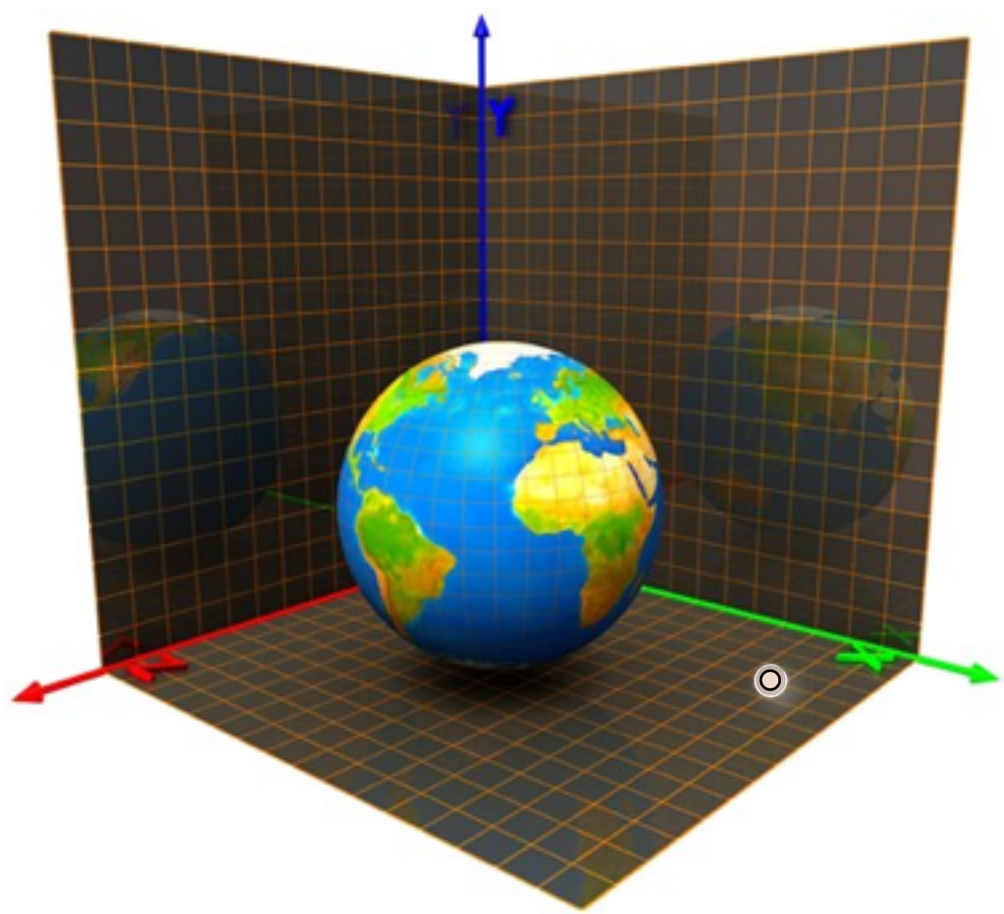
Nuclear Physics from Lattice QCD (part 1)

The why's, what's and how's...

Raúl Briceño

Jefferson Lab



HUGS, June 2014

Outline

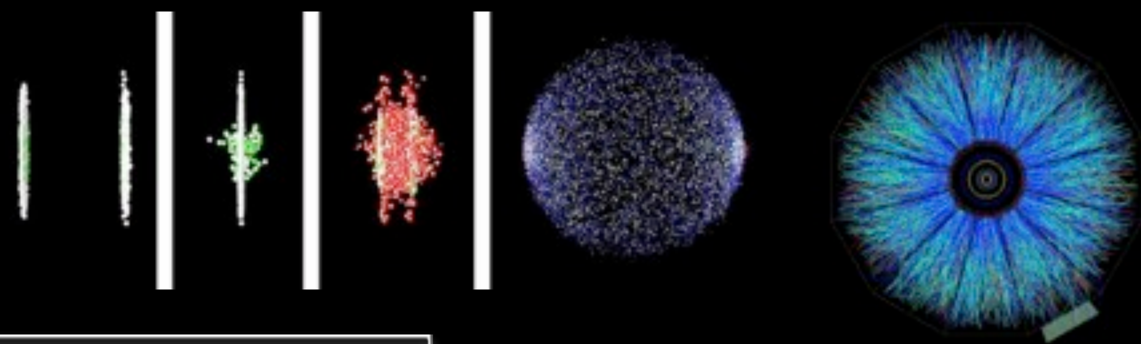
First half:

- Why QCD / Lattice QCD?
- What's Lattice QCD?
- Symmetry?

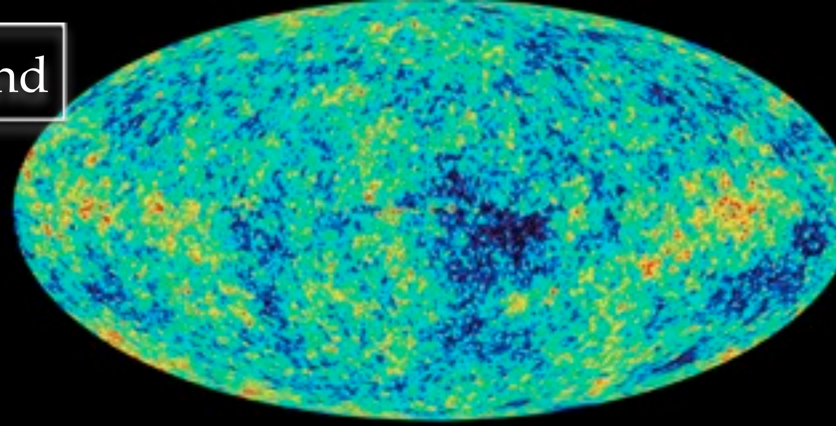
Second half:

- Masses & decay constants of single particles
- Scattering, resonances & bound states
- Decays, form factors, etc.

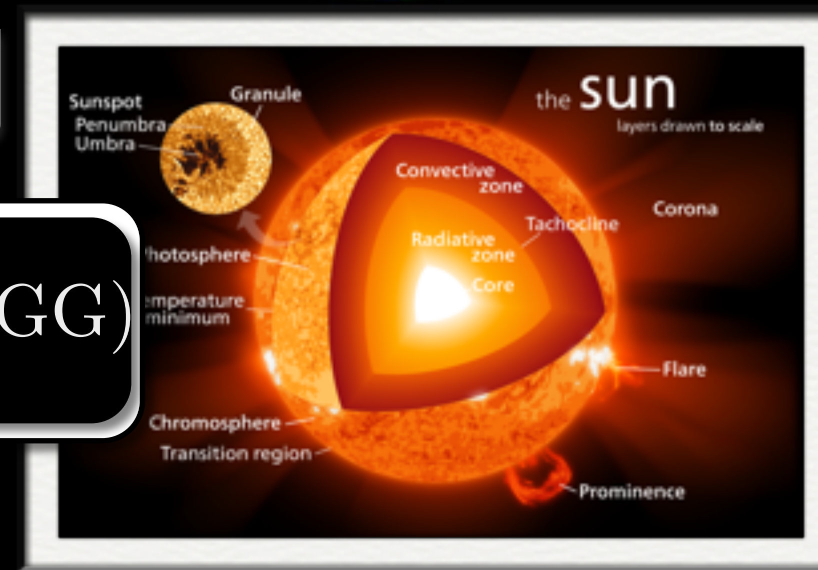
QCD



Cosmic microwave background

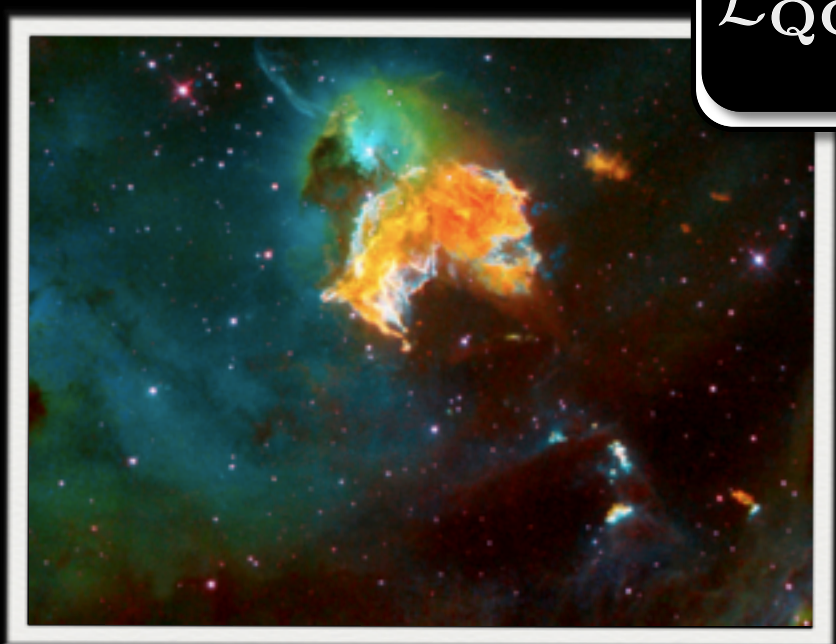


Stellar evolution



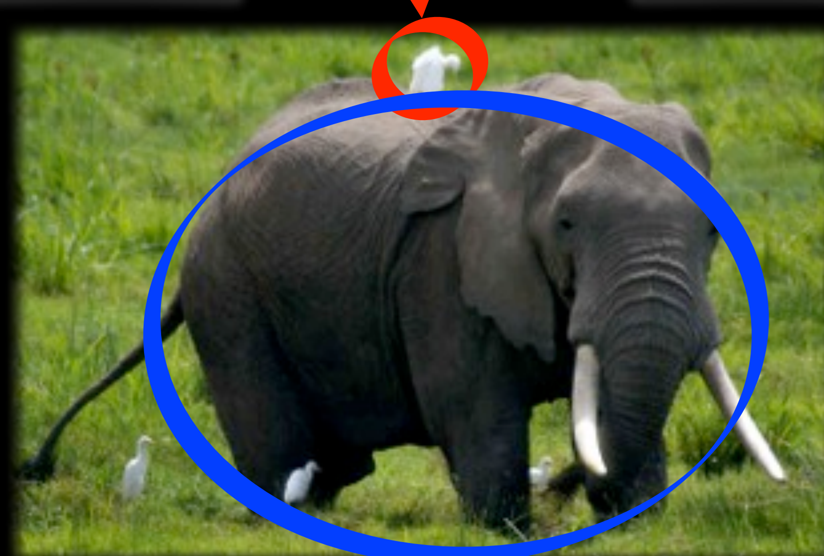
Heavy ion collisions

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_{\mathrm{f}} \left(\mathrm{i} \not{D} - \mathrm{m}_{\mathrm{f}} \right) \psi_{\mathrm{f}} - \frac{1}{4} \mathrm{tr} \left(\mathrm{GG} \right)$$



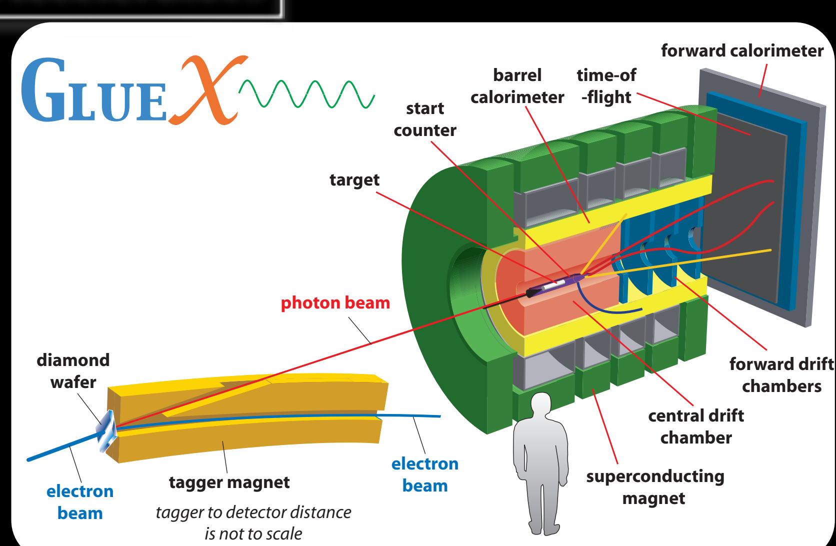
Supernova

Higgs



Today's goal!

Accelerators

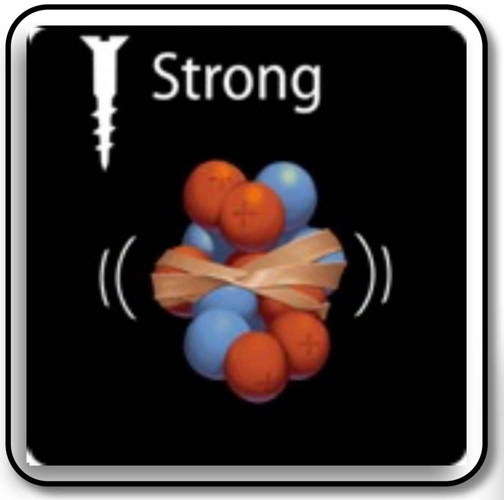


Glue!

Jose Rodriguez (Microsoft)

Unfolding QCD

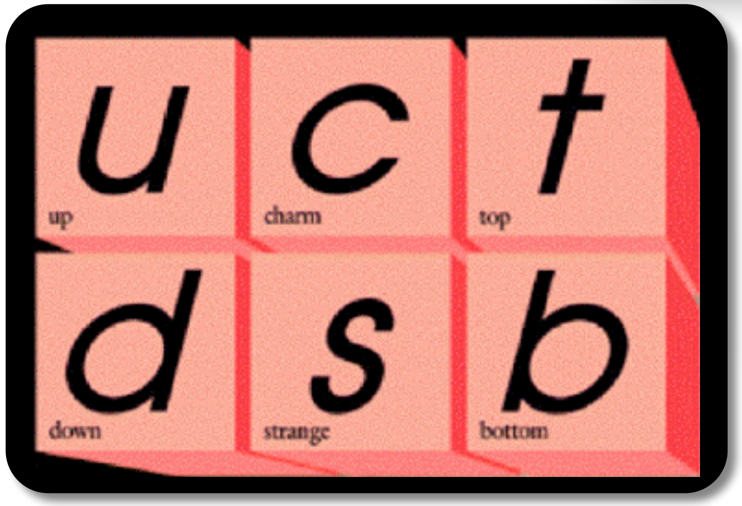
$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_{\mathrm{f}}\,(\mathrm{i}\,\not{D} - \mathrm{m}_{\mathrm{f}})\,\psi_{\mathrm{f}} - \frac{1}{4}\mathrm{tr}\,(\mathrm{GG})$$



"chromo"

quarks & gluons carry "color"!

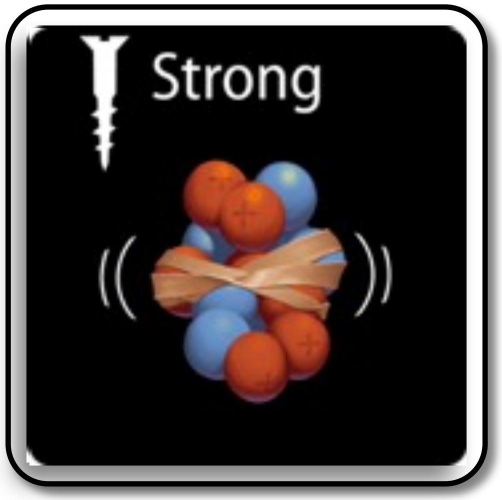
Warning: Not REAL color! It is like charge in QED, there are three types of this "charge": red, blue, green!



quarks come in 6 different types of flavor!

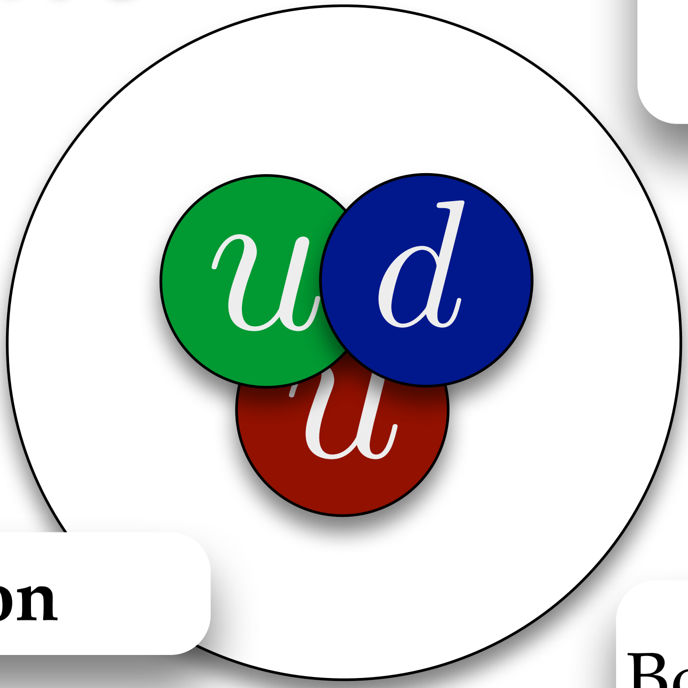
Quantum chromodynamics

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_{\mathrm{f}}\,(\mathrm{i}\,\not{D} - \mathrm{m}_{\mathrm{f}})\,\psi_{\mathrm{f}} - \frac{1}{4}\mathrm{tr}\,(\mathrm{GG})$$



"chromo"

quarks carry color, but bound states of quarks do NOT!



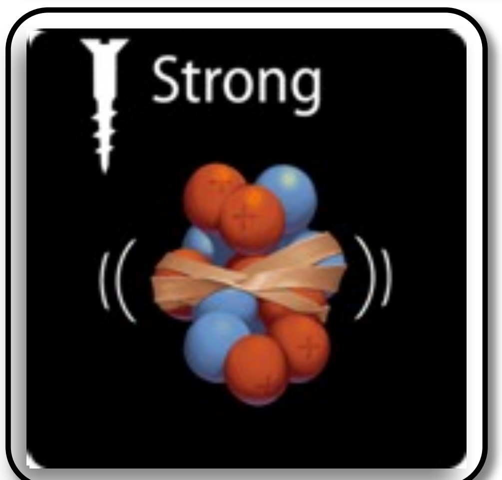
the proton

no free quarks!

Bound states of quarks are "**hadrons**"

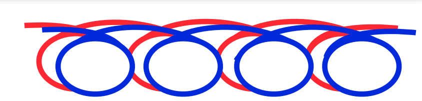
Unfolding QCD

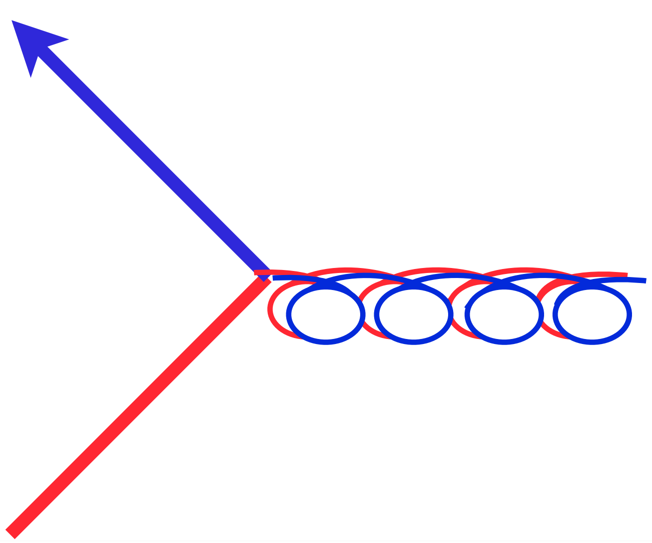
$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_{\mathrm{f}} \left(\mathrm{i} \not{D} - \mathrm{m}_{\mathrm{f}} \right) \psi_{\mathrm{f}} - \frac{1}{4} \mathrm{tr} \left(\mathrm{GG} \right)$$



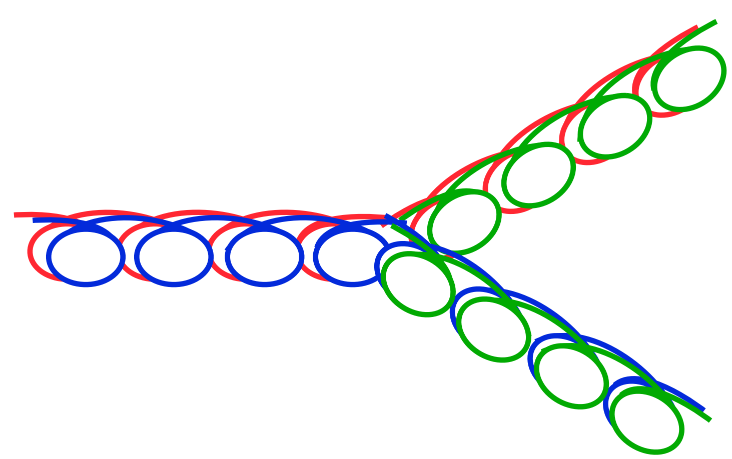
quarks

gluons

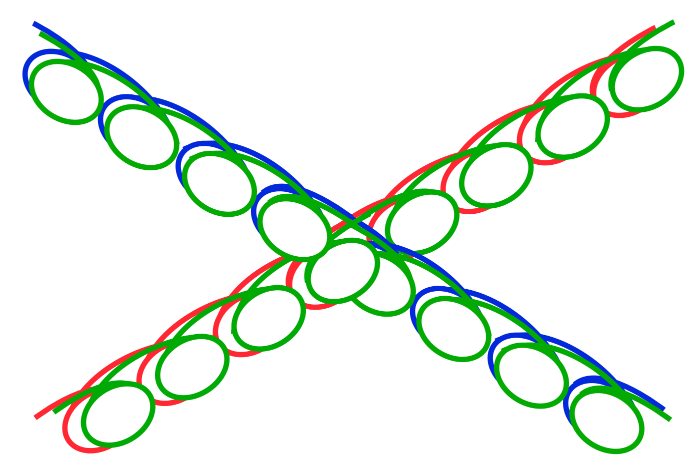




quarks & gluons couple



gluons can decay



gluons can scatter

Unfolding QCD

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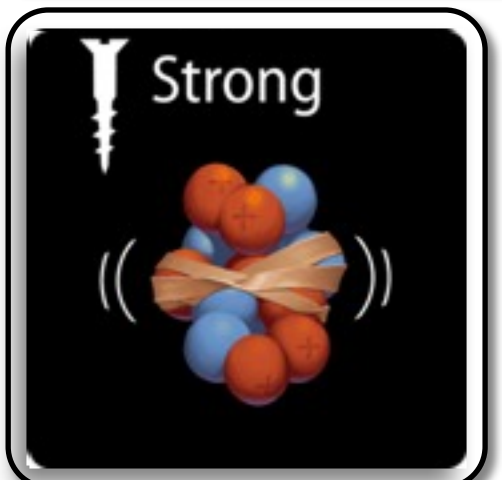
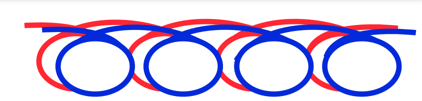
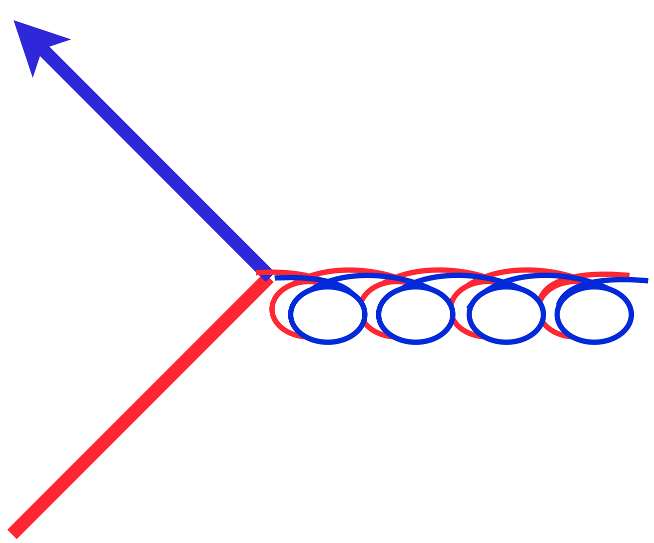


quarks

gluons



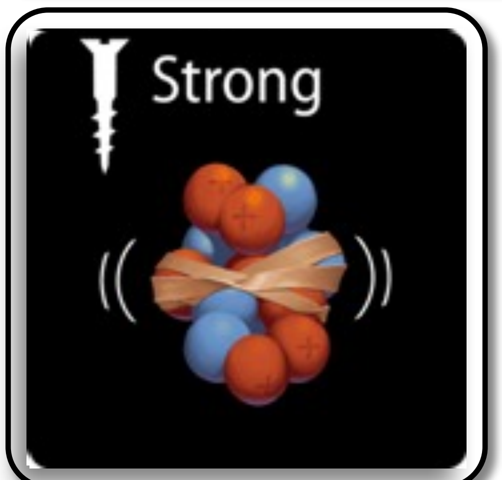


These effects make QCD look remarkably similar to QED!

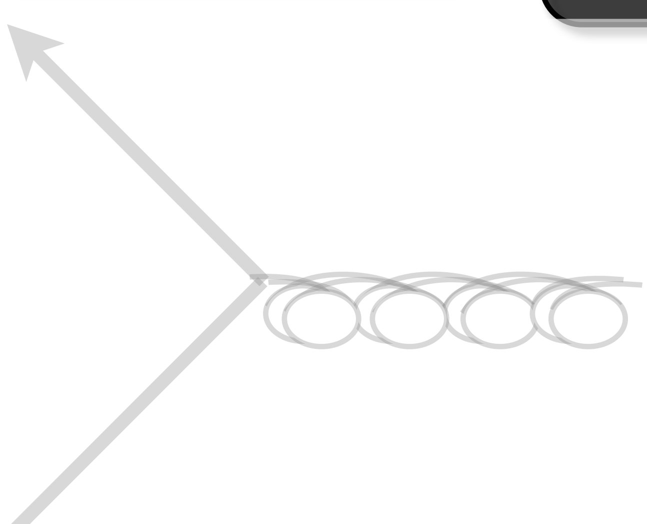
quarks & gluons couple

Unfolding QCD

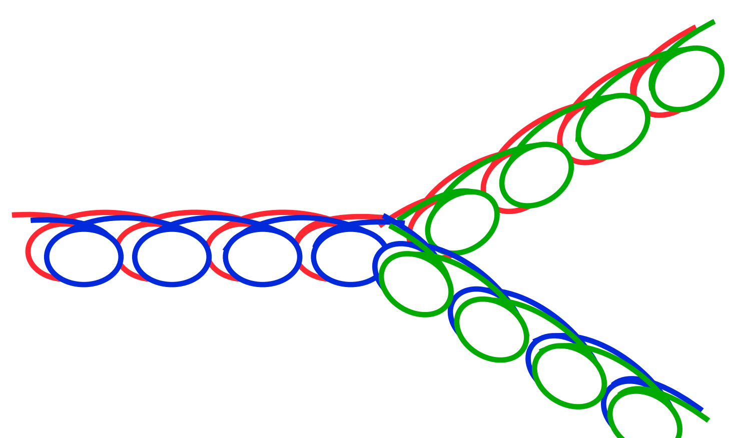
$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_{\mathrm{f}}\left(\mathrm{i}\,\not{D} - \mathrm{m}_{\mathrm{f}}\right)\psi_{\mathrm{f}} - \frac{1}{4}\mathrm{tr}\left(\mathrm{GG}\right)$$



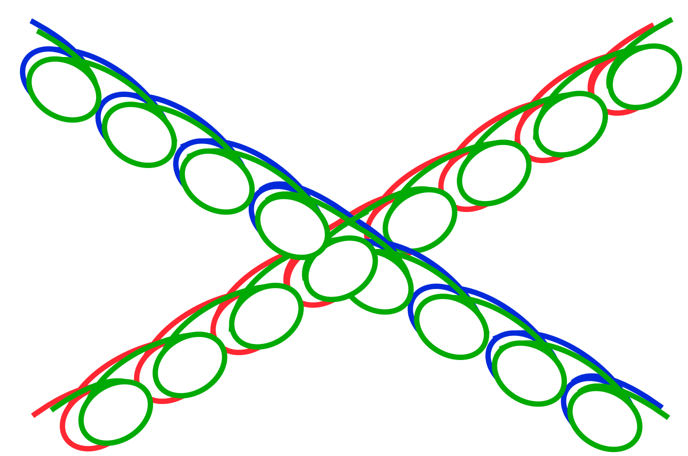
These effects make QCD have remarkably different behavior from QED!



quarks & gluons couple



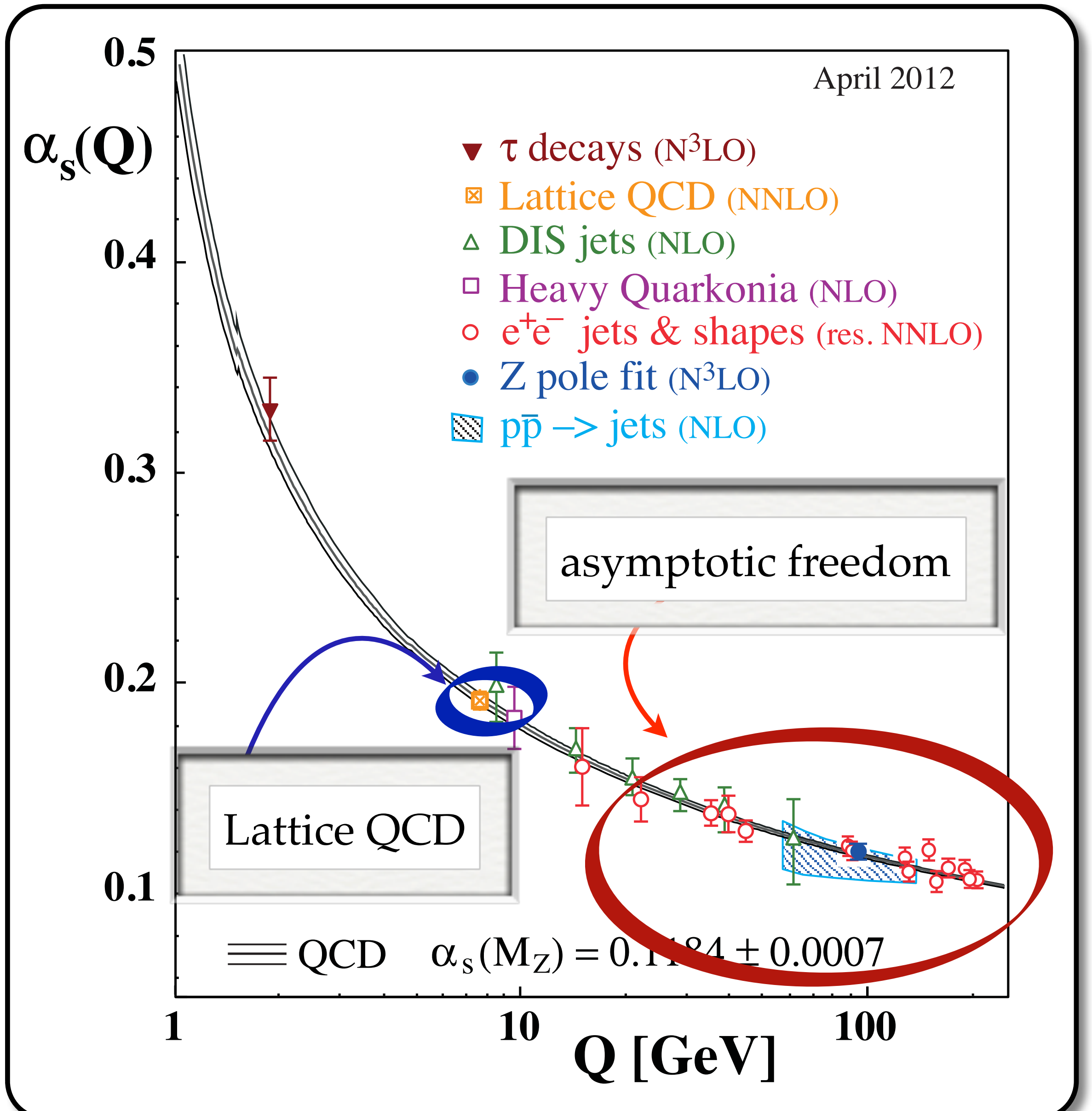
gluons can decay



gluons can scatter

Perturbative vs. non-perturbative

PDG Website



$$\beta(\alpha_s) = Q^2 \frac{\partial g}{\partial Q^2} = -(b_0 \alpha_s^2 + b_1 \alpha_s^3 + b_2 \alpha_s^4 + \cdots)$$

$$b_0 = (33 - 2n_f)/(12\pi)$$

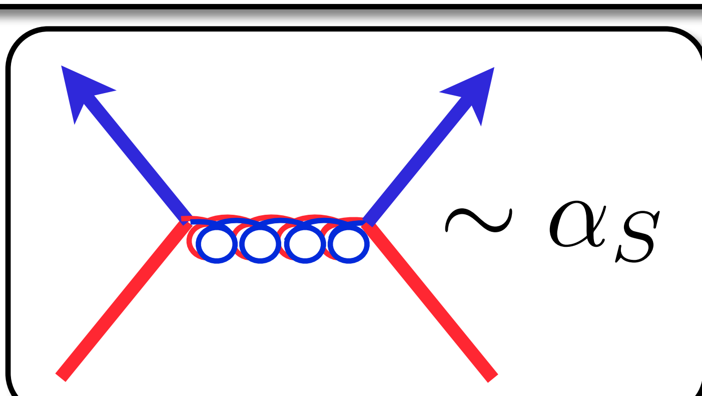
$$b_1 = (153 - 19n_f)/(24\pi^2)$$

$$b_2 = (2857 - \frac{5033}{9} n_f + \frac{325}{27} n_f^2)/(128\pi^3)$$

$$\ldots$$

$$\alpha_s(Q^2) \approx \frac{1}{b_0 ln_Q} \left(1 - \frac{b_1}{b_0^2} \frac{\ln t}{t} + \frac{b_1^2(\ln^2 t - \ln t - 1) + b_0 b_2}{b_0^4 t^2} - \frac{b_1^3(\ln^3 t - \frac{5}{2}\ln^2 t - 2\ln t + \frac{1}{2}) + 3 b_0 b_1 b_2 \ln t - \frac{1}{2} b_0^2 b_3}{b_0^6 t^3} \right)$$

$$\ln_q \equiv \ln \left(\frac{Q^2}{\Lambda_{QCD}^2} \right), \quad \Lambda_{QCD} \sim 200 \text{ MeV}$$



QCD is both!

Non-perturbative QCD

Three significant features of QCD

allows us to write down a theory in terms of quarks & gluons

low-energy degrees of freedom are not quarks & gluons, but rather hadrons

gives insight as to why the long-distance behavior of the strong nuclear force is dominated by pion-exchange, among many other things.

- asymptotic freedom
- confinement
- spontaneous chiral symmetry breaking

The last two are non-perturbative characteristic of QCD. Any hope to understand these, requires us to construct a non-perturbative framework for studying QCD at low-energies.

Non-perturbative QCD

Non-perturbative model-independent QCD tools:

- EFT (See talk by Dr. Danilkin,...)

parametrize analytic behavior of low-energy phenomena, but limited predictive power!

nicely complimentary!

- Lattice QCD

abundant predictive power, at the cost of loosing analytic handle of QCD

Lattice QCD:

- The *only fully predictive* tool we have for low-energy QCD
- Numerical QCD
- Requires introducing *well understood and controlled systematic* errors
- LQCD is not a model! It's simply a way to regularized QCD.

Outline

First half:

- [x] Why QCD / Lattice QCD?
- [ ] What's Lattice QCD?
- [ ] Symmetry?

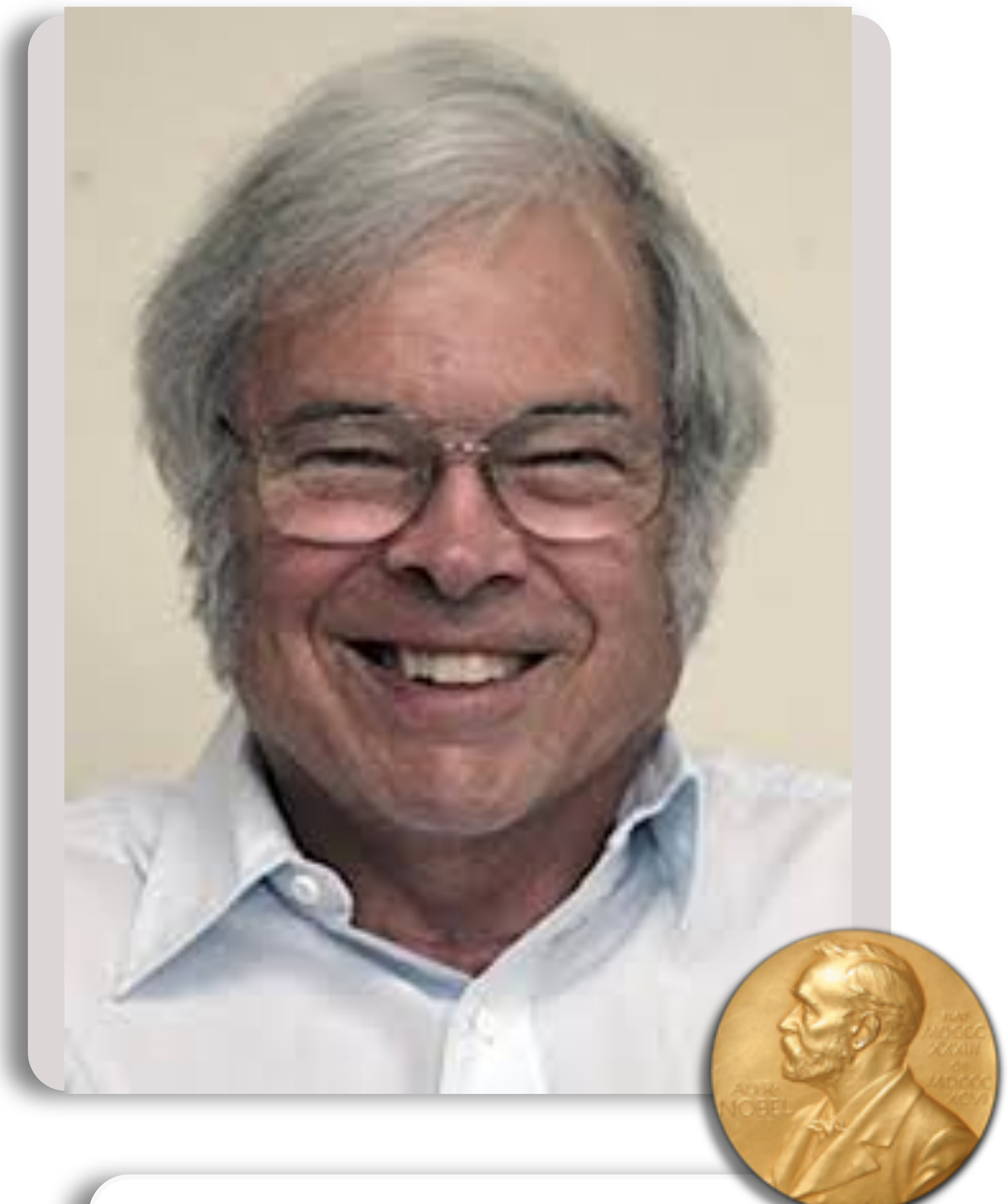
Second half:

- [ ] Masses & decay constants of single particles
- [ ] Scattering, resonances & bound states


Question?

Lattice QCD

Numerical
quantum chromodynamics (QCD)



Ken Wilson
1936-2013

Lattice QCD

Definition #1

- *"Lattice QCD is the formulation of QCD in a finite (L^3 by T), discretized 4D Euclidean spacetime. The basic building block is the numerical 4D Euclidean path integral."*

$$Z_T = \int \mathcal{D}[\psi, \bar{\psi}, U]\ e^{-S_E[\psi,\bar{\psi},U,L,T]}$$

Definition #2

- *"Lattice QCD refers to the numerical evaluation of quantum statistical mechanical properties of QCD in a discretized, finite volume (L^3). The basic building block is the canonical partition function, which is evaluated a finite temperature 1/T."*

$$Z_T = \mathrm{tr}\left[e^{-T\hat{H}_{QCD}[L]}\right]$$

one could also introduce a chemical potential...this is extremely challenging

A sketch for a scalar field theory

I claim that this equality holds for any QFT. To avoid technicalities regarding an SU(3) gauge theory, I will show this equivalence for a standard scalar field theory with an arbitrary set of interactions. We start with the second definition, and we must define the Hamiltonian for this theory:

$$\hat{H} = \int d^3x \left(\frac{1}{2}\hat{\Pi}^2(t,\mathbf{x}) + \frac{1}{2}\left(\nabla\hat{\Phi}(t,\mathbf{x})\right)^2 + \frac{m^2}{2}\hat{\Phi}^2(t,\mathbf{x}) + V(\hat{\Phi}(t,\mathbf{x}))\right)$$

The field operator and its canonical momentum operator, satisfy the standard equal time commutation relations:

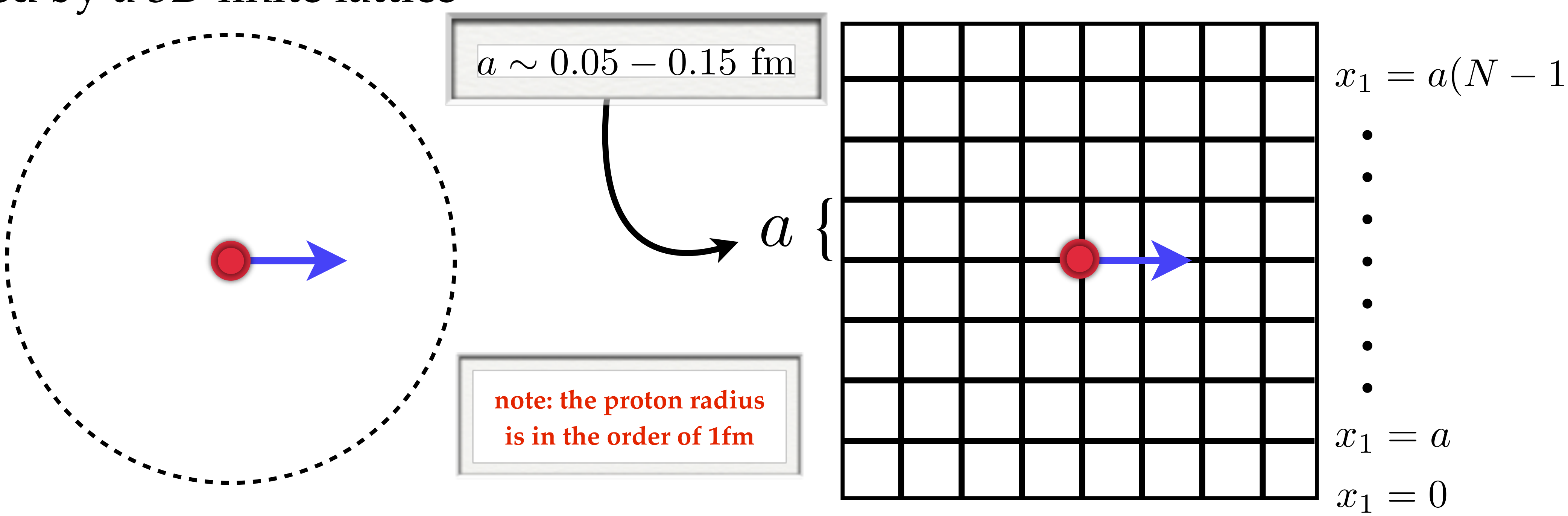
$$\left[\hat{\Phi}(t,\mathbf{x}),\hat{\Pi}(t,\mathbf{y})\right] = i\delta(\mathbf{x}-\mathbf{y}), \qquad \left[\hat{\Phi}(t,\mathbf{x}),\hat{\Phi}(t,\mathbf{y})\right] = 0, \qquad \left[\hat{\Pi}(t,\mathbf{x}),\hat{\Pi}(t,\mathbf{y})\right] = 0$$

Question: What is the relation between the field operator and the canonical momentum?

$$\hat{\Pi}(t,\mathbf{x}) \equiv \frac{\partial\mathcal{L}\left[\hat{\Phi}(t,\mathbf{x}),\partial_\mu\hat{\Phi}(t,\mathbf{x})\right]}{\partial(\partial_t\hat{\Phi}(t,\mathbf{x}))} = \partial_t\hat{\Phi}(t,\mathbf{x})$$

A sketch for a scalar field theory

In order to evaluate any meaningful QFT we must defined a UV regularization scheme. The standard continuum UV regularization is dimensional regularization (*"dim reg"*) since it preserves all the symmetries of the underlying theory, but of course there are many others (e.g., Pauli Villars, hard momentum cutoff, etc.). Alternatively, one could choose to study the QFT on a *lattice*. The basic idea is that the continuous spacetime is replaced by a 3D finite lattice



$$\mathbf{x} \Rightarrow a\mathbf{n}, \quad n_i = 0, 1, \ldots, N-1 \ \text{ for } \ i = 1, 2, 3$$

Boundary conditions needed. Typical choice is periodic boundaries, but one could pick antiperiodic, twisted, Dirichlet, etc.

A sketch for a scalar field theory

In order to write down the lattice scalar Hamiltonian, we must first discretize derivative:

$$\partial_j \hat{\Phi}(t,\mathbf{x}) = \frac{\hat{\Phi}(\mathbf{n}+\hat{j}) - \hat{\Phi}(\mathbf{n}-\hat{j})}{2a} + \mathcal{O}(a^2)$$

Note the change in the arguments of the field operators. With this we write the discretized Hamiltonian as at this order:

$$\hat{H} = \hat{H}_0 + \hat{U}, \qquad \hat{H}_0 = a^3 \sum_{\mathbf{n}} \frac{1}{2}\hat{\Pi}^2(\mathbf{n})$$

$$\hat{U} = a^3 \sum_{\mathbf{n}} \left(\frac{1}{2} \sum_{j=\{1,2,3\}} \left(\frac{\hat{\Phi}(\mathbf{n}+\hat{j}) - \hat{\Phi}(\mathbf{n}-\hat{j})}{2a} \right)^2 + \frac{m^2}{2}\hat{\Phi}^2(\mathbf{n}) + V(\hat{\Phi}(\mathbf{n})) \right)$$

We have neglected high order discretization corrections, but in practice we can keep track of these, and for actual Lattice QCD one *must* include higher order corrections. Having a discretized spacetime, the commutation relations now read:

$$\left[\hat{\Phi}(\mathbf{n}), \hat{\Pi}(\mathbf{n})\right] = \frac{i\delta_{\mathbf{n},\mathbf{n}'}}{a^3}, \qquad \left[\hat{\Phi}(\mathbf{n}), \hat{\Phi}(\mathbf{n}')\right] = 0, \qquad \left[\hat{\Pi}(\mathbf{n}), \hat{\Pi}(\mathbf{n}')\right] = 0$$

Note: take continuum limit and recover delta-function

A sketch for a scalar field theory

In order to evaluate the trace, we us the basis: $\hat{\Phi}(\mathbf{n})|\Phi\rangle = |\Phi\rangle\ \Phi(\mathbf{n})$

Which satisfies: $\langle\Phi'|\Phi\rangle = \delta(\Phi' - \Phi) \equiv \prod_{\mathbf{n}} \delta(\Phi'(\mathbf{n}) - \Phi(\mathbf{n}))$

note: even though we have discretized spacetime, the fields can take on a continuous set of values at each point in space

$$\mathbb{I} = \int \mathcal{D}\Phi |\Phi\rangle\langle\Phi|, \qquad \mathcal{D}\Phi \equiv \prod_{\mathbf{n}} d\Phi(\mathbf{n})$$

Now I will evaluate the trace in the following manner:

$$Z_T = \mathrm{tr}\left[e^{-T\hat{H}}\right] \equiv \int \mathcal{D}\Phi\ \langle\Phi|e^{-T\hat{H}}|\Phi\rangle = \lim_{N_T\to\infty} \int \mathcal{D}\Phi\ \langle\Phi|\widehat{W}_\epsilon^{N_T}|\Phi\rangle$$

$$= \lim_{N_T\to\infty} \int [\prod_j \mathcal{D}\Phi_j]\ \langle\Phi_1|\widehat{W}_\epsilon|\Phi_2\rangle\langle\Phi_2|\widehat{W}_\epsilon|\Phi_3\rangle\cdots\langle\Phi_N - 1|\widehat{W}_\epsilon|\Phi_1\rangle$$

note: the fact that the initial and final states are the same leads to periodic BCs

Where we have introduced: $\widehat{W}_\epsilon \equiv e^{-\epsilon\hat{U}/2} e^{-\epsilon\hat{H}_0} e^{-\epsilon\hat{U}/2}$

correct up to terms that vanish in the continuum limit

Last non-trivial step...

$$\langle\Phi_j|\widehat{W}_\epsilon|\Phi_{j+1}\rangle = \langle\Phi_j|e^{-\epsilon\hat{U}/2} e^{-\epsilon\hat{H}_0} e^{-\epsilon\hat{U}/2}|\Phi_{j+1}\rangle$$

$$= e^{-\epsilon(U[\Phi_j]+U[\Phi_{j+1}])/2}\langle\Phi_j|e^{-\epsilon\hat{H}_0}|\Phi_{j+1}\rangle$$

$$= \sqrt{\frac{a^3}{2\pi\epsilon}}^{N^3} e^{-\epsilon(U[\Phi_j]+U[\Phi_{j+1}])/2-(a^3/2\epsilon)\sum_{\mathbf{n}}(\Phi_{j+1}(\mathbf{n})-\Phi_j(\mathbf{n}))^2}$$

HW: Show the last equality!

A sketch for a scalar field theory

Now we simply need to recognize that...

$$S_E[\Phi] = a^3\epsilon \sum_{\mathbf{n}} \sum_{j=0}^{N_T-1} \left(\frac{1}{2}\left(\frac{\Phi_{j+1}(\mathbf{n}) - \Phi_j(\mathbf{n})}{\epsilon}\right)^2 + \frac{1}{2}\sum_{\hat{e}_k}\left(\frac{\Phi_j(\mathbf{n}+\hat{e}_k) - \Phi_j(\mathbf{n}-\hat{e}_k)}{2a}\right)^2 + \frac{m^2}{2}\Phi_j^2(\mathbf{n}) + V(\Phi_j(\mathbf{n}))\right)$$

Important features to recognize is the fact that the relative sign between the time and spatial derivative is the same. This is due to the fact that in Euclidean spacetime the metric is just the 4D Kronecker delta function. Also, the other signs make sense.

Putting all the pieces together we get:

I've absorbed the overall constant up front onto the measure...

$$\mathrm{tr}\left[e^{-T\hat{H}}\right] = \int [\prod_j \mathcal{D}\Phi_j] e^{-S_E[\Phi]}$$

Perfect time for questions!

Observables

Simplest example is the two-point correlation function. This is related to the probability of creating a state at some initial time, letting it propagate and then annihilating it. Some examples of operators are: $\mathcal{O} = \Phi,\ \mathcal{O} = \Phi^n,\ \mathcal{O} = \Phi\partial_\mu\Phi$

There are three representations for this object.

1

$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle_T \equiv \frac{1}{Z_T} tr[e^{-\hat{H}T}\mathcal{O}(t)\mathcal{O}^\dagger(0)]$$

$$= \frac{1}{Z_T} tr[e^{-\hat{H}(T-t)}\mathcal{O}(0)\ e^{-\hat{H}t}\mathcal{O}^\dagger(0)]$$

$$= \frac{1}{Z_T}\sum_{n,m} e^{-E_n(T-t)-E_m t}\ |\langle E_n|\mathcal{O}(0)|E_m\rangle|^2$$

t=separation time between source and sink. T=temporal extent of the lattice, i.e., *how big is the time part of our spacetime volume...*

This representation explains how to extract observables. For example, we know that by studying the exponential behavior of the correlation function, we can determine the spectrum and the matrix element of operators.

Observables

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1 $$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle_T = \frac{1}{Z_T}\sum_{n,m} e^{-E_n(T-t)-E_m t}\ |\langle E_n|\mathcal{O}(0)|E_m\rangle|^2$$

2 $$C(t) = \frac{1}{Z_T}\int [\prod_j \mathcal{D}\Phi_j]\mathcal{O}(t)\mathcal{O}^\dagger(0)\ e^{-S_E}$$

this representation, as will become apparent shortly, allows us to evaluate correlation functions numerically

Observables

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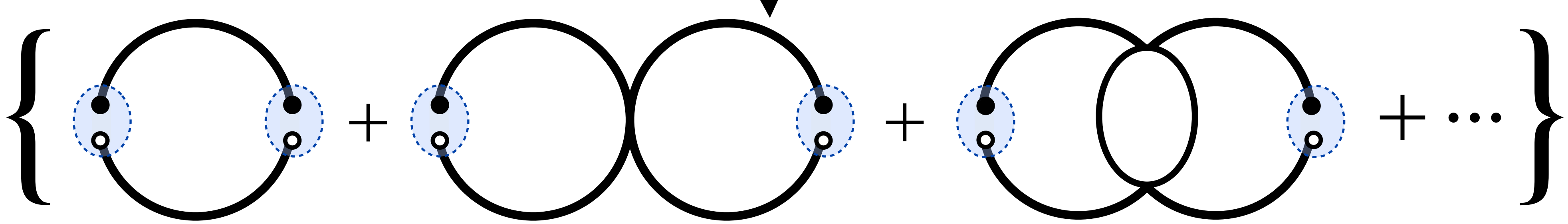
2 $$C(t) = \frac{1}{Z_T}\int [\prod_j \mathcal{D}\Phi_j]\mathcal{O}(t)\mathcal{O}^\dagger(0)\ e^{-S_E}$$

3 Sum over all Feynman diagrams:

hadrons: *the low-energy degrees of freedom*

e.g., $\pi\pi \to \pi\pi$

$C(t) = \text{F.T.}$ 

this representation gives *meaning* to the observables, and it will be the focus of the second lecture

Why Euclidean?

Generically we have to evaluate an integral of the form: $\langle f[\Phi]\rangle_T \equiv \int [\prod_j \mathcal{D}\Phi_j] e^{-S_E[\Phi]}\ f[\Phi]$

We could attempt to evaluate this using brute-force numerical tools, but this is a high-dimensionality integral, e.g. if we have a single scalar field, and we truncate spacetime such that (L^3 x T) = (10^3 x 10), then we have to approximately evaluate 10,000 integrals. Using a mesh of only 10 points per integral, this would require summing over ***~$10^{10,000}$ elements****! Typical LQCD calculations require integrating SU(3) gauge fields, which are functions of 8 parameters in spacetimes that are in the order of (L^3 x T) ~ (40^3 x 100). This would be a complete disaster!!!*

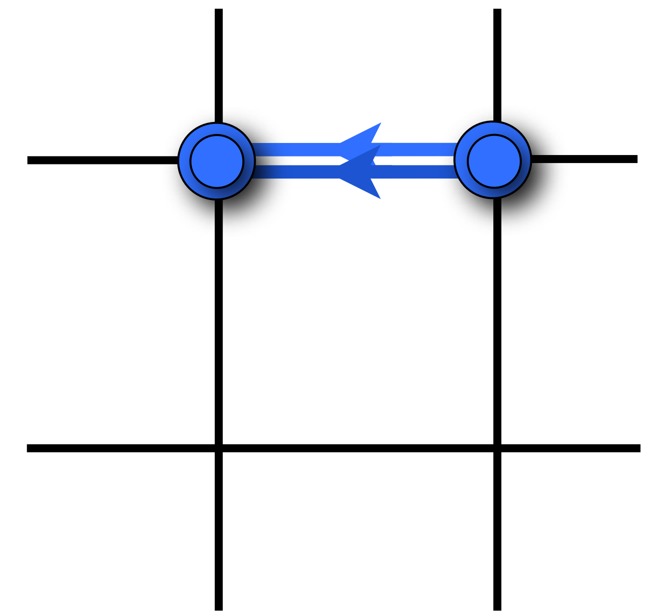
Instead we use **Monte Carlo** techniques. This requires defining a probability density: $e^{-S_E[\Phi]}$ over which we sample the different allowed configurations that the fields can take on. Note, the probability is maximum when the actions is minimized, which leads to classical solutions. Fluctuations away from this lead to quantum fluctuations.

Finally, the expectation value of this observable is the average & uncertainty of the different *measurements* in the this weighted sample.

$$\langle f[\Phi]\rangle_T \approx \bar{f} = \frac{1}{N_G}\sum_{g\in G} f[\Phi_g] \qquad \sigma_{\langle f[\Phi]\rangle_T} \approx \frac{1}{N_G}\sqrt{\sum_{g\in G}\ (f[\Phi_g] - \bar{f})}$$

Some details on the Lattice QCD

Some basics about Lattice QCD



- Quarks *live* in lattice sites
- Gluons *live* in the links between sites
- Fermions are integrated out exactly!

$$\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\; e^{-\bar{\psi}\mathbb{M}\psi} = \det[\mathbb{M}]$$

- Gauge configurations are generated using Monte Carlo
- Calculating propagators of quark at physical quark masses is hard! The majority of calculations are performed at unphysically heavy pion masses. This can be an advantage! Some calculations are performed at the physical point now!

$$\langle \longrightarrow \rangle \sim \mathbb{M}^{-1} \sim \frac{1}{m_q}$$

Nearly divergent eigenvalues!
Numerically noisy!

Outline

First half:

- [x] Why QCD / Lattice QCD?
- [x] What's Lattice QCD?
- [ ] Symmetry?

Second half:

- [ ] Masses & decay constants of single particles
- [ ] Scattering, resonances & bound states

What’s symmetry got to do with it?

We have Wick-rotated our spacetime to have the wrong metric, discretized spacetime and at the end we truncated it. This cannot have been done at zero cost! What did we loose?

anyone?...anyone?

What’s symmetry got to do with it?

We have Wick-rotated our spacetime to have the wrong metric, discretized spacetime and at the end we truncated it. This cannot have been done at zero cost! What did we loose?

- **Gauge symmetry remains intact!**
- No more Poincare symmetry = (translation) + (rotations) + (boost) (in particular we don’t have Lorentz symmetry and reduced rotational symmetry)
    - A continuous Euclidean spacetime has = (translation) + (rotations) + (reflections)
    - Discretized lattice have less allowed rotations (hypercubic for isotropic lattices)
    - Finite volumes have less allowed rotations (cubic for cubic volumes)
- Chiral symmetry (in the massless quark limit) is partially lost . It is modified in a non-trivial way.

Symmetry and physics

Less symmetry!

Something **must** be lost:
angular momentum conservation!

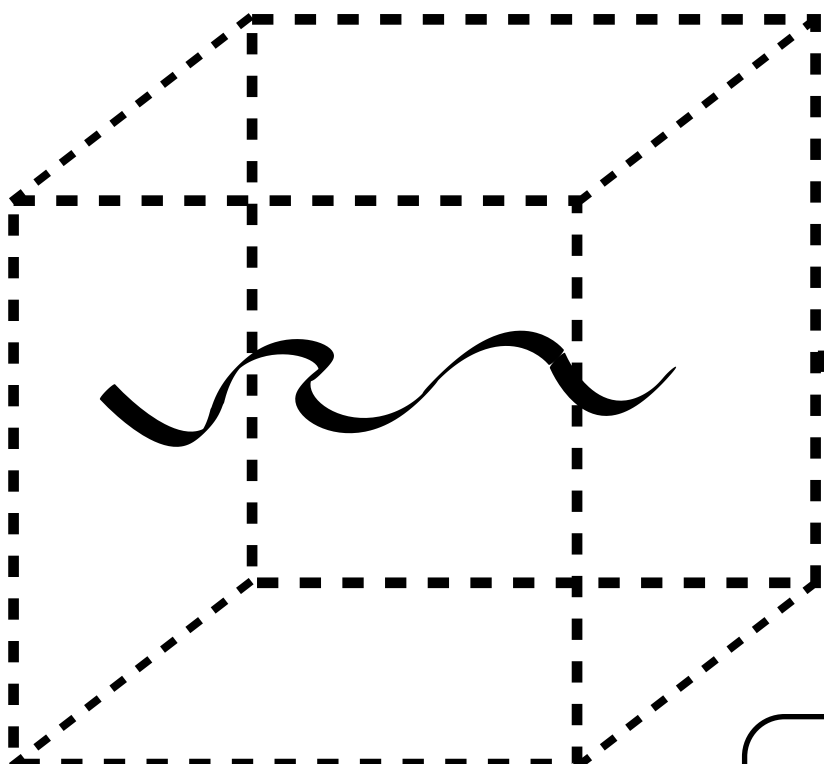
Symmetry and phys

More fun with cats
in a box this afternoon!

Less symmetry!

Something **must** be lost:
angular momentum conservation!

Final remarks



Euclidean Spacetime

- Hadronic spectra: $\mathrm{E}(\mathrm{a}, \mathrm{L}, \mathrm{T}, \mathrm{m_q})$
- Matrix elements: $\mathcal{A}(\mathrm{a}, \mathrm{L}, \mathrm{T}, \mathrm{m_q})$

- **Formalism** *(this afternoon!)*
- Limits: $(\mathrm{a} \to 0, \mathrm{L} \to \infty, \mathrm{T} \to \infty, \mathrm{m_q} \to \mathrm{m_q^{phys}})$

- Physics: hadron masses, decay constants, scattering parameters, form factors,...

Minkowski Spacetime

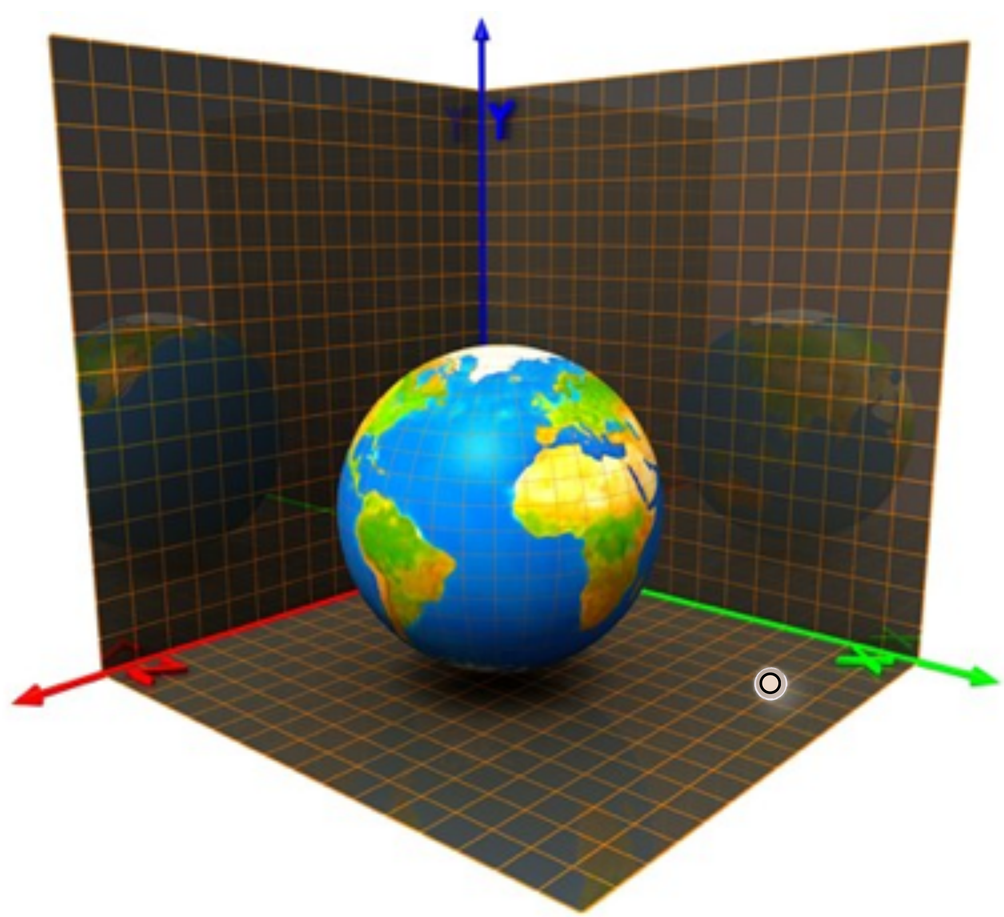

Question?

Nuclear Physics from Lattice QCD (part 2)

The why's, what's and how's...

Raúl Briceño

Jefferson Lab



HUGS, June 2014

Outline

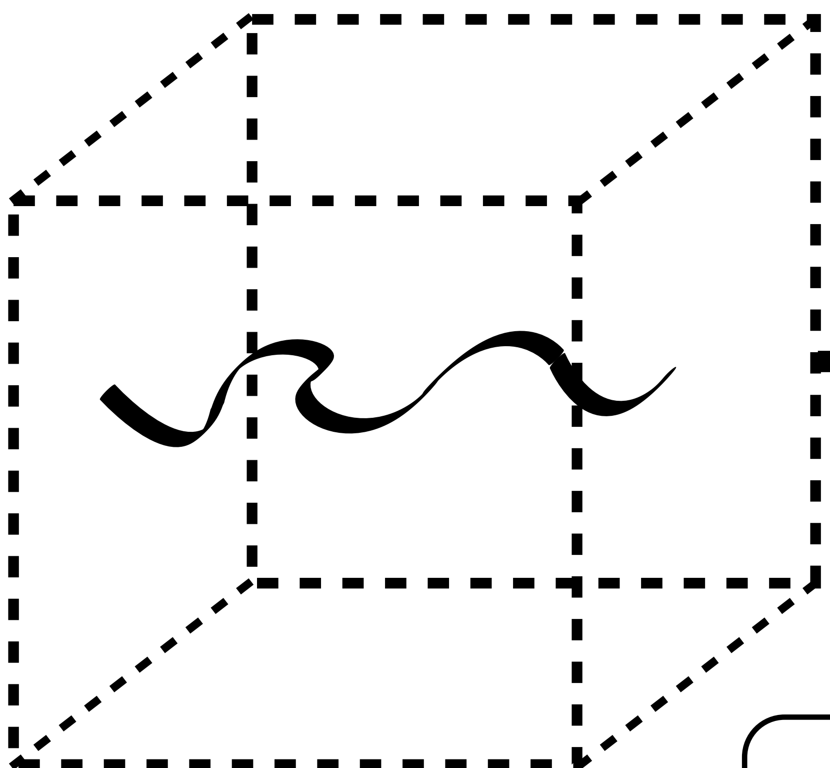
First half:

- ☑ Why QCD / Lattice QCD?
- ☑ What's Lattice QCD?
- ☑ Symmetry?

Second half:

- ☐ Masses & decay constants of single particles
- ☐ Scattering, resonances & bound states

Recap



Euclidean Spacetime

- Hadronic spectra: $\mathrm{E(a, L, T, m_q)}$
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- **Formalism**
- Limits: $(\mathrm{a} \to 0, \mathrm{L} \to \infty, \mathrm{T} \to \infty, \mathrm{m_q} \to \mathrm{m_q^{phys}})$

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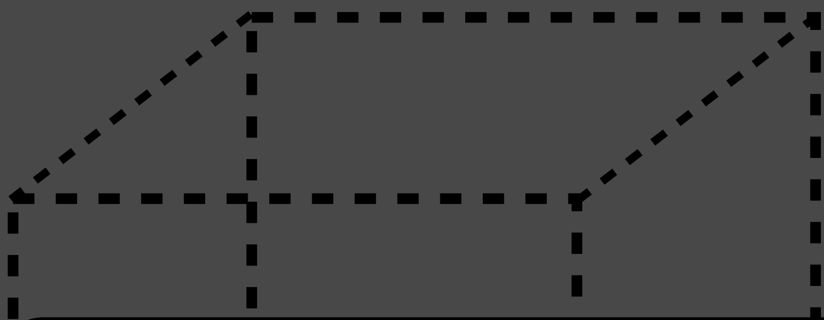
Minkowski Spacetime

Recap



Hadronic spectra: $E(a, L, T, m_q)$

Disclaimer: for the remainder of today, I will forget about discretization effects...

Limits: $(a \to 0, L \to \infty, T \to \infty, m_q \to m_q^{phys})$

Physics: hadron masses, decay constants, scattering parameters, form factors,...

Minkowski Spacetime

Recap

Simplest example is the two-point correlation function. This is related to the probability of creating a state at some initial time, letting it propagate and then annihilating it. Some examples of operators are: $\mathcal{O} = \Phi, \; \mathcal{O} = \Phi^n, \; \mathcal{O} = \Phi \partial_\mu \Phi$

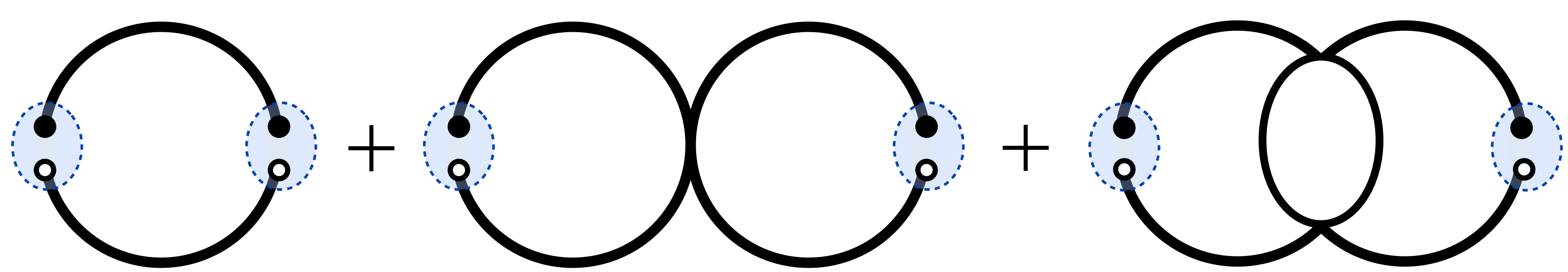
There are three representations for this object.

1 $$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle_T = \frac{1}{Z_T}\sum_{n,m} e^{-E_n(T-t)-E_m t} \; |\langle E_n|\mathcal{O}(0)|E_m\rangle|^2$$

2 $$C(t) = \frac{1}{Z_T}\int [\prod_j \mathcal{D}\Phi_j] \mathcal{O}(t)\mathcal{O}^\dagger(0) \; e^{-S_E}$$

3 Sum over all Feynman diagrams:

e.g., $\pi\pi \to \pi\pi$

$C(t) = \text{F.T.} \Big\{$  $+ \cdots \Big\}$

Physics ~~Kittens~~ in a box

One particle in a finite volume

(developing some intuition)

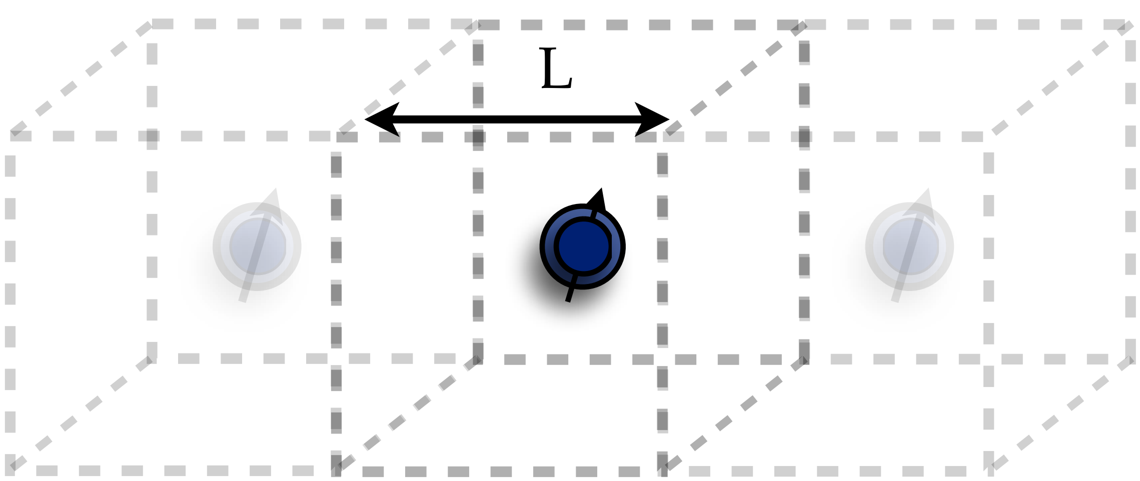
Before diving into details, what should we expect? Consider the simple case when the ground state is much lighter than the first excited state, or when $t, T >> 1/E_n$:

$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle_T = \frac{1}{Z_T}\sum_{n,m} e^{-E_n(T-t)-E_m t}\, |\langle E_n|\mathcal{O}(0)|E_m\rangle|^2 \to \mathcal{A}_T \cosh[E_0(t-T/2)]$$

a constant that depends on the temporal extent

From the asymptotic behavior of the correlation function we get the energy of a single particle in a periodic box! How should we interpret this?
We should expect finite volume effects from the interaction of the particle with its various mirror images.
How large does the box need to be to be able to neglect finite volume effects? 1cm,1m,1km...? What sets this scale?

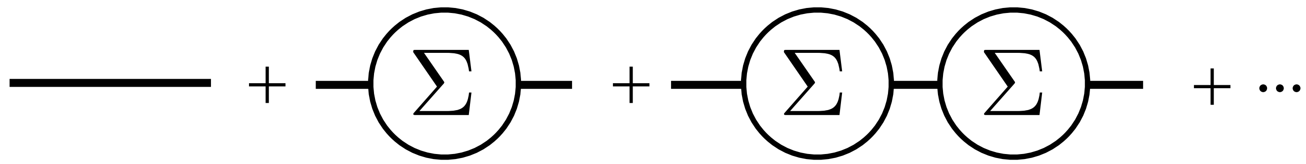
Hint: what dictates the long range piece of the nuclear force?



One particle in a finite volume

(mathematical tools)

Remember the third representation of the correlation functions? Just go ahead and calculate the correlation function:

$C(P) =$ 

$$= \frac{i}{P^2 - m_0^2 + \Sigma(L,T,P^2) + i\epsilon} \equiv \frac{i\ Z_h(L,T)}{P^2 - m_h(L,T)^2 + i\ \epsilon}$$

This result is generic and independent about the nature of the particle of interest. If we want to obtain the spectrum, for example, then we simply need to look at the pole of the propagator, which we can relate to the self-energy in the following self-consistent and perturbative fashion

$$p^2 = m_0^2 - \Sigma(L,T,p^2) = m_0^2 - \Sigma(L,T,m_0^2) + \cdots = \underbrace{m_0^2 - \Sigma(\infty,\infty,m_0^2)}_{(m_h^{\text{phys}})^2} - \underbrace{(\Sigma(L,T,m_0^2) - \Sigma(\infty,\infty,m_0^2))}_{\delta\Sigma(L,T,m_0^2)}$$

$$= (m_h^{\text{phys}})^2 - \delta\Sigma(L,T,(m_h^{\text{phys}})^2) + \cdots \equiv (m_h(L,T))^2$$

finite volume correction: if we can show that this quantity is small, then we are in business!

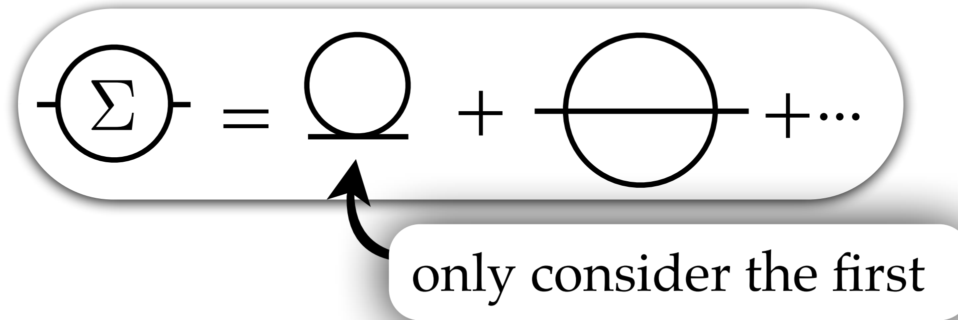
infinite volume mass

One particle in a finite volume

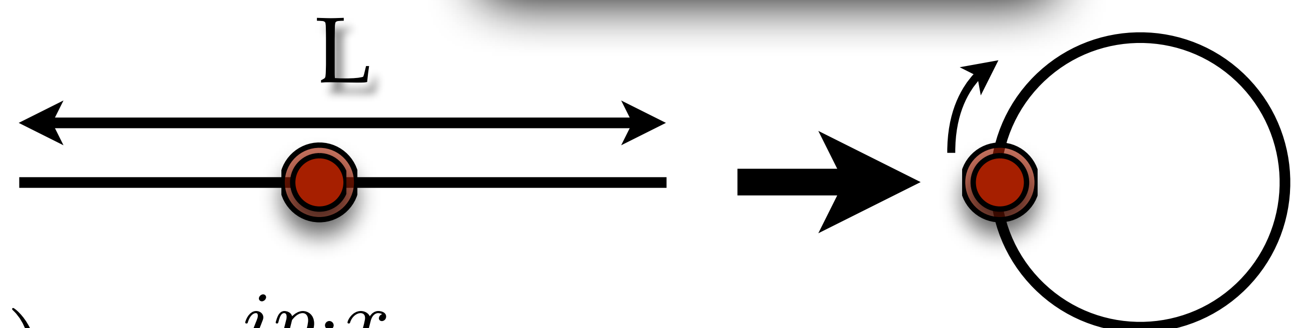
(mathematical tools)

In order to calculate self-energy consider a toy low-energy Lagrangian, say for some stable scalar meson (there's no such a thing, all stable mesons are pseudoscalars, but bare with me)

$$\mathcal{L}_{toy} = \frac{1}{2}\phi\left(-\partial^2 - m^2\right)\phi - \frac{\lambda}{4!}\phi^4$$



Remember, we live in a periodic volume:



Field operators will have the form: $\phi(x) \sim e^{ip\cdot x}$

Imposing period boundary conditions: $\phi(T, L) = \phi(0)$

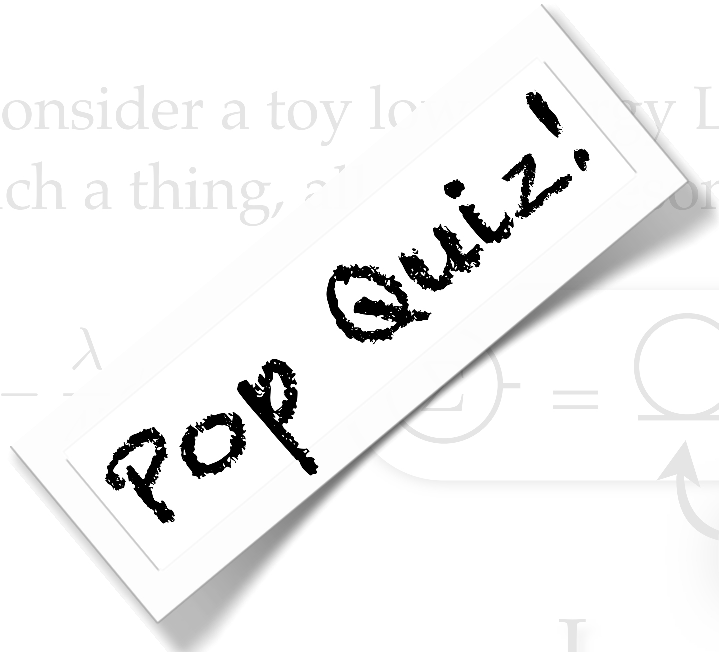
Discretized momenta: $\mathbf{p} = \dfrac{2\pi\mathbf{n}}{L}$ where $\mathbf{n} = [\{000\}, \{001\}, \{00-1\}, \{010\}, \ldots]$

Matsubara frequencies: $\omega_{n_0} = \dfrac{2\pi n_0}{T}$

Due to time constraint, I will neglect finite T effects and make it infinite. This is a good approximation since one can show that corrections scale like *exp(-Tm*$_\pi$) ~ *exp(-10)*

One particle in a finite volume

(mathematical tools)



only consider the first

L

Answer: These are the numerical values that **n²** can take from 0 to 9.

Remember, we live in a periodic volume.

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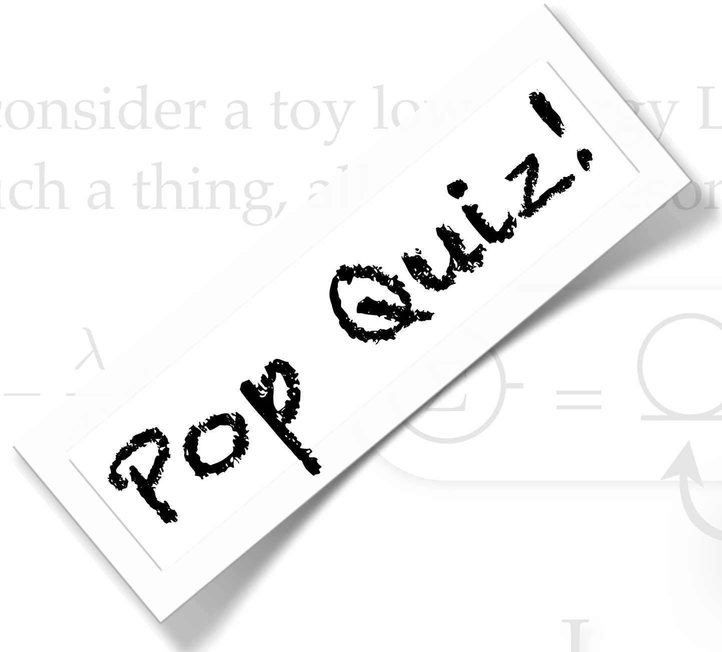
One particle in a finite volume

(mathematical tools)



Answer: These are the numerical values that $\mathbf{n}^2$ can take from 0 to 9.

Question: What are 0,1,2,3,4,5,6,8,9?

Proof (?): n={000}, n²=0

n= [{001},{00-1}...,{-100}], n²=1

n= [{011},{011}...,{-1-10}], n²=2

n= [{111},{11-1}...,{-1-1-1}], n²=3

n= [{002},{00-2}...,{-200}], n²=4

n= [{201},{20-1}...,{-10-2}], n²=5

n= [{211},{21-1}...,{-1-1-2}], n²=6

n= [{022},{02-2}...,{-2-20}], n²=8

n= [{122},{12-2}...,{-2-2-1}], n²=9

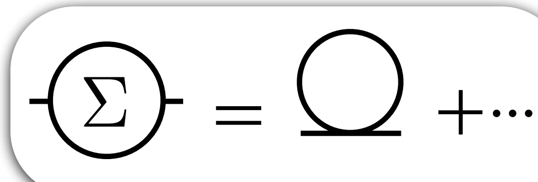
$$\mathbf{n} = [\{000\}, \{001\}, \{00-1\}, \{010\}, \ldots]$$

Due to time constraint, I will neglect finite T effects and make it infinite. This is a good approximation since one can show that corrections scale like *exp(-Tmπ) ~ exp(-10)*

One particle in a finite volume

(mathematical tools)

Finally we can write down the self-energy of our *"toy pion"*:



$$i\Sigma(L) = \frac{\lambda}{L^3}\sum_{\mathbf{n}}\int\frac{dk_0}{2\pi}\,\frac{1}{k_0^2 - (\frac{2\pi\mathbf{n}}{L})^2 - m^2 + i\epsilon}$$

Using the Poisson resummation formula: $\frac{1}{L^3}\sum_{\mathbf{k}=\frac{2\pi\mathbf{n}}{\mathbf{L}}} f(\mathbf{k}) = \int\frac{d^3k}{(2\pi)^3}f(\mathbf{k}) + \sum_{\mathbf{n}\neq 0}\int\frac{d^3k}{(2\pi)^3}f(\mathbf{k})\ e^{iL\mathbf{n}\cdot\mathbf{k}}$

We find:

$$\boxed{\delta m^2(L) \equiv -\delta\Sigma(L) = \frac{\lambda}{2m}\sum_{\mathbf{n}\neq 0}\left(\frac{m}{2\pi L\ n}\right)^{3/2} e^{-nmL}}$$

We want this to be zero!

Again, this is exponentially suppressed, except *exp*(-*Lm*π) ~ *exp*(-4) (nevertheless small).

Punch line: *"get a big enough box and you might as well forget about the fact that you performed calculations in a finite Euclidean spacetime"*

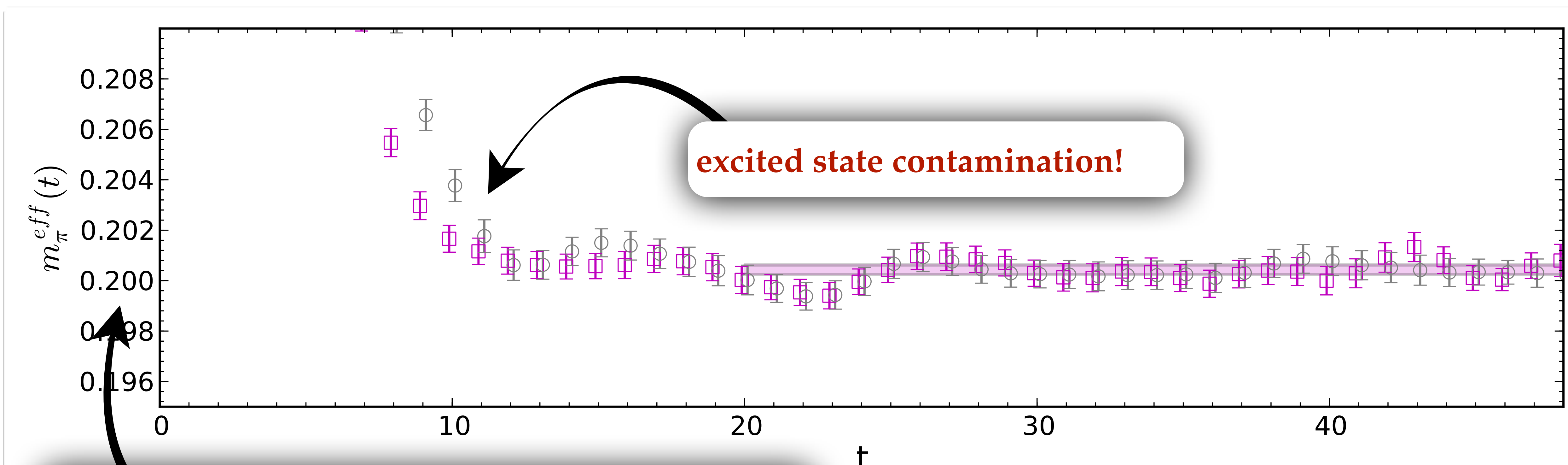
One example!

Too much math, let's look at some pretty plot!

This is work by the NPLQCD Collaboration. You can find the electronic copy of the paper in this [link].

Remember: $C_\pi(t) \to \mathcal{A}_{T,\pi} \cosh[m_\pi(t - T/2)]$

Effective mass plot: $m_\pi^{eff}(t) \equiv \cosh^{-1}\left[\frac{C_\pi(t-1) + C_\pi(t+1)}{2C_\pi(t)}\right] \to m_\pi$



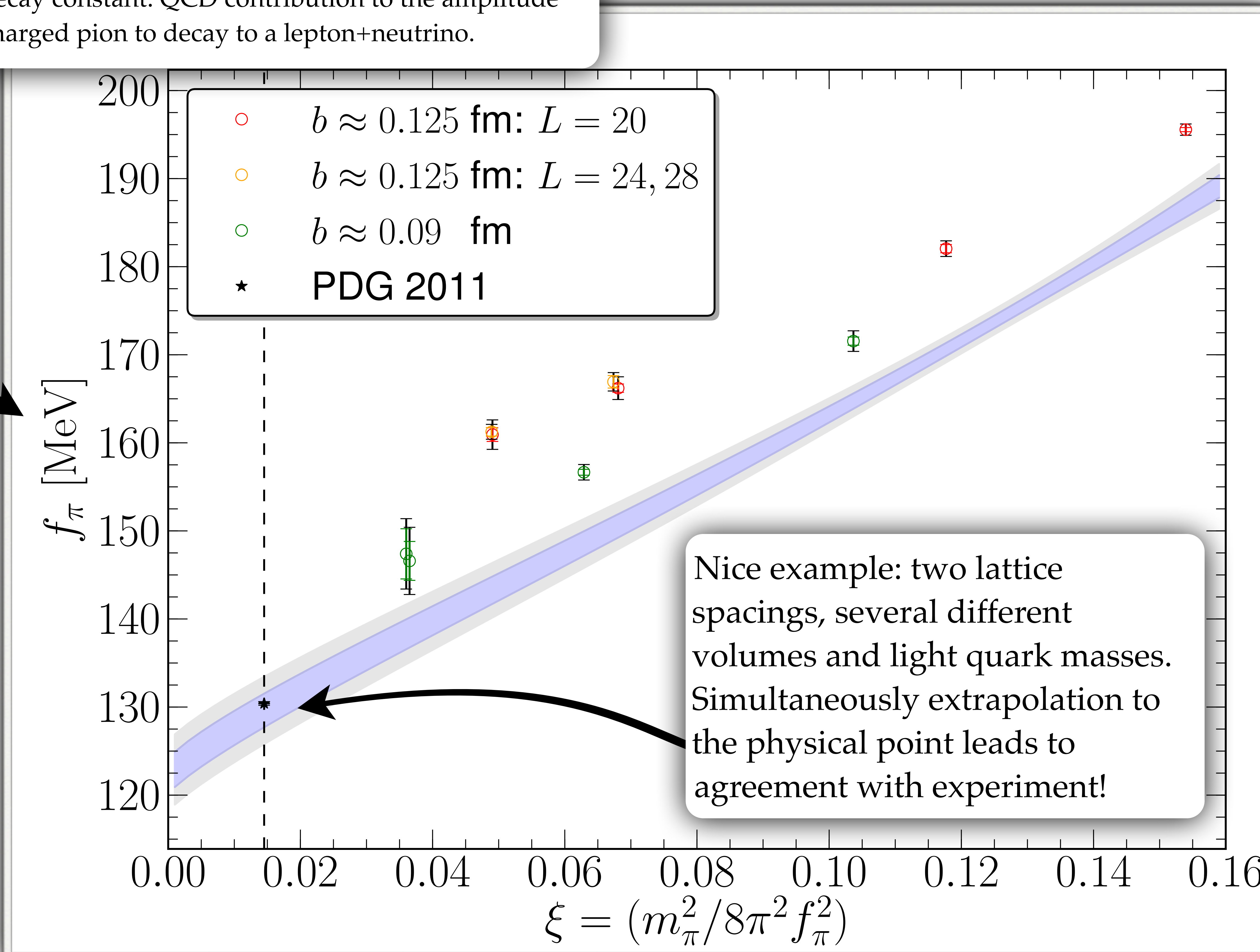
define in lattice spacing units. Lattice spacing is a~0.09fm, so this corresponds to a physical value of m_π~0.2x197/0.09 MeV ~440 MeV.

Question: Why 197?

One example!

Too much math, let's look at some pretty plot!

Pion decay constant: QCD contribution to the amplitude for a charged pion to decay to a lepton+neutrino.



Nice example: two lattice spacings, several different volumes and light quark masses. Simultaneously extrapolation to the physical point leads to agreement with experiment!

Outline

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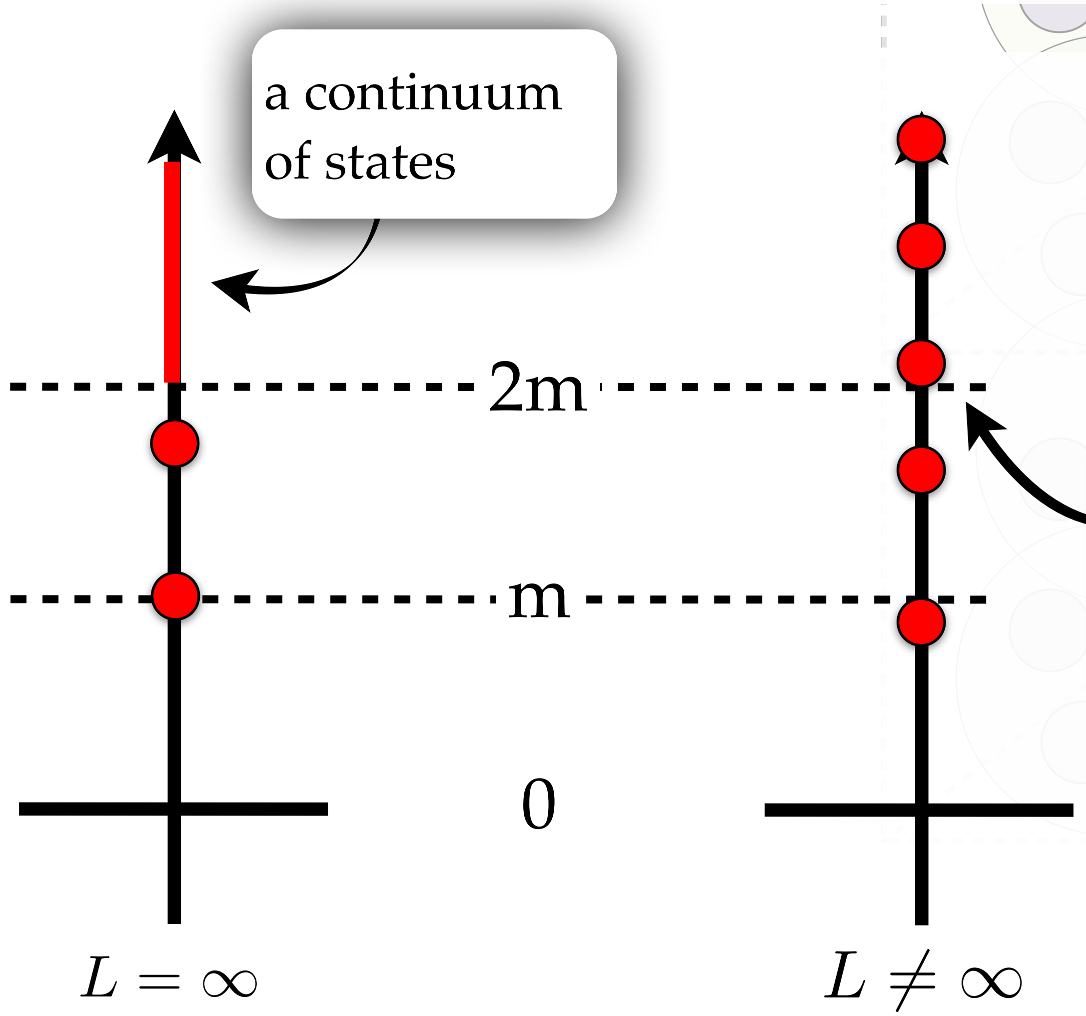
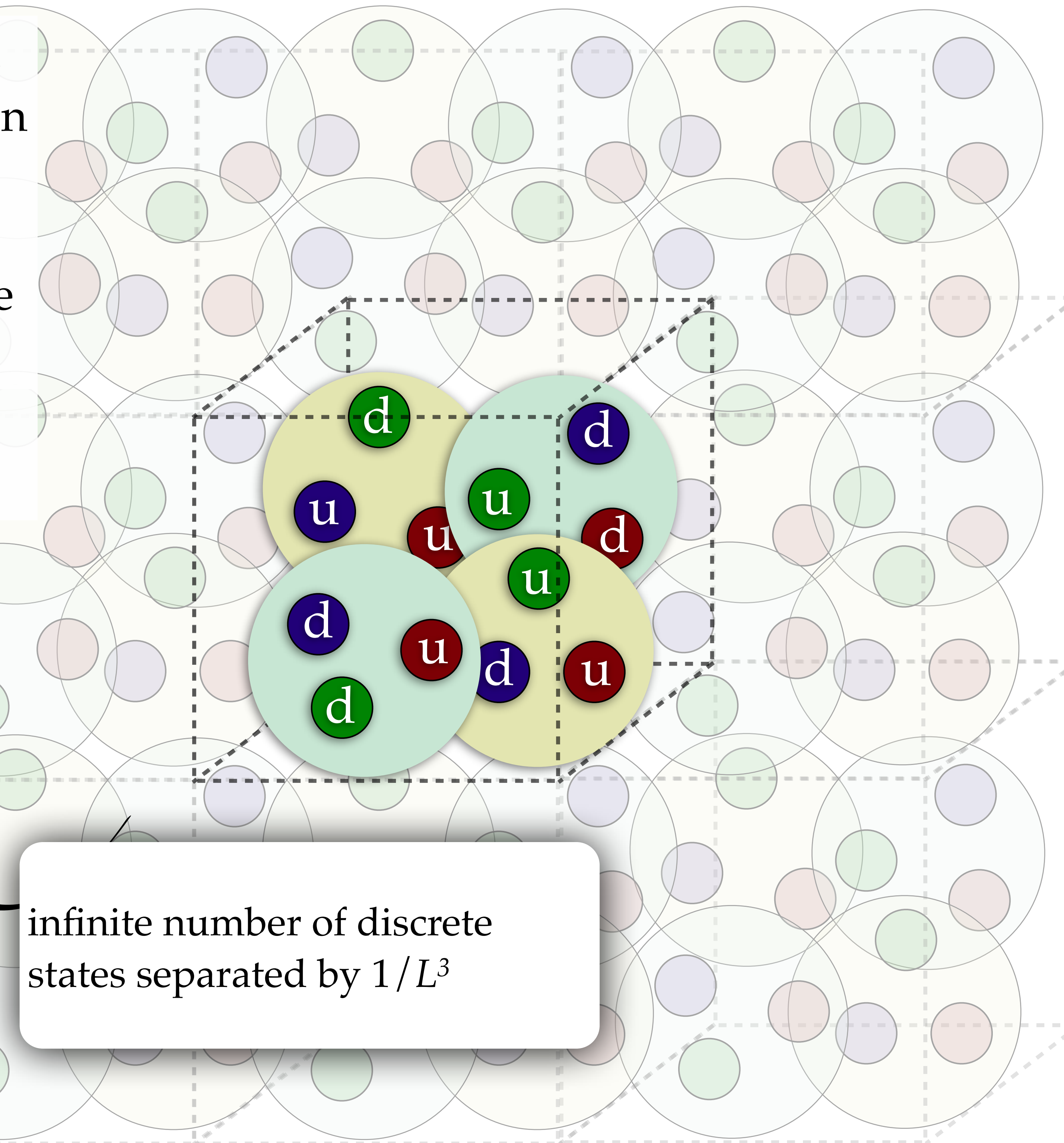
Many-particles a finite volume?

With such success in the one-body sector, we would be tempted to just jump right in to study many-body physics! Unfortunately, physics is not as kind to us...life get hard really quickly as you pile more and more particles in a box.

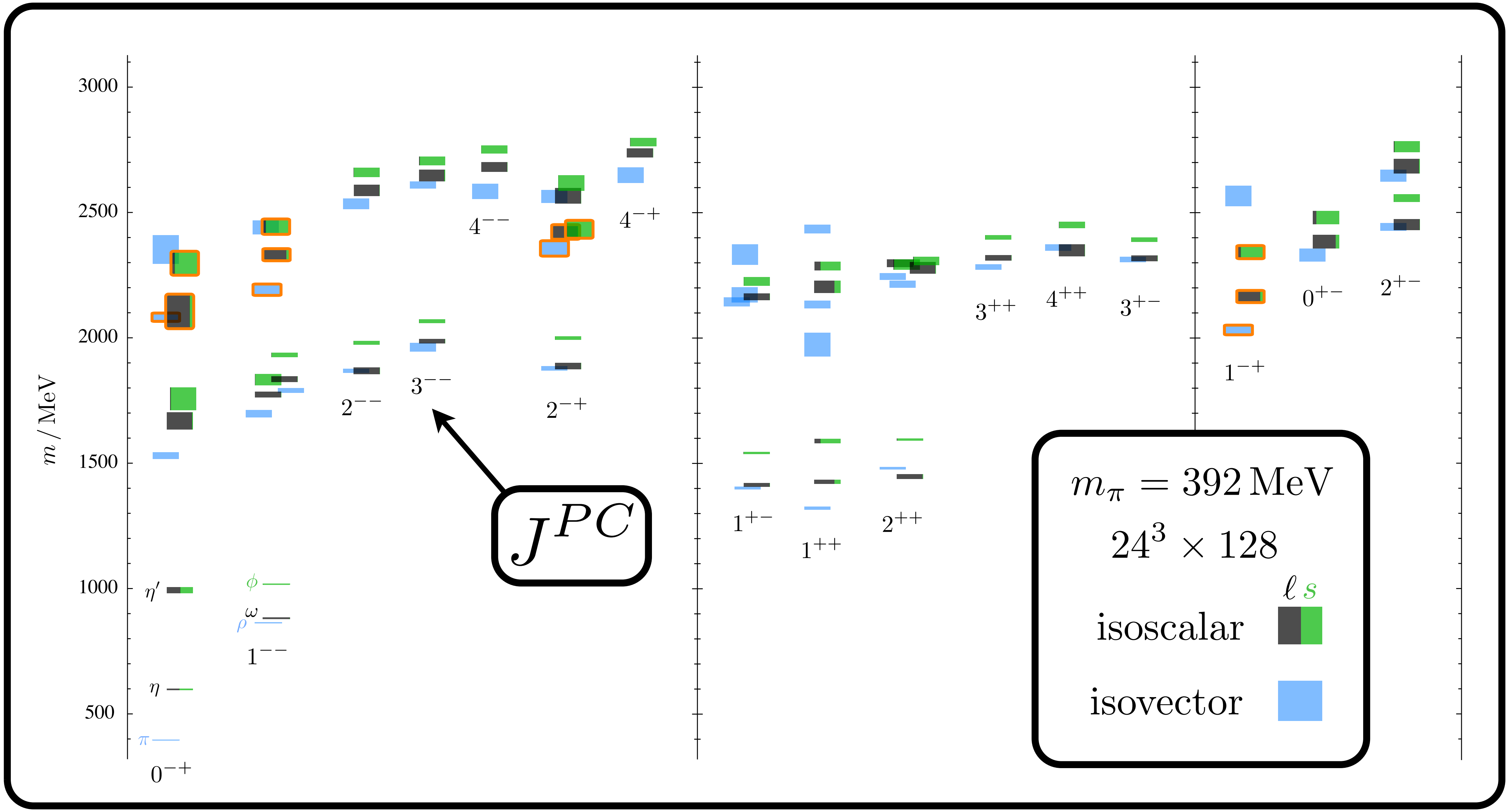
To start: if we calculate a two-particle energy, what would it mean?





Actual lattice results

in the meson sector



Hadron Spectrum Collaboration: [PRD] arXiv:1309.2608 [hep-lat]
J. Dudek, R. Edwards, P. Guo & C. Thomas (2013)

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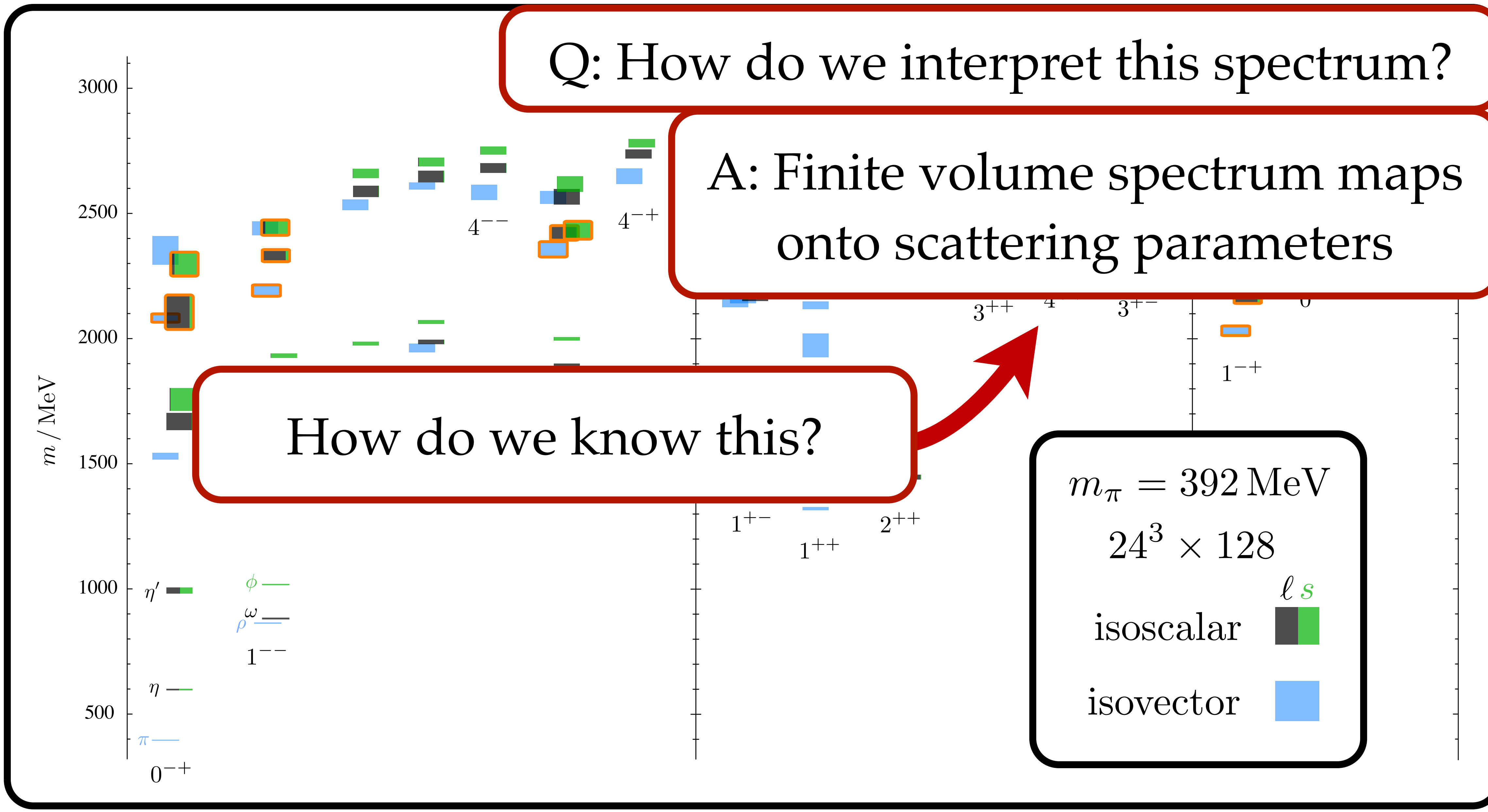

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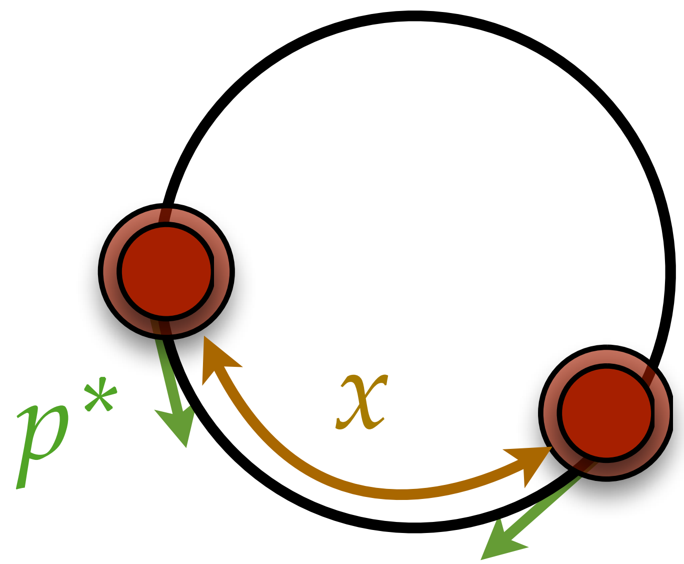
Reinventing the *quantum-mechanical* wheel

Two particles:



- Probability conservation
- Infinite volume scattering phase shift

$$\psi(x) \sim e^{ip^* x + i2\delta(p^*)}$$

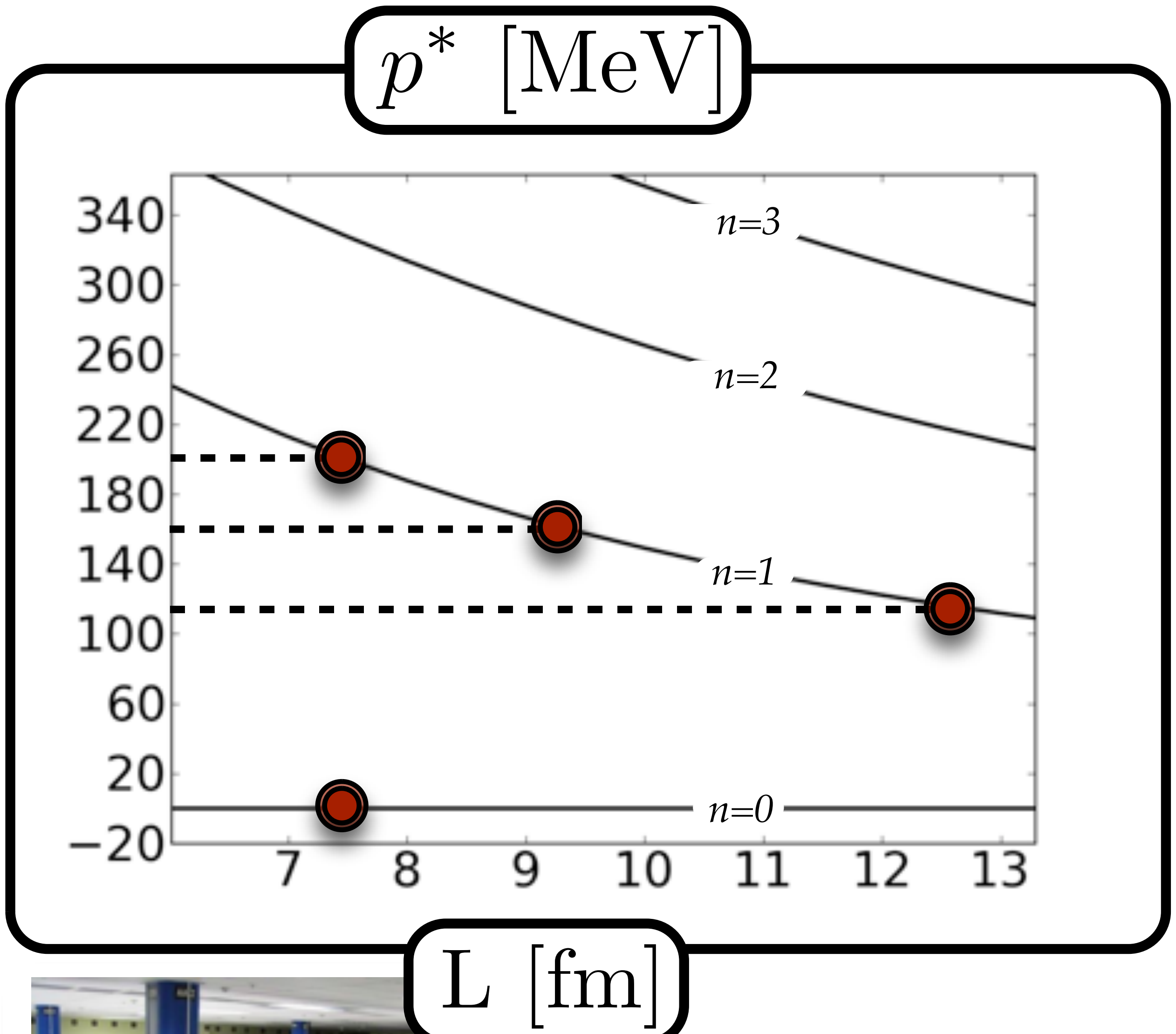
Asymptotic wavefunction

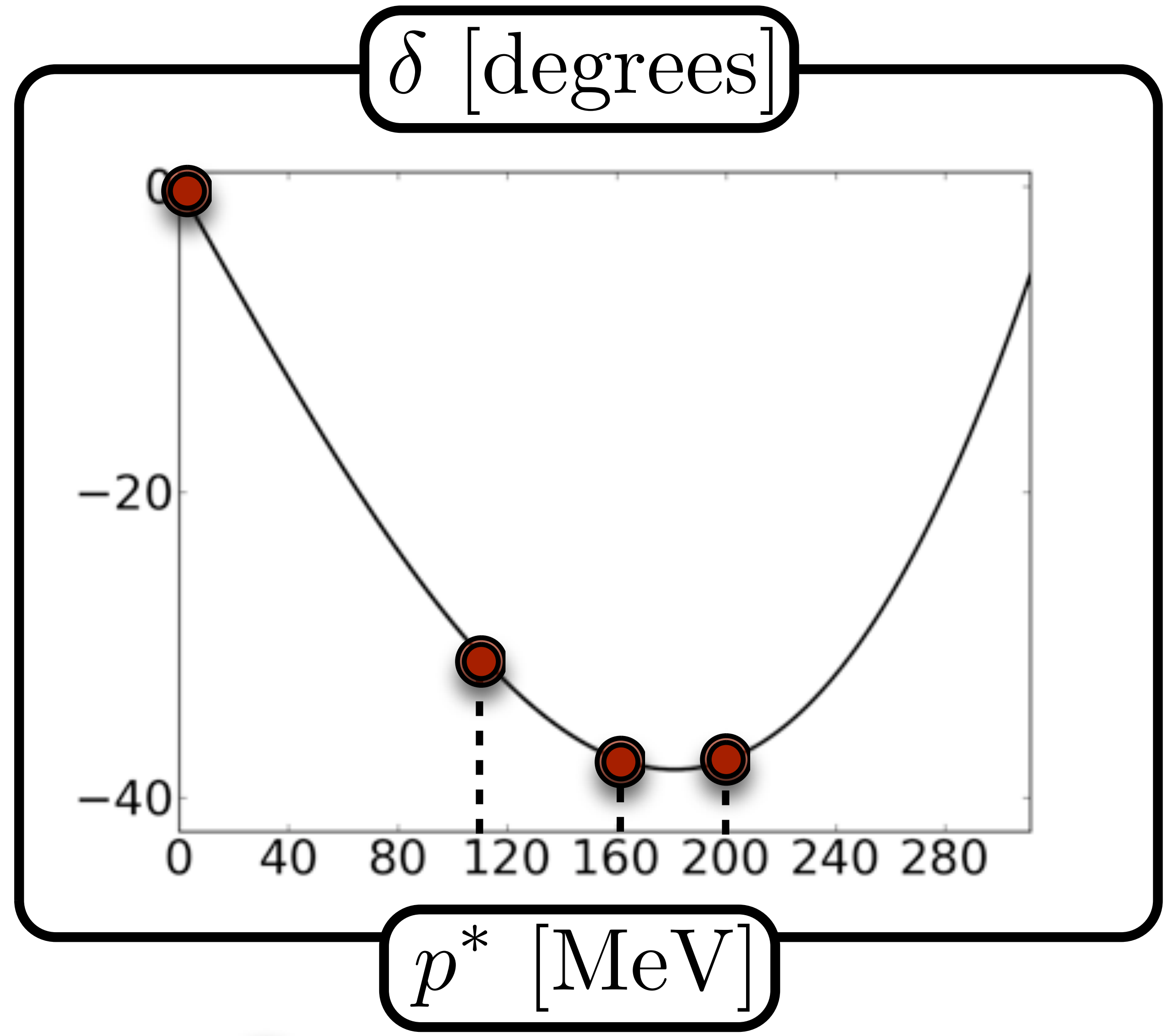
Periodicity: $\psi(L) = \psi(0)$

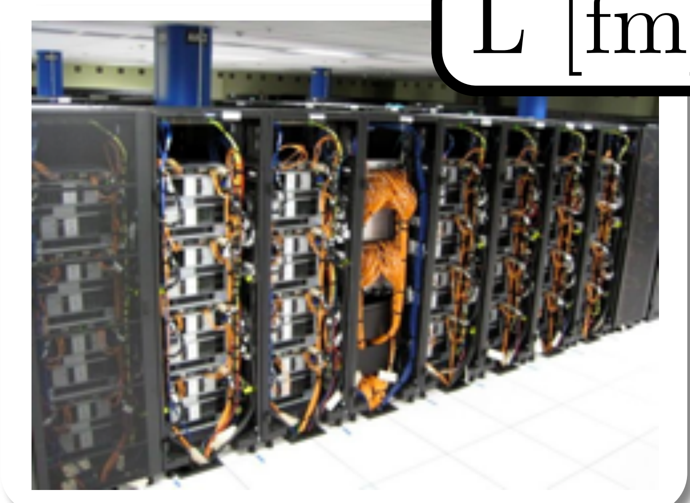
Quantization condition: $\boxed{L\ p_n^* + 2\delta(p_n^*) = 2\pi n}$

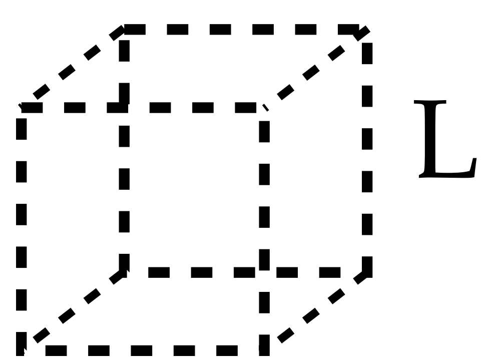
Reinventing the *quantum-mechanical* wheel

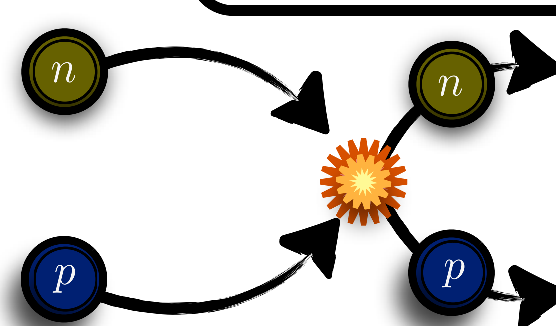
$$\boxed{L\, p_n^* + 2\delta(p_n^*) = 2\pi n}$$







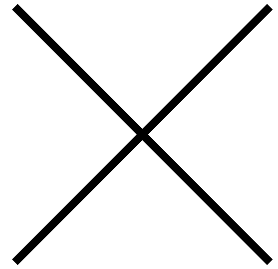




$\sim (\sin\delta)^2$

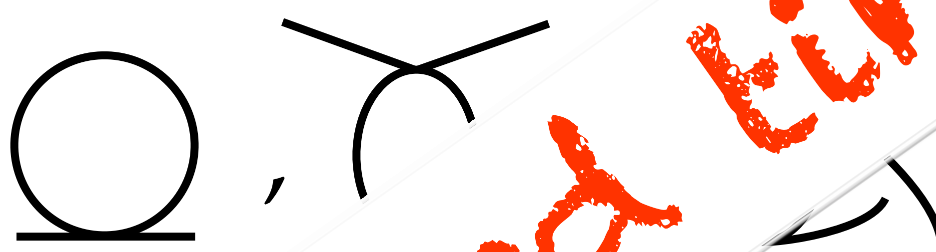
Sketch of 3+1D resu

Consider a non-relativistic toy problem:



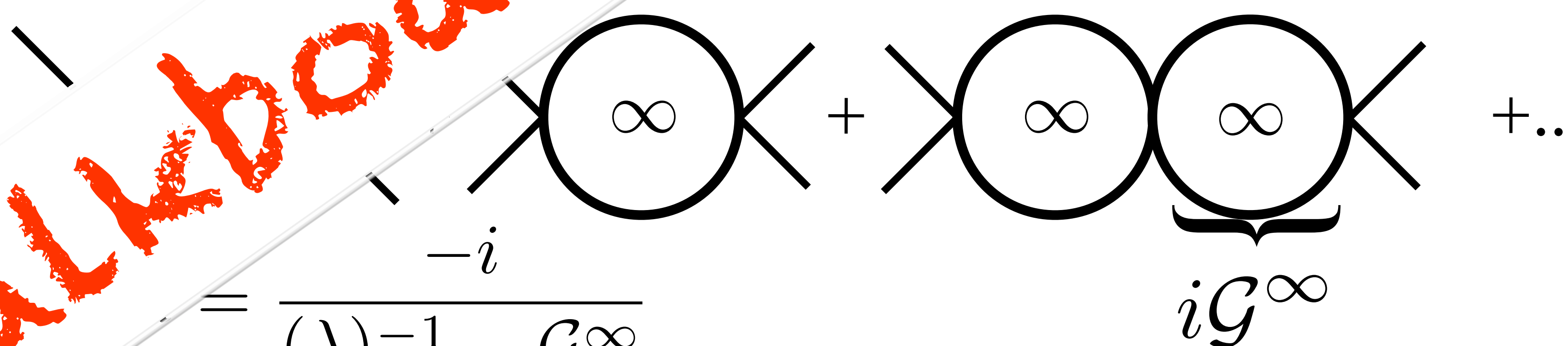
$= -i\lambda$ mom ent

In non-relativistic limit:



$\longrightarrow 0$

Scattering amplitude:



$$= \frac{-i}{(\lambda)^{-1} - \mathcal{G}^{\infty}}$$

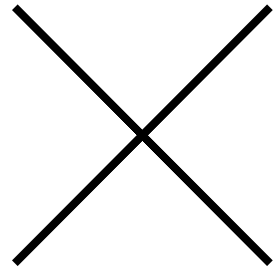
$$(\lambda)^{-1} = -(\mathcal{M})^{-1} + \mathcal{G}^{\infty}$$

note: I have avoided having to talk about renormalization. This equality is exact: however I choose to renormalize the RHS will lead to a different definition of the LHS.

Chalkboard time!

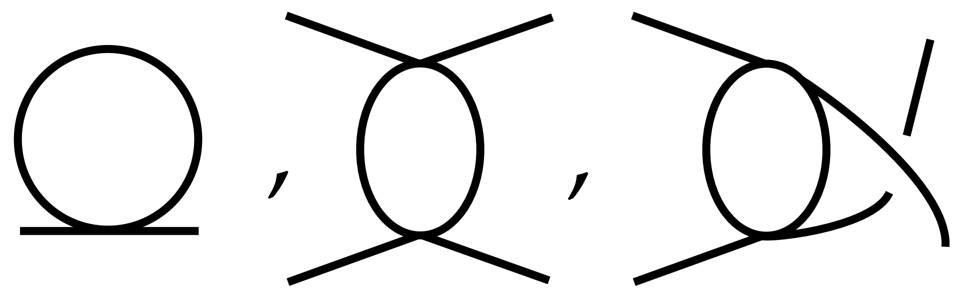
Sketch of 3+1D result

Consider a non-relativistic toy problem:



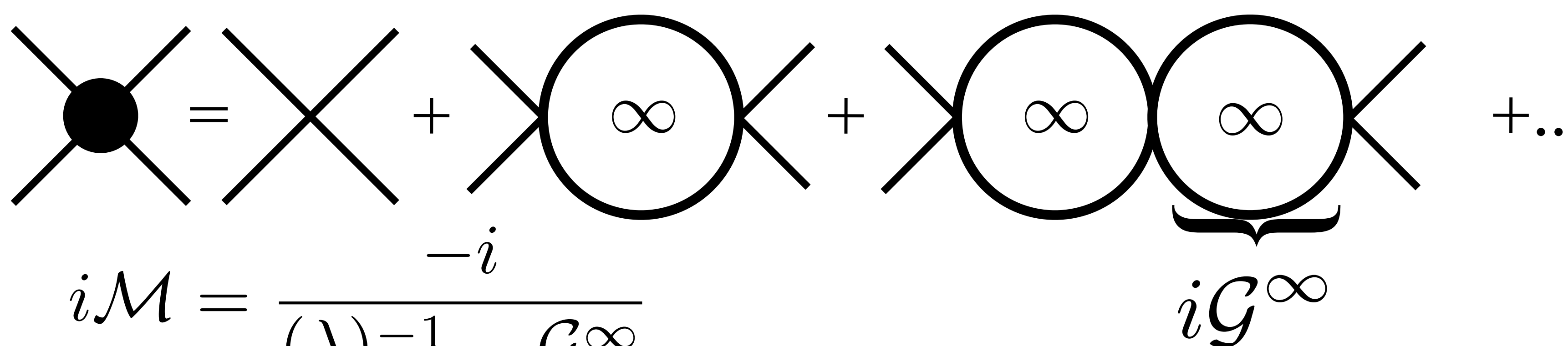
$= -i\lambda$ momentum independent

In non-relativistic limit:



$\longrightarrow 0$

Scattering amplitude:



$$i\mathcal{M} = \frac{-i}{(\lambda)^{-1} - \mathcal{G}^{\infty}}$$

$$\Rightarrow (\lambda)^{-1} = -(\mathcal{M})^{-1} + \mathcal{G}^{\infty}$$

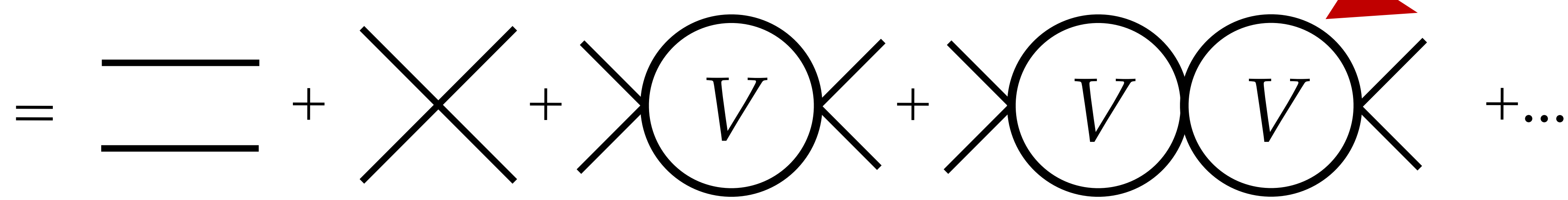
note: I have avoided having to talk about renormalization. This equality is exact: however I choose to renormalize the RHS will lead to a different definition of the LHS.

Sketch of 3+1D result

We have: $(\lambda)^{-1} = -(\mathcal{M})^{-1} + \mathcal{G}^{\infty}$

Now, lets make the volume finite and obtain the spectrum. This can be obtained from the poles of the momentum-space correlation function:

discretized momenta are summed over



$$= G_{free} + (G_{free})^2 \frac{-i}{(\lambda)^{-1} - \mathcal{G}^V} = G_{free} + (G_{free})^2 \frac{i}{(\mathcal{M})^{-1} + \delta\mathcal{G}^V}$$

this has poles at *free* energies

this diverges at the free energies as well, with the same magnitude but opposite sign!

Therefore the poles satisfy: $(\mathcal{M})^{-1} + \delta\mathcal{G}^V = 0$

Remember: $(\mathcal{M})^{-1} \sim \#(p\cot\delta - ip)$

We finally arrive at: $$p\cot\delta = \left[\frac{1}{L^3}\sum_{\mathbf{k}=2\pi\mathbf{n}/L} - P.V.\int\frac{d^3k}{(2\pi)^3}\right]\frac{4\pi}{k^2-p^2}$$

Sketch of 3+1D result

We have: $(\lambda)^{-1} = -(\mathcal{M})^{-1} + \mathcal{G}^{\infty}$

Now, lets make the volume finite and obtain the spectrum. This can be obtained from the poles of the momentum-space correlation function:

discretized momenta are summed over

$= G_{free} +$ ... $G_{free} + (G_{free})^2 \dfrac{i}{(\mathcal{M})^{-1} + \delta\mathcal{G}^{V}}$

ies

Therefore the poles sa ... 0

Remember: $(\mathcal{M})^{-1} \sim \#(p\cot\delta - ip)$

This relative simple equation encodes quite a bit of physics:

- phase shift
- bound states
- resonances
- ....

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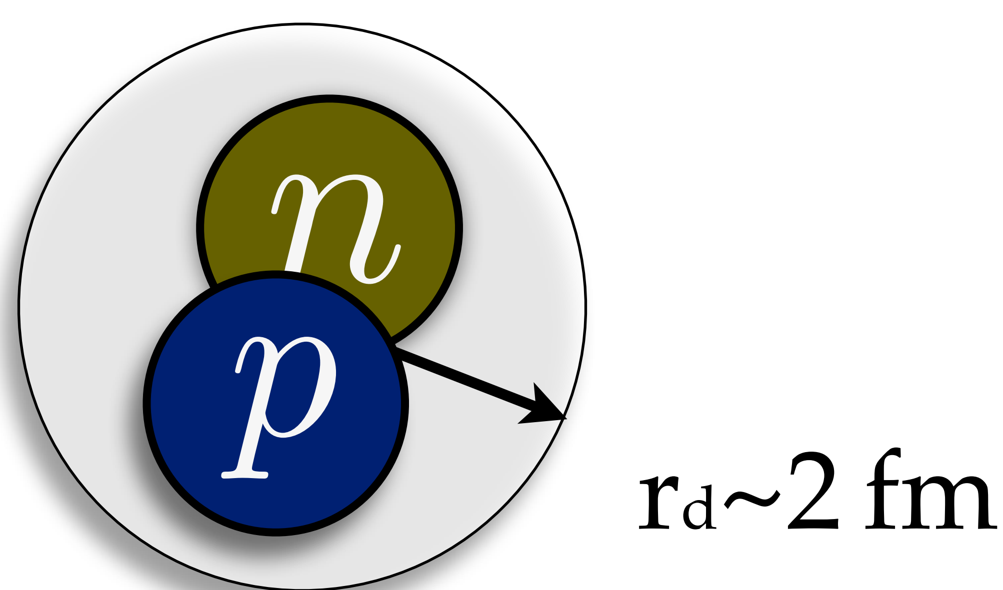
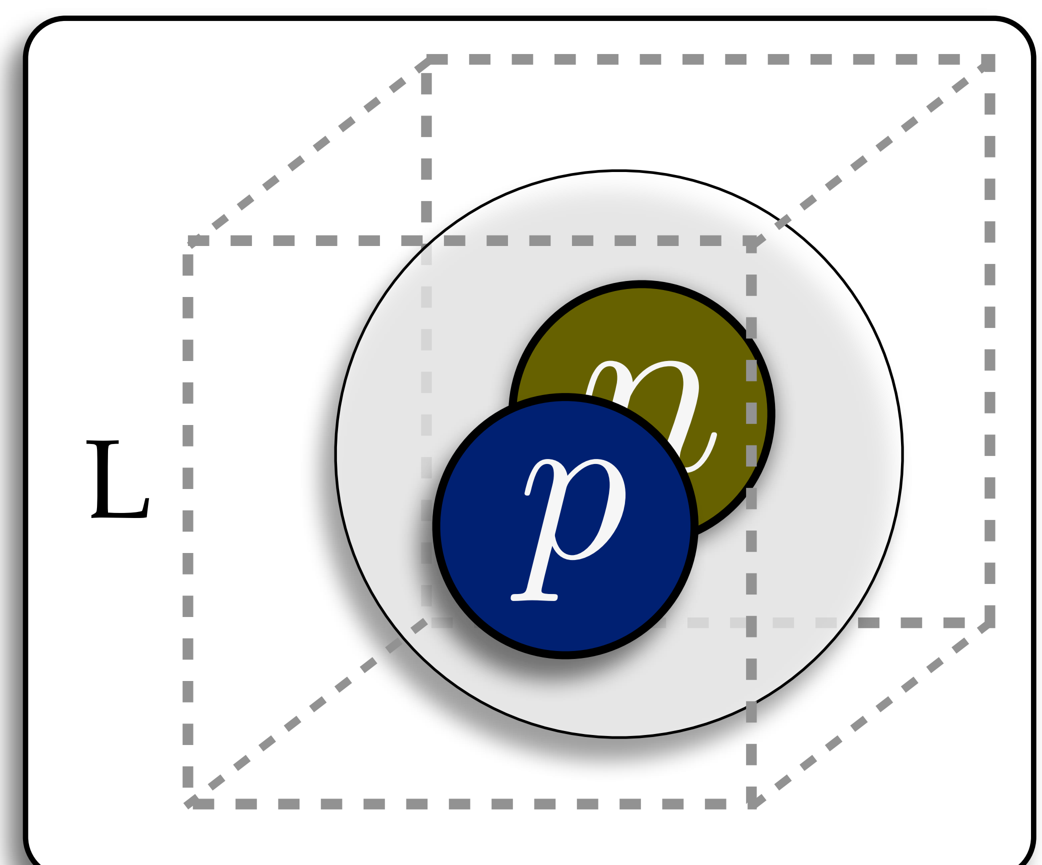
Remember the deuteron?

- Lightest bound nucleus
- Composed of one proton and one neutron
- Finely tuned?
- Can we study it in a box?





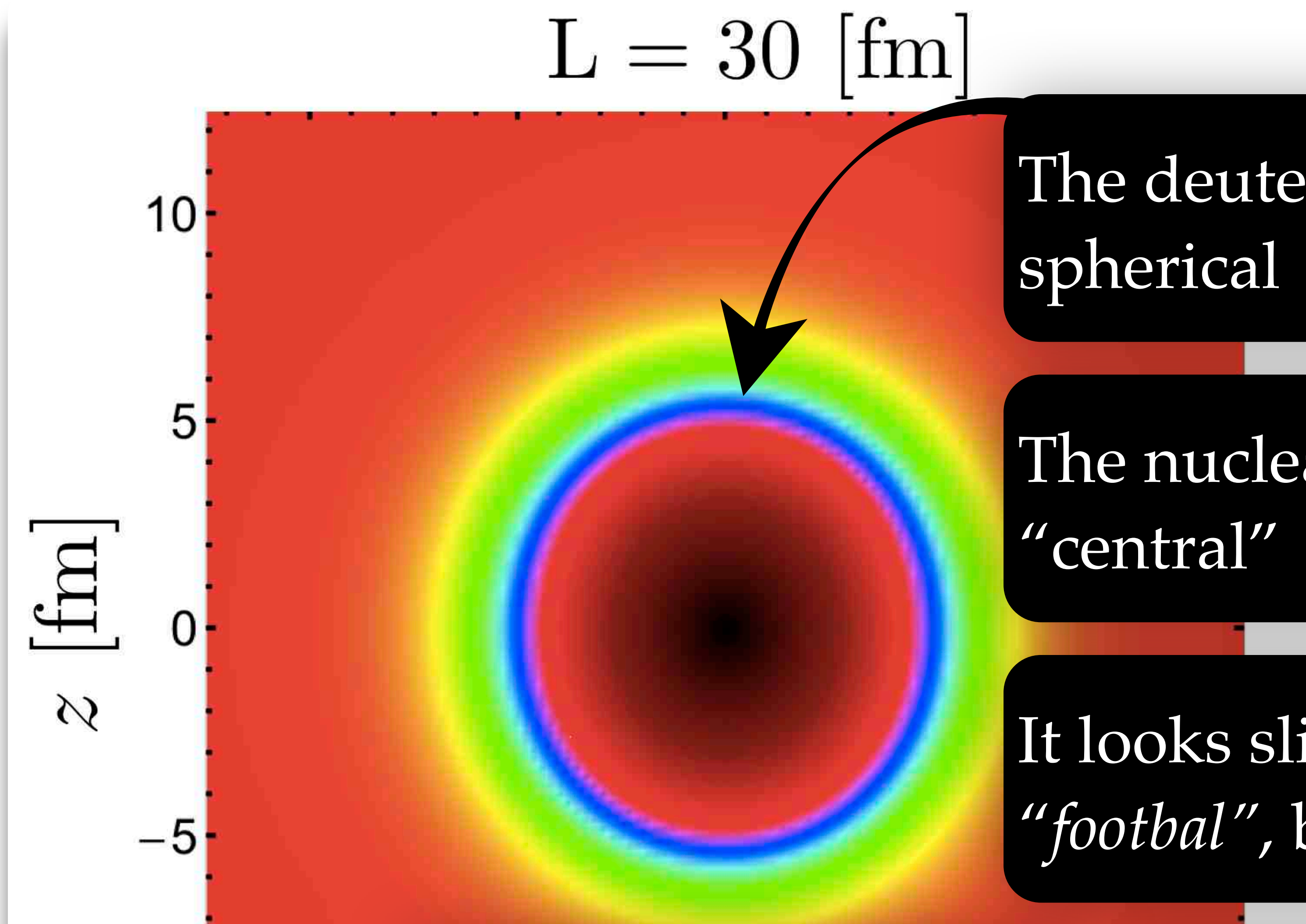
Symmetry and physics

Remember these guys?

Less symmetry!

Something **must** be lost:
angular momentum conservation!

The deuteron in a box



The deuteron is nearly spherical

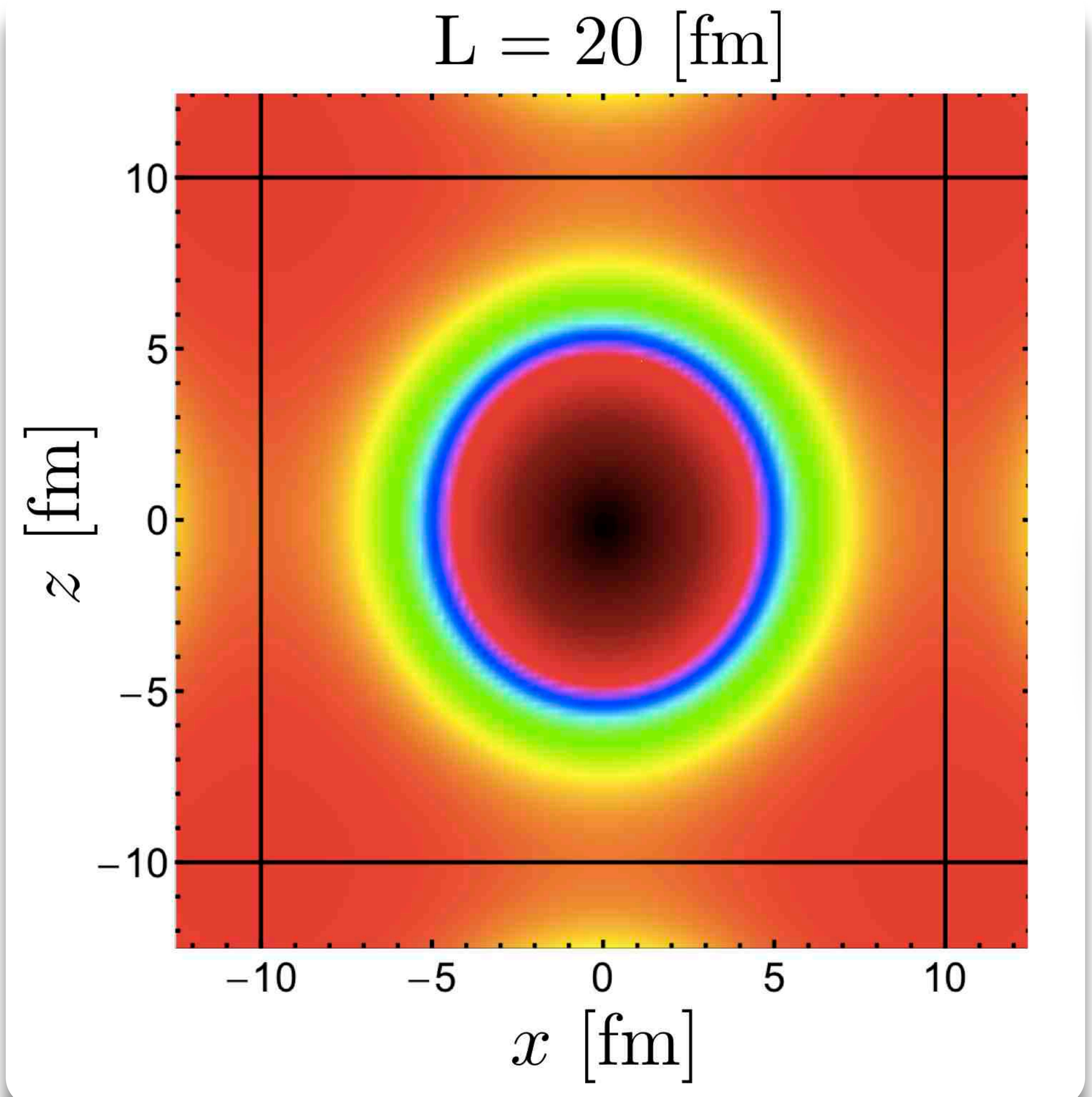
The nuclear force is not "central"

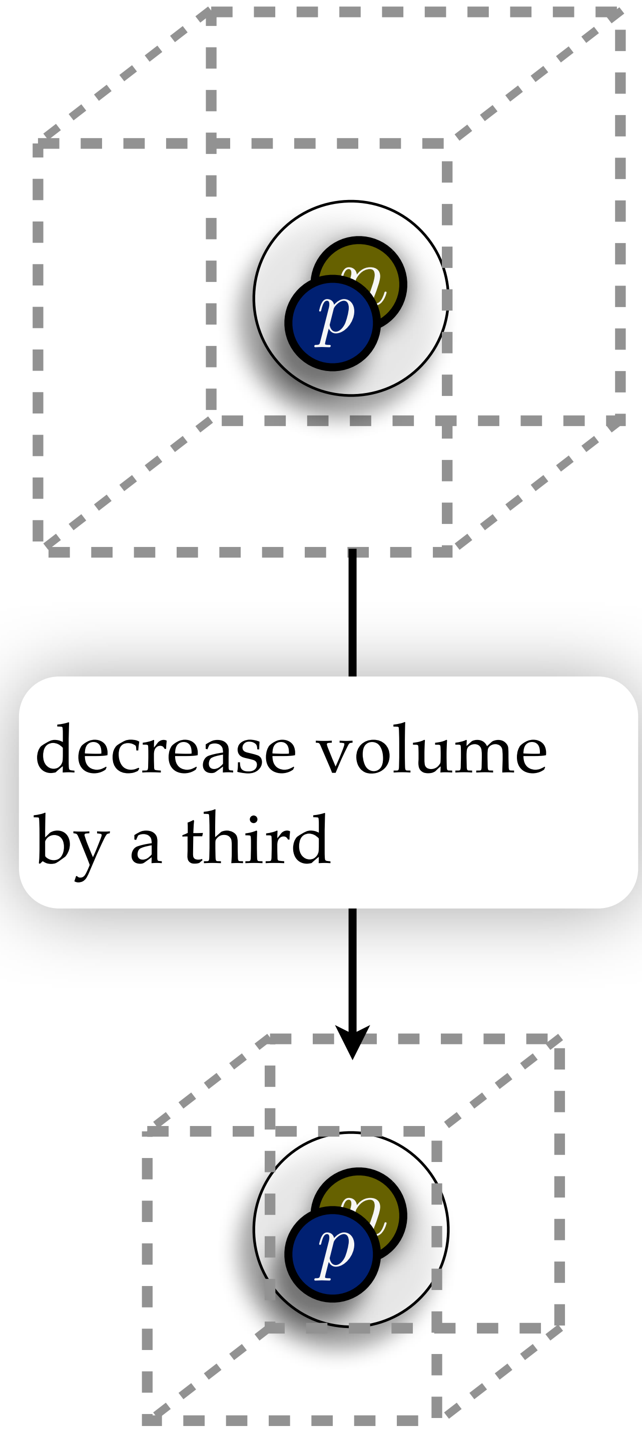
It looks slightly like a *"footbal"*, but almost spherical

?

RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

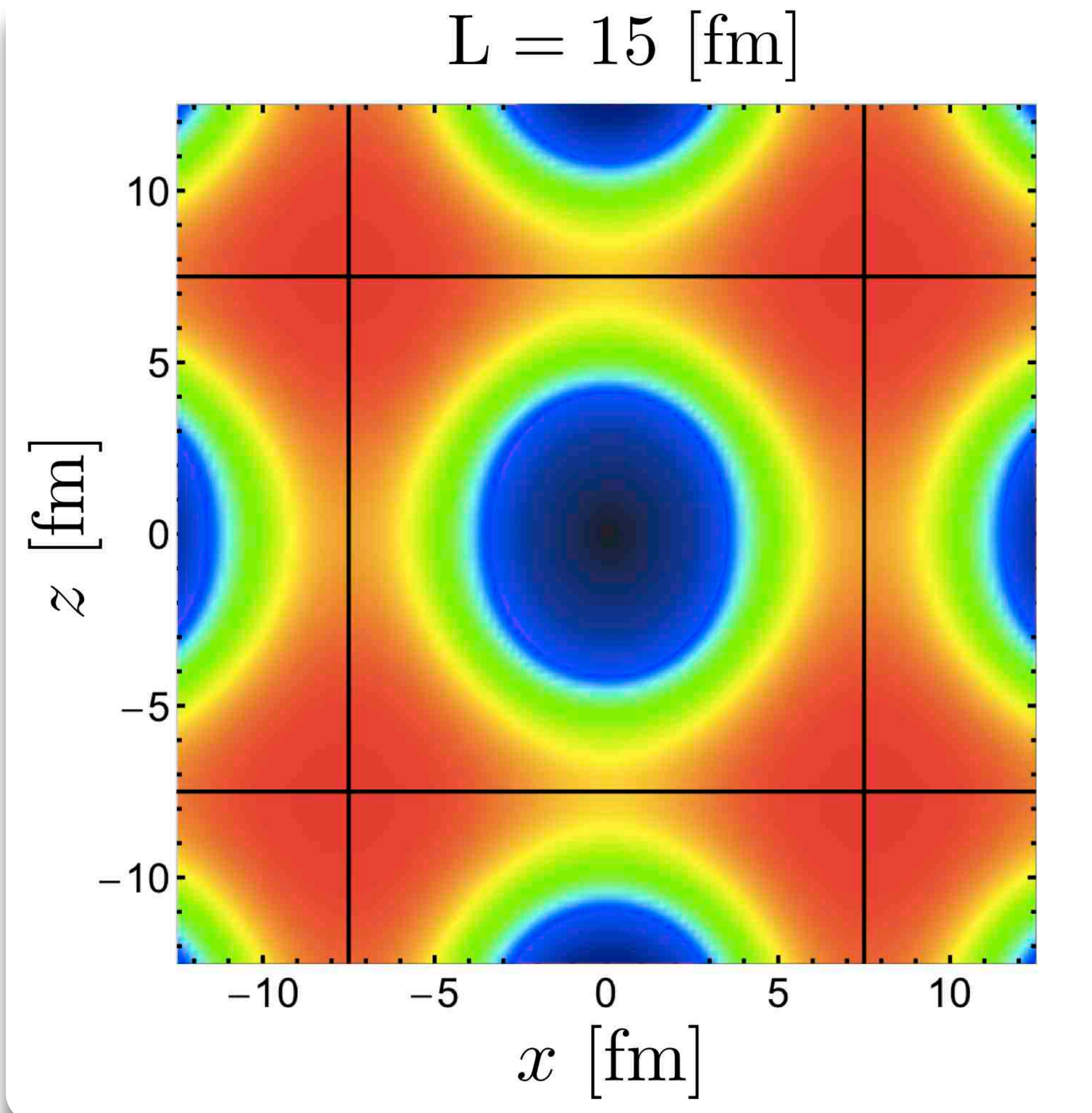
The deuteron in a box





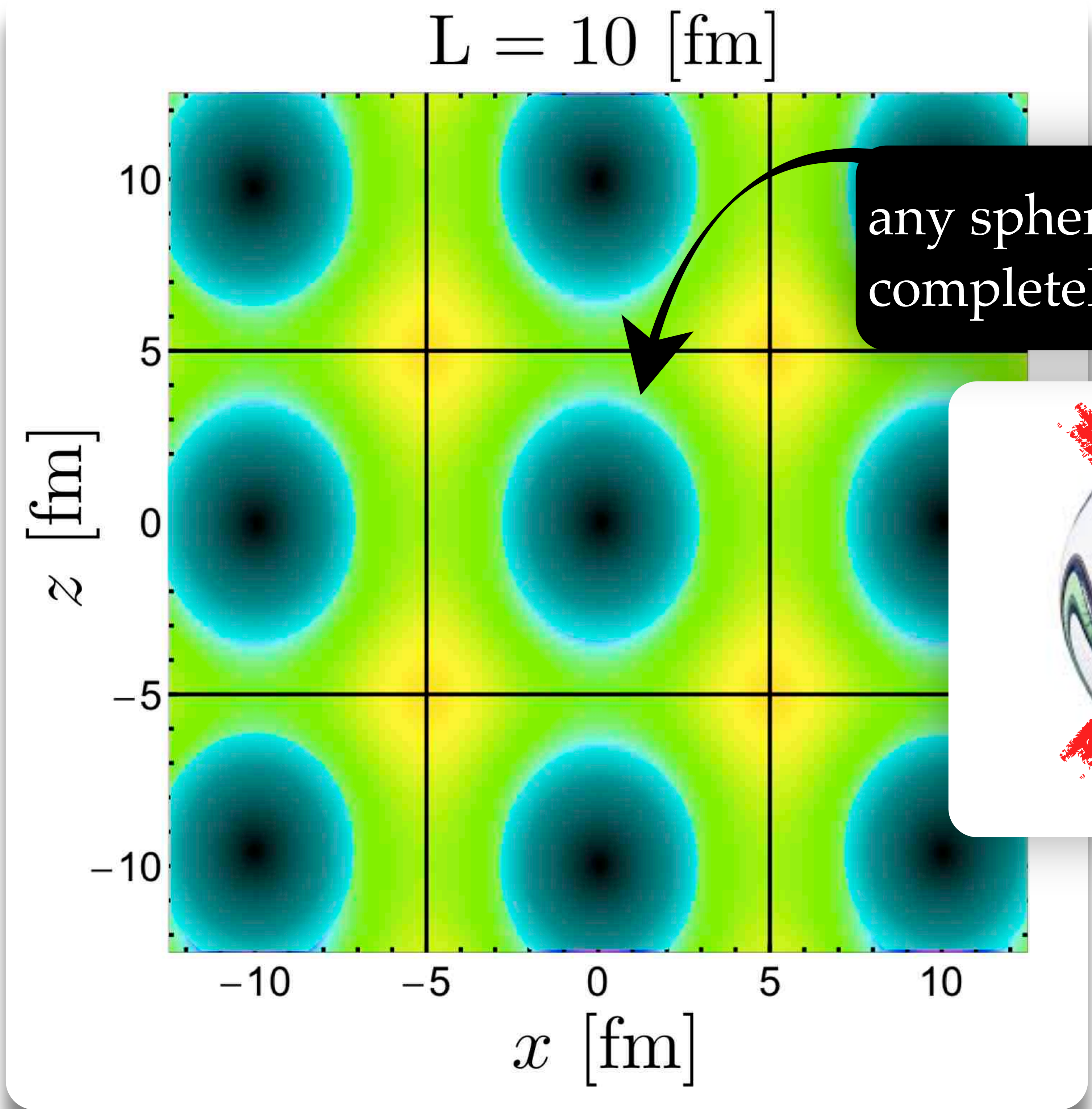
RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

The deuteron in a box



RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

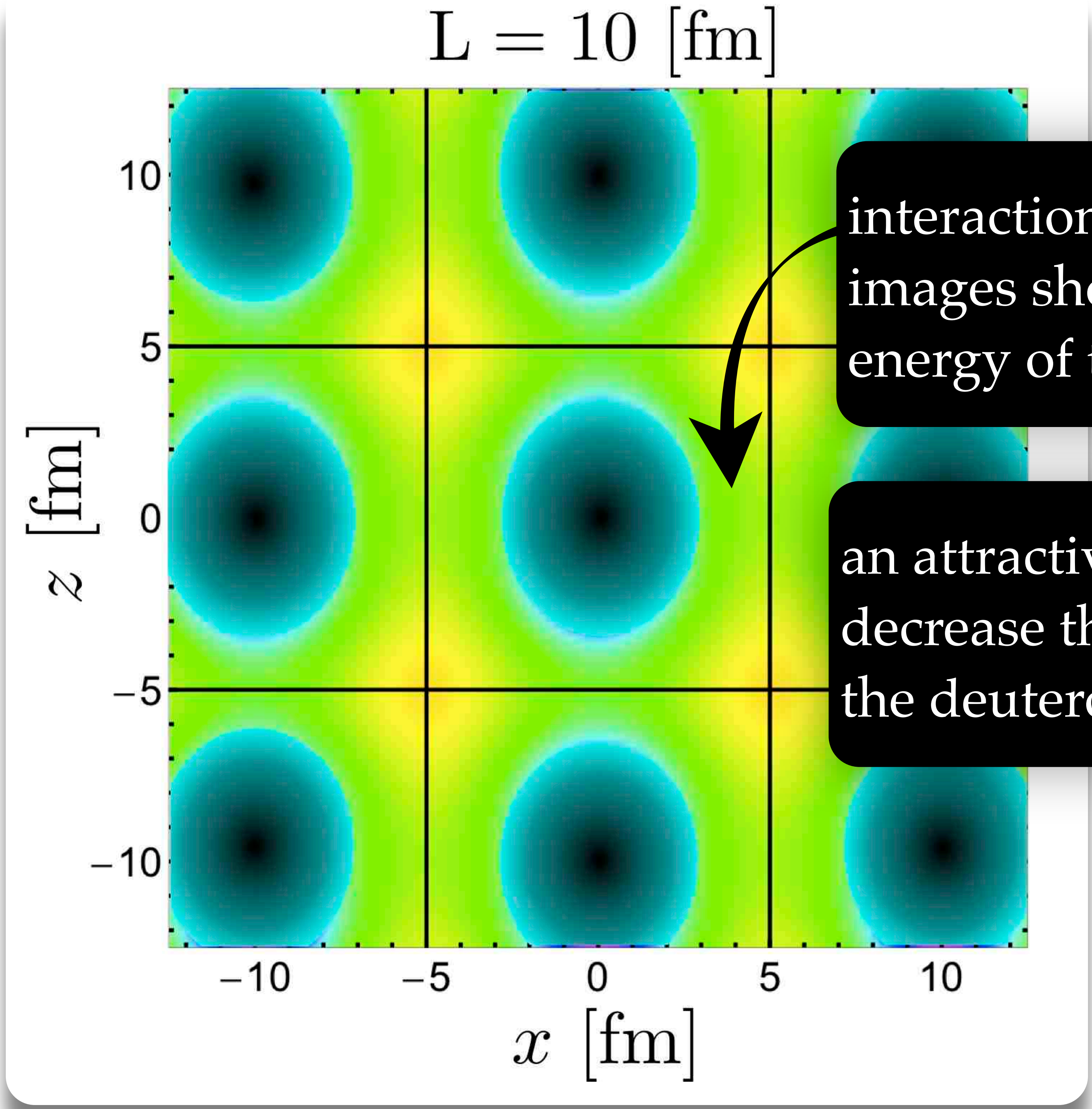
The deuteron in a box



any spherical symmetry is completely lost!

RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

The deuteron in a box



interaction with mirror images should change the energy of the system

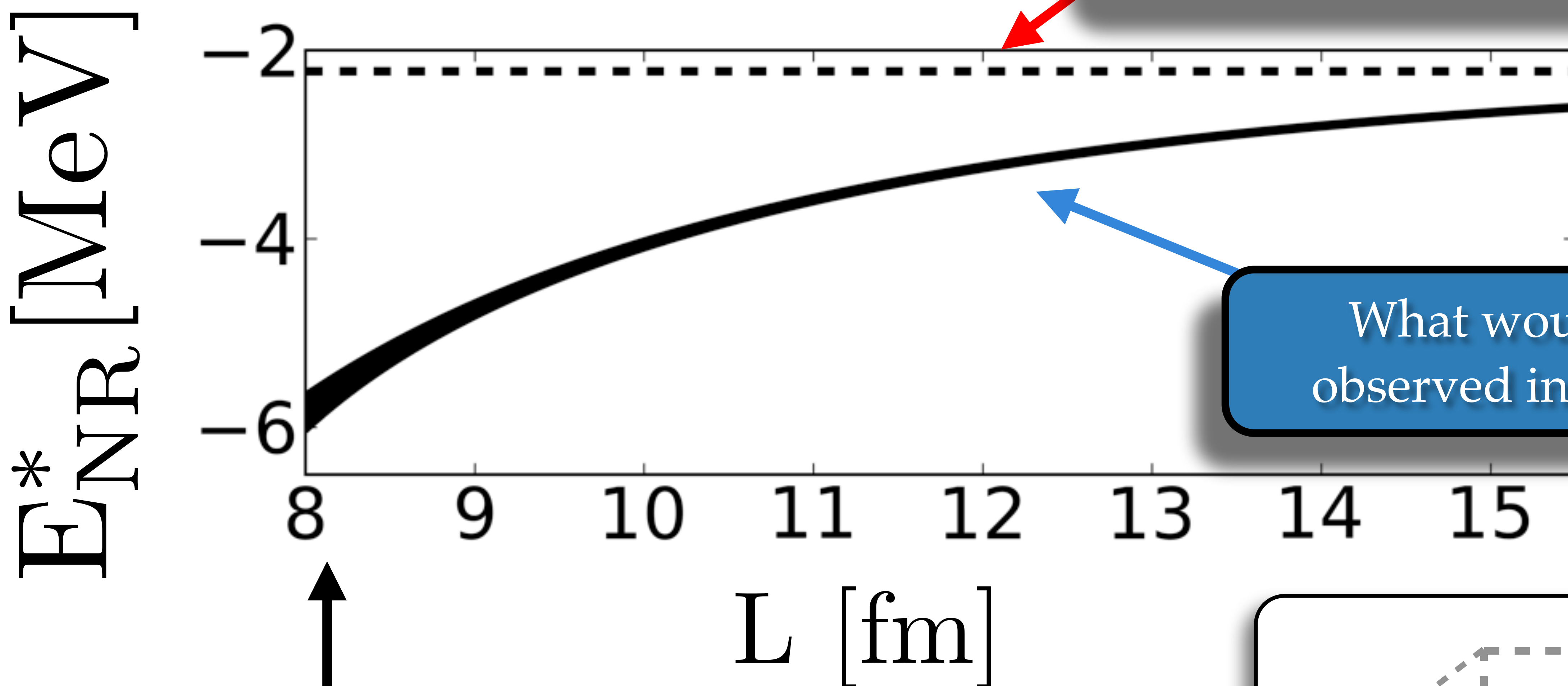
an attractive interaction will decrease the energy and make the deuteron more bound

RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

The deuteron in a box

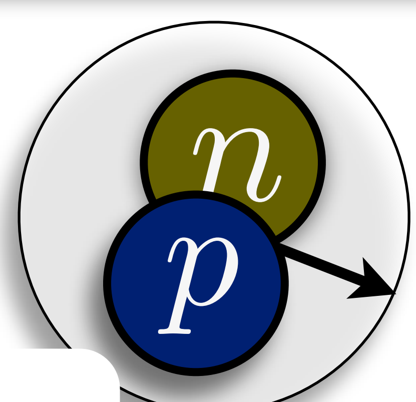
$E^*_{NR} = E^* - 2\ m_N$

Infinite volume deuteron

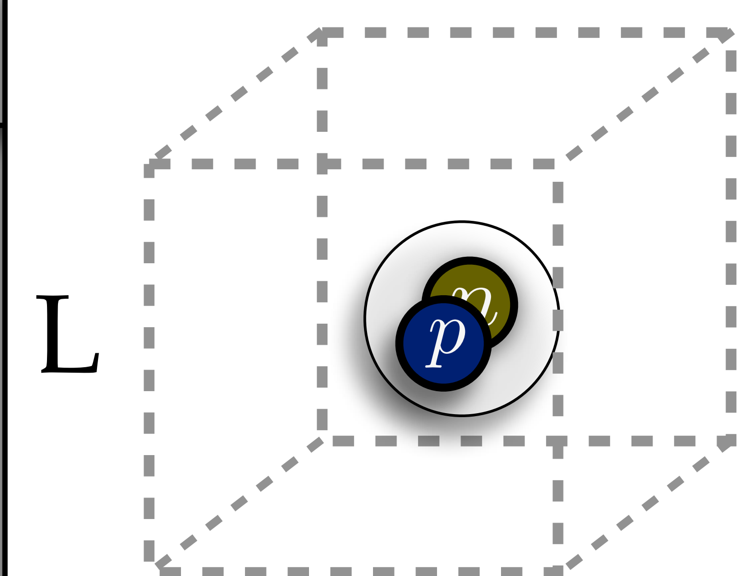


What would be observed in LQCD

Note: only twice as big as the deuteron!



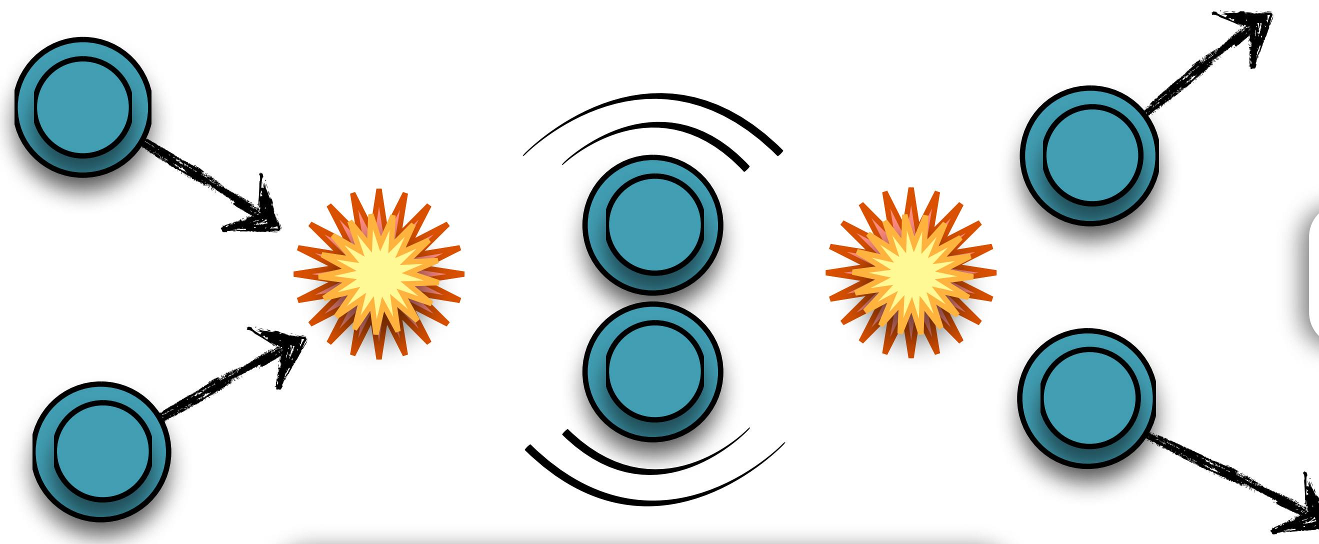
$r_d \sim 2$ fm



RB, Z. Davoudi, T. C. Luu and M. J. Savage [PRD] (2013)

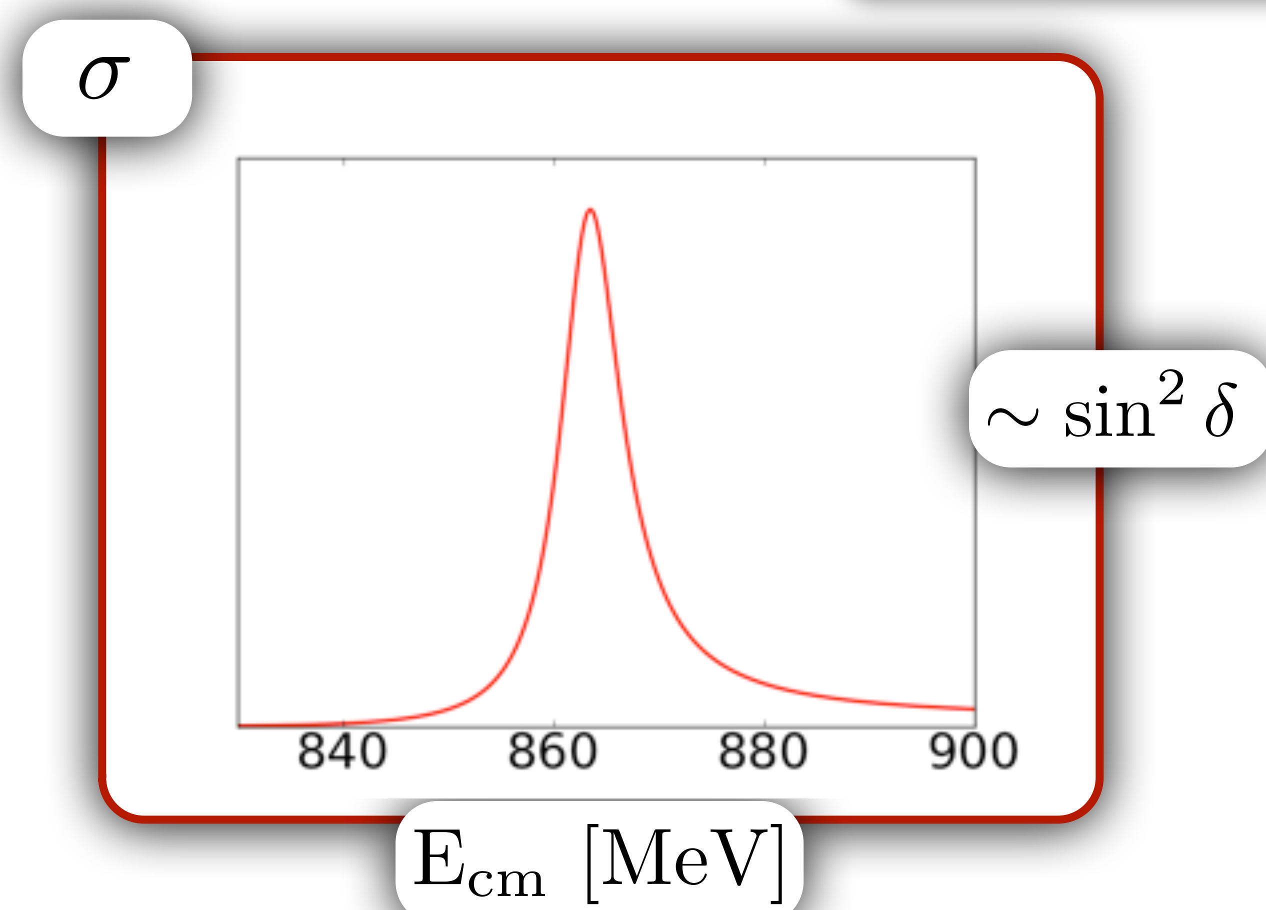
Another example: resonances

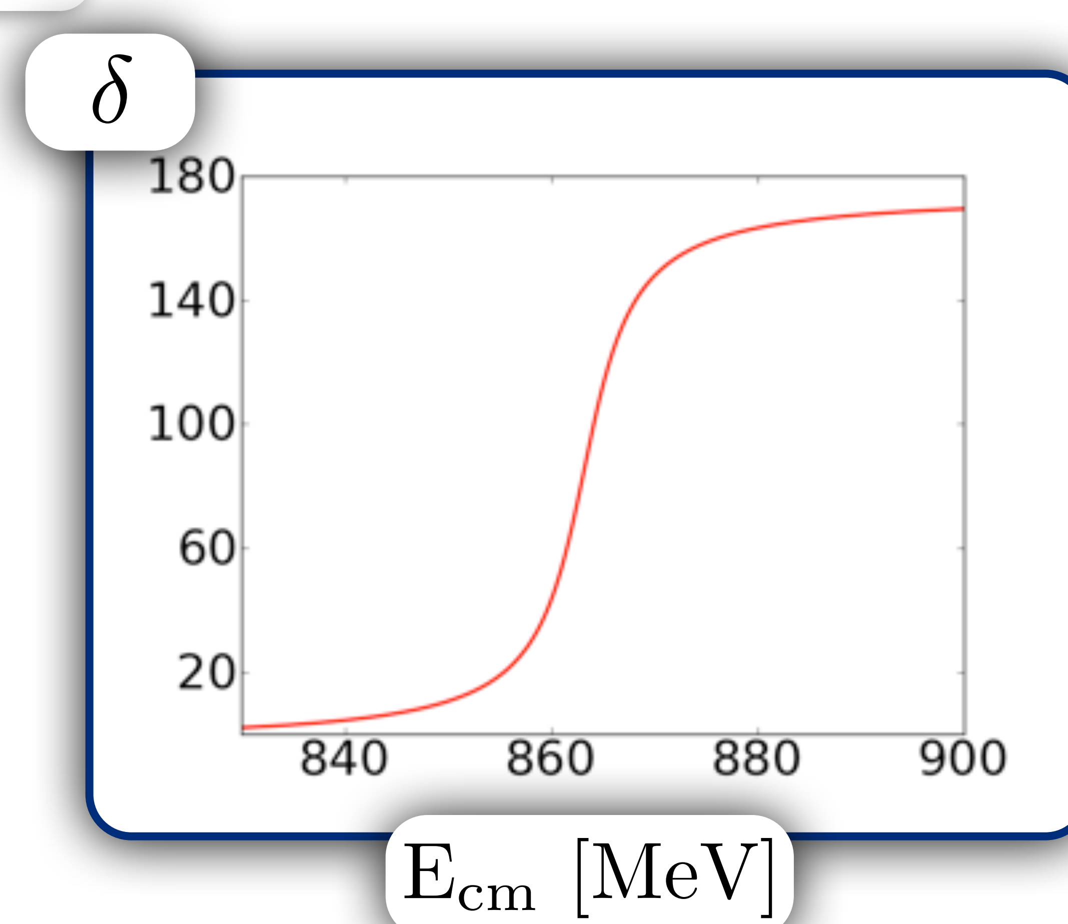
Incoming states



"States scatter off"

Resonance ~ short lived bound state

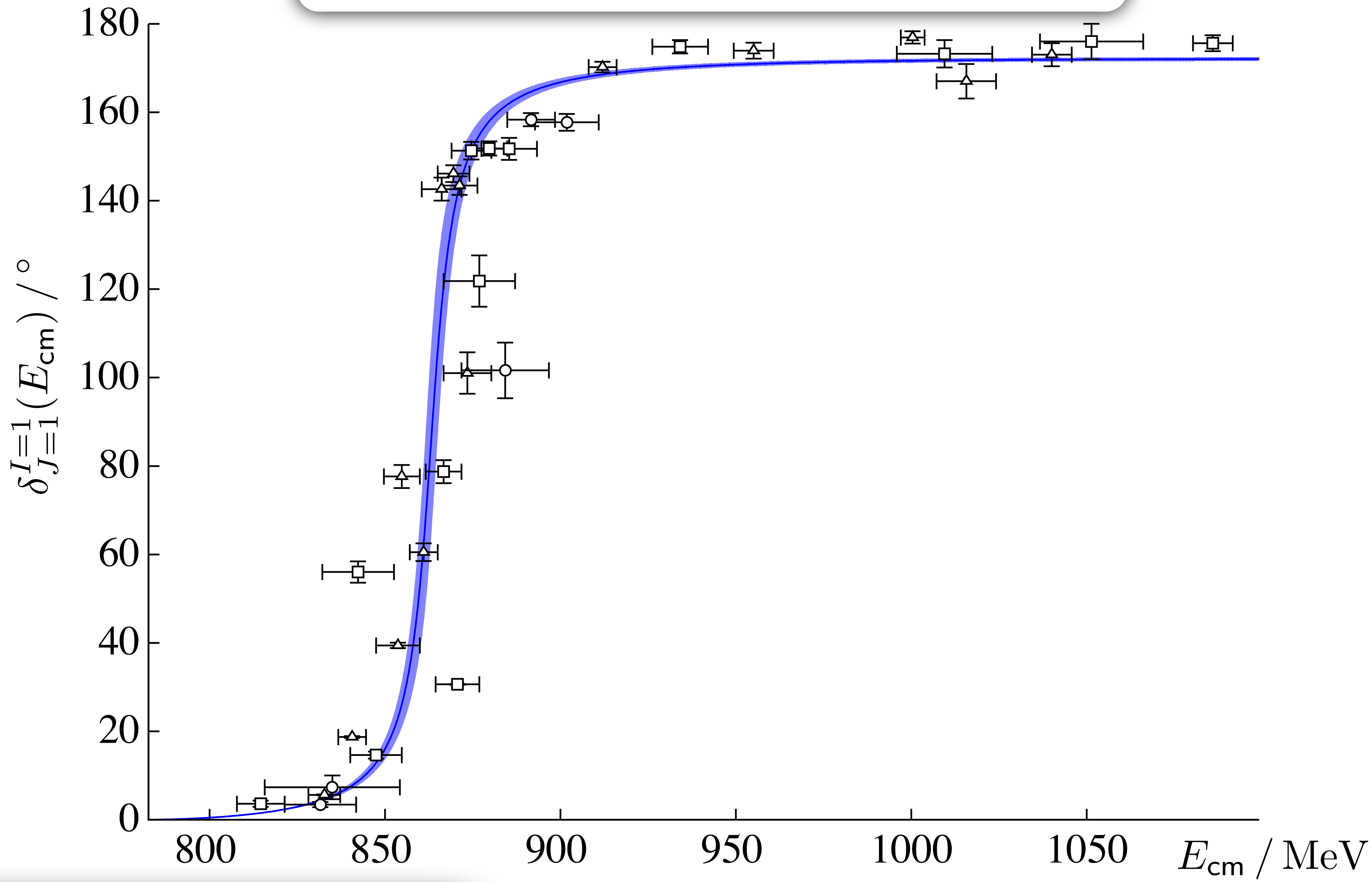




Another example: resonances

“ ρ ” resonance in $\pi\pi$ scattering

$m_\pi = 392\,\mathrm{MeV}$



arXiv:1212.0830 [hep-ph] [PRD]
Hadron Spectrum Collaboration (2012)

Using a simplified version of the master equation derived in RB arXiv:1401.3312 [hep-lat] [PRD]

Outline

First half:

- ☑ Why QCD / Lattice QCD?
- ☑ What's Lattice QCD?
- ☑ Symmetry?

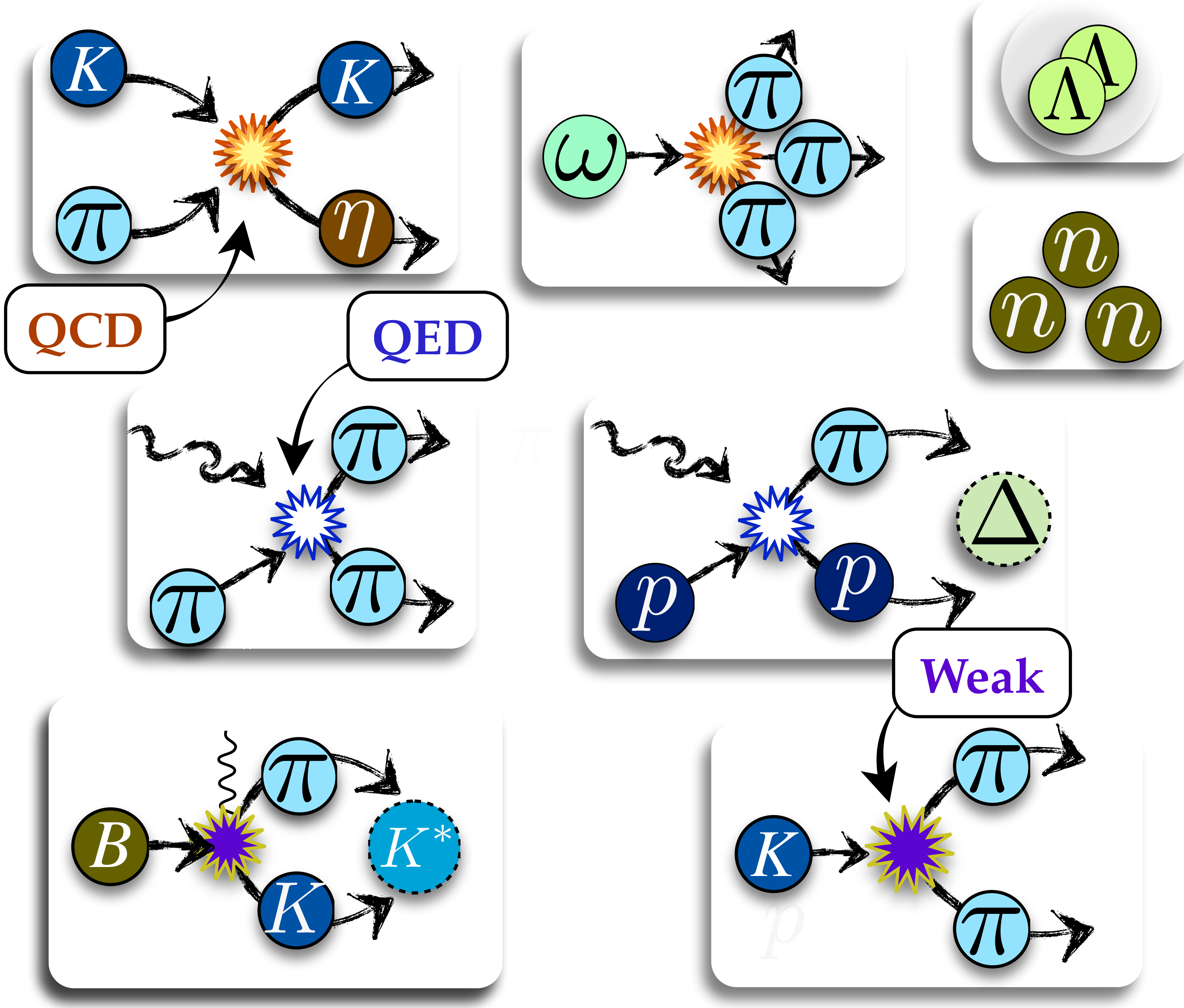
Second half:

- ☑ Masses & decay constants of single particles
- ☑ Scattering, resonances & bound states

Status of formalism

(a very bias estimate)

- Spectroscopy / scattering:
- Form factors:
- Fundamental symmetries:

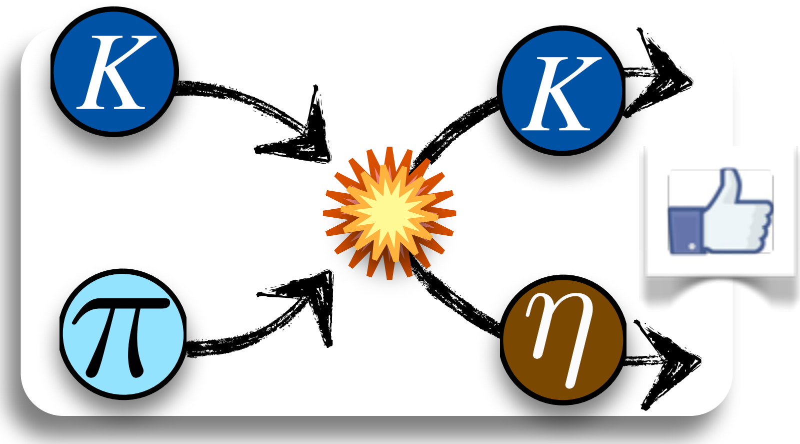


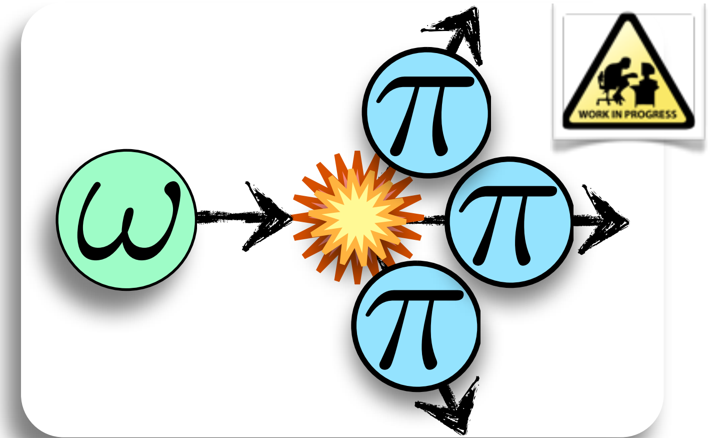
Status report
(a very bias estimate)

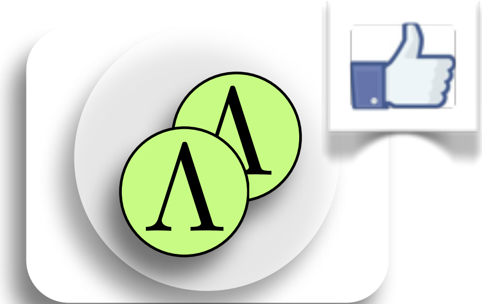

: Under control

: progress made / more to come

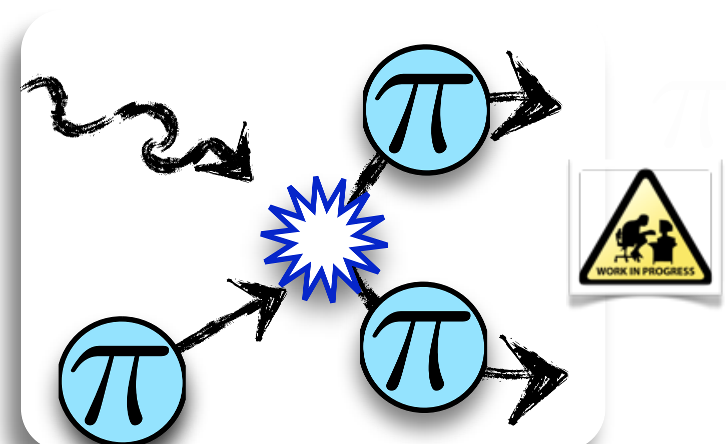
- Spectroscopy / scattering:

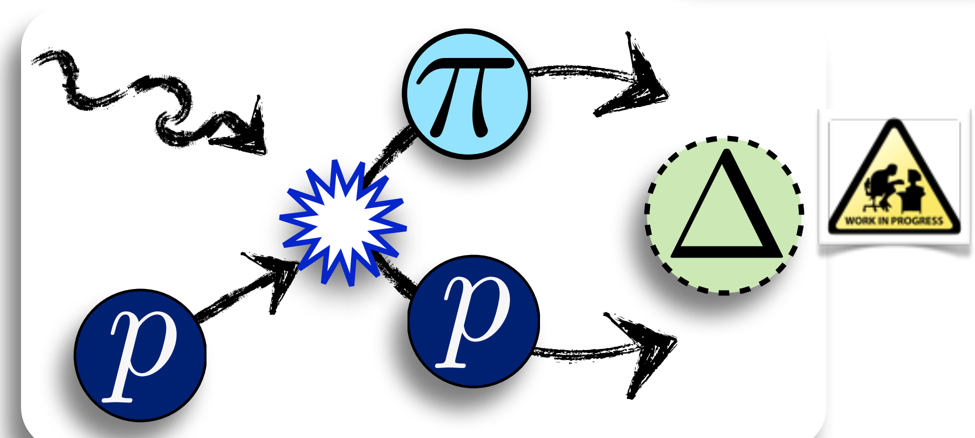




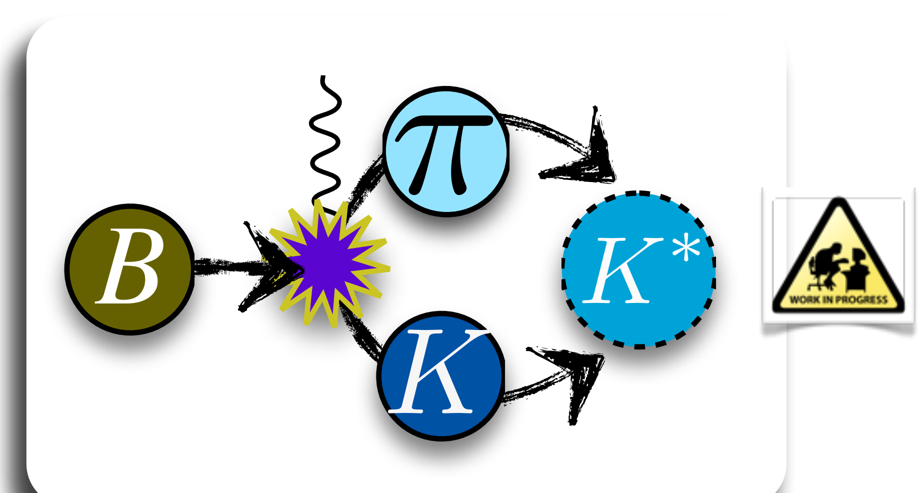


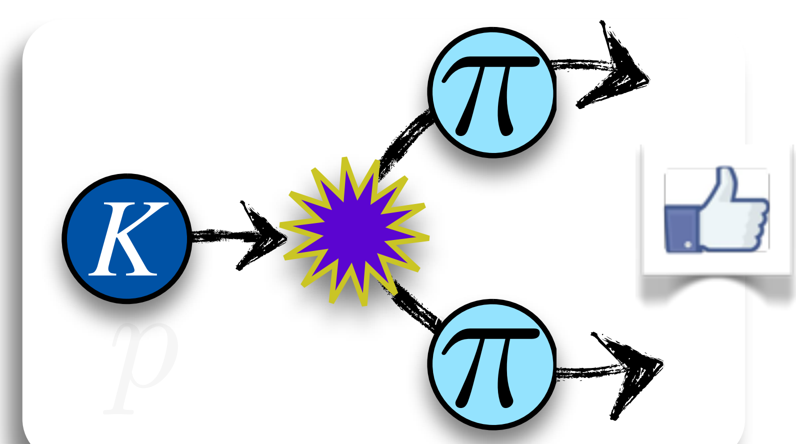
- Form factors:





- Fundamental symmetries:





Final remarks

Lattice QCD is a vast field, with many intricacies and subtleties, here all I can give is a taste of the exciting and challenging aspects of this ever growing field. Lattice QCD has proven to be the most reliable first principles tool for studying low-energy QCD. In recent years it has become evident that we can actually study fundamental nuclear processes directly via LQCD, but just as in anything else in nuclear physics, this has proven to be technically challenging. Furthermore, it has forced us to think outside the box and come up with scheme to achieve our basic scientific goals. I hope that in the past two hours I have conveyed just that.