lambda) - I_0(q,\Lambda)$$

The poles of this object correspond to isolated energy eigenvalues in the FV volume: $1 - \delta I_0^V T = 0 \Rightarrow (T)^{-1} + \delta I_0^V = 0 \Rightarrow \boxed{q \cot \delta_s = \frac{1}{\pi L} S\left(\frac{q^2 L^2}{4\pi^2}\right)}$ (*)

$\sim q \cot \delta_s - \cancel{iq}$ $\qquad \sim \cancel{iq} + \cdots$

what is calculated from LQCD? $E_{NR}^{(-1)}$, $E_{NR}^{(0)}$, $E_{NR}^{(1)}$, ...

Bound state energy $\qquad$ The first excited state

Now input q into (*) and get $\delta(q)$

This is a direct calculation of S-wave nucleon phase shift from LQCD.

Understanding luscher formula better:

- Systematics of luscher: It only applies to elastic scattering and is valid up to pion production threshold: $2m_\pi$

- Even below the inelastic threshold there are exponential correction to the luscher formula that scale like: $e^{-m_\pi L}$.

□ Discussion point: How large the lattice volume should be to get phase shifts from luscher formula up to 1% error? at physical pion mass? How about $m_\pi = 800$ MeV and $m_\pi = 300$ MeV?

- If interactions are turned off, luscher formula gives $\delta = 0$.

  □ How can you see this directly from luscher formula?.

- luscher formula indicate that the volume dependene of bound states is governed by exponential and not power-law.

$$k^{(V)} = \underbrace{k^{(0)}}_{\text{infinite volume value for binding momentum}} + A\,\frac{e^{-k^{(0)}L}}{L} + \cdots$$

You can easily check this from S function by analytically continuing to $q^2 \to -k^2$.

□ Discussion point: How large the lattice volume should be to get deuteron binding momentum up to 2% level? (Note: $k_d^{(0)} \simeq 45.7$ MeV)

- Luscher formula has been generalized to arbitrary CM momentum, higher partial-wave, unequal masses - two-particle coupled channel, two-nucleon systems with arbitrary spin and parity and so on.

- The other systematic in Luscher calculation is that due to broken rotational symmetry, higher partial-waves contribute to for example s-wave phase shift. So as long as the energy is low, one can neglect those higher partial-waves. (For a system of two identical particle with zero CM boost, $\ell=4$ scattering contaminates the s-wave scattering in this FV formula.)

Slides: The plot of S-function

NPLQCD extraction of NN phase-shifts

" " of the light nuclei spectra

" Study of Hyperon (Y) - Nucleon (N) interaction phase shifts

NPLQCD and JLab extraction of $\pi\pi$ phase-shifts