CalLat
(California Lattice)

I. CalLat overview, effective theory, Bigstick: WH

II. Lattice QCD, NN phase shifts: André Walker-Loud

California Lattice (CalLat)

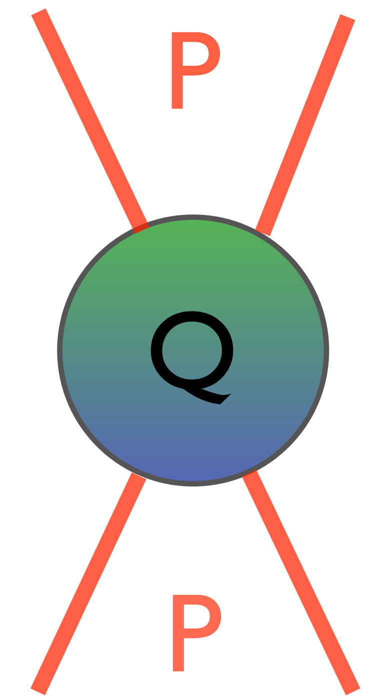
- CalLat structure
  - new group, small, centered around LBL/Berkeley and LLNL
  - focused on a single problem: construct a controlled theory of nuclear structure and reactions, and link that theory directly to LQCD

- Nuclear physics: difficulty of traditional approaches in truncated spaces
  - results that depend on parameters with no obvious physical significance, such as "starting energies", oscillator parameters, number of shells
  - wave functions evaluated in truncated Hilbert space (P- or "included" space) which have no precise connection to the exact wave function in P+Q, with properties (like orthogonality) that should not persist under P

- The lattice QCD challenge:
  - the fermion sign problem endemic to Monte Carlo many-body theory

CalLat: these problems may have a common solution

The Conventional Nuclear Physics Approach



- Conceptually want to go from LQCD to an effective non-relativistic many-nucleon calculation in a truncated Hilbert space **= P**

- Know from effective field theory this is a well-posed problem

- What is actually done is the following "two-step"

experimental NN phase shifts δ(E) $\xrightarrow{P+Q}$ NN potential quite singular at small r $\xrightarrow{P}$ an effective potential for the nucleus

- The resulting NN interaction is highly singular and nonperturbative

- Consequently the reduction P+Q to P is challenging, forcing uncontrolled approximations, e.g., a plane-wave basis (momentum is not a valid cutoff for P), with scattering limited to two nucleons

CalLat's Unconventional Approach

Idea #1

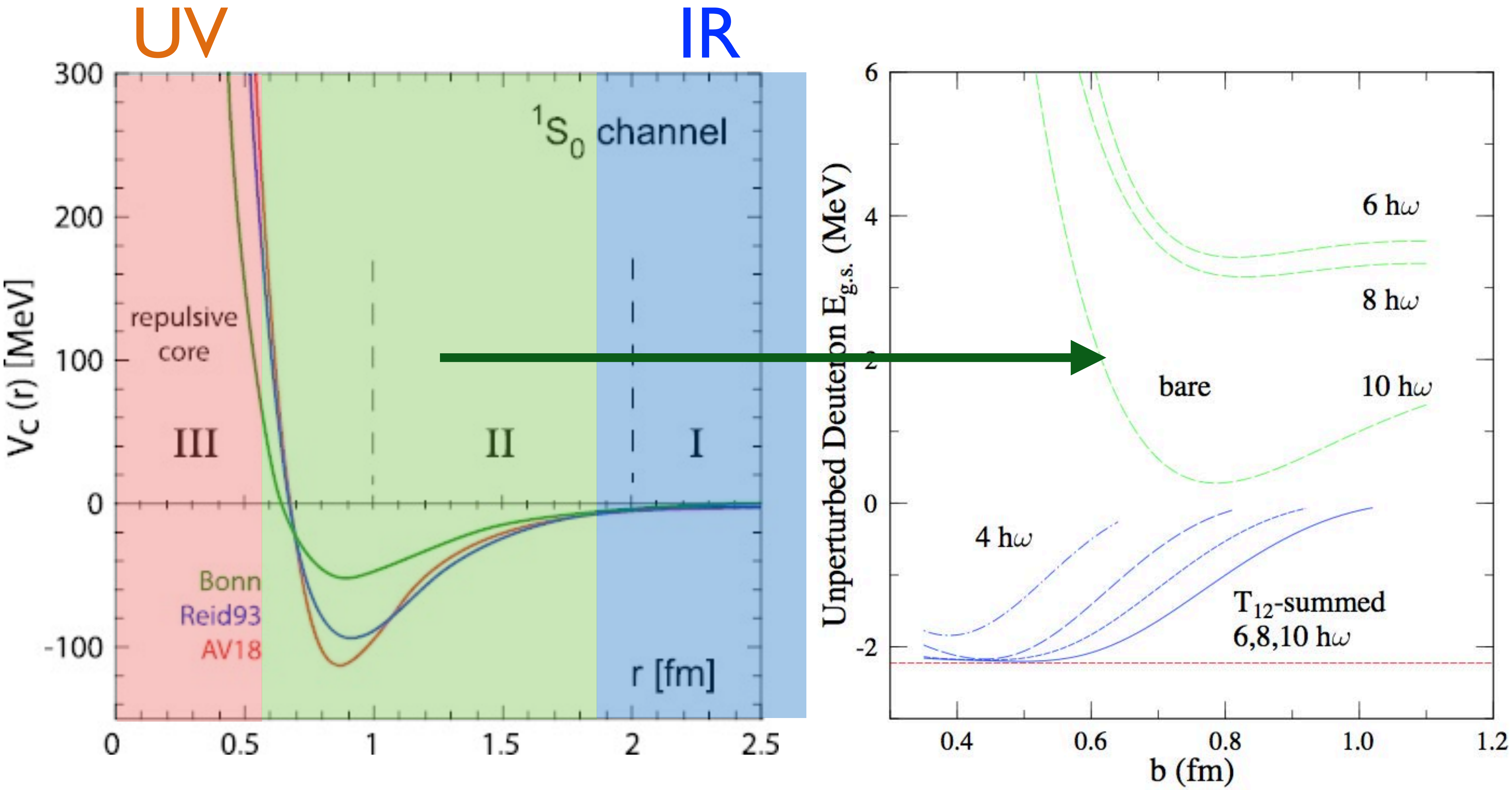
- Effective theories should not be executed in two steps, especially if step one produces a largely intractable step two!

- There is a unique, finite, compact Hilbert space P for solving the non-relativistic many-nucleon problem: the HO (translational invariance)

- The effective interaction H^{eff} in that space is NOT a potential, but something far more interesting — Q contains large corrections in both the infra-red and ultra-violet

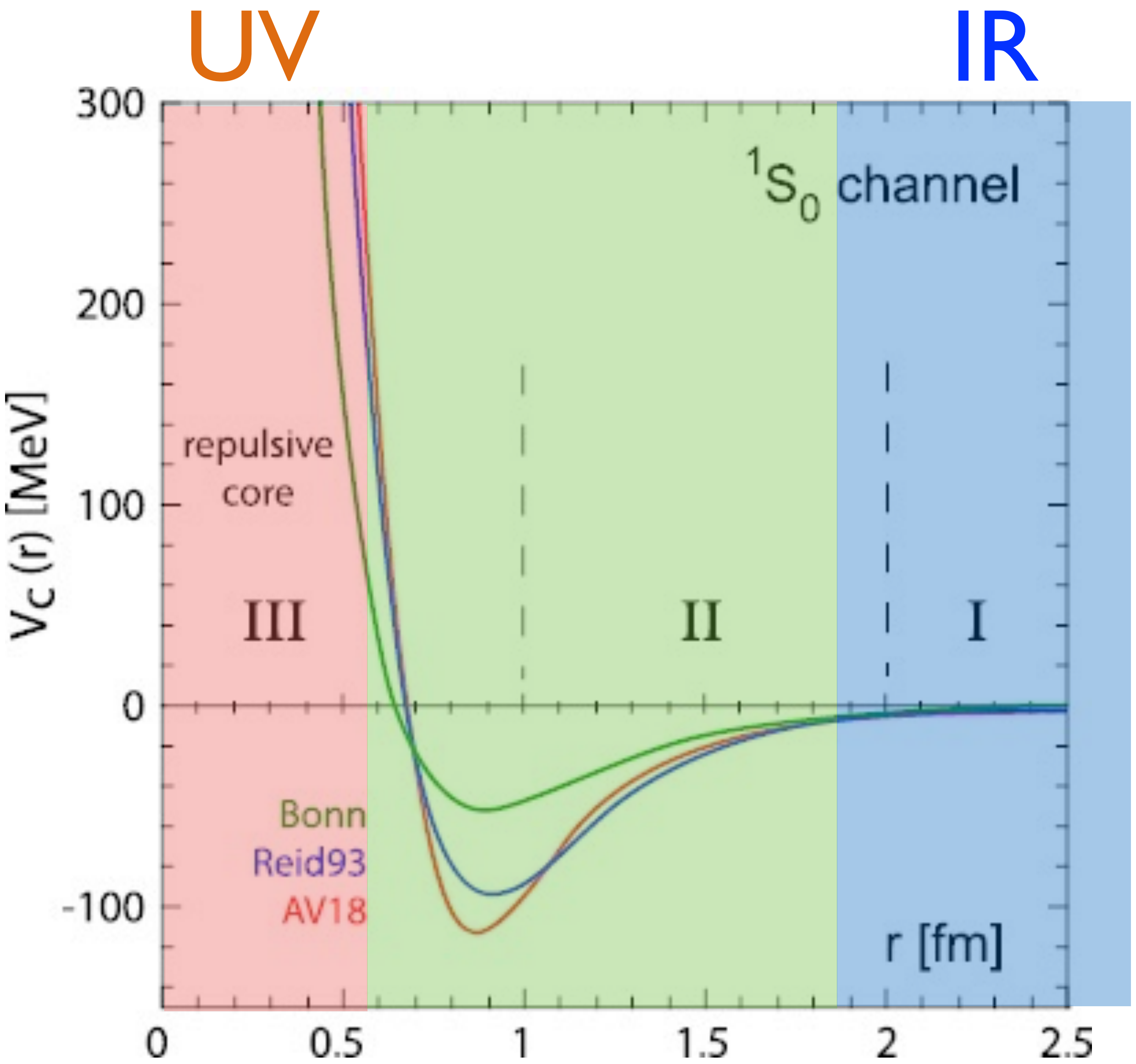
- This multi-scale problem can be factored into its UV/IR components. The UV components connected with the singular nature of the short-range interaction can be very accurately represented by a few low-energy constants (LECs)

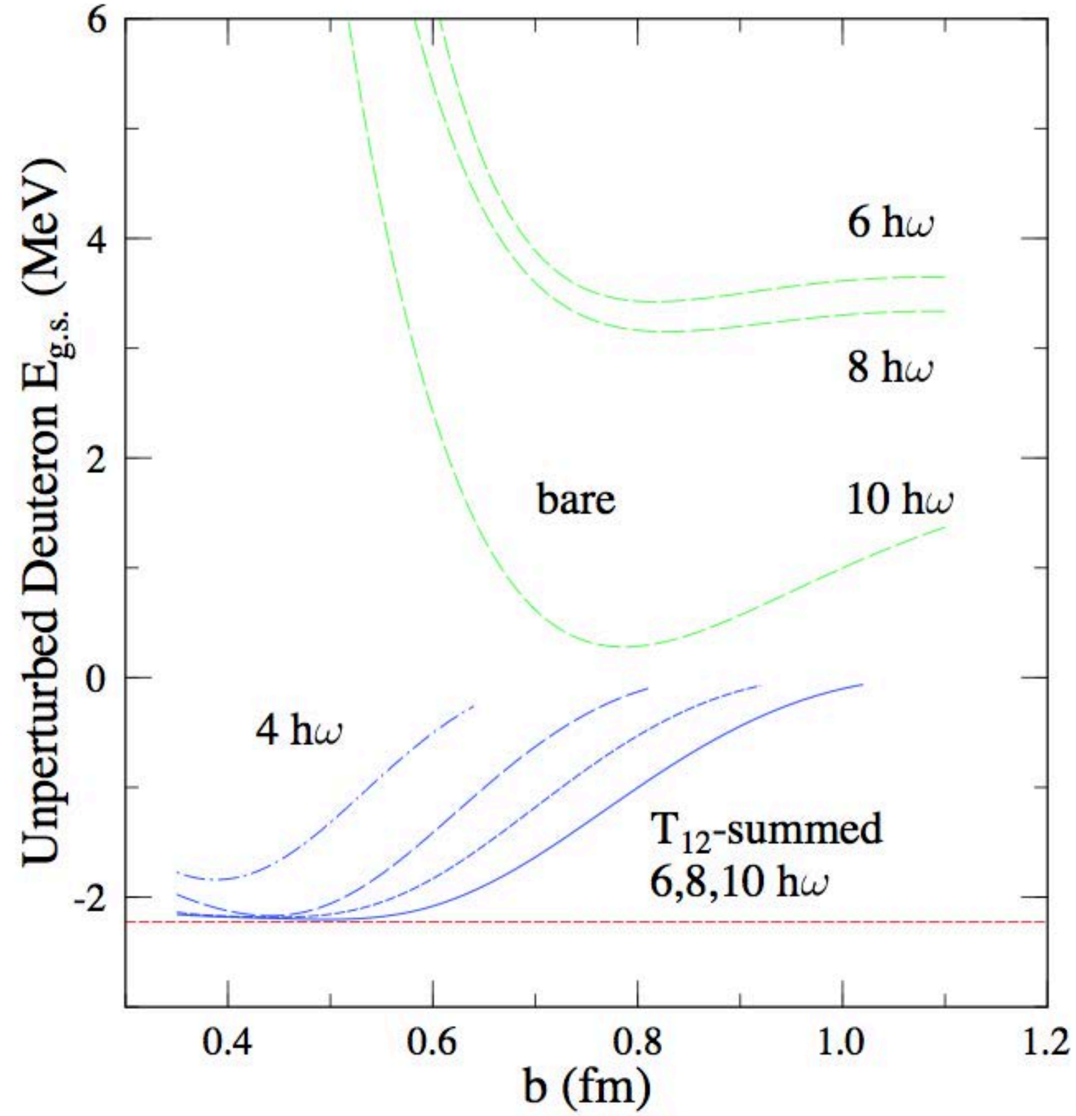
- Question: Working in a *compact* Hilbert space, can one in a determine the LECs from the available experimental information, the NN phase shifts?



Simple example: the deuteron with av18 potential

standard C.I. approach requires ~100 $\hbar\omega$ to achieve 1 keV accuracy





$$H^{\rm eff} = PH \frac{1}{E-QH} QHP \rightarrow P \frac{E}{E-TQ} \left[T - T\frac{Q}{E}T + V + V \frac{1}{E-QH} QV \right] \frac{E}{E-QT} P$$

$$V \frac{1}{E-H} V \rightarrow V_\delta \equiv \; a_{LO}^{3S1} \delta(\vec{r}) + a_{NLO}^{3S1} (\overleftarrow{\nabla}^2_{HO} \delta(\vec{r}) + \delta(\vec{r}) \overrightarrow{\nabla}^2_{HO}) + \cdots$$

with the energy-dependent IR physics now correct, a rapidly convergent short-range expansion for the missing UV physics, encoded in a few *energy-independent LECs*

Idea #2

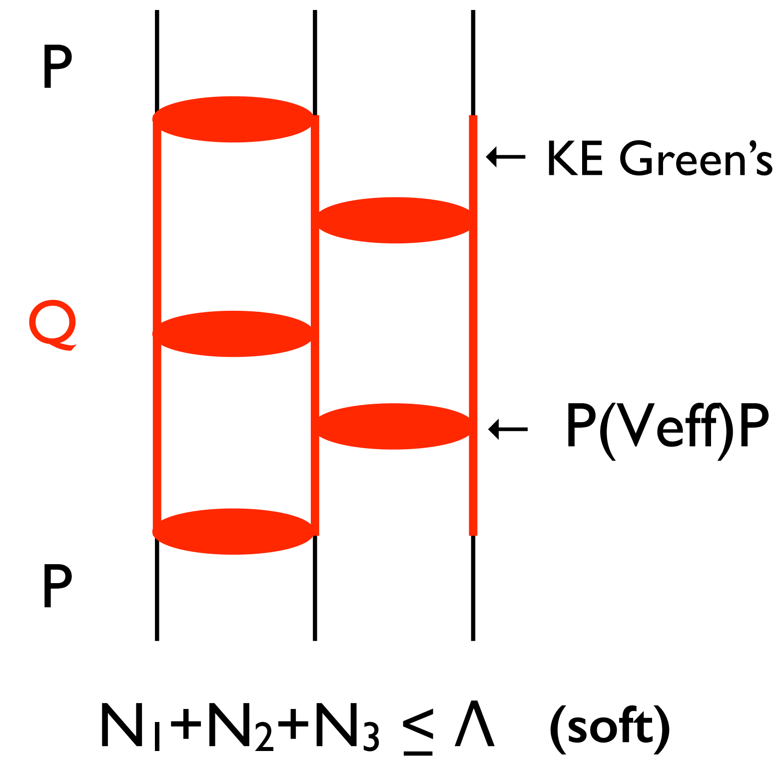
- If one can solve step #1, then one a procedure for exactly propagating the two-body physics through an N-body system:

- The exact result is obtained by the substitution of

$$V \to P\left[\frac{E}{E-TQ}(V+V_\delta)\frac{E}{E-QT}\right]P$$

in the Bloch-Horowitz equation

- The interaction now is *soft and restricted to P* — no longer highly nonperturbative (great!)



- But it is many-body (not so great): soft, strong-interaction scattering, separated by enhanced IR energy-dependent propagation

- Thus we have challenge #2:
  Adapt the numerical machinery of nuclear physics — Lanczos-based direct diagonalizations in P — to handle the more complex many-body interactions that HOBET generates

Idea #3

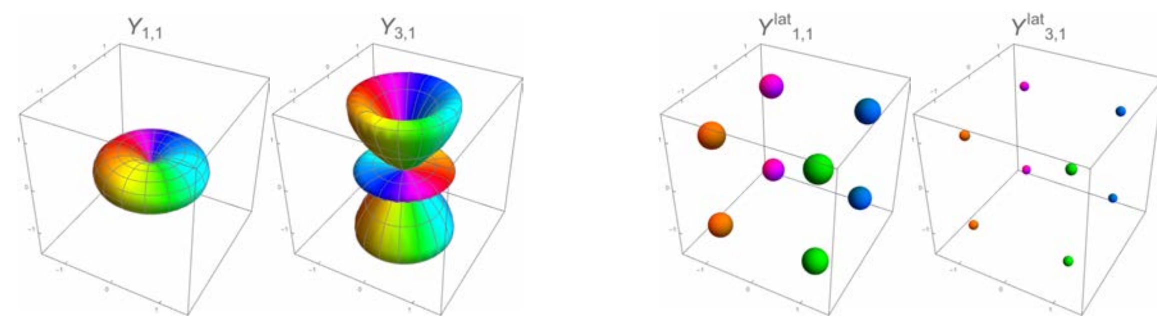
- If one completes steps #1, #2, then one will have also rigorously connected LQCD to conventional many-body theory

- Just replace experiment by LQCD

$$\{a^{3S1}_{LO},\ a^{3S1}_{NLO}\} \leftrightarrow \text{exp, or}$$

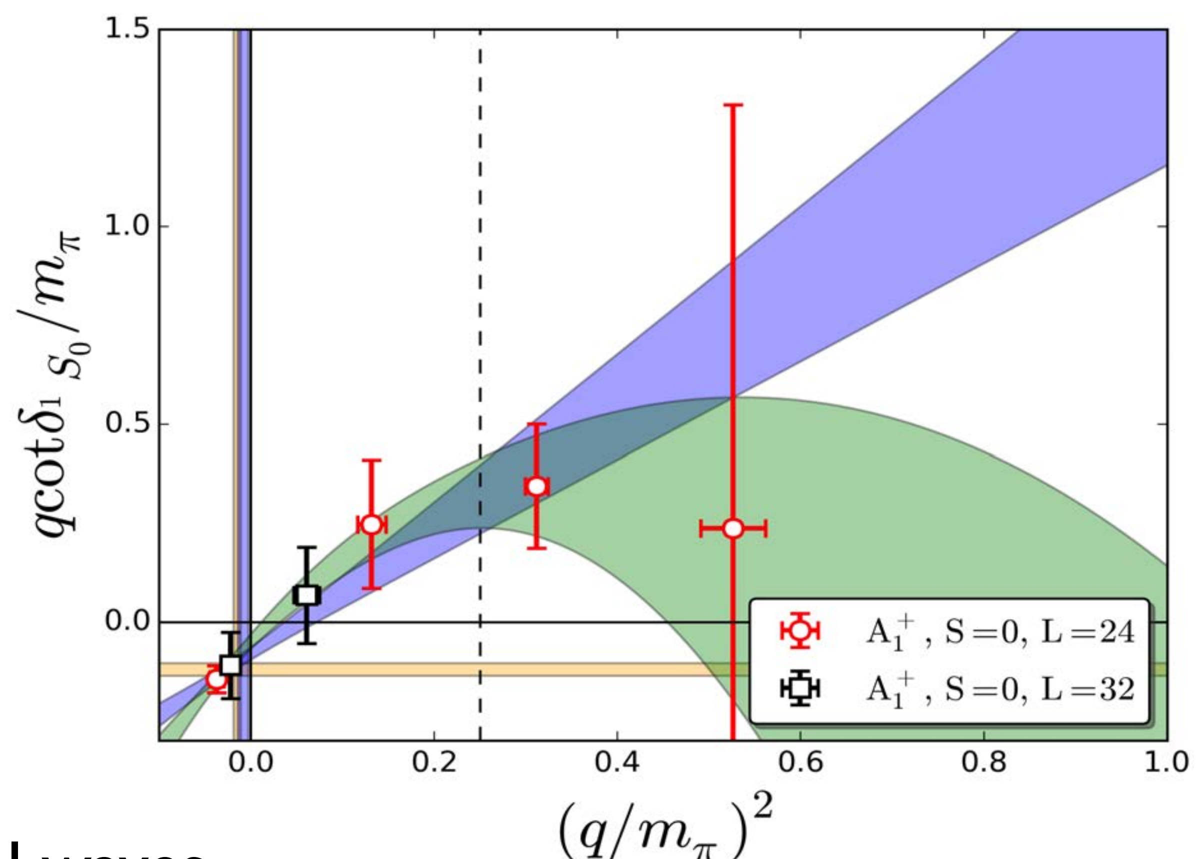
$$\{a^{3S1}_{LO},\ a^{3S1}_{NLO}\} \leftrightarrow \text{LQCD}$$

  in the Bloch-Horowitz equation



(a) continuum (b) discretized

- This effectively is an end-run around the *LQCD fermion sign problem*: the non-relativistic theory HOBET is explicitly antisymmetric



- Opens up wonderful opportunities to "mix and match" LQCD, experiment

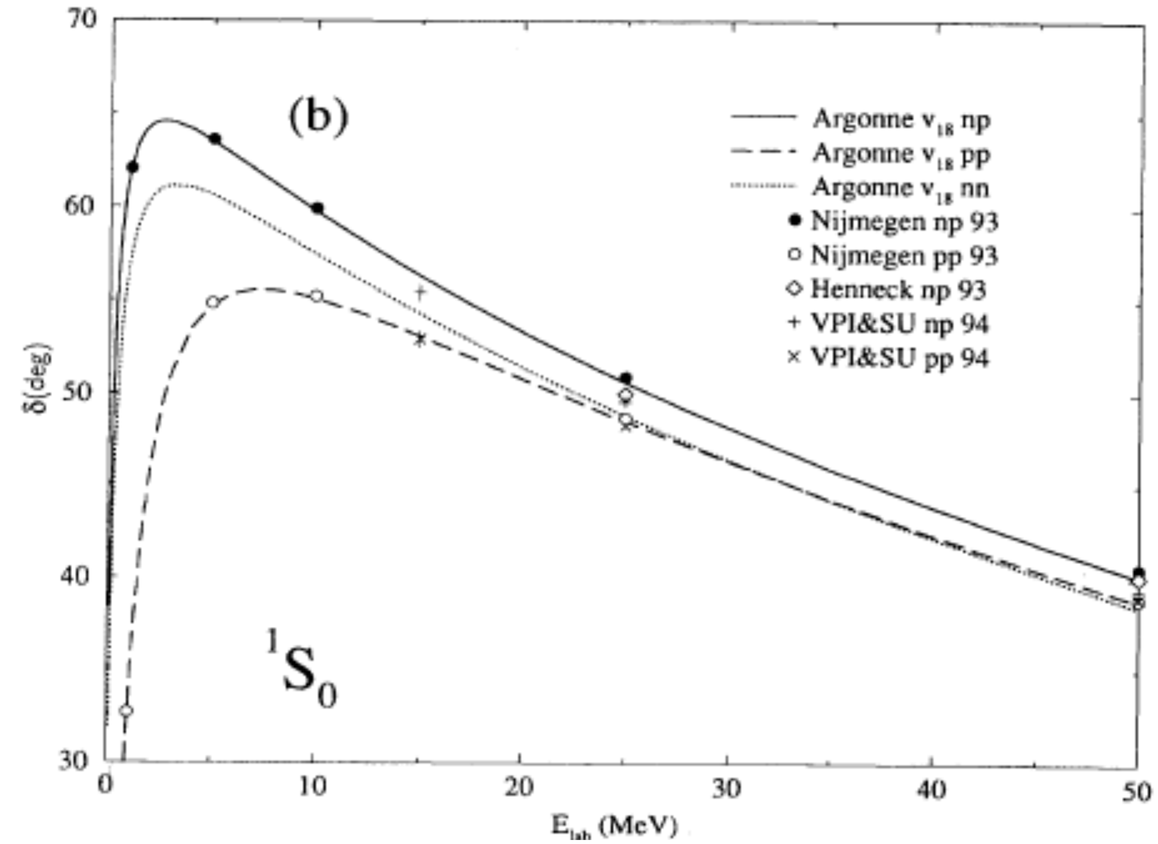
- Challenge #3: Develop LQCD NN scattering techniques beyond point s-wave: spatially extended sources, partial waves

Three Key Advances this Past Year

- Development of a simple method to construct the effective interaction directly from phase-shift input
- Development of Bigstick into a very powerful Lanczos engine for solving HOBET's C.I. problem, in large spaces
- Completion of the first LQCD calculations of s-wave scattering beyond the scattering length limit, and the first calculations of higher partial wave scattering (Andre Walker-Loud)

These map onto the three components of our program

1. Doing scattering in an compact Hilbert space



- there exists a solution for any E>0: the projection of a continuum wave function onto a discrete HO basis is well defined

- the IR/UV separation yields the following HOBET equation

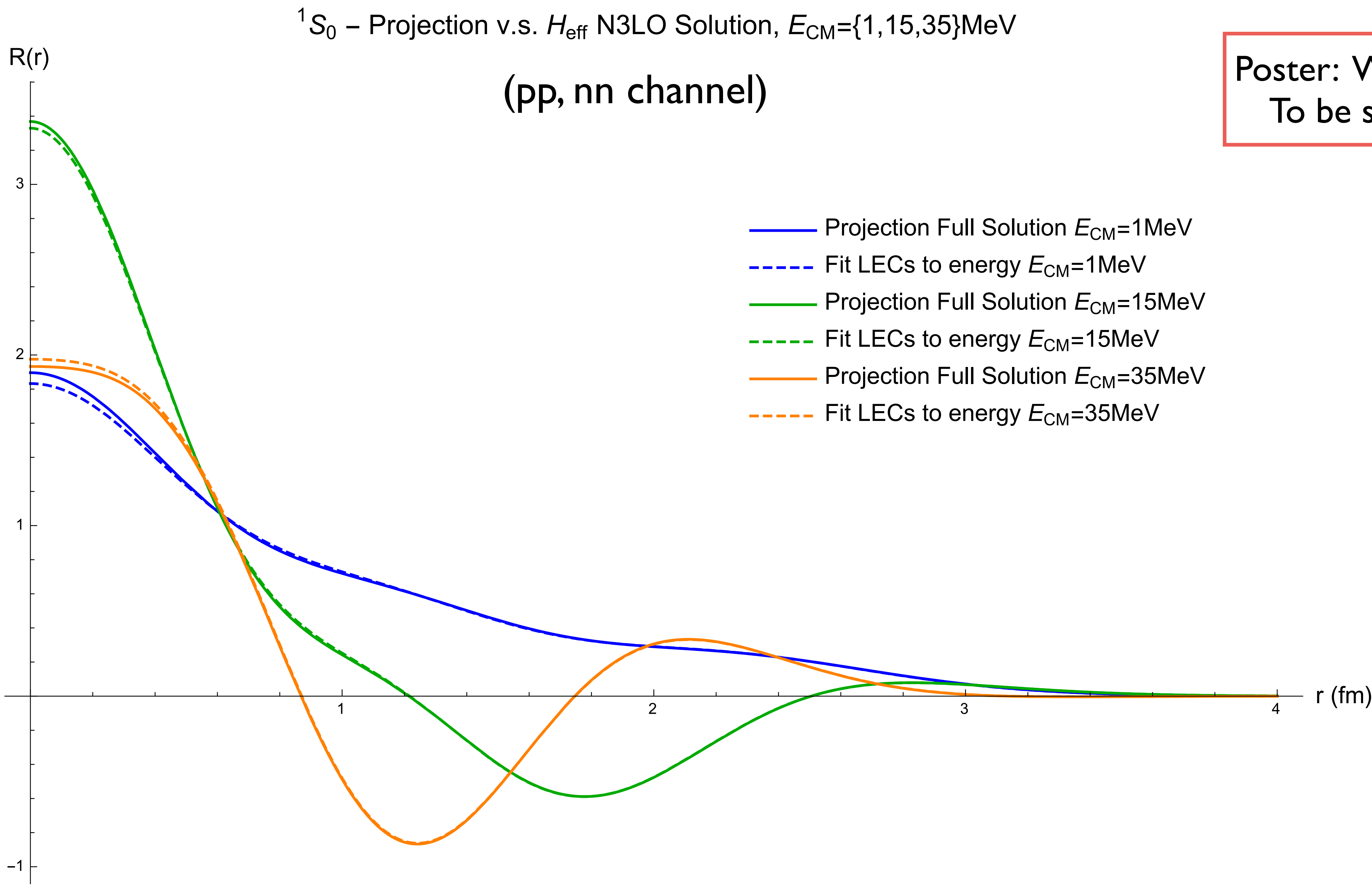
$$H^{\text{eff}} P\Psi = EP\Psi$$

$$H^{\text{eff}} = P \frac{E}{E - TQ} \left[T - T\frac{Q}{E}T + V + V^{UV}(a_{LO}^{3S1}, \ldots) \right] \frac{E}{E - QT} P$$

- the Green's function goes to the free Green's function asymptotically; we pick an E and define that function by inserting the known experimental δ(E), building in the right IR behavior

- we solve the eigenvalue equation in P — and fail to get a solution at E

- the only missing physics is UV: we adjust a_{LO}^{3S1} until we get a self-consistent solution at E — thereby determining the LECs — simple and direct!



Poster: WH + Ken McElvain
To be submitted to PRL

Six energy-independent constants in N3LO (four in NNLO) are determined

Yield (nearly) exact projection P of the true wave function as a continuous function of r and as a continuous function of E<50 MeV

Done without any knowledge of the "potential" outside of P — a true ET

If one has the exact Heff and the exact P,
one has the exact full-space eigenvalue

$^3S_1$ (deuteron) channel: deuteron binding energy prediction

Order	E_{BND}	$\sum(\Delta E/E)^2$
LO	-2.1886	3.0e-2
NLO	-2.2075	3.8e-4
NNLO	-2.2249	1.5e-7
Full	-2.2245	-

sub-keV binding energy accuracy at NNLO (4 LECs)

(without LECs and without our IR summation,
the deuteron would not even bind)

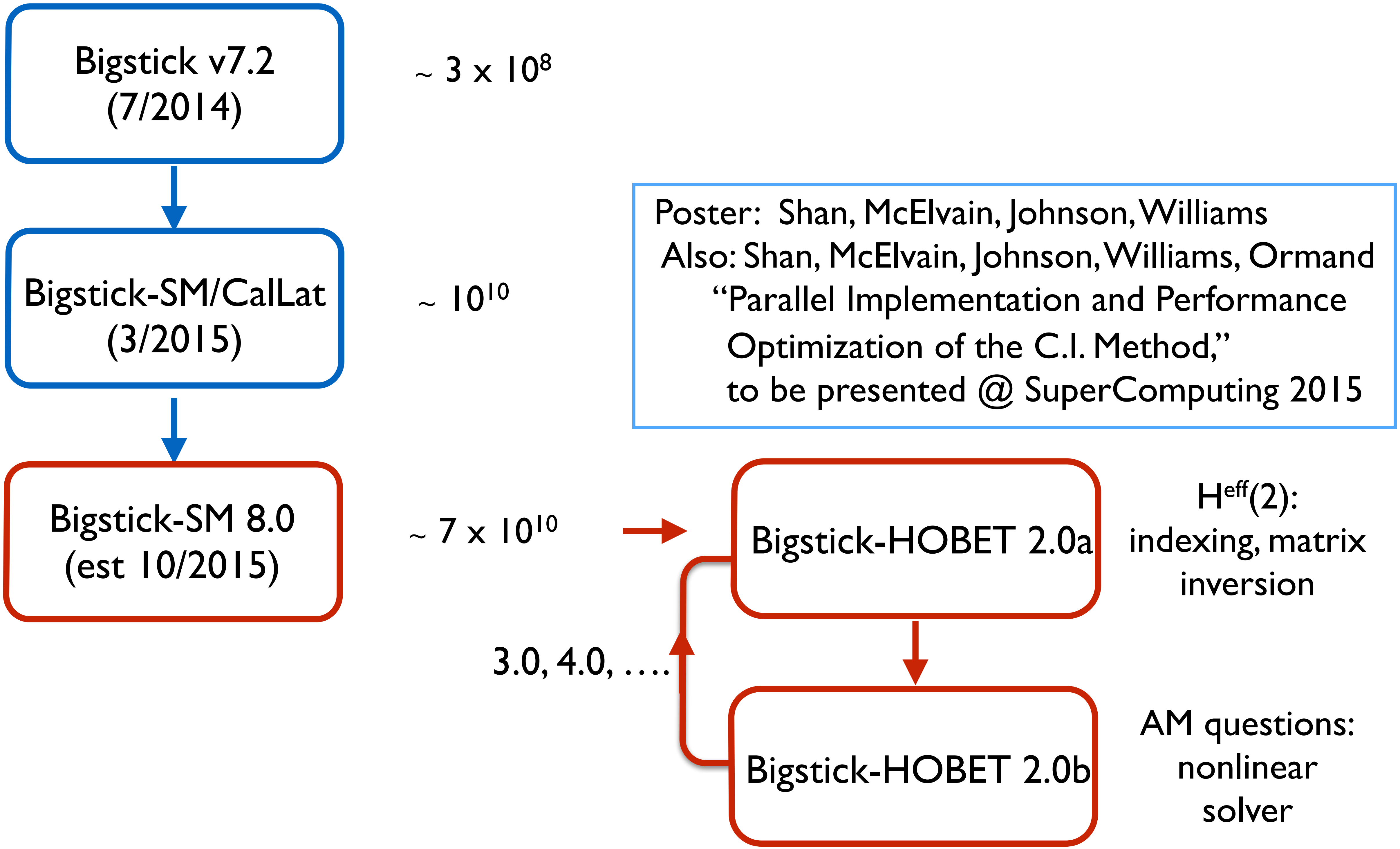
2. Bigstick development: our Lanczos engine

- HOBET's IR-UV scale separation is provided by the diagonalization in P: we need to be able to handle $\Lambda = 8\hbar\omega$ calculations for nontrivial nuclei
- the interaction is spectator-dependent and many-body
- the eigenvalue problem must be solved self-consistently — at each energy

Examined existing Lanczos engines to see which could provide the best starting point

Bigstick was selected

- developed under SciDACII/UNEDF to a level where bases $\sim 3 \cdot 10^8$ reached (C. Johnson, E. Ormand)
- clean, logical, modular structure - published algorithm review, and a helpful internals document
- on-the-fly Hamiltonian construction optimizing memory requirements, speed
- existing capabilities for a three-body H^{eff}. Most modules needed for an extension to four bodies present
- a build-in indexing scheme that can be exploited to treat HOBET's spectator dependence



Bigstick-HOBET — One Year into a 3-year program

Big Picture

Nonrelativistic Nuclear Structure
(model dependent)

Cold Lattice QCD
(exact, but with a sign problem growing with A)

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Nonrelativistic Nuclear Structure
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⇓

CalLat

$LECs$

δ^{LQCD}

A Controlled Nonrelativistic ET applicable to nuclei ↔ ↔ Cold Lattice QCD focused on NN scattering observables

experimental observables

connect to fundamental theory

Associated Math and CS Challenges

- large-basis Lanczos diagonalization, complex Hamiltonian
- nonlinear eigenvalue problem
- linear operator inversion

- inversion of the LQCD Dirac operator requiring solvers for 4D complex lattices
- contractions for operator evaluation
- I/O

$LECs$ ← CalLat ← δ^{LQCD}

A Controlled Nonrelativistic ET described by LECs ↔ ↔ Cold Lattice QCD focused on NN scattering observables

experimental observables

connect to fundamental theory

Ken McElvain
(Berkeley NP grad student)

Thorsten Kurth
(LBNL NP postdoc)

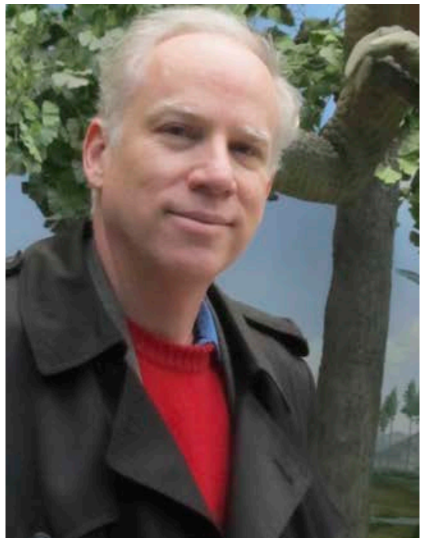
Amy Nicholson
(Berkeley postdoc)

Wick Haxton
(Berkeley/LBNL)

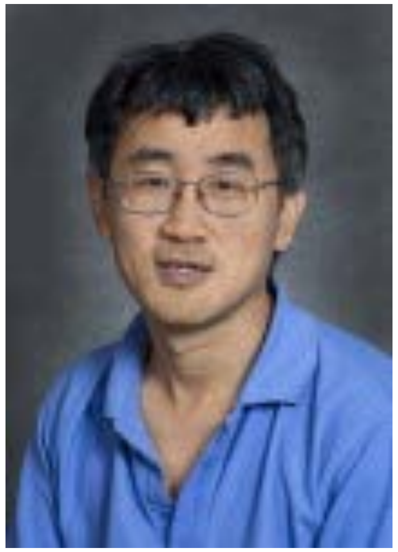
HOBET effective interactions development

Bigstick performance

Ken McElvain
(Berkeley NP grad student)



Calvin Johnson
(CalState SD)



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Bigstick solvers/math

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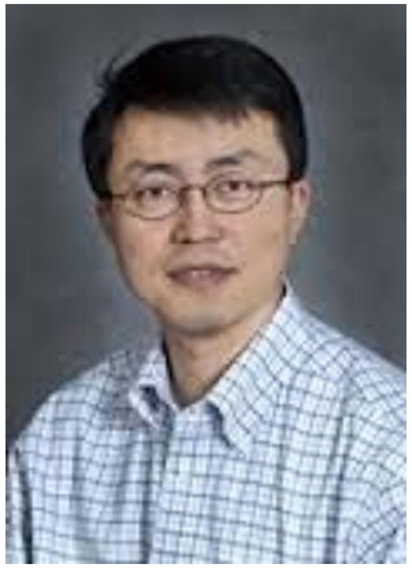

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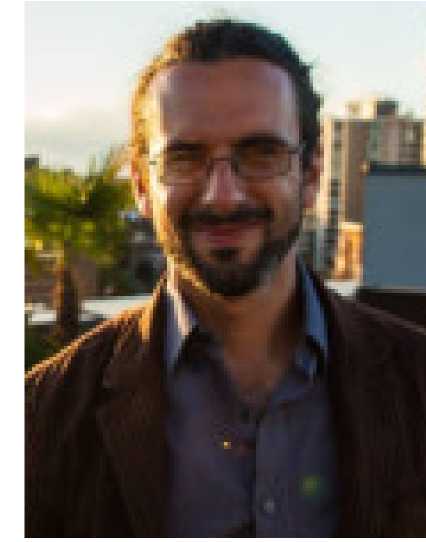

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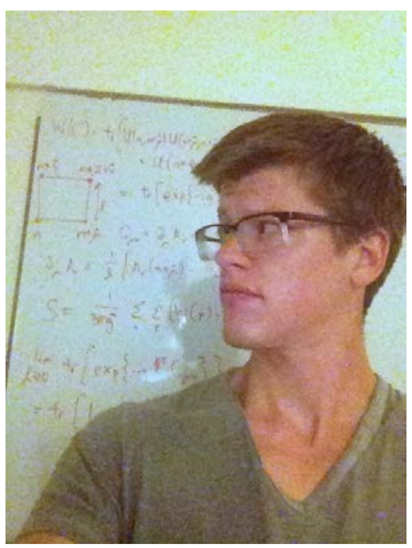


Mark Strother
(Berkeley NP
grad student)

Tom Scogland
(LLNL CS

Performance

Bronis de
Supinski

Performance

Ron Falgout
(LLNL CS)

Multi-Grid

Abhinav Sarje
(LBNL CRD

I/O

and collaborators Michael Buchoff, Philip Powell, Enrico Rinaldi, Sergey Syritsyn, Joe Wasem

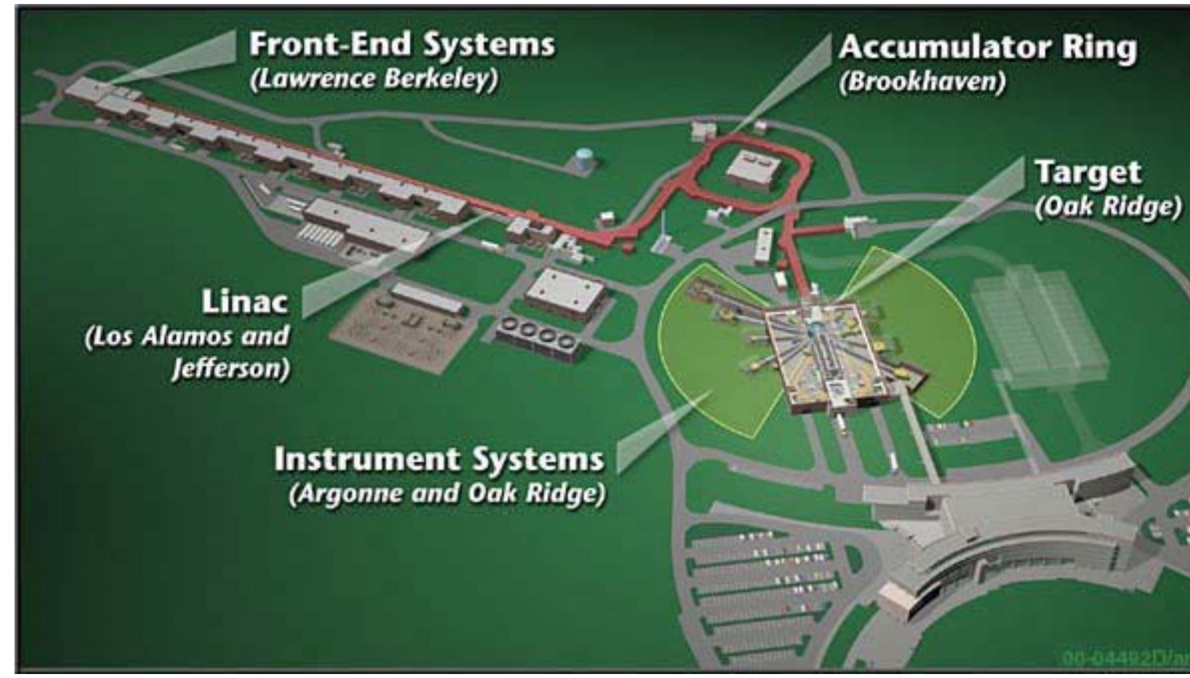
II. Lattice QCD, NN phase shifts

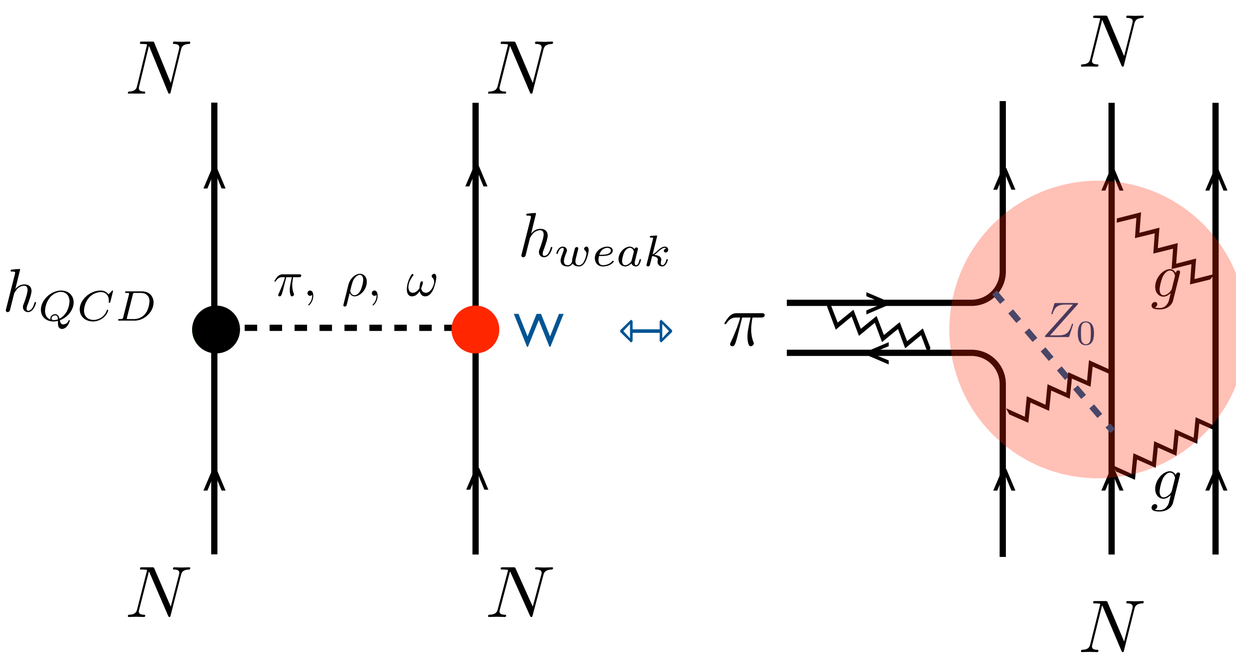
André Walker-Loud

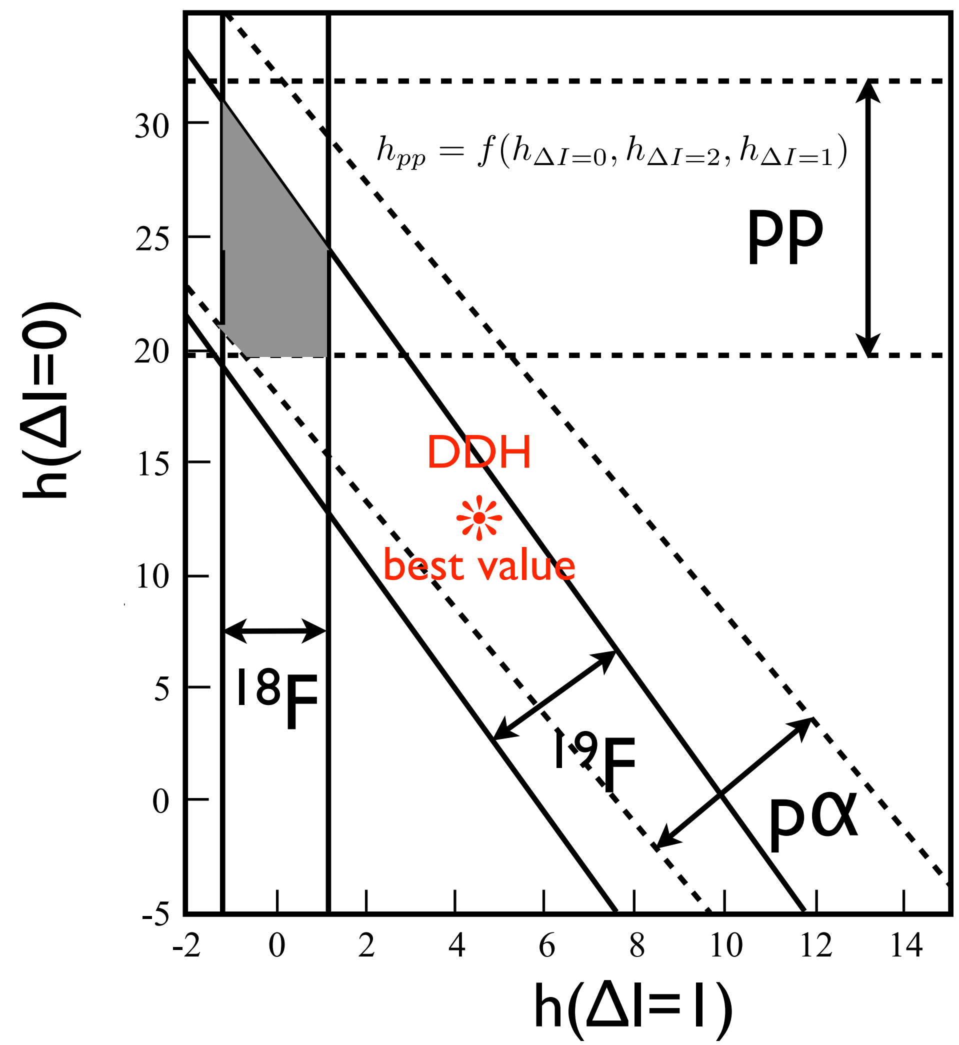
II. Lattice QCD, NN phase shifts

One of our main goals is to compute *weak parity-violating* two-nucleon amplitude

NPDGamma Experiment
SNS @ ORNL



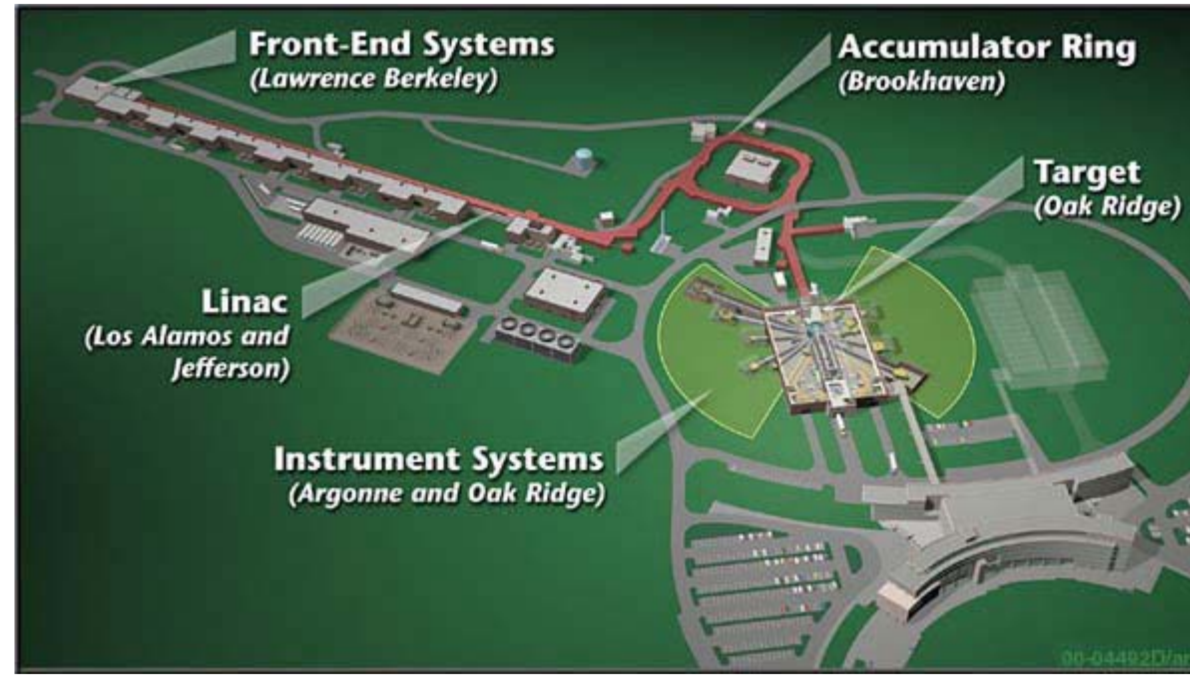




$$h_{weak} \sim 10^{-7} h_{QCD}$$

II. Lattice QCD, NN phase shifts

One of our main goals is to compute *weak parity-violating* two-nucleon amplitude



NPDGamma Experiment
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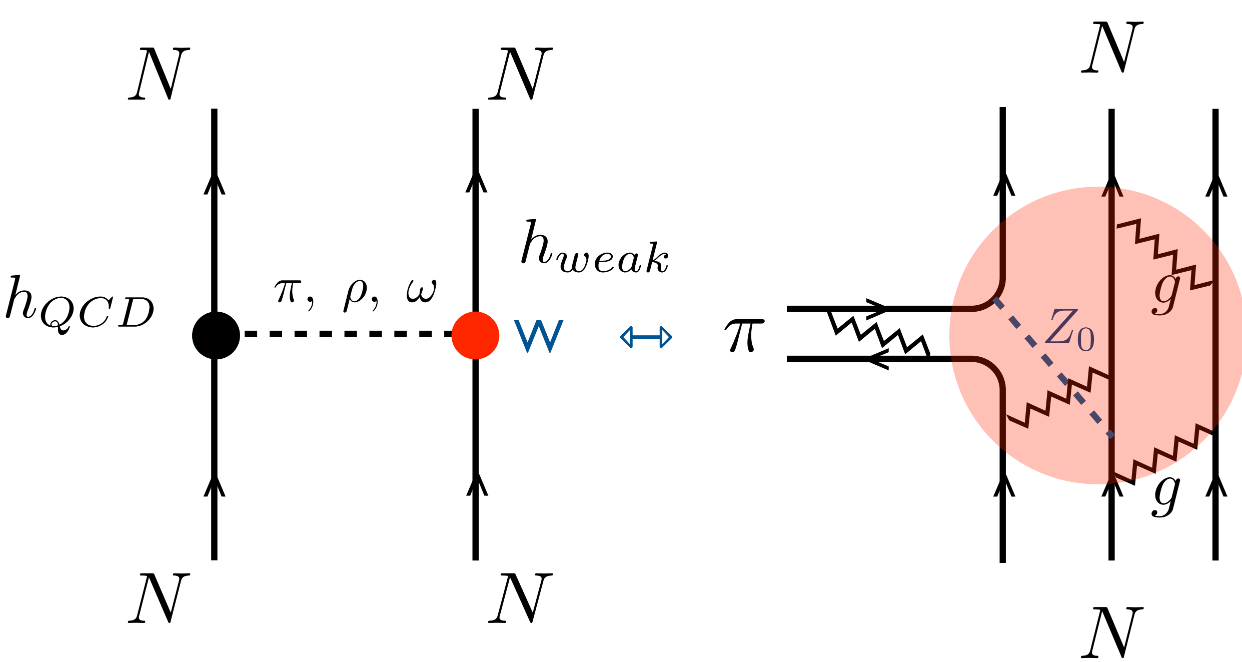
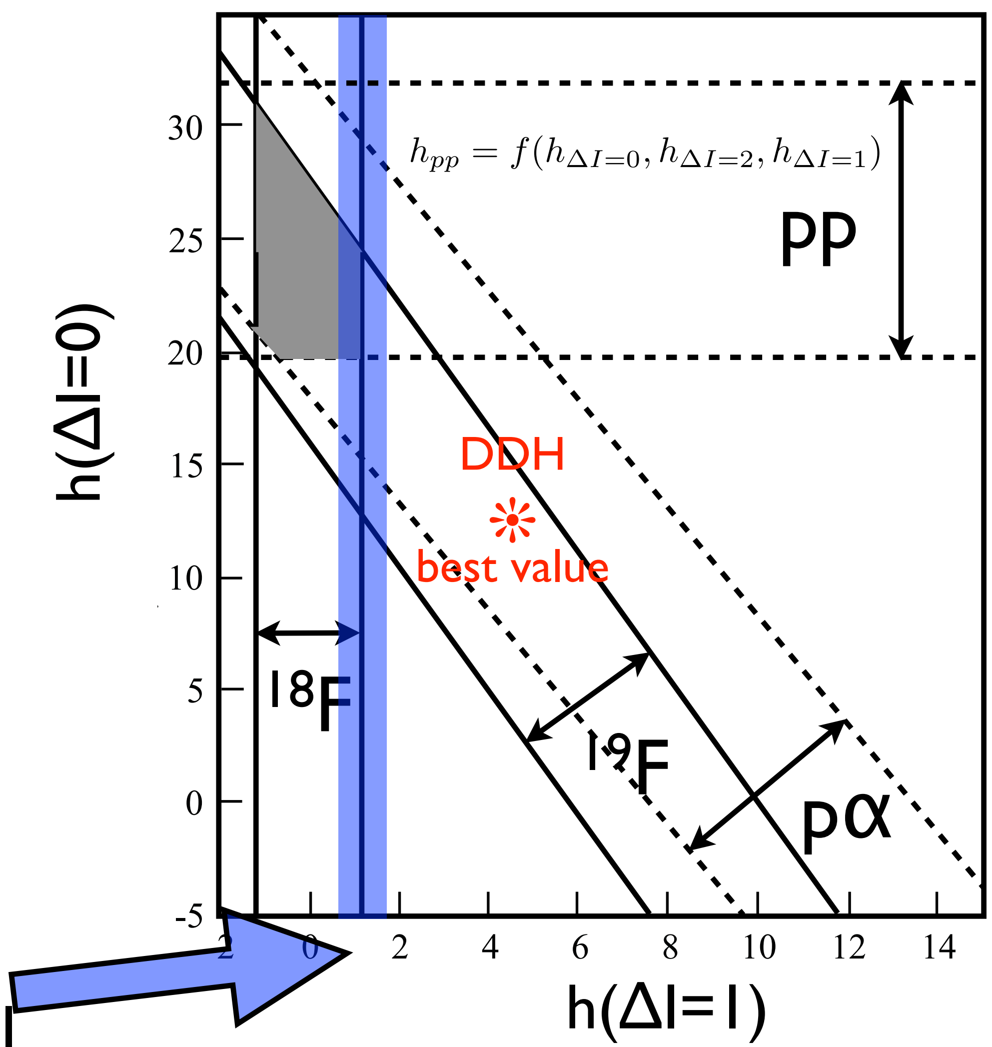
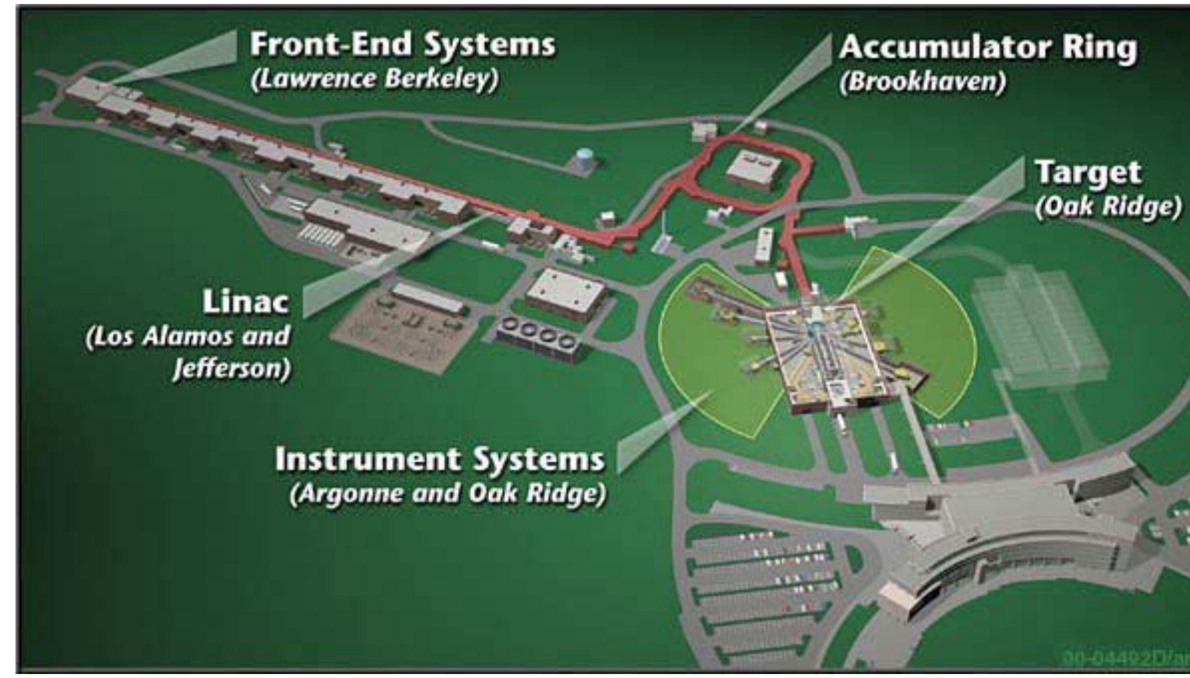




first LQCD calculation of for
L=2.5 f a=0.123f m_π= 389 MeV
systematic approximations
J.Wasem Phys. Rev. C85 (2012) 022501

II. Lattice QCD, NN phase shifts

One of our main goals is to compute *weak parity-violating* two-nucleon amplitude



NPDGamma Experiment
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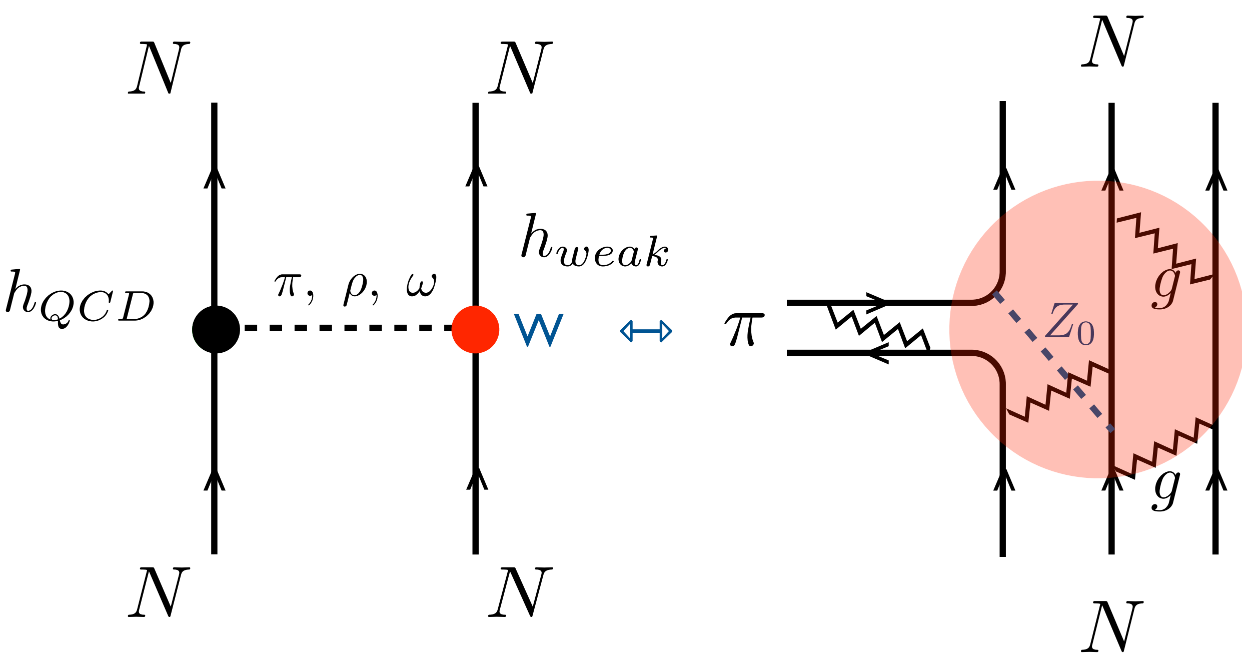
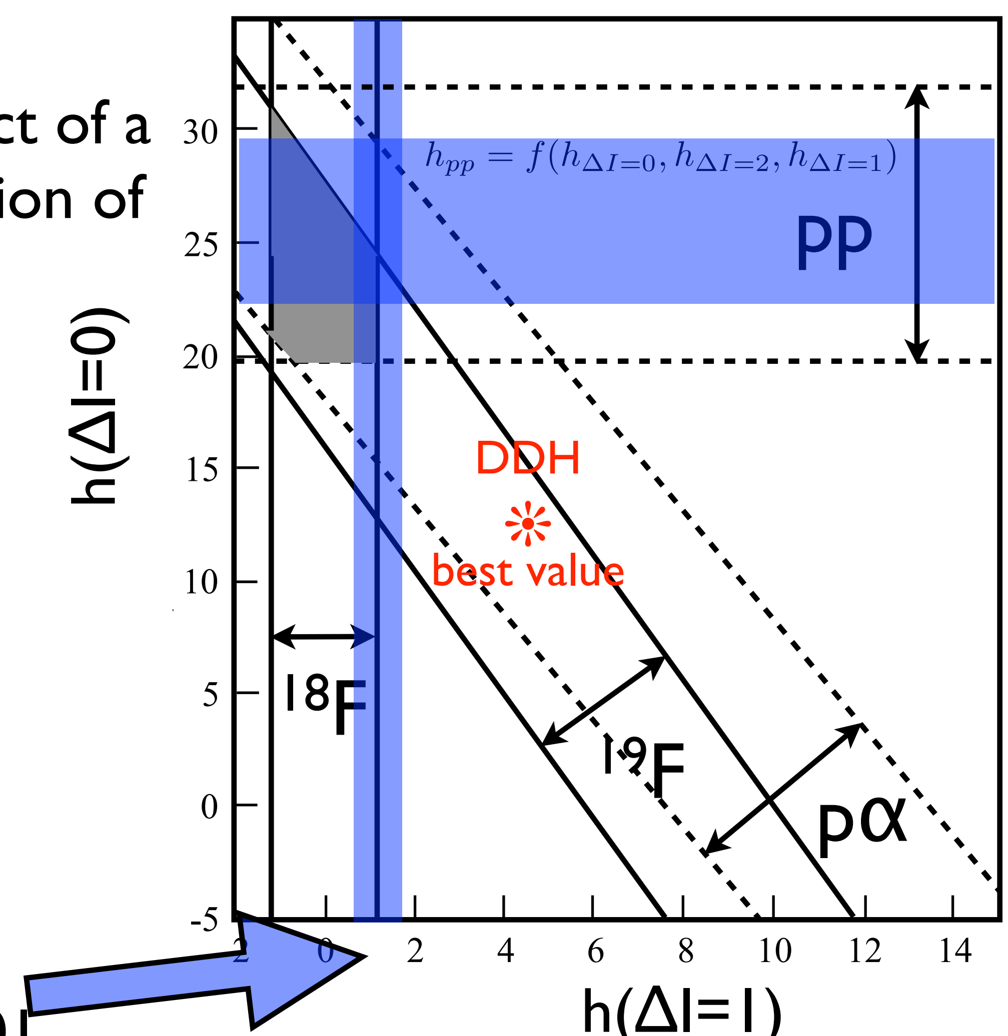


potential impact of a future calculation of h_ρ^2



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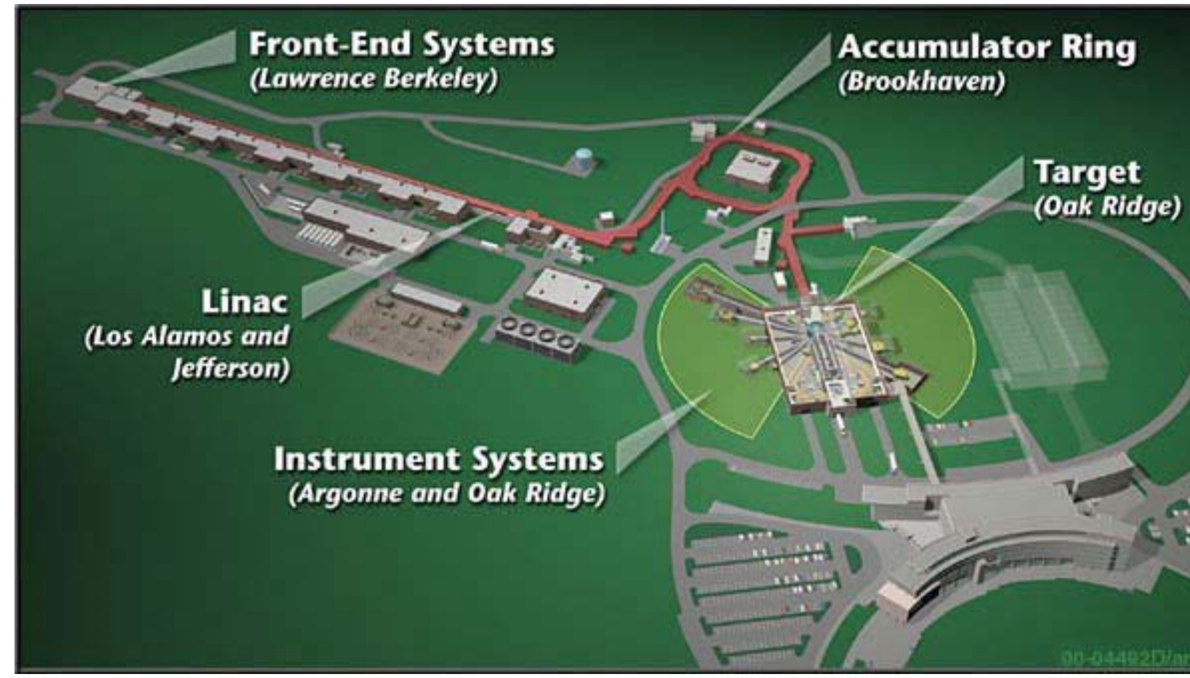
II. Lattice QCD, NN phase shifts

One of our main goals is to compute *weak* parity-violating two-nucleon amplitude



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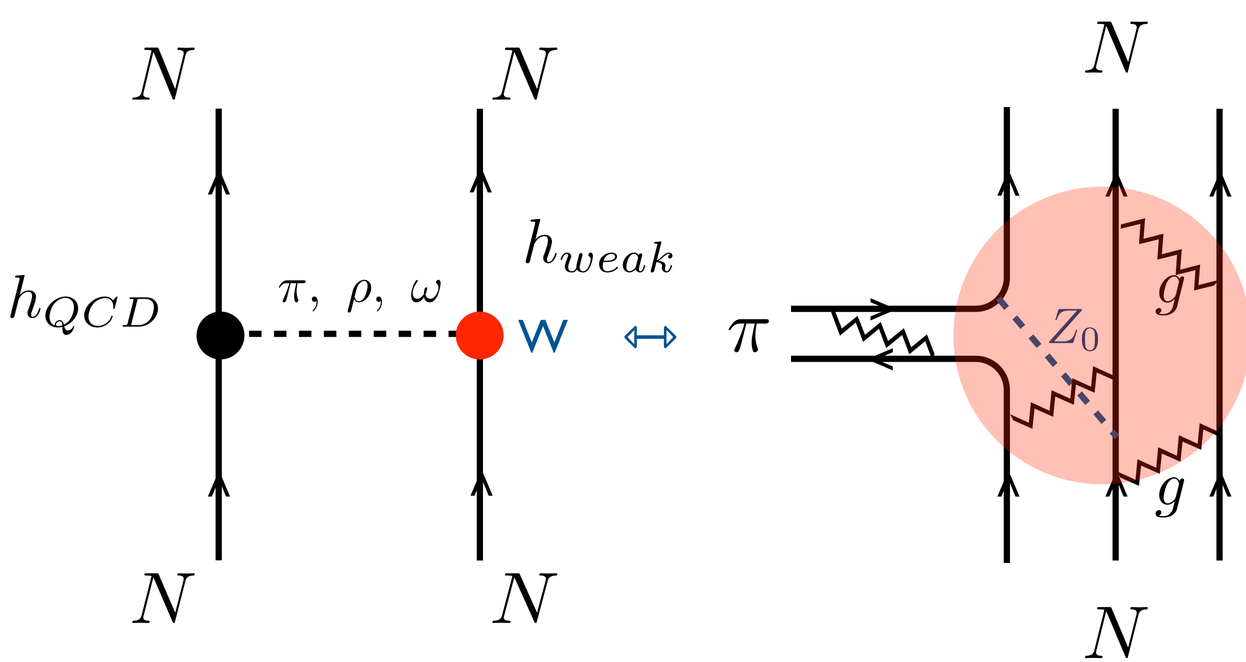
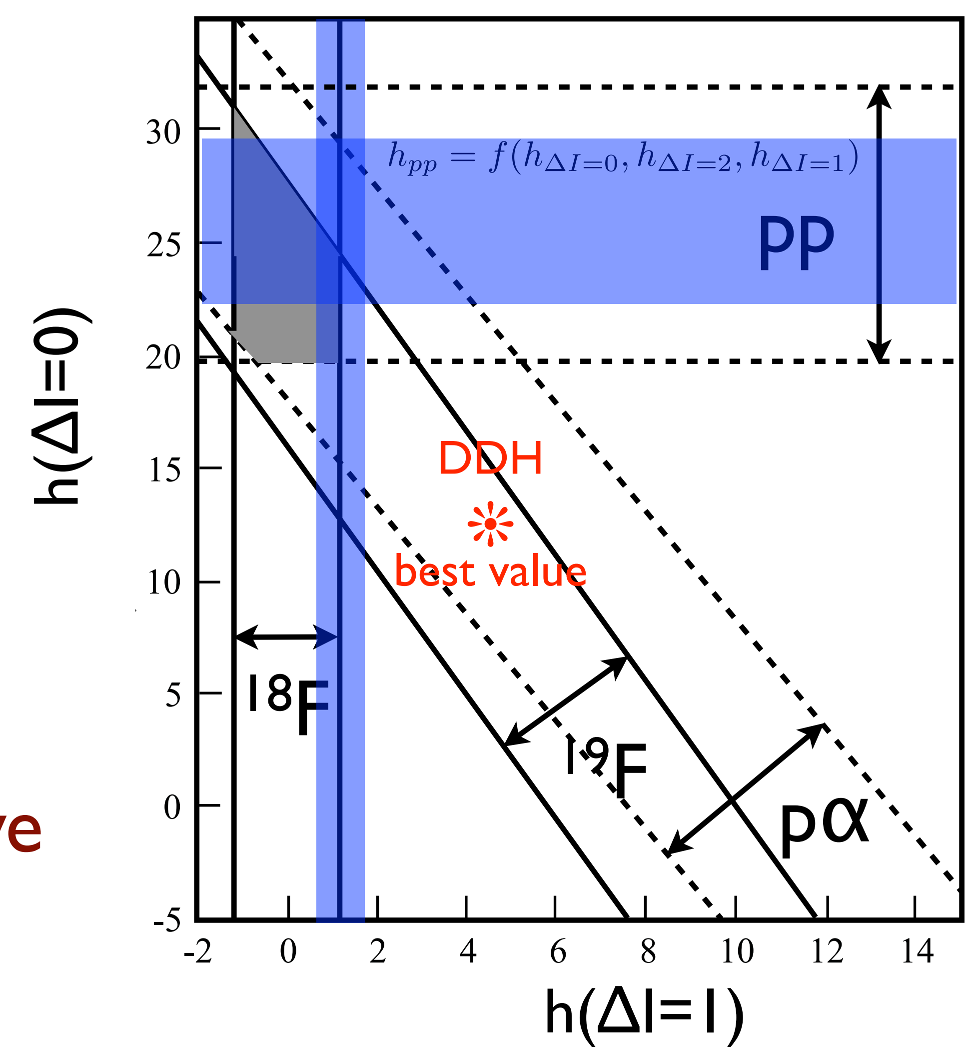
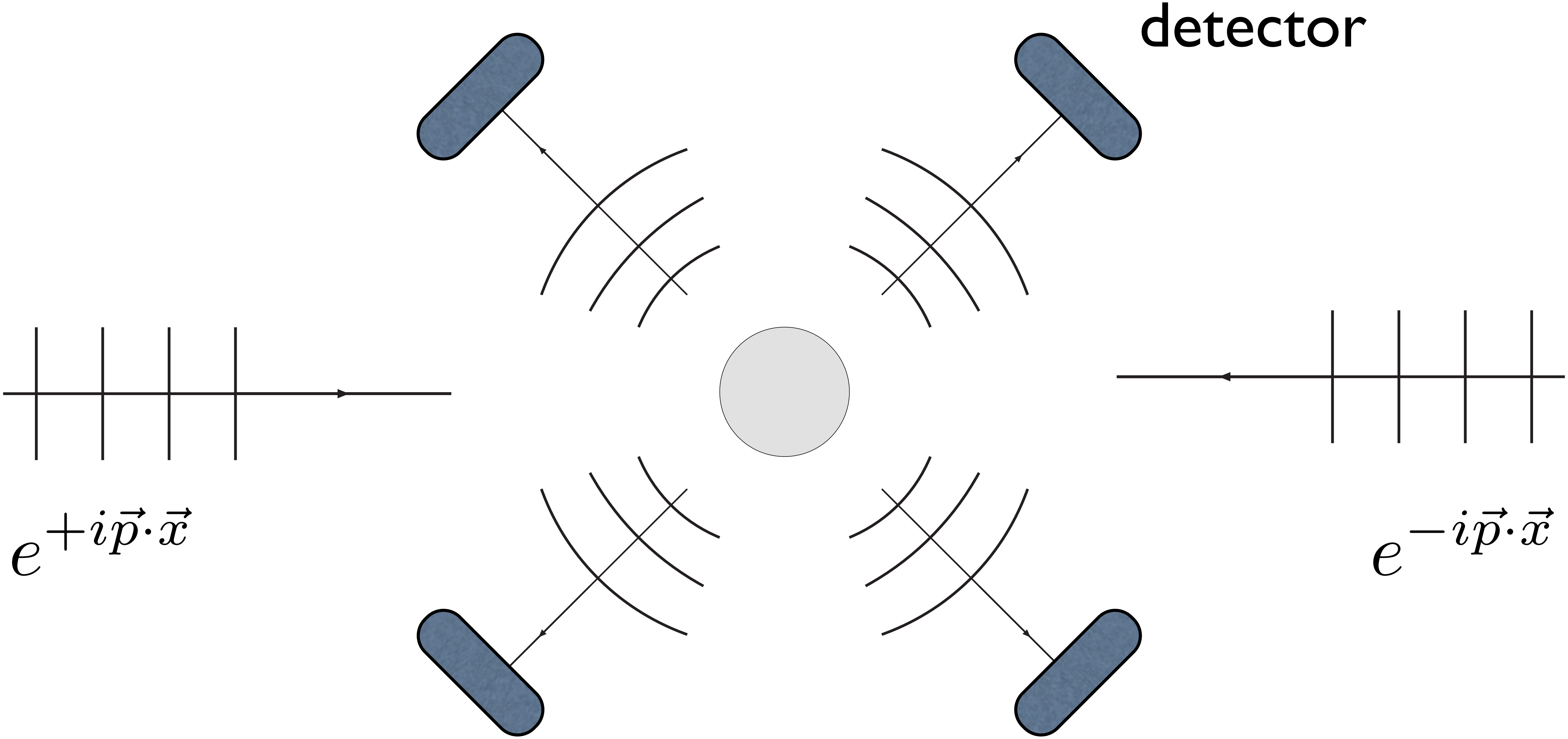




In order to understand this *weak* interaction (and other Standard Model and Beyond interactions) we must understand the NN interaction from QCD

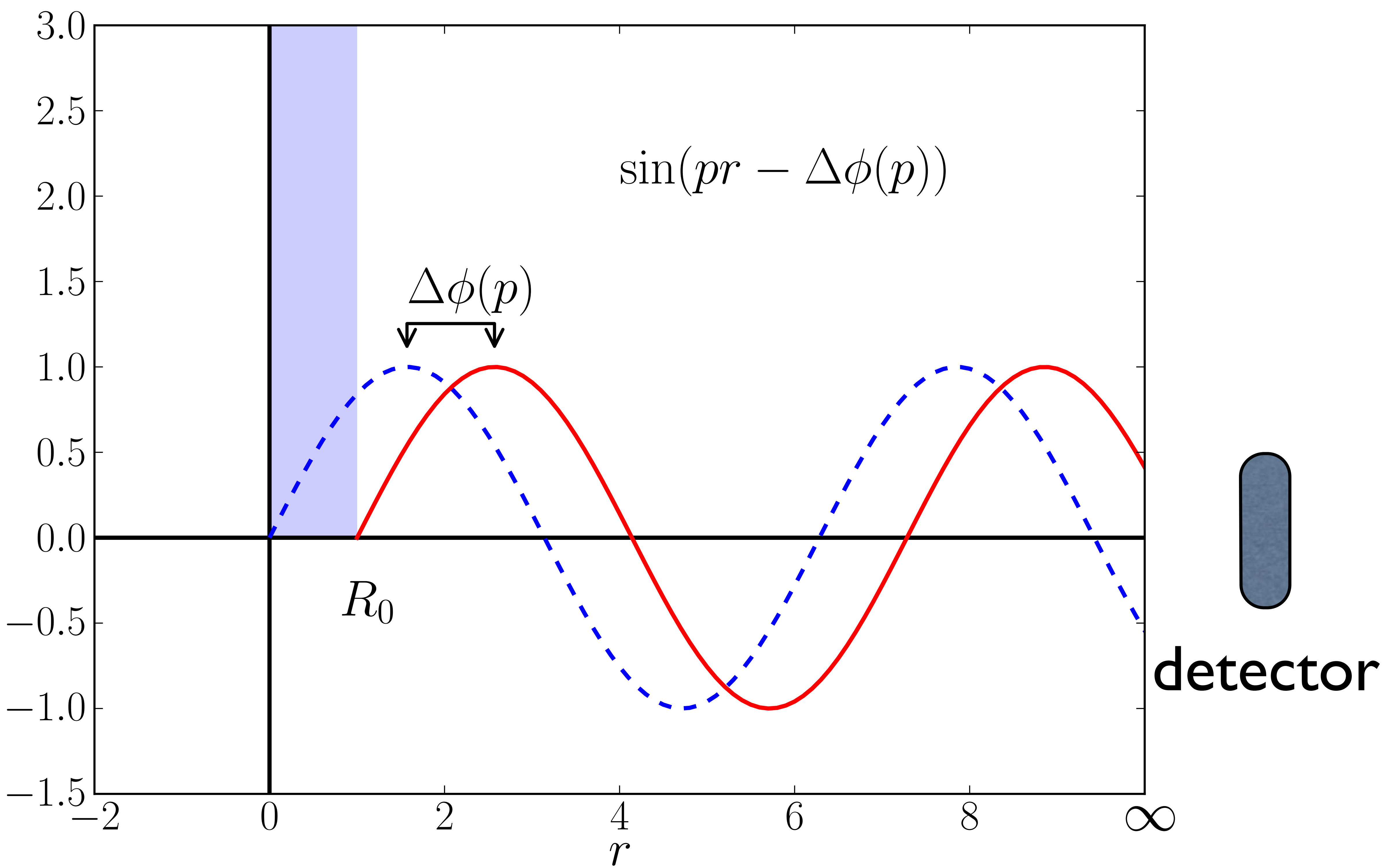
Scattering



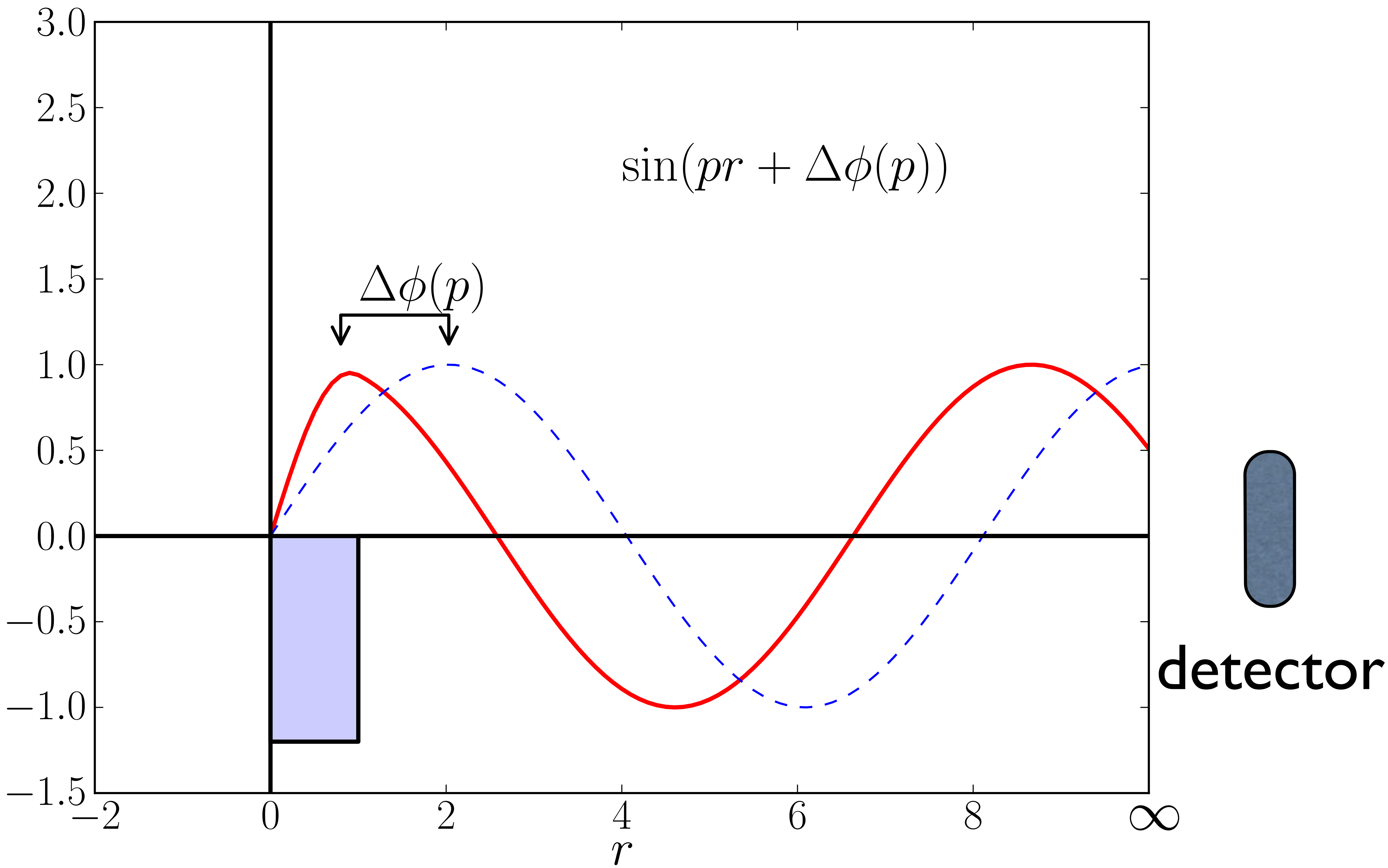
$$S_l(p) = e^{2i\delta_l(p)}$$

Scattering Phase Shift

Scattering off “Hard Sphere”

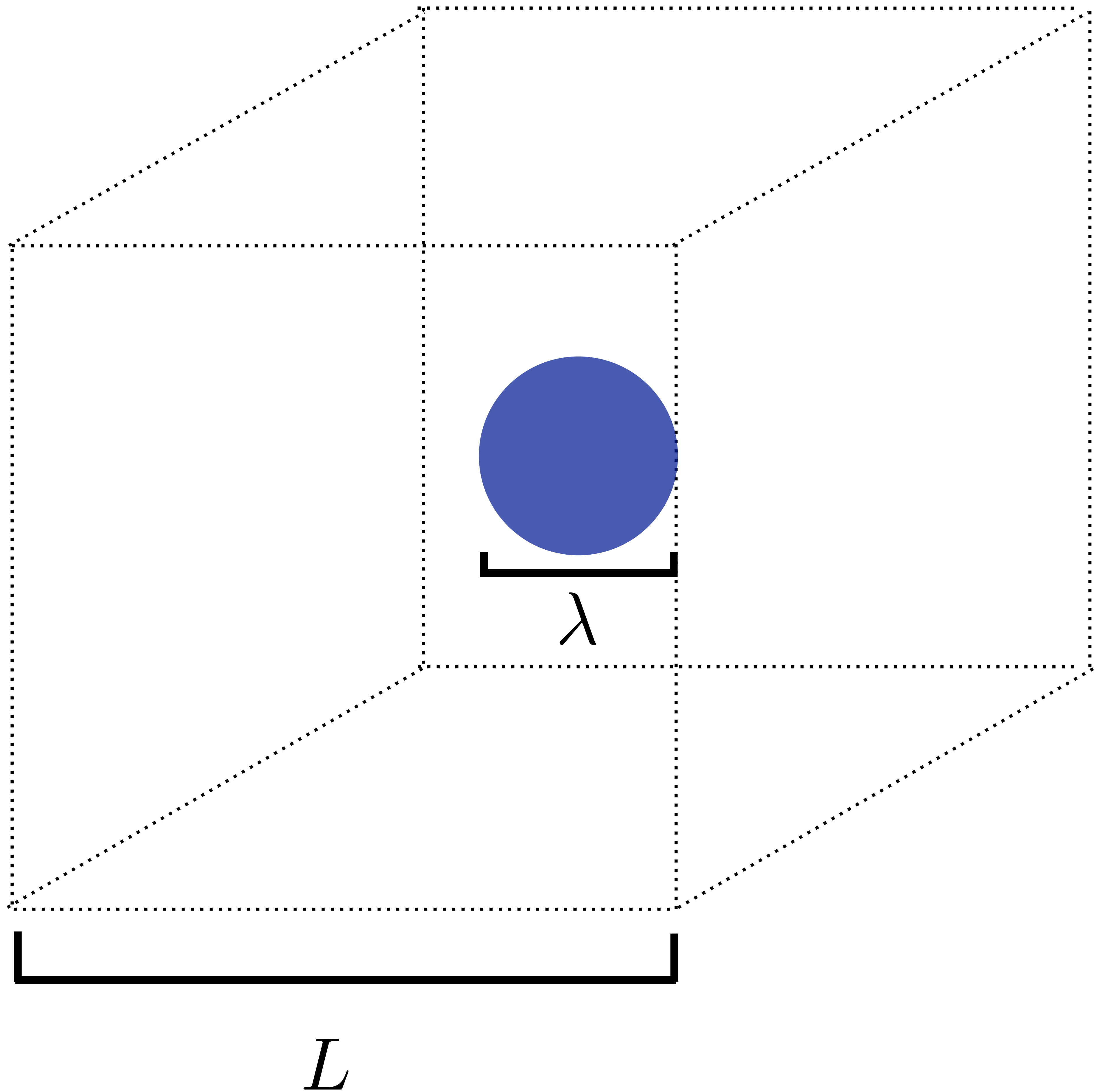


Scattering off "Soft Sphere"

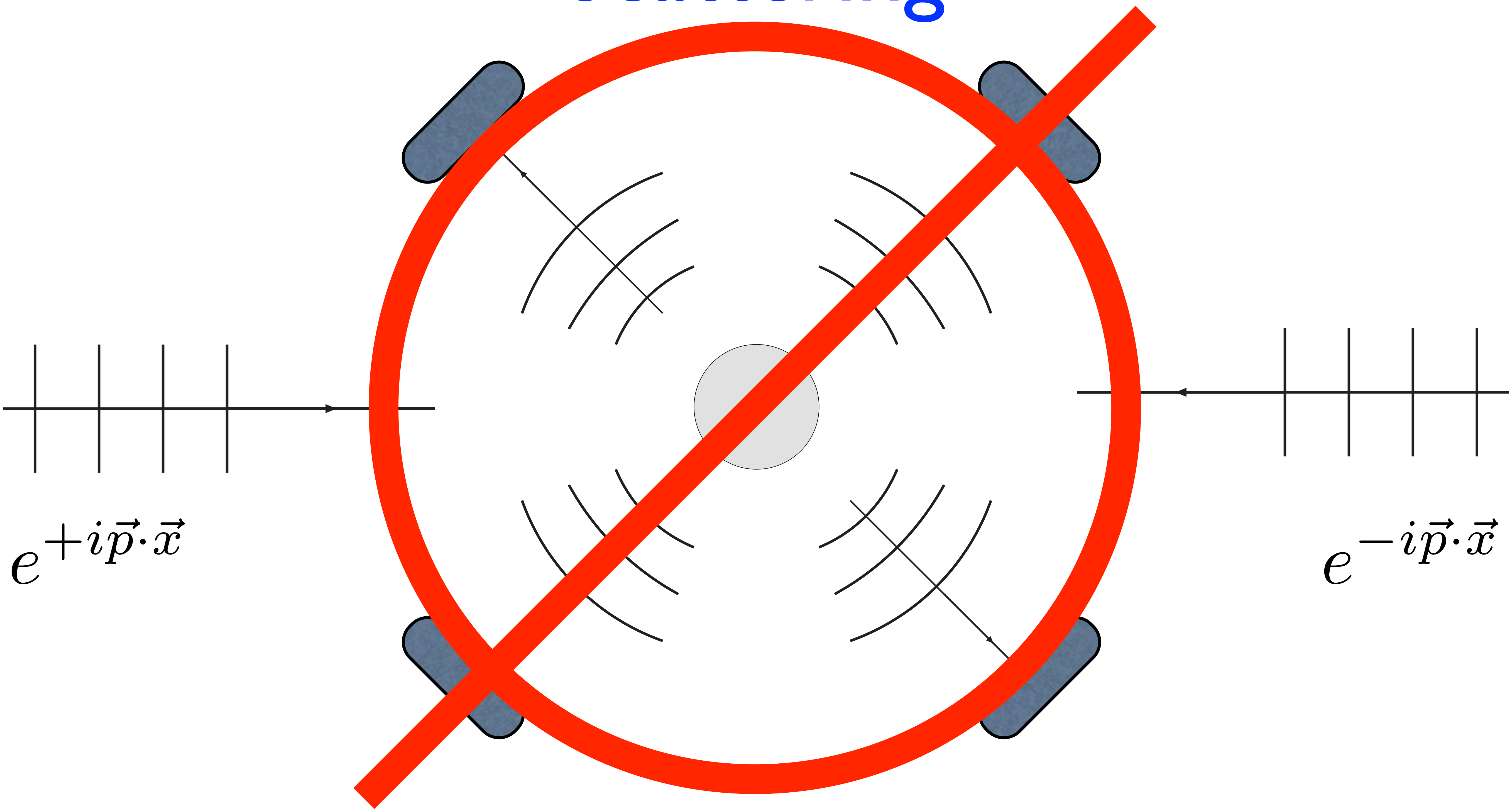


State of the art lattice QCD calculations

$$\frac{L}{\lambda} \sim 4 - 6$$



Scattering

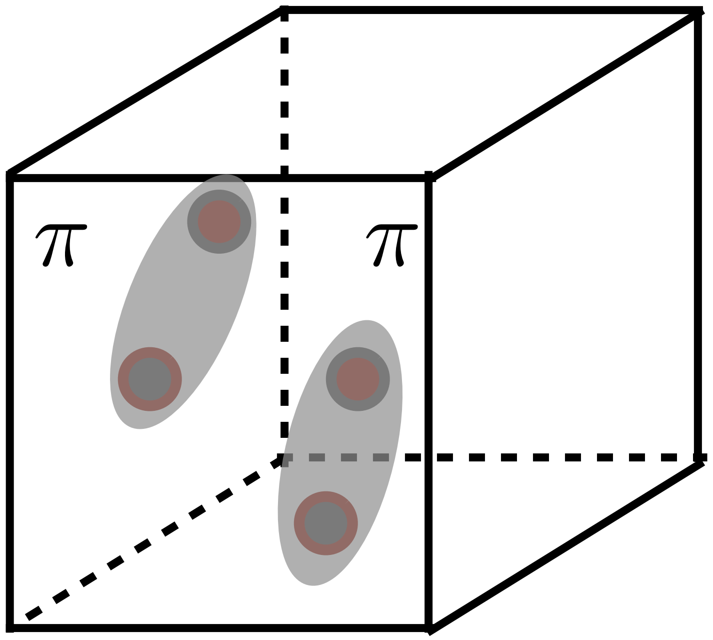


$$S_l(p) = e^{2i\delta_l(p)}$$

Scattering Phase Shift

lattice QCD calculations performed in finite volume

infinite volume scattering phase shifts



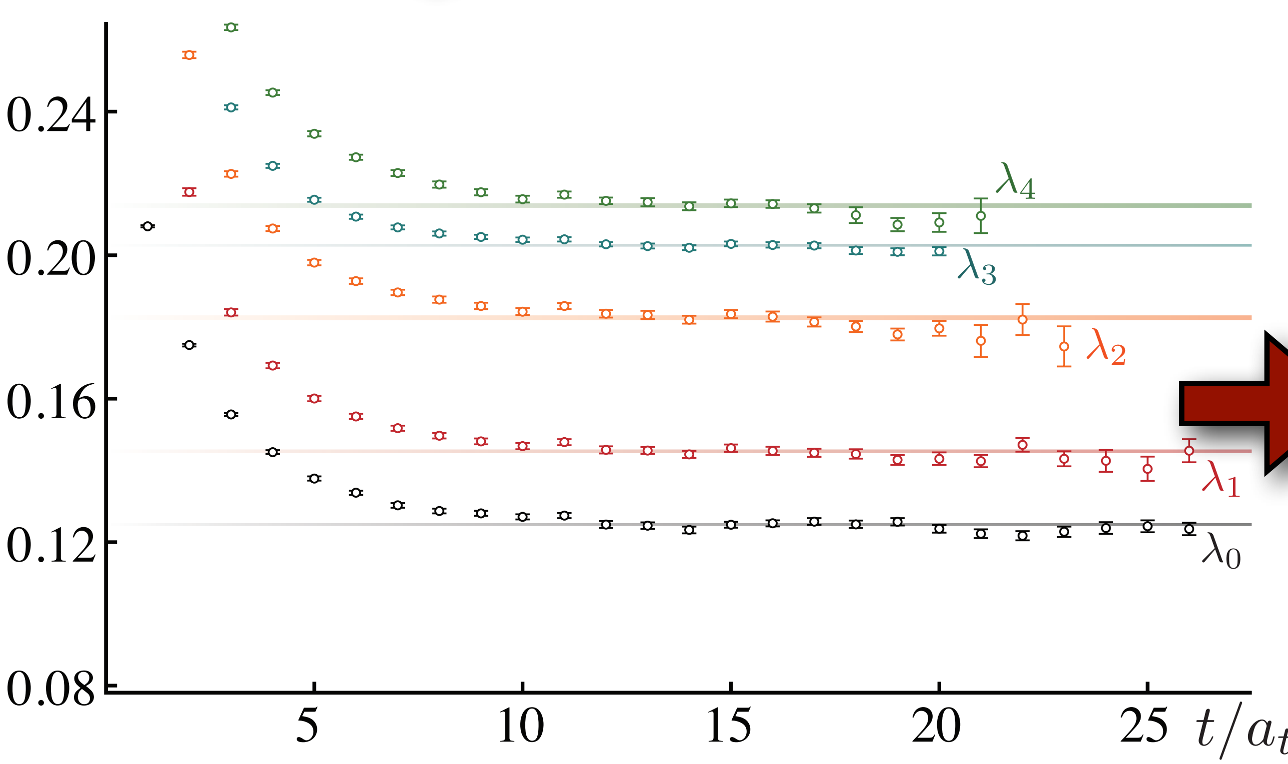
$$E = 2\sqrt{m^2 + p^2}$$ (two particles)

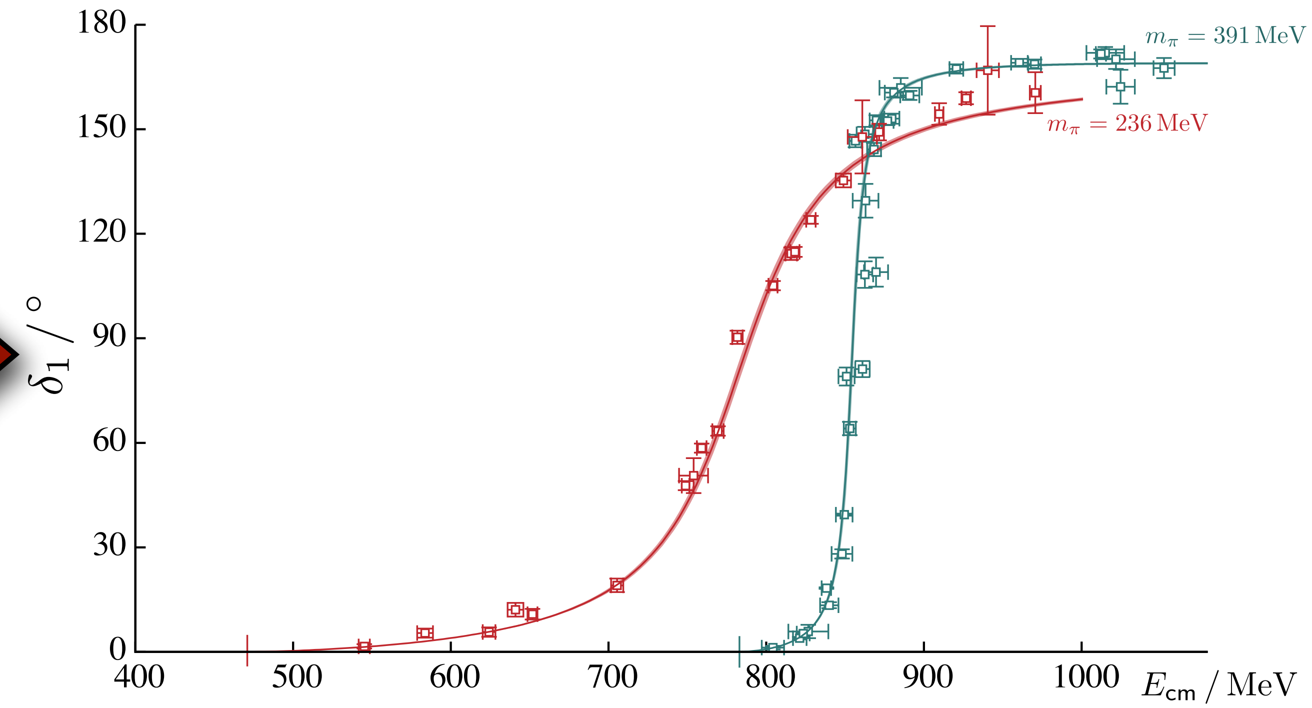
$$p \cot \delta(p) = \frac{1}{\pi L} \sum_{|\vec{n}|<\Lambda} \frac{1}{|\vec{n}|^2 - \frac{p^2 L^2}{4\pi^2}} - 4\pi\Lambda$$

(includes bound states)

Lüscher Formalism

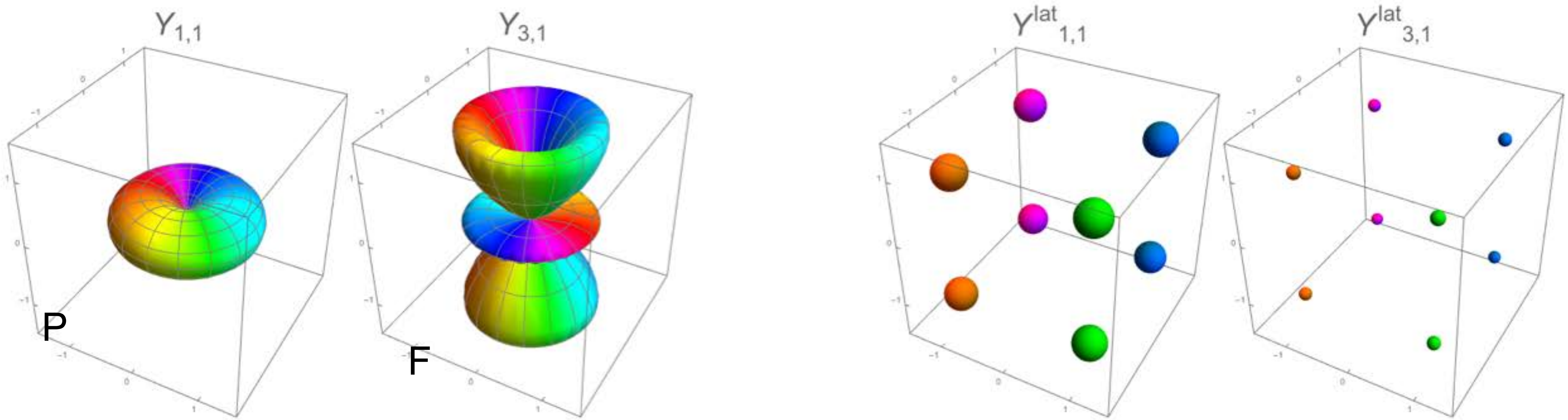
Wilson et al (HSC)
[supported by USQCD]
arXiv:1507.02599





Rotational symmetry and the lattice
(How to map a sphere into a cube)

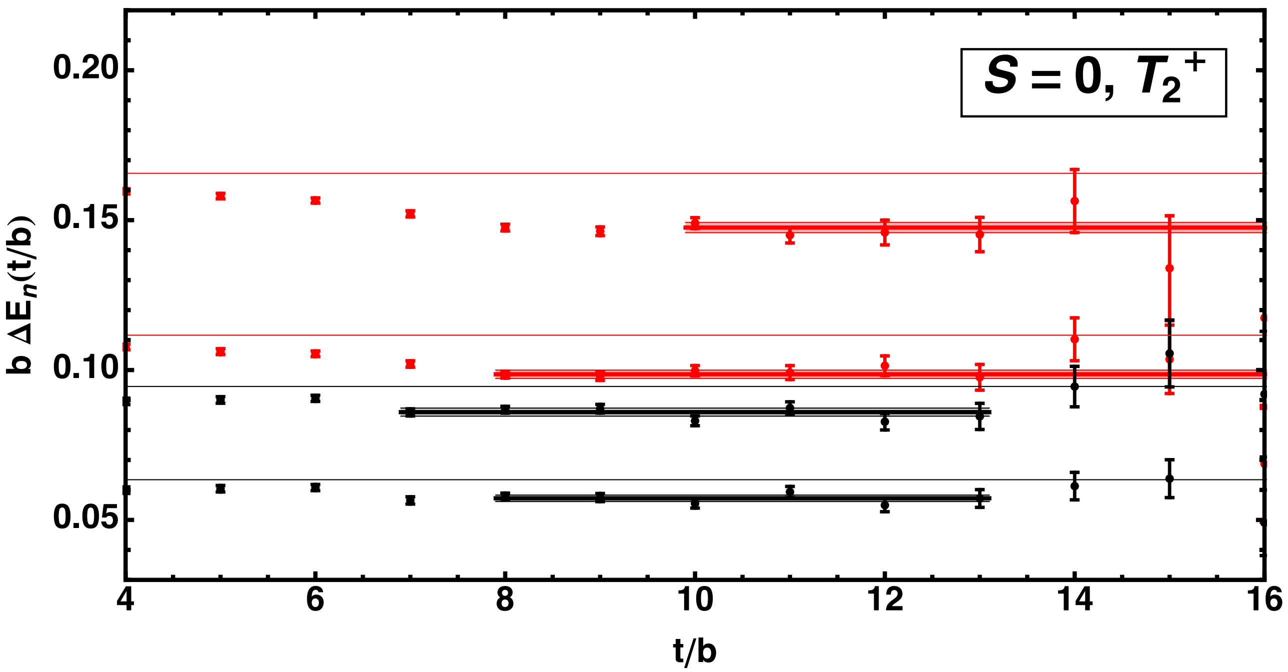
- Finite volume cubic lattice breaks rotational symmetry
- In continuum one has orthonormal states with definite Angular Momentum
- Not so on the lattice

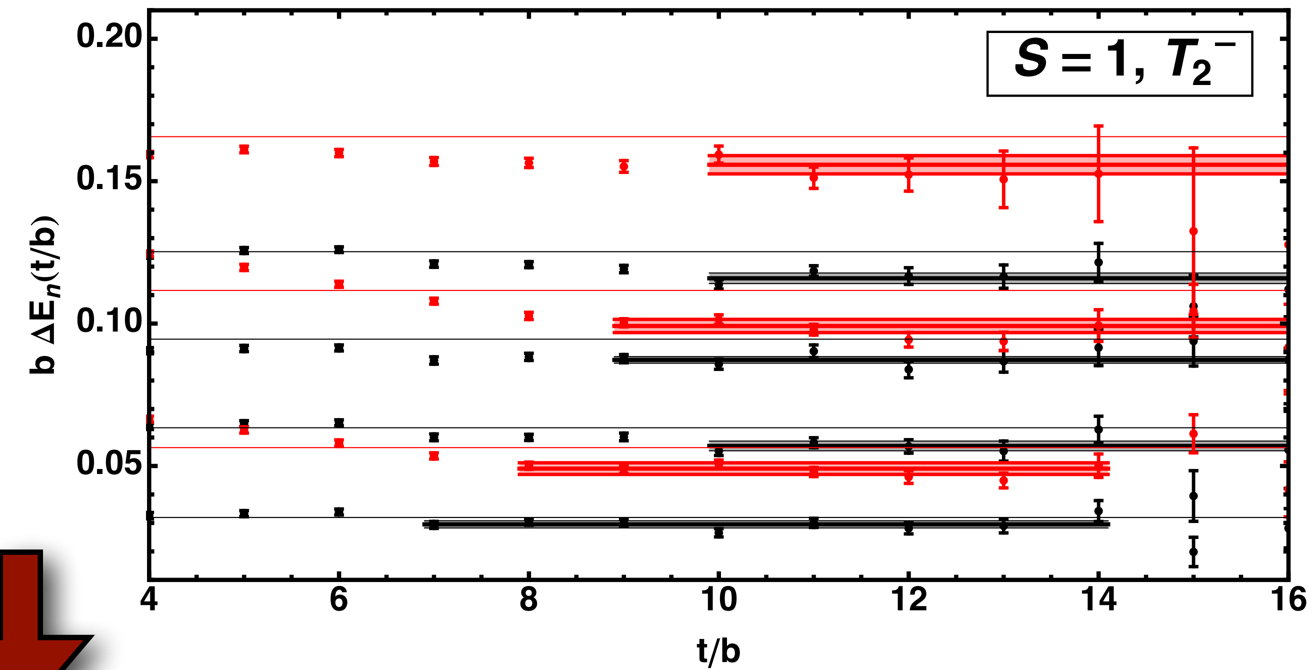


(a) continuum — orthogonal angular momentum basis

(b) discretized — Not orthogonal in angular momentum

- One obtains unphysical mixing of partial waves of same parity
- Luscher disentangles unphysical mixing (solve complicated det eq. - Raúl Briceño et al
- Need many finite volume energy levels to high precision
- Need SOURCES that couple to P,D,F waves (can not be local operators)



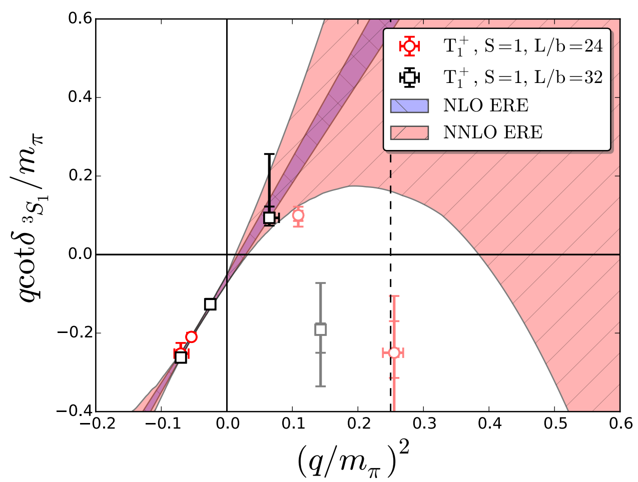


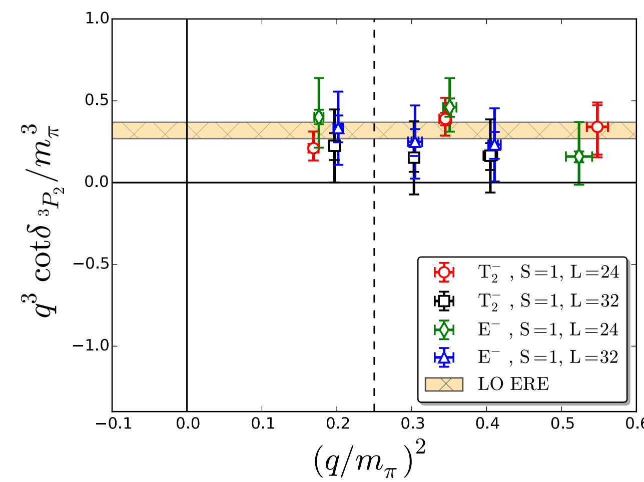
Evan Berkowitz
Thorsten Kurth
Amy Nicholson

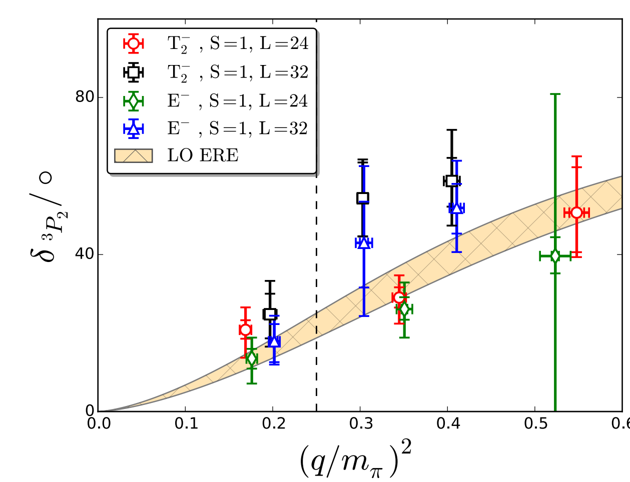
S

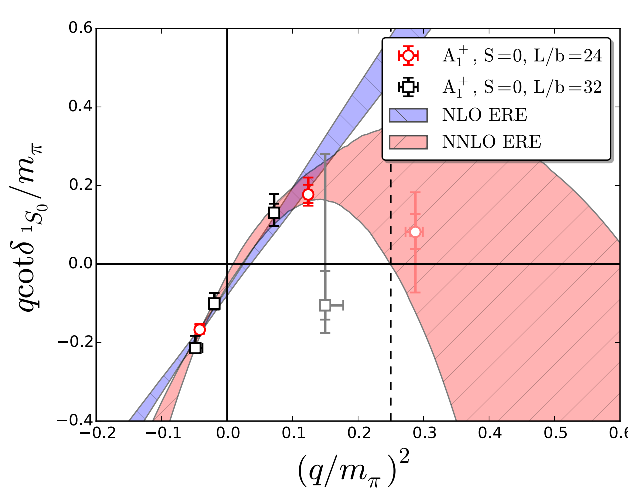
P

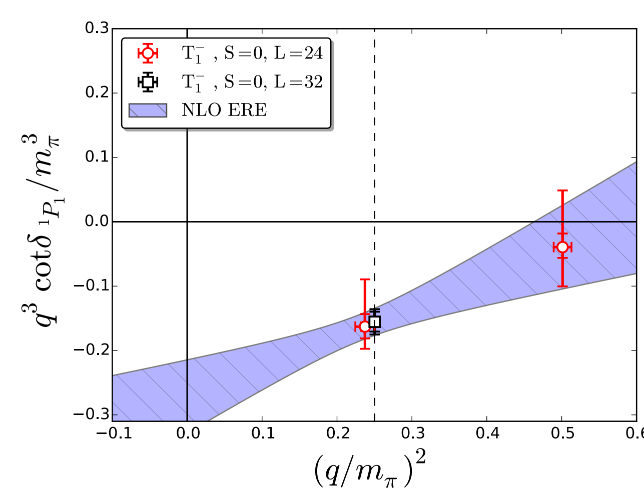
First LQCD calculation of P,D(,F) wave NN

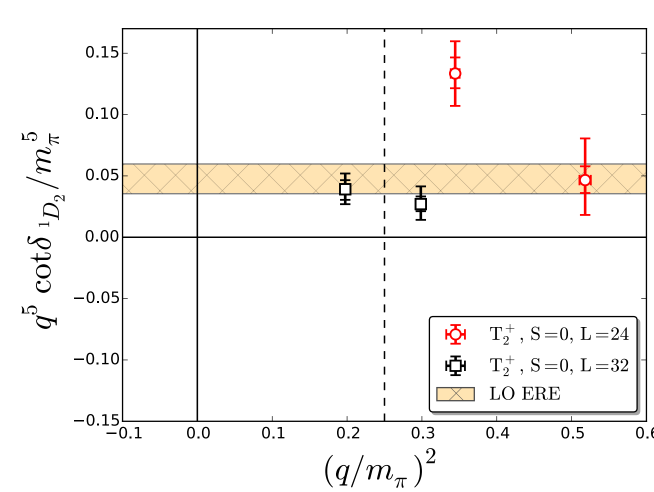












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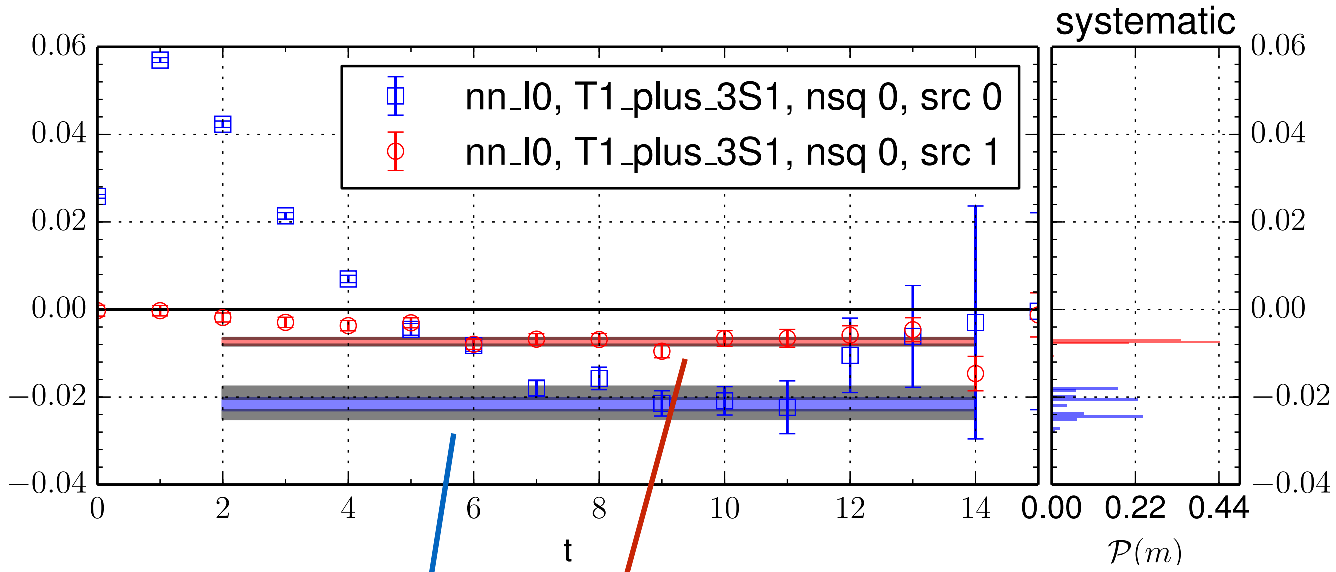
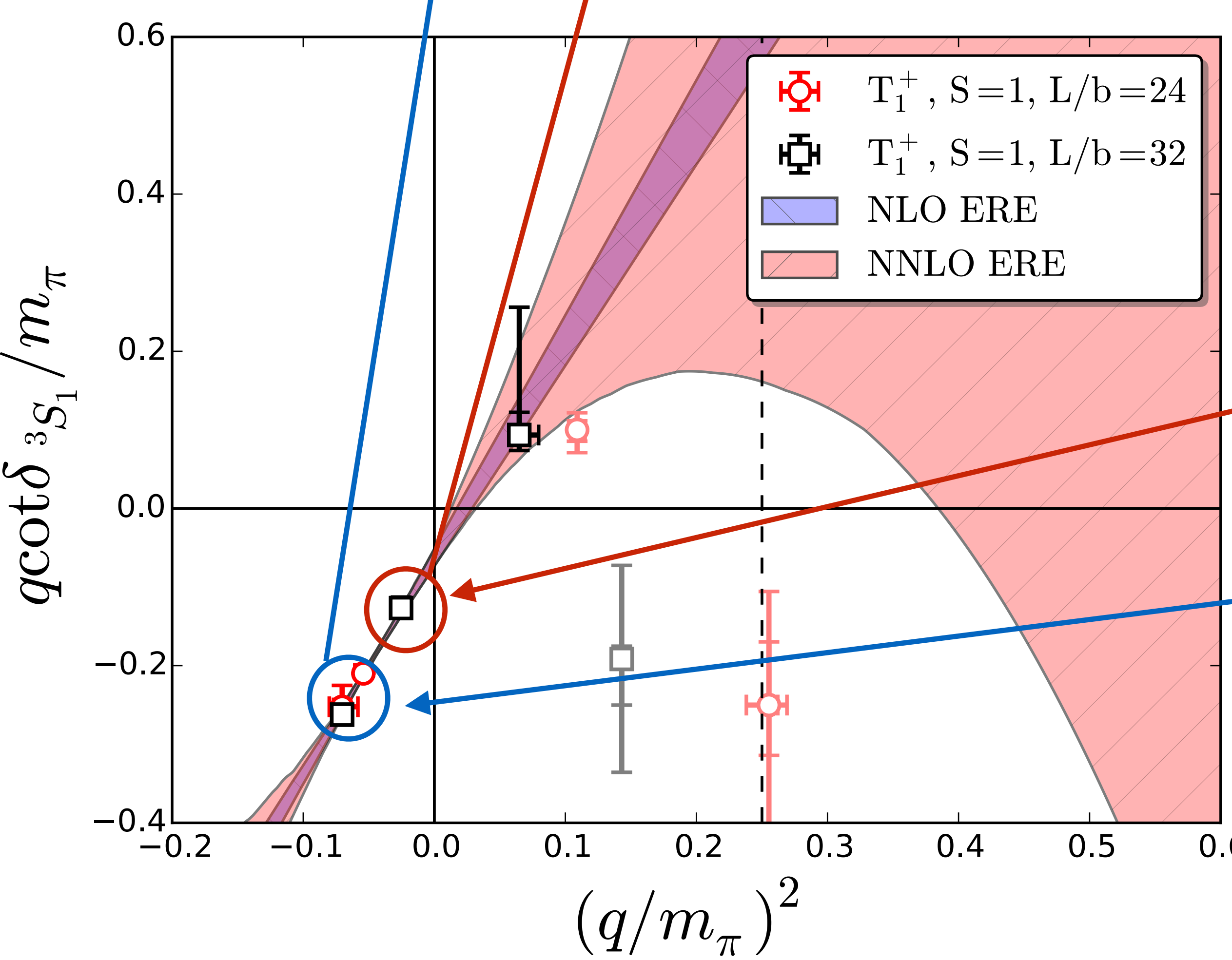


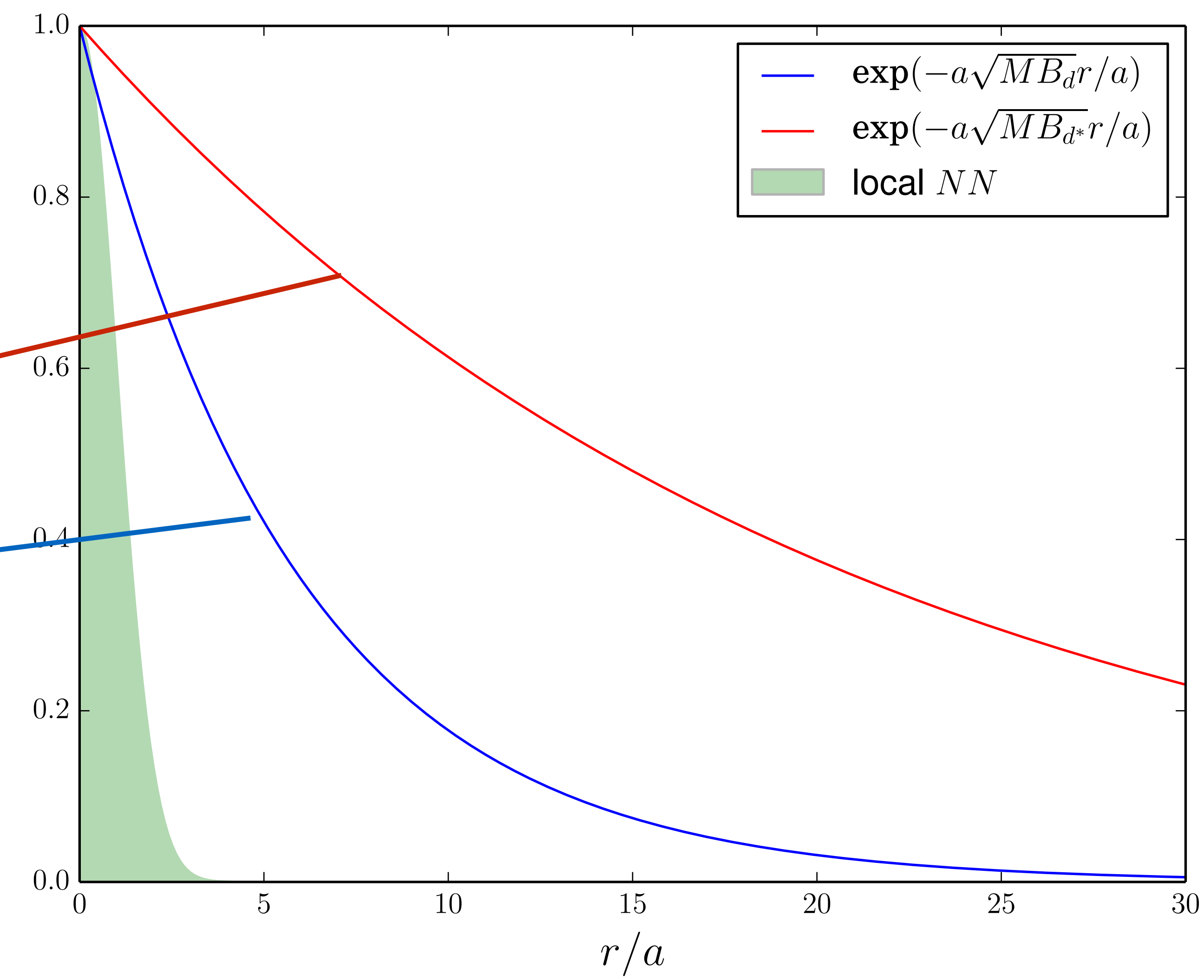
Our improved basis of operators gives sensitivity to more states in the spectrum

$$N^\dagger\left(\mathbf{x}-\frac{1}{2}\mathbf{r}\right)N^\dagger\left(\mathbf{x}+\frac{1}{2}\mathbf{r}\right)|0\rangle$$

Two bound states in deuteron channel, $m_\pi \sim 800$ MeV

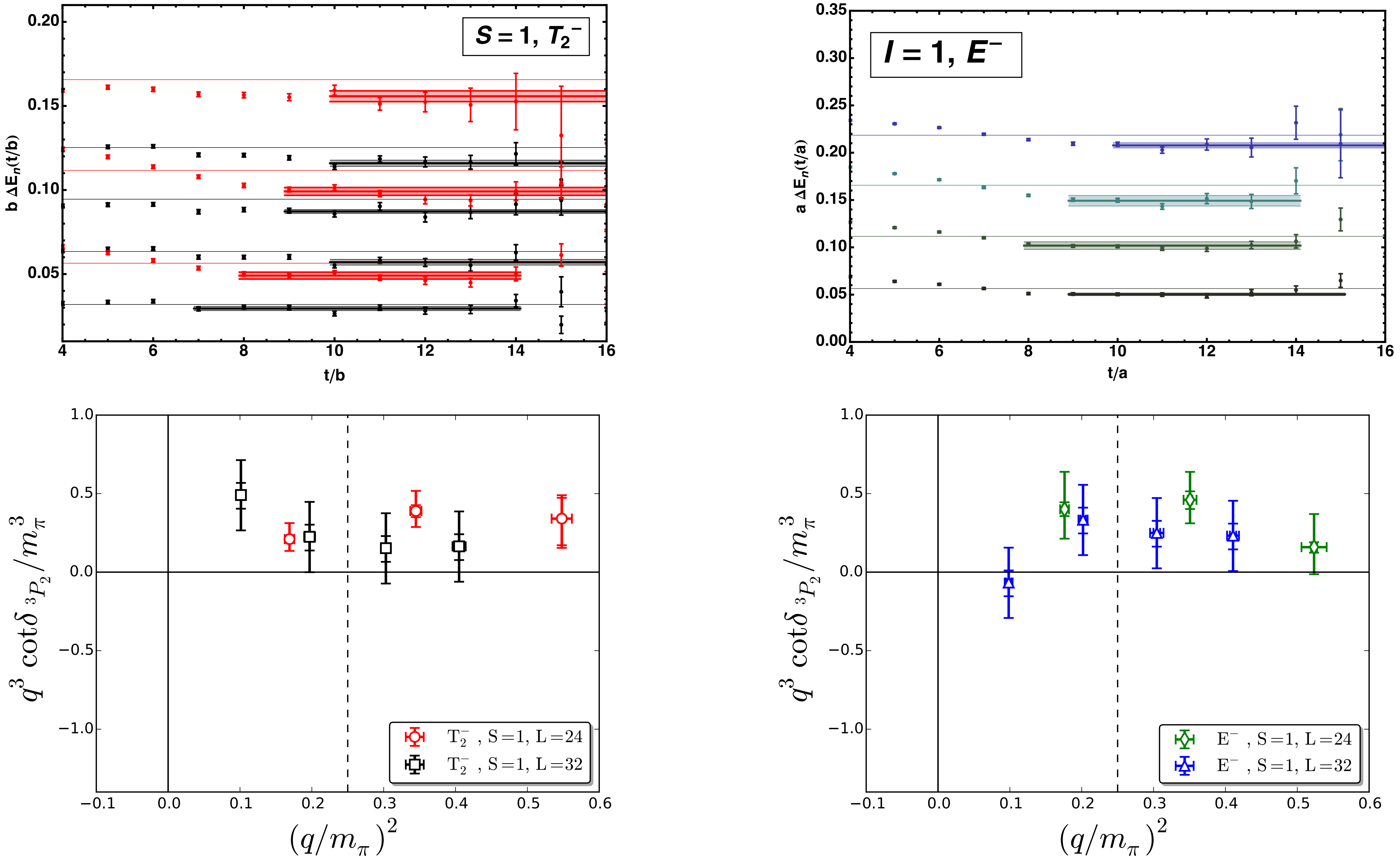
all prior calculations used local operators, $\mathbf{r}=\mathbf{0}$





Significant test of finite-volume formalism:

T_2^- and E^- both couple to the ${}^3P_2$ scattering channel



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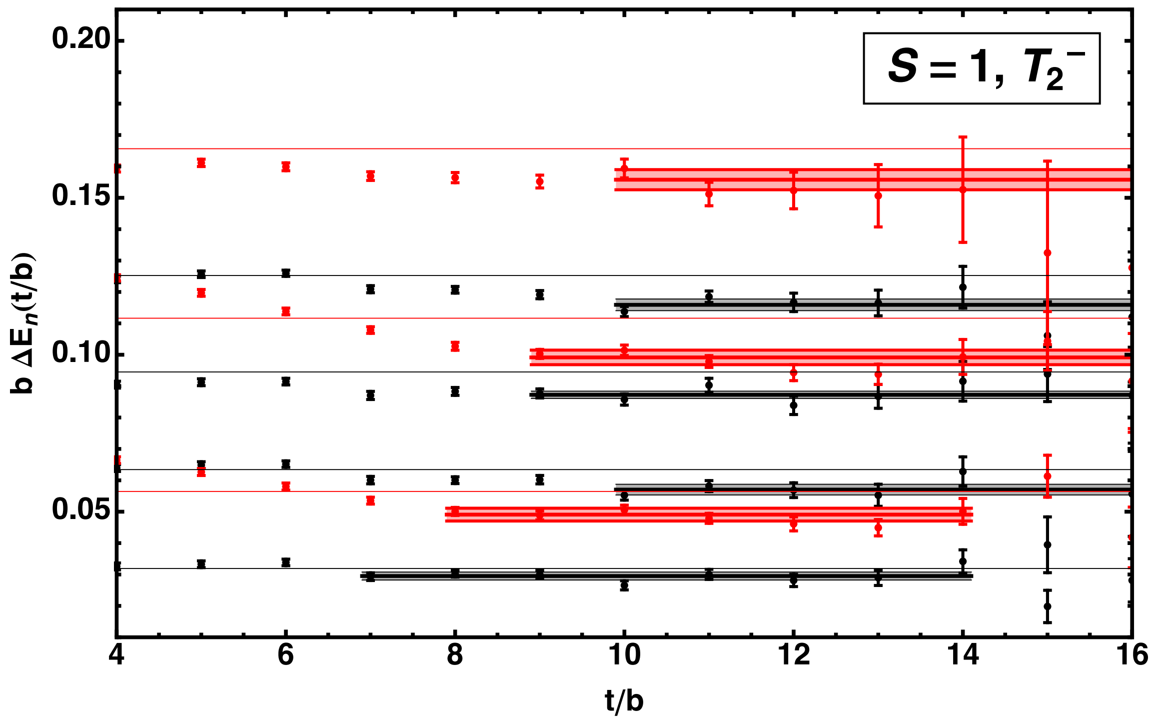
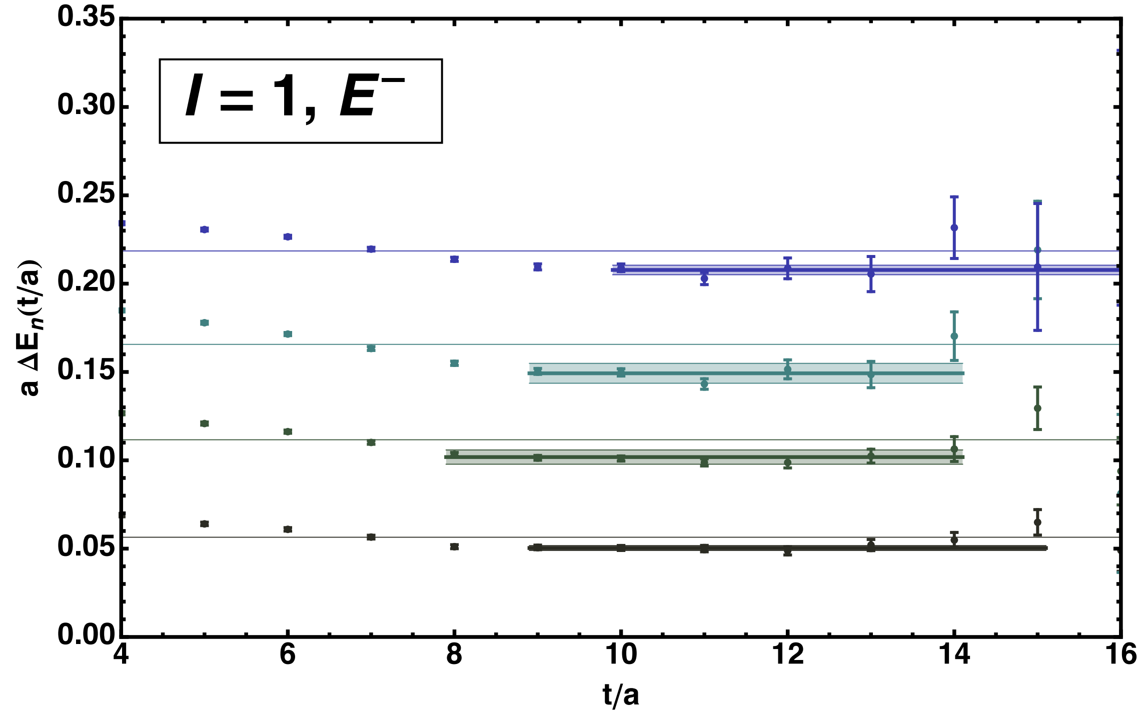
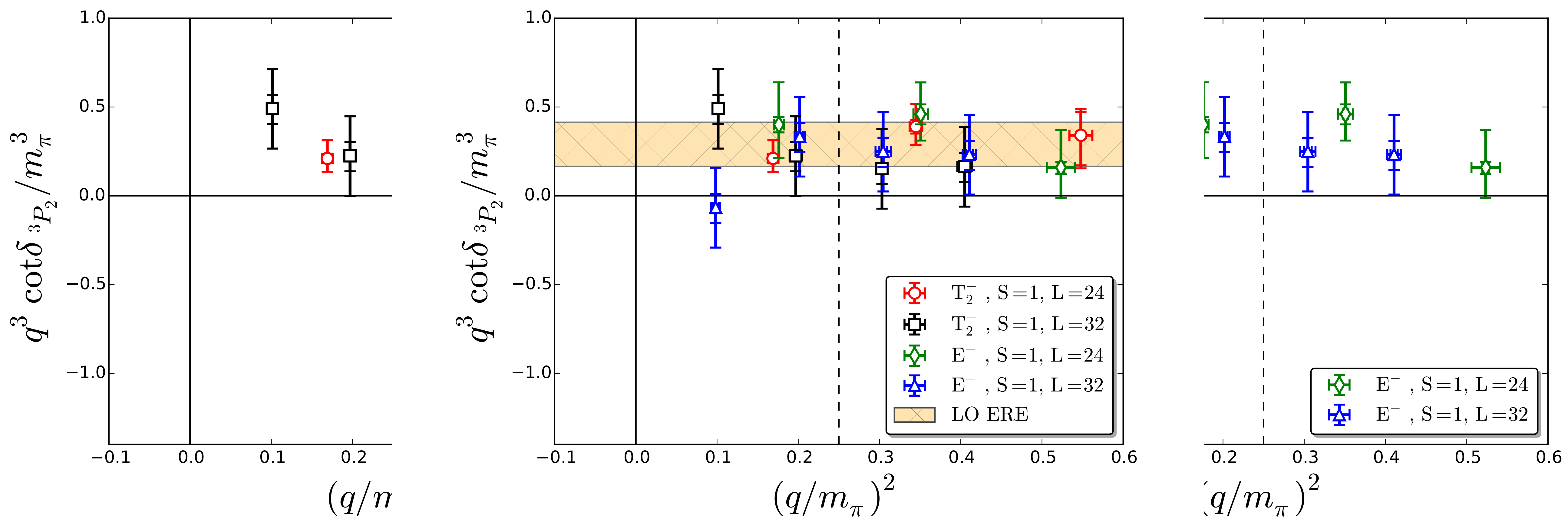
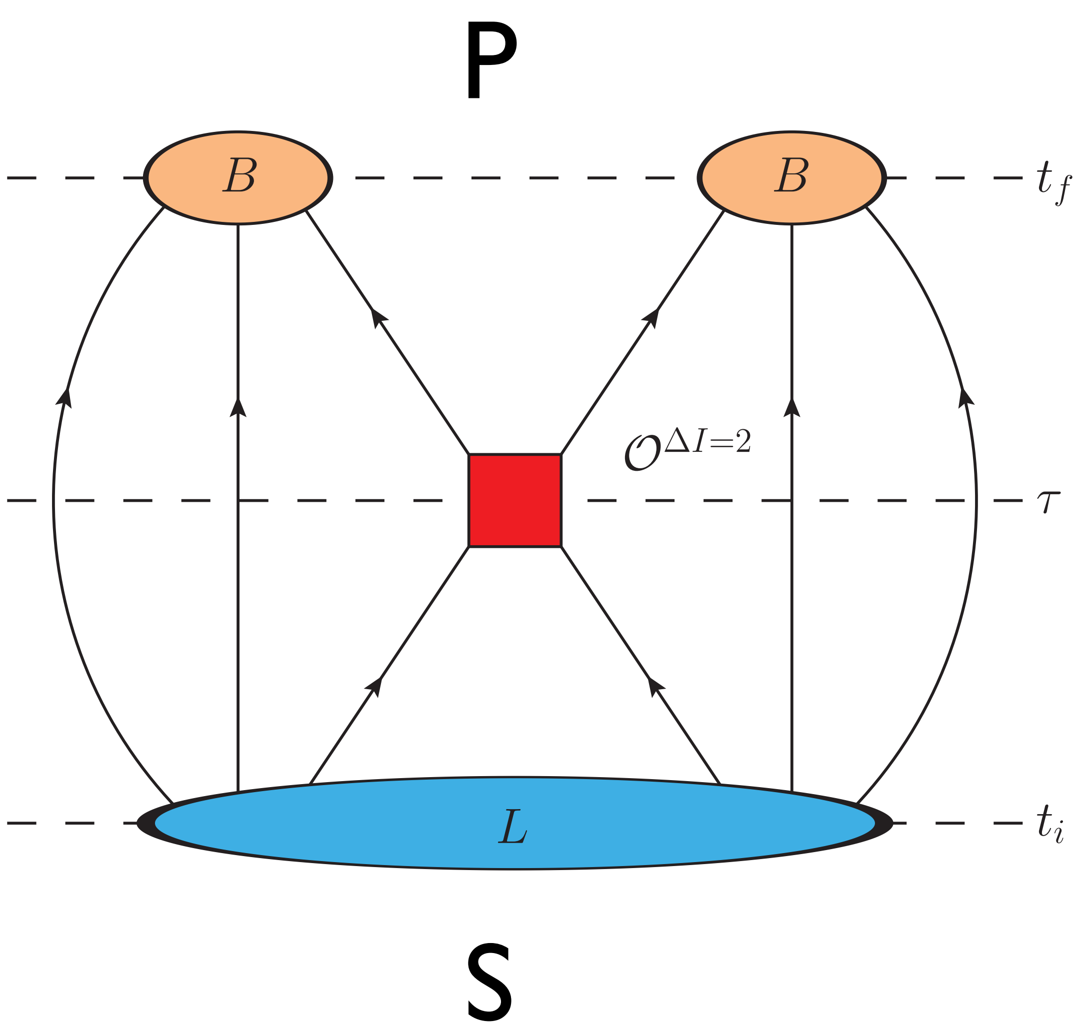






Finally - progress on the parity violating amplitude



$$\langle pp(^3P_1)|\mathcal{O}^{\Delta I=2}|pp(^1S_0)\rangle_{V=\infty} = LL\left(\delta_{^1S_0}, \frac{\partial \delta_{^1S_0}}{\partial E}, \delta_{^3P_1}, \frac{\partial \delta_{^3P_1}}{\partial E}\right)\langle pp(^3P_1)|\mathcal{O}^{\Delta I=2}|pp(^1S_0)\rangle_{V=L^3}$$

Known Lellouch-Lüscher (LL) function

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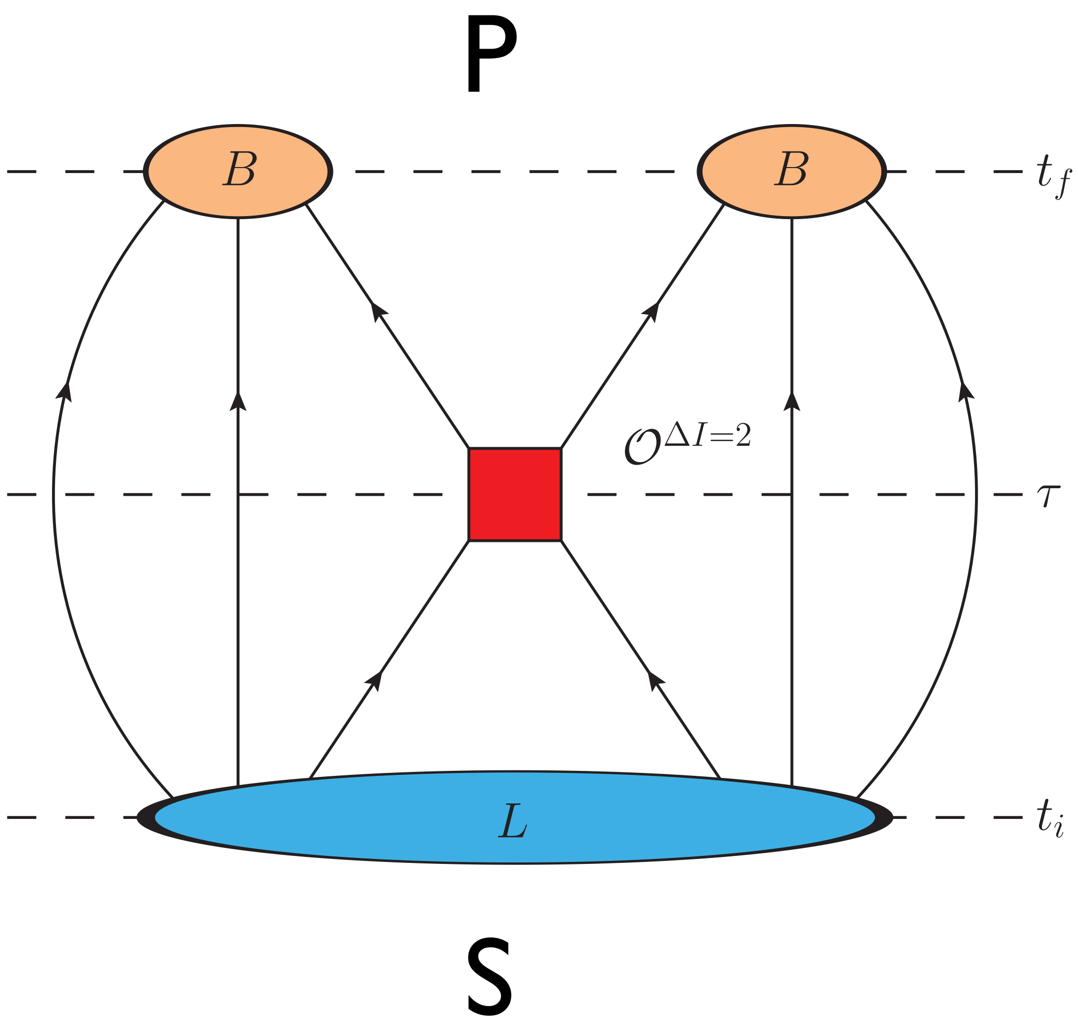
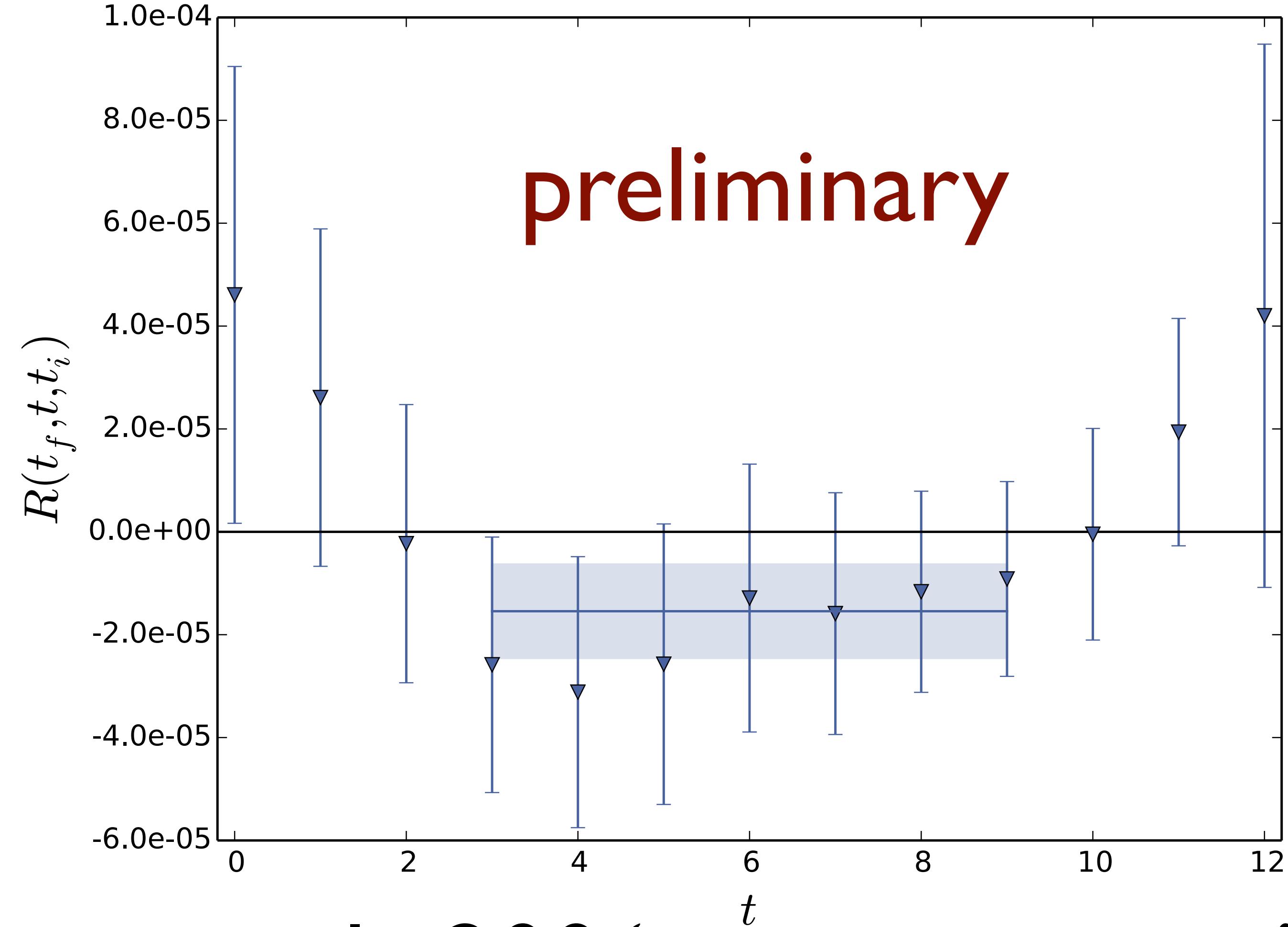


'bare' lattice matrix element



only 200 'measurements'

$$\langle pp(^3P_1)|\mathcal{O}^{\Delta I=2}|pp(^1S_0)\rangle_{V=\infty} = LL\left(\delta_{^1S_0}, \frac{\partial \delta_{^1S_0}}{\partial E}, \delta_{^3P_1}, \frac{\partial \delta_{^3P_1}}{\partial E}\right) \langle pp(^3P_1)|\mathcal{O}^{\Delta I=2}|pp(^1S_0)\rangle_{V=L^3}$$

Known Lellouch-Lüscher (LL) function

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Summary

- Significant investment to developing best methods and software
- Testing of methods has produced first results
- Results are a first for LQCD: NN partial waves [S],P, D,F - paper to appear in 1 week
- First results for I=2 parity violating amplitude - need to increase statistics for publishable result
- For the Lattice QCD effort so far, we have worked closely with Abhinav Sarje (LBNL CRD) and Balint Joó (JLab) to optimize various aspects of our code.

Going Forward

- NN scattering phase shifts at m_pi = 600, 400 MeV for S,P,D,F partial waves
- NN scattering with PV operator insertion with m = 800,600,400 MeV
- Insert to HOBET directly and also extrapolate and test extrapolation to physical pion mass (140 MeV)
- Implement efficient Fast Fourier Transform (slowest part of code)
- Explore multigrid methods to reach lower pion mass