From chiral effective field theory to a lattice Hamiltonian

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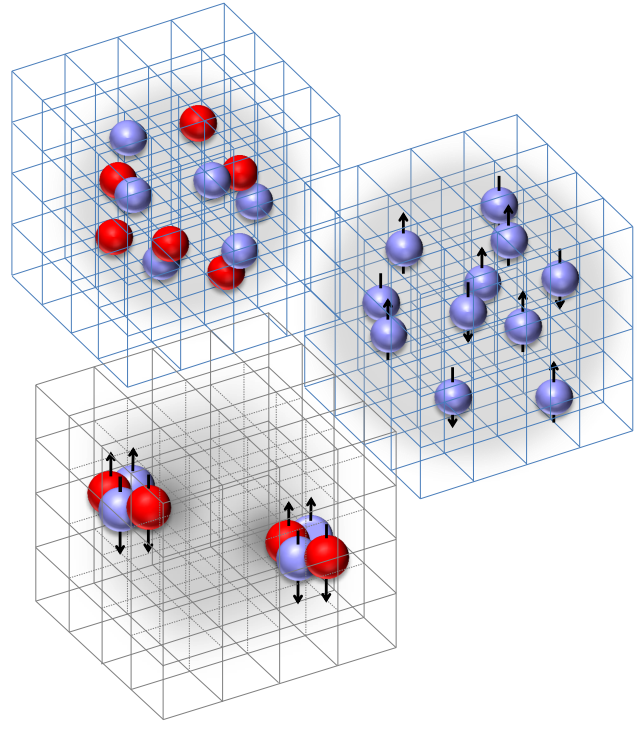
Lectures on Nuclear Lattice EFT:
School of Physics,
Beihang University, Beijing
August 24-28, 2026



Nuclear Scattering on the Lattice

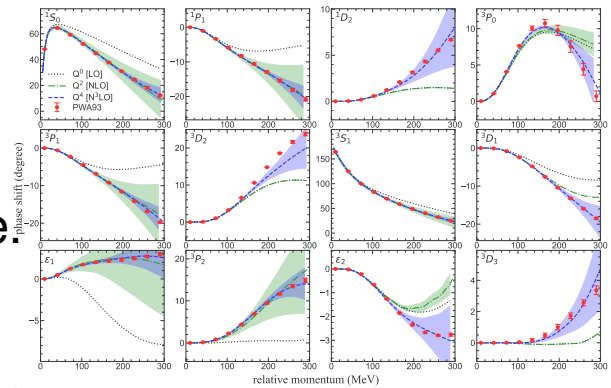
$H \longrightarrow$ scattering information $\longrightarrow \delta_\ell(p)$

How can a finite lattice describe an infinite-volume scattering process?

Scattering wave functions → phase shifts → the determination of LECs

Given a two-nucleon interaction on a spatial lattice, how do we calculate its scattering observables and adjust the interaction so that they reproduce physical NN scattering?

- From scattering wave functions to observables
  - ☐ continuum asymptotic wave functions and phase shifts;
  - ☐ scattering amplitude and effective-range expansion.
- How do we extract phase shifts on a lattice?
  - ☐ Lüscher finite-volume method;
  - ☐ spherical-wall and auxiliary-potential methods.
- From a simple interaction to chiral NN forces
  - ☐ benchmark continuum–lattice calculations;
  - ☐ improved contact interactions and pion exchange.
- How are the LECs determined?
  - ☐ construct partial-wave operators;
  - ☐ fit lattice phase shifts to empirical NN scattering data.



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SE et al. *Nature* 630, 8015, 59-63 (2024)

Li, SE, Epelbaum, Lee, Lu, Meissner, *Phys. Rev. C*, 98 (2018) 4, 044002

How is scattering information encoded in a wave function?

Two-body Schrödinger equation

For two nucleons interacting through a potential $V(\mathbf{r}_1 - \mathbf{r}_2)$,

$$H = -\frac{\nabla_1^2}{2m_N} - \frac{\nabla_2^2}{2m_N} + V(\mathbf{r}_1 - \mathbf{r}_2).$$

The center-of-mass and relative coordinates,

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,$$

so that the relative motion is governed by

$$H_{\rm rel} = -\frac{\nabla^2}{2\mu} + V(\mathbf{r}), \qquad \mu = \frac{m_N}{2}.$$

For a central interaction, expand the relative wave function in partial waves,

$$\psi(\mathbf{r}) = \sum_{\ell m} \frac{u_\ell(r)}{r} Y_{\ell m}(\hat{\mathbf{r}}),$$

What does the interaction do?

Suppose the nuclear interaction has a finite range $R_{\rm int}$. For

$$r > R_{\rm int}, \qquad V_\ell(r) = 0,$$

the radial wave again satisfies the *free* Schrödinger equation.

$$u_\ell^{(0)}(r) \propto \sin\left(pr - \frac{\ell\pi}{2}\right).$$

With the interaction present,

$$\boxed{u_\ell(r) \underset{r>R_{\rm int}}{\longrightarrow} A_\ell \sin\left(pr - \frac{\ell\pi}{2} + \delta_\ell(p)\right)}$$

where

$$E = \frac{p^2}{2\mu}.$$

How is scattering information encoded in a wave function?

For $r > R_{\rm int}$, $\quad u_\ell(r) \propto \sin\left(pr - \dfrac{\ell\pi}{2} + \delta_\ell(p)\right).$

Using $\sin x = \dfrac{1}{2i}\left(e^{ix} - e^{-ix}\right)$, we obtain the asymptotic radial wave as

$$u_\ell(r) \propto \frac{e^{-i\delta_\ell}}{2i}\left[\underbrace{e^{2i\delta_\ell}e^{\,i(pr-\ell\pi/2)}}_{\text{outgoing wave}} - \underbrace{e^{-i(pr-\ell\pi/2)}}_{\text{incoming wave}}\right].$$

Therefore the interaction changes the relative phase between the outgoing and incoming waves:

$$\boxed{S_\ell(p) = e^{2i\delta_\ell(p).}}$$ For elastic scattering, $|S_\ell| = 1,$

so the entire effect of the interaction in each partial wave is encoded in the phase shift $\delta_\ell(p)$.

Scattering converts: $\boxed{V(\mathbf{r}) \longrightarrow u_\ell(r) \longrightarrow \delta_\ell(p) \longrightarrow S_\ell(p)}$

From phase shifts to measurable scattering

On the previous slide, the effect of the interaction in each partial wave was encoded in

$$\boxed{S_\ell(p) = e^{2i\delta_\ell(p)}.}$$

But what is observed in a scattering experiment? Far from the interaction region, the full wave function has the asymptotic form

$$\boxed{\psi(\mathbf{r}) \underset{r\to\infty}{\longrightarrow} \underbrace{e^{ipz}}_{\text{incident plane wave}} + \underbrace{f(\theta)\frac{e^{ipr}}{r}}_{\text{outgoing scattered wave}}.}$$

The function $f(\theta)$ is the **scattering amplitude:**

- ☐ determines the measurable angular distribution,
- ☐ can be decomposed into partial waves for a central interaction.

$$\boxed{f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)\, f_\ell(p)\, P_\ell(\cos\theta),} \quad \Longrightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2.}$$

Each partial-wave amplitude is completely determined by the phase shift,

$$\boxed{f_\ell(p) = \frac{S_\ell(p)-1}{2ip} = \frac{e^{2i\delta_\ell(p)}-1}{2ip} = \frac{1}{p\cot\delta_\ell(p) - ip}.}$$

From phase shifts to scattering observables

Low-energy S-wave scattering
At sufficiently low momentum, the S wave ($\ell = 0$) dominates. The quantity $p \cot \delta_0(p)$ is analytic near threshold and can be expanded as

$$\boxed{p \cot \delta_0(p) = -\frac{1}{a_0} + \frac{1}{2} r_0 p^2 + v_2 p^4 + \cdots}$$

This is the **effective-range expansion**, where

$$a_0 \ : \ \text{scattering length}, \qquad r_0 \ : \ \text{effective range}.$$

In particular,

$$\boxed{a_0 = -\lim_{p \to 0} \frac{\tan \delta_0(p)}{p}}$$

and therefore

$$p \cot \delta_0(p) \underset{p \to 0}{\longrightarrow} -\frac{1}{a_0}.$$

Our next problem is therefore:

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

A toy-model scattering problem: the spherical square-well

Before extracting phase shifts from a lattice calculation, it is useful to start from a problem for which the continuum answer is known exactly.

Consider two particles with reduced mass μ interacting through an attractive spherical square-well potential,

$$\boxed{V(r) = \begin{cases} -V_0, & r < R, \\ 0, & r > R, \end{cases} \qquad V_0 > 0.}$$

For the S wave $(\ell = 0)$, the radial Schrödinger equation is

$$\left[-\frac{1}{2\mu} \frac{d^2}{dr^2} + V(r) \right] u_0(r) = E\, u_0(r), \qquad E = \frac{p^2}{2\mu}.$$

Inside the interaction region $(r < R)$ $\quad u_{\text{in}}(r) = A \sin(qr), \quad q = \sqrt{p^2 + 2\mu V_0}.$

Outside the interaction region $(r > R)$ $\quad u_{\text{out}}(r) = B \sin\left(pr + \delta_0(p)\right).$

Simple enough $\implies$ $\delta_0(p)$ can be obtained analytically in the continuum

Nontrivial enough $\implies$ support scattering, resonant behavior, and bound-state.

A toy-model scattering problem: the spherical square-well

For the spherical square well,

$$u_{\text{in}}(r) = A\sin(qr), \qquad u_{\text{out}}(r) = B\sin(pr + \delta_0).$$

The wave function and its derivative must be continuous at $r = R$:

$$A\sin(qR) = B\sin(pR + \delta_0), \qquad \text{and} \qquad Aq\cos(qR) = Bp\cos(pR + \delta_0).$$

Eliminating the normalization constants A and B: $\boxed{q\cot(qR) = p\cot(pR + \delta_0)}$

$$\Longrightarrow \qquad \tan(pR + \delta_0) = \frac{p}{q}\tan(qR) \qquad \Longrightarrow \qquad \boxed{\delta_0(p) = \tan^{-1}\left[\frac{p}{q}\tan(qR)\right] - pR}$$

The interaction acts only for $r < R$, but its effect is encoded entirely in the phase $\delta_0(p)$ of the free wave for $r > R$.

$$\boxed{V_0,\ R \quad \longrightarrow \quad u_0(r) \quad \longrightarrow \quad \delta_0(p)}$$

The square well as a benchmark for lattice scattering

For the spherical square well we know the continuum answer analytically,

$$\boxed{\delta_0(p) = \tan^{-1}\left[\frac{p}{q}\tan(qR)\right] - pR, \qquad q = \sqrt{p^2 + 2\mu V_0}.}$$

At low momentum this phase shift determines the scattering length,

$$\boxed{a_0 = -\lim_{p\to 0}\frac{\tan\delta_0(p)}{p} = R - \frac{\tan(q_0 R)}{q_0}, \qquad q_0 = \sqrt{2\mu V_0}.}$$

Thus the continuum problem provides a complete benchmark:

$$\boxed{V_0,\ R \quad \longrightarrow \quad \delta_0(p) \quad \longrightarrow \quad a_0,\ r_0, \ldots}$$

But on a finite periodic lattice we do **not** have access to the $r \to \infty$ asymptotic wave function.
Instead, the calculation gives a discrete spectrum,

$$\boxed{H_{\rm lat} \quad \longrightarrow \quad E_1(L_{\rm box}),\ E_2(L_{\rm box}),\ E_3(L_{\rm box}), \ldots}$$

The central question is now

$$\boxed{E_n(L_{\rm box}) \qquad \stackrel{?}{\longrightarrow} \qquad \delta_0(p_n).}$$

Finite-Volume Scattering: Lüscher's Method

$$\boxed{E_n(L_{\rm box}) \quad \longleftrightarrow \quad \delta_\ell(p_n)}$$

The scattering wave disappears at infinity, but its information survives in the finite-volume spectrum.

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

Infinite volume: $r \to \infty \quad \Longrightarrow \quad u_0(r) \propto \sin\left(pr + \delta_0(p)\right) \qquad u_0(r) \quad \longrightarrow \quad \delta_0(p)$

In finite volume: $\psi(\mathbf{r} + L_{\rm box}\hat{\mathbf{e}}_i) = \psi(\mathbf{r}) \quad \longrightarrow$ there is **no** region $r \to \infty$

There is no freely outgoing scattering wave extending to infinity.

Instead, the finite system has only a discrete set of energy eigenvalues,

$$E_0(L_{\rm box}), \quad E_1(L_{\rm box}), \quad E_2(L_{\rm box}), \quad \ldots$$

The central question: If the phase shift is defined from an asymptotic scattering wave in infinite volume, how can a set of discrete energies in a finite box possibly tell us $\delta_0(p)$?

Lüscher's idea: $\quad E_n(L_{\rm box}) \quad \Longleftrightarrow \quad \delta_0(p_n)$

Note: Lüscher's method is fundamentally a *finite-volume* method. The spatial lattice spacing a is an additional regulator and needs to be discussed separately.

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

1: What does the periodic box do to the free particles?

$\psi(\mathbf{r} + L_{\text{box}}\hat{\mathbf{e}}_i) = \psi(\mathbf{r})$ requires $e^{i\mathbf{q}\cdot(\mathbf{r}+L_{\text{box}}\hat{\mathbf{e}}_i)} = e^{i\mathbf{q}\cdot\mathbf{r}}$, and therefore

$$\boxed{\mathbf{q_n} = \frac{2\pi}{L_{\text{box}}}\mathbf{n}, \qquad \mathbf{n} = (n_x, n_y, n_z) \in \mathbb{Z}^3.}$$

For two particles in the center-of-mass frame ($\mathbf{p}_1 = \mathbf{q}, \mathbf{p}_2 = -\mathbf{q}$), and the relative energy and the free two-particle energies are

$$E^{(0)}_{\text{rel}} = \frac{q^2}{2\mu} \quad \text{and} \quad \boxed{E^{(0)}_{\mathbf{n}} = \frac{1}{2\mu}\left(\frac{2\pi}{L_{\text{box}}}\right)^2 |\mathbf{n}|^2.}$$

$$\underbrace{\int \frac{d^3q}{(2\pi)^3}}_{\text{continuous momenta}} \longrightarrow \underbrace{\frac{1}{L^3_{\text{box}}}\sum_{\mathbf{q}}}_{\text{discrete momenta}} .$$

The finite box converts the continuous scattering spectrum into a set of discrete standing-wave energies.

The remaining question is quantitative: $E_n(L_{\text{box}}) \quad \xrightarrow{?} \quad \delta_0(p_n)$.

2: Turn on the interaction $H = H_0 + V$.

For the free system: $$E_{\mathbf{n}}^{(0)} = \frac{1}{2\mu}\left(\frac{2\pi}{L_{\text{box}}}\right)^2 |\mathbf{n}|^2,$$

When the particles interact: $$E_{\mathbf{n}}^{(0)} \quad \Longrightarrow \quad E_n(L_{\text{box}}).$$

The interaction changes the standing wave that can fit inside the periodic box, and consequently shifts the allowed energies.

But in infinite volume we already know how the interaction changes a wave:

$$u_0(r) \propto \sin(pr) \qquad \longrightarrow \qquad u_0(r) \propto \sin\left(pr + \delta_0(p)\right).$$

Therefore,

interaction changes the phase $\iff$ interaction shifts the finite-volume energies.

The basic physical idea of Lüscher's method: The phase shift cannot be measured directly inside the finite box, but its effect survives in the displacement of the discrete two-particle energy levels.

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

3: Reveal the "magic" with the simplest interaction

Consider the simplest short-range interaction $\boxed{V = C_0.}$

The free two-body Green's operator is $\boxed{G_0^{(+)}(E) = \dfrac{1}{E - H_0 + i0^+}.}$

For a contact interaction, successive interactions occur at zero relative separation. Therefore define

$$\boxed{I_\infty(E) \equiv \langle \mathbf{r} = 0 | G_0^{(+)}(E) | \mathbf{r} = 0 \rangle = \int \frac{d^3q}{(2\pi)^3} \frac{1}{E - \dfrac{q^2}{2\mu} + i0^+}.}$$

The repeated-scattering series is then

$$\begin{aligned} T_\infty(E) &= C_0 + C_0 I_\infty(E) C_0 + C_0 I_\infty(E) C_0 I_\infty(E) C_0 + \cdots \\ &= C_0 \left[1 + C_0 I_\infty + (C_0 I_\infty)^2 + \cdots \right]. \end{aligned}$$

Summing the geometric series, $\boxed{T_\infty(E) = \dfrac{1}{C_0^{-1} - I_\infty(E)}.}$

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

4: Where is the phase shift hidden in T_∞?

For S-wave elastic scattering, $$f_0(p) = \frac{1}{p \cot \delta_0(p) - ip}.$$

Scattering state	Outgoing free Green's function behaves as	Standard momentum-state normalization
$\psi^{(+)} = \lvert\mathbf{p}\rangle + G_0^{(+)} T \lvert\mathbf{p}\rangle$	$G_0^{(+)}(\mathbf{r}; E) \underset{r\to\infty}{\longrightarrow} -\frac{\mu}{2\pi}\frac{e^{ipr}}{r}.$	$\langle\mathbf{p}'\lvert\mathbf{p}\rangle = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p}),$

Comparing with the asymptotic scattering wave gives $$\boxed{f_0(p) = -\frac{\mu}{2\pi} T_\infty(p).}$$

Therefore, we obtain, $$T_\infty^{-1}(p) = -\frac{\mu}{2\pi}\left[p \cot \delta_0(p) - ip\right] = -\frac{\mu}{2\pi} p \cot \delta_0(p) + i\frac{\mu p}{2\pi}.$$

$$\Longrightarrow \qquad \boxed{\operatorname{Re} T_\infty^{-1}(p) = -\frac{\mu}{2\pi} p \cot \delta_0(p).}$$

But remember what we obtained from the repeated-scattering series,

$$T_\infty^{-1}(p) = C_0^{-1} - I_\infty(p). \qquad \Longrightarrow \qquad \boxed{C_0^{-1} - \operatorname{Re} I_\infty(p) = -\frac{\mu}{2\pi} p \cot \delta_0(p).}$$

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

5: Put exactly the same interaction in the finite box

$$V = C_0.$$

Only the free propagation changes,

$$\boxed{\int \frac{d^3q}{(2\pi)^3} \quad \longrightarrow \quad \frac{1}{L^3_{\text{box}}} \sum_{\mathbf{q}}.} \quad \Longrightarrow \quad \boxed{I_L(E) = \frac{1}{L^3_{\text{box}}} \sum_{\mathbf{q}} \frac{1}{E - \dfrac{q^2}{2\mu}}.}$$

The repeated-contact series has exactly the same structure,

$$T_L(E) = C_0 + C_0 I_L(E) C_0 + C_0 I_L(E) C_0 I_L(E) C_0 + \cdots$$

$$= \boxed{\frac{1}{C_0^{-1} - I_L(E)}.}$$

A finite-volume eigenenergy occurs when this denominator vanishes,

$$\boxed{C_0^{-1} = I_L(E_n).}$$

$$\boxed{\text{same interaction} \; + \; \text{different propagation} \quad \Longrightarrow \quad \text{finite-volume spectrum.}}$$

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

6: Eliminate the unknown short-distance coupling

In infinite volume we found: $$C_0^{-1} - \mathrm{Re}\, I_\infty(p) = -\frac{\mu}{2\pi} p \cot \delta_0(p).$$

At a finite-volume energy eigenvalue, $$C_0^{-1} = I_L(p).$$

The same C_0 appears in both equations. Therefore it cancels:

$$\boxed{p \cot \delta_0(p) = -\frac{2\pi}{\mu} \left[I_L(p) - \mathrm{Re}\, I_\infty(p) \right].}$$

The "mystery" begins to disappear:

The same short-distance interaction C_0 appears in the finite- and infinite-volume problems. When the two are compared, C_0 cancels.

scattering information $=$ finite-volume sum $-$ infinite-volume integral.

The remaining quantity depends only on the finite-volume geometry and on the physical momentum p.

How do we determine $p \cot \delta_\ell(p)$ from a finite lattice calculation?

7: Write the finite-volume sum in dimensionless form

For a finite-volume energy E define $E = \dfrac{p^2}{2\mu}, \qquad \mathbf{q_n} = \dfrac{2\pi}{L_{\rm box}}\mathbf{n}, \qquad \boxed{\eta = \left(\dfrac{pL_{\rm box}}{2\pi}\right)^2}$

$$I_L(p) = \frac{1}{L_{\rm box}^3}\sum_{\mathbf{n}} \frac{1}{\dfrac{p^2}{2\mu} - \dfrac{q_{\mathbf{n}}^2}{2\mu}} = \frac{2\mu}{L_{\rm box}^3}\sum_{\mathbf{n}} \frac{1}{p^2 - \left(\dfrac{2\pi}{L_{\rm box}}\right)^2 |\mathbf{n}|^2} = \boxed{-\frac{\mu}{2\pi^2 L_{\rm box}}\sum_{\mathbf{n}} \frac{1}{|\mathbf{n}|^2 - \eta}}$$

But this sum is ultraviolet divergent $\Longrightarrow$ For $|\mathbf{n}| \gg 1$ $\quad \dfrac{1}{|\mathbf{n}|^2 - \eta} \simeq \dfrac{1}{|\mathbf{n}|^2}.$

A thin spherical shell of radius n contains approximately $\boxed{dN \simeq 4\pi n^2\, dn}$

integer vectors, so the shell contributes $\quad dN\,\dfrac{1}{n^2} \simeq 4\pi\, dn.$

$$\boxed{\sum_{|\mathbf{n}|<\Lambda} \frac{1}{|\mathbf{n}|^2 - \eta} = 4\pi\Lambda + \text{finite part.}}$$

Note: The divergence is not a physical finite-volume effect. It is the same short-distance divergence that is present in the infinite-volume momentum integral.

Lüscher's quantization condition

Use the same ultraviolet regulator in the finite- and infinite-volume expressions.

$$I_L(p) = -\frac{\mu}{2\pi^2 L_{\text{box}}} \sum_{|\mathbf{n}|<\Lambda} \frac{1}{|\mathbf{n}|^2 - \eta} \qquad \text{Re}\, I_\infty(p) = -\frac{2\mu\Lambda}{\pi L_{\text{box}}} + \mathcal{O}(\Lambda^{-1})$$

Use $$-\frac{2\pi}{\mu}\left[I_L - \text{Re}\, I_\infty\right] \implies \boxed{p \cot \delta_0(p) = \frac{1}{\pi L_{\text{box}}} \lim_{\Lambda\to\infty} \left[\sum_{|\mathbf{n}|<\Lambda} \frac{1}{|\mathbf{n}|^2 - \eta} - 4\pi\Lambda\right]}$$

where

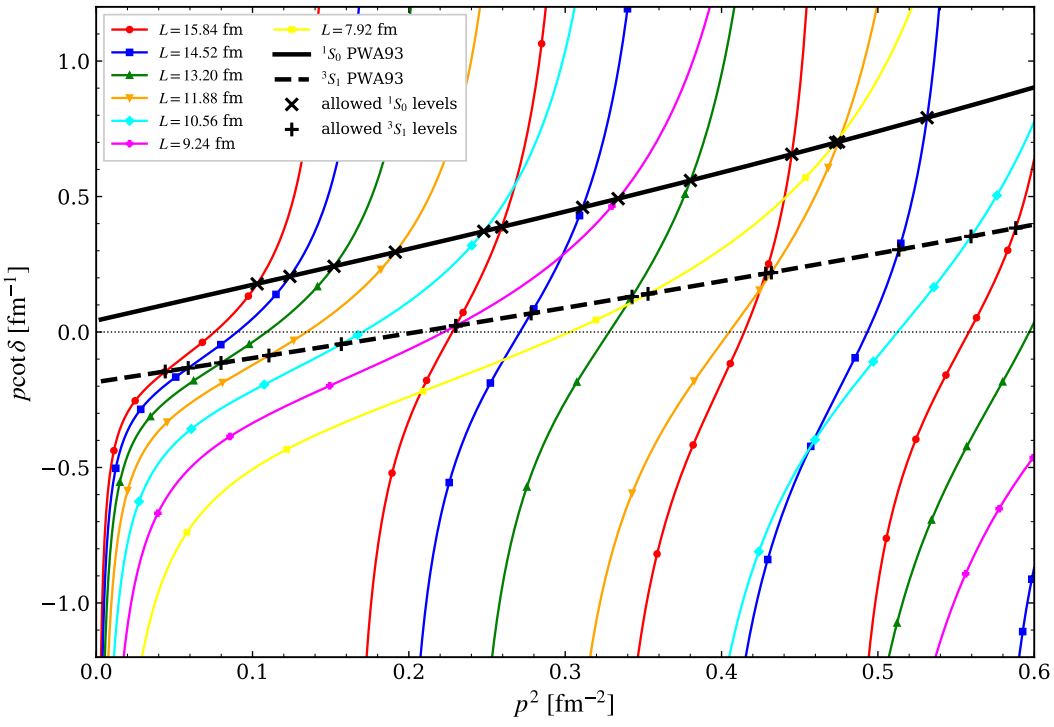
$$S(\eta) = \lim_{\Lambda\to\infty} \left[\sum_{|\mathbf{n}|<\Lambda} \frac{1}{|\mathbf{n}|^2 - \eta} - 4\pi\Lambda\right] \qquad \eta = \left(\frac{pL_{\text{box}}}{2\pi}\right)^2$$

$S(\eta)$ is **not** part of the nuclear interaction. It describes the geometry of a periodic cubic box.

$$\boxed{E_n(L_{\text{box}}) \to p_n \to \eta_n \to S(\eta_n) \to p_n \cot \delta_0(p_n) \to \delta_0(p_n)}$$

Lüscher's method: finite-volume energies $\longleftrightarrow$ phase shifts

$$p \cot \delta_0(p) = \frac{1}{\pi L_{\text{box}}} S(\eta), \qquad \eta = \left(\frac{p L_{\text{box}}}{2\pi} \right)^2$$



What does the figure tell us?

For a given box size L_{box},

- The colored curves depend only on the **periodic-box geometry**.
- The black curves contain the **physical scattering information**.
- Only momenta satisfying the Lüscher quantization condition can appear as finite-volume energy eigenstates.

$$\text{intersection} \iff p_n \iff E_n(L_{\text{box}})$$

How do we use this in an actual lattice calculation?

$$E_n(L_{\text{box}}) \longrightarrow p_n \longrightarrow \eta_n \longrightarrow S(\eta_n) \longrightarrow p_n \cot \delta_0(p_n) \longrightarrow \delta_0(p_n)$$

The Spherical-Wall Method

Hamiltonian $\longrightarrow$ $R_\ell(r)$ $\longrightarrow$ $S_\ell(p)$ $\longrightarrow$ $\delta_\ell(p)$

Carlson, Pandharipande, Wiringa *Nucl. Phys. A* 424, 47-59 (1984)
Borasoy, Epelbaum, Krebs, Lee, Meissner *Eur. Phys. J. A* 34, 185-196 (2007).
Rokash, Pine, SE, Lee, Epelbaum, Krebs, *Phys. Rev. C*, 92 (2015) 5, 054612
Lu, Lahde, Lee, Meissner, *Phys. Lett. B*, 760 (2016) 309-313
Li, SE, Epelbaum, Lee, Lu, Meissner, *Phys. Rev. C*, 98 (2018) 4, 044002

An alternative approach: the spherical-wall method

In Lüscher's method: $E_n(L_{\text{box}}) \longrightarrow p_n \longrightarrow p_n \cot \delta_\ell(p_n) \longrightarrow \delta_\ell(p_n)$

Remember how the phase shift originally appeared:

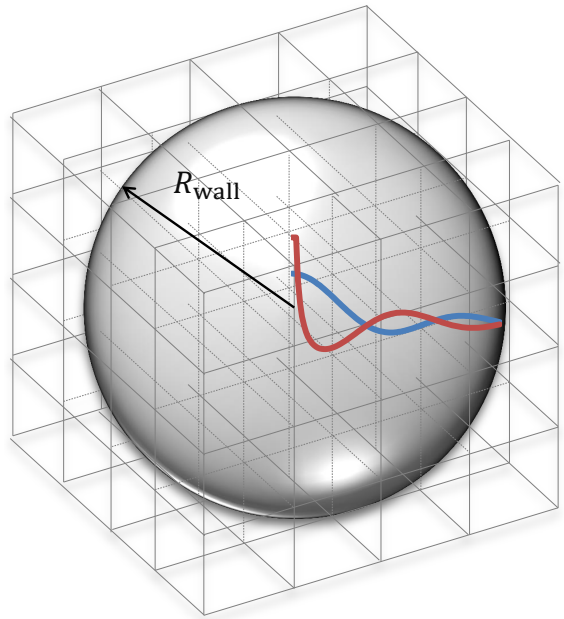
$$r > R_{\text{int}} \qquad \Longrightarrow \qquad u_\ell(r) \propto \sin\left(pr - \frac{\ell\pi}{2} + \delta_\ell(p)\right).$$

This suggests another possibility: Can we construct a finite-volume problem in which we can directly examine the asymptotic radial wave function?

The spherical-wall idea Instead of allowing the particles to propagate through the periodic boundaries, impose a hard boundary on their **relative separation**,

$$r < R_W, \qquad R_W > R_{\text{int}}.$$

The phase shift can then be extracted from the standing wave inside the spherical wall.



Hamiltonian $\longrightarrow$ radial wave function $\longrightarrow \delta_\ell(p)$

The hard spherical wall

Consider the relative-coordinate Hamiltonian,

$$H_{\rm rel} = -\frac{\nabla^2}{2\mu} + V(r) + \Lambda_W\,\Theta(r - R_W),$$

$\Lambda_W \to \infty$ so that the wave function is strongly suppressed for $r > R_W$,

$$\boxed{\psi(r = R_W) = 0}$$

Write the partial-wave decomposition as

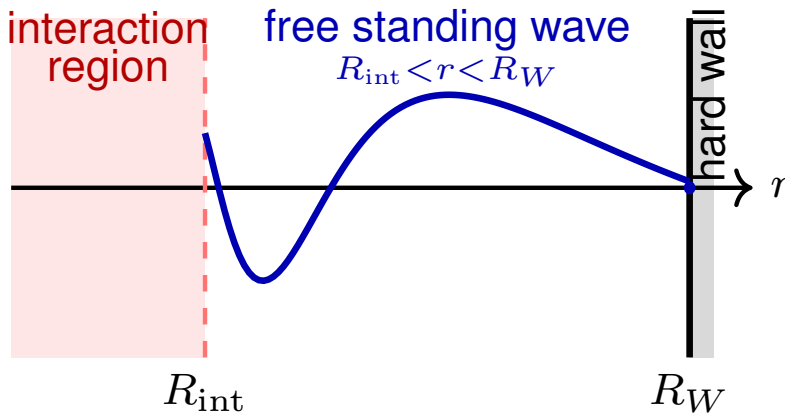
$$\psi(\mathbf{r}) = R_\ell(r) Y_{\ell m}(\hat{\mathbf{r}}), \qquad u_\ell(r) = r R_\ell(r)$$

$$\boxed{R_\ell(r) = \mathcal{N}\left[\cos\delta_\ell(p)\, j_\ell(pr) - \sin\delta_\ell(p)\, y_\ell(pr)\right].}$$

Applying the wall condition,

$$\cos\delta_\ell\, j_\ell(pR_W) - \sin\delta_\ell\, y_\ell(pR_W) = 0,$$

$$\Longrightarrow \qquad \boxed{\delta_\ell(p) = \tan^{-1}\left[\frac{j_\ell(pR_W)}{y_\ell(pR_W)}\right]}$$



For the S wave,

$$j_0(x) = \frac{\sin x}{x}, \quad y_0(x) = -\frac{\cos x}{x},$$

$$\Longrightarrow \qquad R_0(r) \propto \frac{\sin(pr + \delta_0)}{pr}.$$

At the wall $\boxed{\delta_0(p) = n\pi - pR_W.}$

The interaction shifts the standing-wave nodes; the wall turns that shift directly into $\delta_\ell(p)$.

The spherical wall on a spatial lattice

Where is a "sphere" on a cubic lattice?
In the continuum, the hard wall can be imposed at an exact radius

$$r = R_W .$$

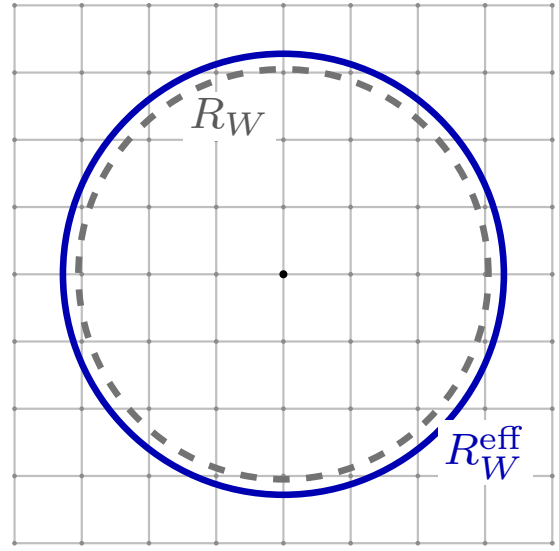
On a cubic spatial lattice,

$$\boxed{r = a\sqrt{n_x^2 + n_y^2 + n_z^2},}$$

so the available lattice sites do **not** form a perfectly smooth spherical surface. Therefore the numerical wall behaves as if it were located at

$$\boxed{R_W \quad \longrightarrow \quad R_W^{\text{eff}} = R_W + \epsilon.}$$

The shift ϵ is a finite-a geometrical effect and must be **calibrated**.



Use the free problem to determine R_W^{eff}
For a free eigenstate,

$$E_n^{(0)} \quad \longrightarrow \quad p_n^{(0)}.$$

The effective wall radius is therefore defined by

$$j_\ell\left(p_n^{(0)} R_W^{\text{eff}}\right) = 0$$

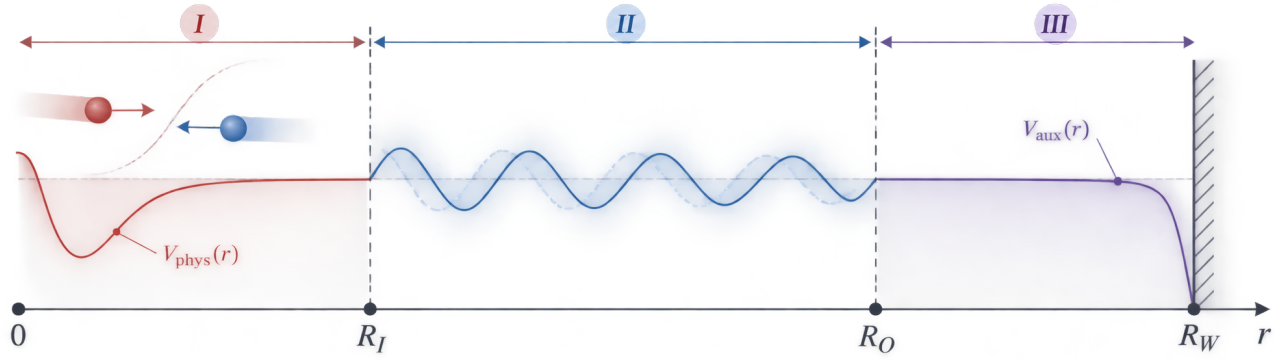
$$\boxed{\text{free spectrum} \quad \longrightarrow \quad R_W^{\text{eff}} \quad \longrightarrow \quad \text{interacting spectrum} \quad \longrightarrow \quad \delta_\ell(p).}$$

The auxiliary-potential method: three radial regions

The hard-wall boundary condition $(R_\ell(R_W) = 0)$ allows only a discrete set of standing waves, $p_1,\ p_2,\ p_3,\ \ldots$ and therefore only a discrete set of phase-shift points,

$$p_1, \quad p_2, \quad p_3, \quad \ldots \qquad \Longrightarrow \qquad \delta_\ell(p_1), \quad \delta_\ell(p_2), \quad \delta_\ell(p_3), \quad \ldots$$

For an S wave the approximate momentum spacing is $\boxed{\Delta p \sim \dfrac{\pi}{R_W}.}$



Region I $0 < r < R_I$
Physical interaction:

$$V_{\rm phys}(r) \neq 0.$$

This is where the particles scatter.

Region II $R_I < r < R_O$
Free propagation:

$$V_{\rm phys} = V_{\rm aux} = 0.$$

This is where we extract $\delta_\ell(p)$.

Region III $R_O < r < R_W$
Auxiliary potential:

$$V_{\rm phys} = 0,\ V_{\rm aux}(r) \neq 0.$$

This is used only to tune the energy.

Use an auxiliary potential to select the scattering energy

Idea: The hard spherical wall gives only a discrete set of standing-wave energies. To obtain the phase shift at a chosen momentum, we add a localized auxiliary potential only in Region III and use it as an **energy dial**.

$$R_O \le r \le R_W, \qquad \boxed{V_{\rm aux}(r) = V_0 \exp\left[-\frac{(r-R_W)^2}{\sigma^2}\right]}$$

Tune the energy $\quad H_{\rm free} + V_{\rm phys} + V_{\rm wall} + V_{\rm aux}(V_0) \implies \boxed{E_n(V_0) = E_{\rm target}.}$

$$R_I < r < R_O, \qquad V_{\rm phys} = V_{\rm aux} = 0.$$

This is the **free propagation region**, so the radial wave function can be fitted as

Fit the wave function in Region II $\quad \boxed{R_\ell(r) \simeq A\, h_\ell^{(-)}(pr) - B\, h_\ell^{(+)}(pr),}$

$$h_\ell^{(\pm)}(x) = j_\ell(x) \pm i\, y_\ell(x),$$

Since the outgoing amplitude differs from the incoming amplitude by the scattering matrix,

$$\boxed{B = S_\ell\, A, \qquad S_\ell = \frac{B}{A}.} \implies S_\ell = e^{2i\delta_\ell} \implies \boxed{\delta_\ell(p) = \frac{1}{2}\arg\left(\frac{B}{A}\right).}$$

Two ways to extract scattering phase shifts on the lattice

Lüscher's method

Keep the **periodic cubic box** and calculate its discrete energy spectrum,

$$E_n(L_{\rm box}).$$

The periodic-box geometry is encoded in

$$\boxed{p\cot\delta_0(p) = \frac{1}{\pi L_{\rm box}} S(\eta), \qquad \eta = \left(\frac{pL_{\rm box}}{2\pi}\right)^2}$$

Therefore,

$$\boxed{E_n(L_{\rm box}) \longrightarrow p_n \longrightarrow \delta_0(p_n).}$$

The scattering information is extracted from **the energy spectrum**.

Spherical-wall method

Replace the periodic boundary condition on the relative motion by a **spherical wall**,

$$R_\ell(R_W) = 0, \qquad R_W > R_{\rm int}.$$

$$R_\ell(r) \simeq A h_\ell^{(-)}(pr) - B h_\ell^{(+)}(pr),$$

with

$$\boxed{S_\ell(p) = \frac{B}{A}, \qquad \delta_\ell(p) = \frac{1}{2}\arg\left(\frac{B}{A}\right)}$$

Therefore,

$$\boxed{\psi_\ell(r) \longrightarrow S_\ell(p) \longrightarrow \delta_\ell(p).}$$

The scattering information is extracted from **the radial wave function**.

From Phase Shifts Back to the Nuclear Interaction

$$\underbrace{H \longrightarrow \delta_\ell(p)}_{\text{forward problem}}$$

$$\boxed{\underbrace{\delta_\ell^{\text{physical}}(p) \longrightarrow \{C_i\} \longrightarrow H}_{\text{inverse problem}}}$$

From phase shifts back to the nuclear interaction

So far we solved the forward problem:

$$\boxed{H \quad \longrightarrow \quad \psi_\ell(r) \quad \longrightarrow \quad \delta_\ell^{\rm lat}(p).}$$

But a realistic nuclear interaction contains parameters that are **not known a priori**.

In chiral EFT we write schematically $\boxed{H_\chi = H_{\rm kin} + V_{\rm long} + V_{\rm short}}$

with $V_{\rm long} = V_{1\pi} + V_{2\pi} + \cdots\,, \qquad V_{\rm short} = \sum_i C_i\, O_i.$

What is known and what must be determined?

The long-range interaction is constrained by pion physics and chiral symmetry.

The allowed operators O_i are fixed by symmetries and power counting, but their strengths C_i must be determined.

Now we solve the inverse problem:

$$\boxed{H(\{C_i\}) \longrightarrow \delta_\ell^{\rm lat}(p;\{C_i\}) \stackrel{!}{\simeq} \delta_\ell^{\rm physical}(p).}$$

Chiral power counting: what enters at each order?

Chiral EFT organizes the nuclear interaction in powers of a small low-energy scale,

$$\frac{Q}{\Lambda_\chi} \ll 1, \qquad Q \sim p,\ m_\pi.$$

For the two-nucleon interaction $V_{NN} = V^{(Q^0)} + V^{(Q^2)} + V^{(Q^3)} + V^{(Q^4)} + \cdots$

Order	Long-range physics	Short-range physics
Q^0 [LO]	one-pion exchange	contacts with no derivatives
Q^2 [NLO]	two-pion exchange begins	contacts with two derivatives
Q^3 [N^{2}LO]	subleading two-pion exchange	no new NN contact structures
Q^4 [N^{3}LO]	higher-order long-range terms	contacts with four derivatives

```
# maximum chiral order
nQord = 4

# orders to be fitted
Qorders = ['Q' + str(x) for x in range(0, nQord + 1, 2)]
```

As the chiral order increases, additional long-range and/or short-range structures enter, systematically improving the description of the scattering amplitude.

From chiral power counting to a contact operator

For a fixed spin–isospin channel, construct a momentum-space partial-wave building block,

$$\Phi^{JJ_z}_{Ln,S}(\mathbf{p}) = (-i)^{L+2n}\sqrt{\frac{4\pi}{2L+1}}\, f_\Lambda(p)\, p^{L+2n} \sum_{m,S_z} \langle Lm, SS_z|JJ_z\rangle\, Y_{Lm}(\hat{\mathbf{p}})\, |SS_z\rangle$$

$L =$ orbital angular momentum,

$n = 0, 1, 2, \ldots$ additional powers of p^2,

$f_\Lambda(p) =$ smooth regulator used in the numerical implementation.

The physics rule

A contact operator connects an initial and final partial-wave structure,

$$V^{(\nu)}_{fi} \sim C^{(\nu)}_{fi} \left|\Phi^{JJ_z}_{L_f n_f,S}\right\rangle \left\langle\Phi^{JJ_z}_{L_i n_i,S}\right| + \text{h.c.}$$

The total momentum order is

$$\boxed{\nu = L_i + 2n_i + L_f + 2n_f.}$$

$\nu = 0 \Rightarrow Q^0, \quad \nu = 2 \Rightarrow Q^2, \quad \nu = 4 \Rightarrow Q^4.$

The same rule in the code

```
for npow in range(0, nQord + 1, 2):

    pairs = [(l0, lap0) for l0 in l
             for lap0 in
             range(0, npow // 2 + 1)]

    for lf, lapf in pairs:
        for li, lapi in pairs:

            if li + 2*lapi + lf + 2*lapf !=
      npow:
                continue
```

What operators appear at Q^0, Q^2, and Q^4?

The momentum-counting rule $\boxed{L_i + 2n_i + L_f + 2n_f = \nu}$

determines which **orbital** structures can occur at a given chiral order. **Spin**, **isospin**, and the Pauli principle then determine the physical NN channels.

Q^0

$\nu = 0$ requires

$$L_i = L_f = 0, \quad n_i = n_f = 0.$$

Therefore only S waves occur:

$$\boxed{{}^1S_0, \qquad {}^3S_1.}$$

Schematically,

$$V_S^{(0)} = C_S^{(0)}.$$

Q^2

Examples:

$$\boxed{V_S^{(2)} \sim C_S^{(2)}(p'^2 + p^2)}$$

$$\boxed{V_P^{(2)} \sim C_P^{(2)} p' p}$$

giving

$${}^1P_1,\ {}^3P_0,\ {}^3P_1,\ {}^3P_2,$$
$${}^3S_1 - {}^3D_1$$

Q^4

Examples;

$$V_S^{(4)} \sim p'^4 + p^4, \quad p'^2 p^2,$$

$$V_P^{(4)} \sim p' p (p'^2 + p^2),$$

$$\boxed{V_D^{(4)} \sim p'^2 p^2,}$$

since

$$L_i = L_f = 2 \quad \Rightarrow \quad L_i + L_f = 4$$

```
# keep only operators of order npow
if li + 2*lapi + lf + 2*lapf != npow:
    continue
```

Regulate and put the interaction on the momentum lattice

Higher order contact operators become increasingly sensitive to the ultraviolet region of the lattice. We therefore introduce an additional smooth regulator.

A convenient smooth regulator is $$f_\Lambda(p) = \exp\left(-\frac{p^2}{2\Lambda^2}\right).$$

Schematically $$\langle p', LSJ|V_{\text{contact}}|p, LSJ\rangle \sim C\, f_\Lambda(p')\, p'^{\,L_f+2n_f}\, p^{\,L_i+2n_i}\, f_\Lambda(p).$$

The angular dependence is supplied by the LSJ projector,

$$p^L Y_{Lm}(\hat{\mathbf{p}}) \quad \text{and} \quad \langle Lm, Sm_s|JJ_z\rangle.$$

On a finite periodic lattice, $$\mathbf{p_n} = \frac{2\pi}{L_{\text{box}}}\mathbf{n}.$$

The momentum-space operator is then transformed to the spatial lattice,

$$O(\mathbf{r}', \mathbf{r}) = \frac{1}{L_{\text{box}}^6} \sum_{\mathbf{p}', \mathbf{p}} e^{i\mathbf{p}'\cdot\mathbf{r}'} O(\mathbf{p}', \mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{r}}.$$

```
# Gaussian regulator
S0_p1 = exp(-qr1**2/(2*Lambda**2))
S0_p2 = exp(-qr2**2/(2*Lambda**2))

# partial-wave projector
oprojL1_p = (
    cg(...)
    * S0_p1
    * qr1**lt
    * spf.sph_harm(m, lt, qp1, qt1)
    * qsq1**lap
    * S0_p2)
```

```
# momentum -> spatial lattice
oprojL1 = np.fft.ifftn(
    oprojL1_p.reshape((L,L,L))
).reshape(L**3)
```

Add pion exchange to the chiral Hamiltonian

The leading long-range force is generated by **one-pion exchange**.

$$\mathbf{q} = \mathbf{p}' - \mathbf{p}, \qquad \boxed{V_{1\pi}(\mathbf{q}) = -\left(\frac{g_A}{2f_\pi}\right)^2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \frac{(\boldsymbol{\sigma}_1\cdot\mathbf{q})(\boldsymbol{\sigma}_2\cdot\mathbf{q})}{\mathbf{q}^2+m_\pi^2} F_\pi(\mathbf{q})}$$

with the smooth regulator used in the calculation $\boxed{F_\pi(\mathbf{q}) = \exp\left[-\frac{\mathbf{q}^2+m_\pi^2}{\Lambda_\pi^2}\right].}$

What the equation contains

$$\underbrace{\frac{1}{\mathbf{q}^2+m_\pi^2}}_{\text{pion propagator}}$$

$$\underbrace{(\boldsymbol{\sigma}_1\cdot\mathbf{q})(\boldsymbol{\sigma}_2\cdot\mathbf{q})}_{\text{spin–momentum structure}}$$

$$\underbrace{\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}_{\text{isospin structure}}$$

For a state of definite total isospin,

$$\boxed{\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 = 2I(I+1) - 3.}$$

The same ingredients in the code

```
# momentum-space lattice
qx = dx * (2*pi) / L
qy = dy * (2*pi) / L
qz = dz * (2*pi) / L
q2 = qx**2 + qy**2 + qz**2

# regulated pion propagator
Yukawa = 1.0/(q2 + Mpi**2) \
       * exp(-(q2 + Mpi**2)/LamPi**2)
```

```
# momentum -> spatial lattice
Vpi = np.fft.ifftn(Vpi.reshape((L, L, L, 3, 3)), \
            axes=(0, 1, 2)).reshape((L**3, 3, 3))

# coupling and isospin factor
Vpi *= -(gA/(2*fpi))**2 \
       * (2*Isospin*(Isospin+1) - 3)
```

How do we determine the low-energy constants?

$$H(\mathbf{C}) = H_{\text{kin}}^{\text{imp}} + V_{\text{long}} + \sum_{i=1}^{N_{\text{LEC}}} C_i O_i,$$

$$\mathbf{C} = (C_1, C_2, \ldots, C_{N_{\text{LEC}}})$$

```
def getphase_wcr_HO(pin, cdict):

    HH = MM.copy()

    for opname, lec in cdict.items():
        HH += lec * opdict[opname].M

    return getphase_wcr(HH, pin)
```

For any trial set $\mathbf{C}$, we now know how to calculate the lattice phase shifts,

Forward calculation $\Longrightarrow$ $\mathbf{C} \longrightarrow H(\mathbf{C}) \longrightarrow \delta_\alpha^{\text{lat}}(p;\mathbf{C})$

Inverse problem $\Longrightarrow$ $\delta_\alpha^{\text{physical}}(p) \longrightarrow \{C_i\}.$

Reference phase shifts $\delta_\alpha^{\text{PWA}}(p_j) \Longleftrightarrow$ partial-wave analyses of physical NN scattering data.

Define the normalized residual

$$r_{\alpha j}(\mathbf{C}) = \frac{\delta_\alpha^{\text{lat}}(p_j;\mathbf{C}) - \delta_\alpha^{\text{PWA}}(p_j)}{\sigma_{\alpha j}}.$$

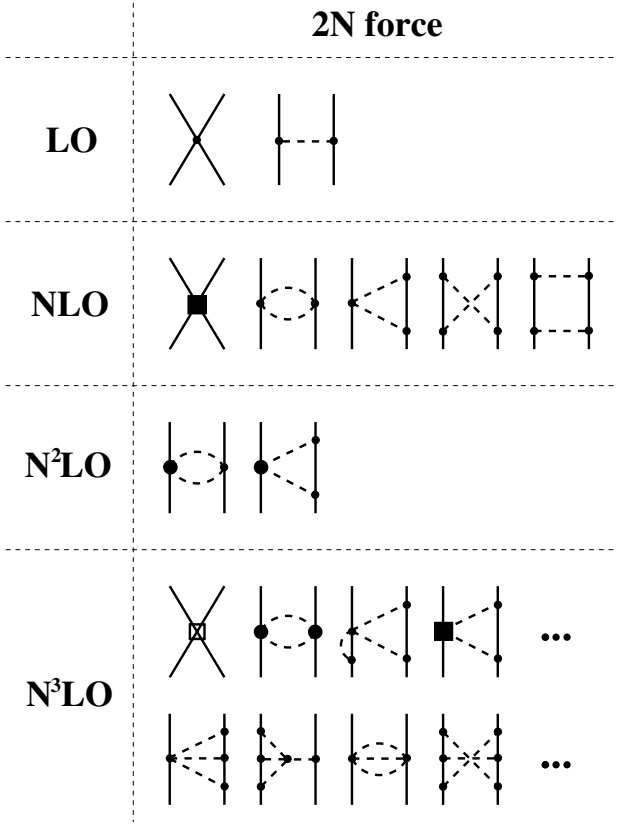
Then minimize $\chi^2(\mathbf{C}) = \sum_{\alpha,j} r_{\alpha j}^2(\mathbf{C}).$

```
cc, pcov = curve_fit(
    func,
    pfit,
    pwa93[mask_fig].flat[:],
    sigma=pwa93_err[mask_fig].flat[:],
    p0=cc,
    absolute_sigma=True
)
```

Which phase shifts constrain which contact interactions?

The contact operators are organized in definite partial-wave channels.

- a simpler decomposition into spin channels
- accurate phase shifts and binding energies.



$\Longleftrightarrow$ $V_{0,^1S_0}$ $V_{0,^3S_1}$

$\Longleftrightarrow$ $V_{2,^1S_0}$ $V_{2,^3S_1}$ $V_{2,^3SD}$ $V_{2,^1P_1}$ $V_{2,^3P_0}$ $V_{2,^3P_1}$ $V_{2,^3P_2}$

$\Longleftrightarrow$ $V^{(1)}_{4,^1S_0}$ $V^{(2)}_{4,^1S_0}$ $V^{(1)}_{4,^3S_1}$ $V^{(2)}_{4,^3S_1}$ $V^{(1)}_{4,^3SD}$ $V^{(2)}_{4,^3SD}$ $V_{4,^1P_1}$ $V_{4,^3P_0}$ $V_{4,^3P_1}$ $V_{4,^3P_2}$ $V_{4,^3PF}$ $V_{4,^1D_2}$ $V_{4,^3D_1}$ $V_{4,^3D_2}$ $V_{4,^3D_3}$

But several operators may contribute to the same channel:

$$\delta_{^1S_0}(p) = \delta_{^1S_0}\left(p; C^{(0)}_{^1S_0}, C^{(2)}_{^1S_0}, C^{(4)}_{^1S_0}, \dots\right).$$

Determine the LECs order by order

Chiral power counting tells us not only which operators exist, but also the order in which they should enter the fit.

$$\boxed{Q^0 \quad \longrightarrow \quad Q^2 \quad \longrightarrow \quad Q^4 \quad \longrightarrow \quad \cdots}$$

Q^0 **[LO]:** $$H^{(0)} = H^{\rm imp}_{\rm kin} + V^{(\leq\nu)}_{\rm long} + \sum_{i\in Q^0} C^{(0)}_i O_i,$$

and determine the leading S-wave LECs.

Q^2 **[NLO]:** Add the two-derivative contact operators,

$$H^{(2)} = H^{\rm imp}_{\rm kin} + V^{(\leq\nu)}_{\rm long} + \sum_{i\in Q^0, Q^2} C_i O_i,$$

and refit the complete set of LECs included through Q^2.

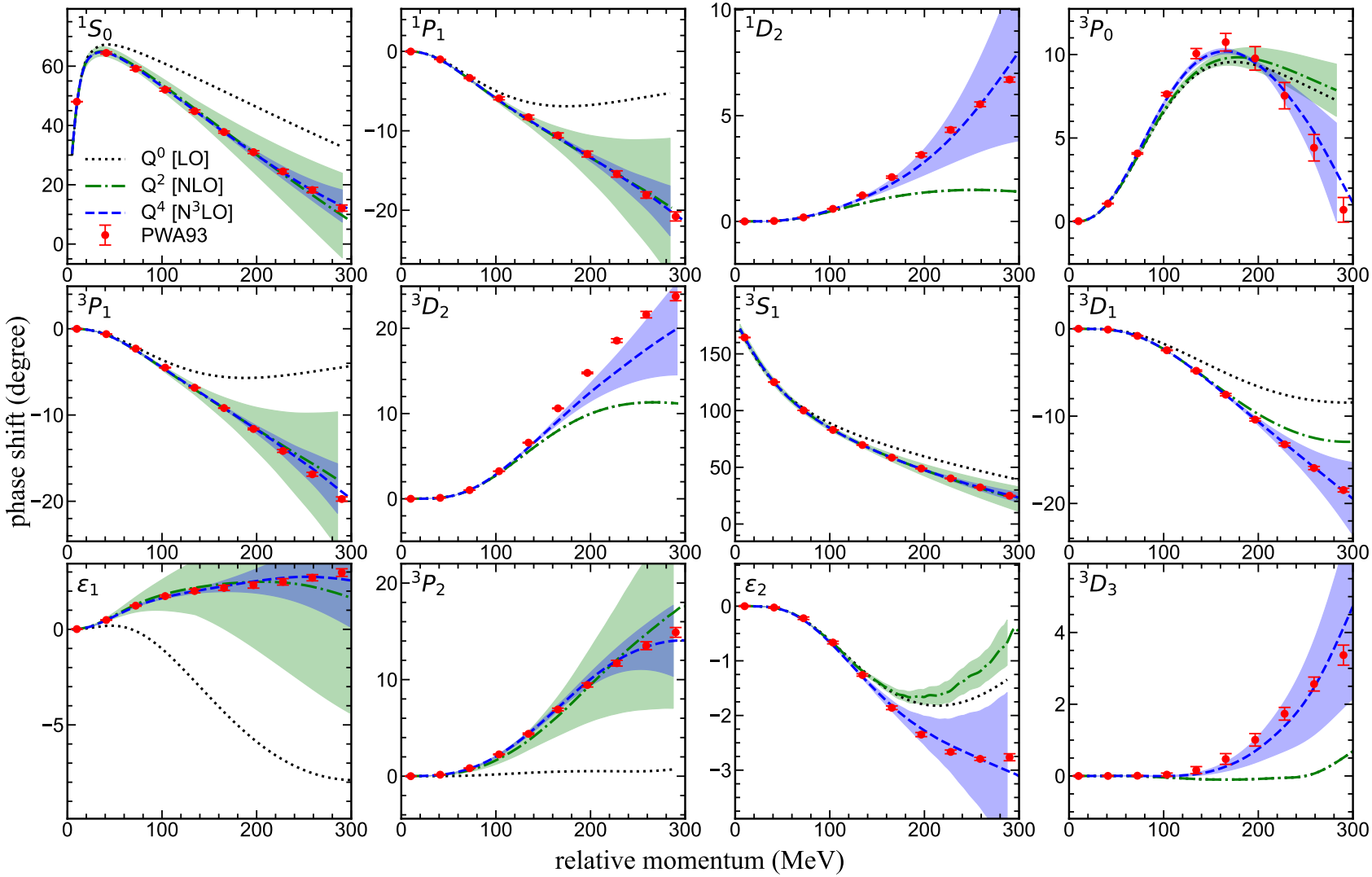
Q^4 **[N^{3}LO]:**

$$H^{(4)} = H^{\rm imp}_{\rm kin} + V^{(\leq\nu)}_{\rm long} + \sum_{i\in Q^0, Q^2, Q^4} C_i O_i,$$

and refit all included LECs.

$$\boxed{\text{add new operators} \quad \longrightarrow \quad \text{refit} \quad \longrightarrow \quad \text{improve the phase shifts.}}$$

Putting everything together: from the lattice Hamiltonian to physical NN scattering



symmetry and power counting $\longrightarrow$ operators $\longrightarrow$ LECs $\longrightarrow$ physical scattering.

EPILOGUE
Beyond Exact Diagonalization

---

few-body exact diagonalization $\longrightarrow$ Euclidean-time projection

$\longrightarrow$ many-body methods

Beyond exact diagonalization: Euclidean-time projection

For the few-body problems $\Longrightarrow$ construct the Hamiltonian matrix $\Longrightarrow$ diagonalize

For larger many-body systems $\Longleftrightarrow$ Hilbert space grows exponentially.

Introduce the Euclidean-time evolution operator $\Longrightarrow$ $\boxed{M =: e^{-a_t H} : .}$

If $H|\Psi_n\rangle = E_n|\Psi_n\rangle, \qquad |\Psi_{\rm trial}\rangle = \sum_n c_n|\Psi_n\rangle,$

then after L_t Euclidean-time steps $\boxed{M^{L_t}|\Psi_{\rm trial}\rangle = \sum_n c_n e^{-a_t E_n L_t}|\Psi_n\rangle.}$

Since $E_n > E_0$ for excited states $\boxed{L_t \to \infty \qquad \Longrightarrow \qquad M^{L_t}|\Psi_{\rm trial}\rangle \propto e^{-a_t E_0 L_t}|\Psi_0\rangle}$

Euclidean time acts as an energy filter: high-energy components are exponentially suppressed.

This is the basic bridge from few-body exact calculations to scalable many-body lattice methods.