# From chiral effective field theory to a lattice Hamiltonian

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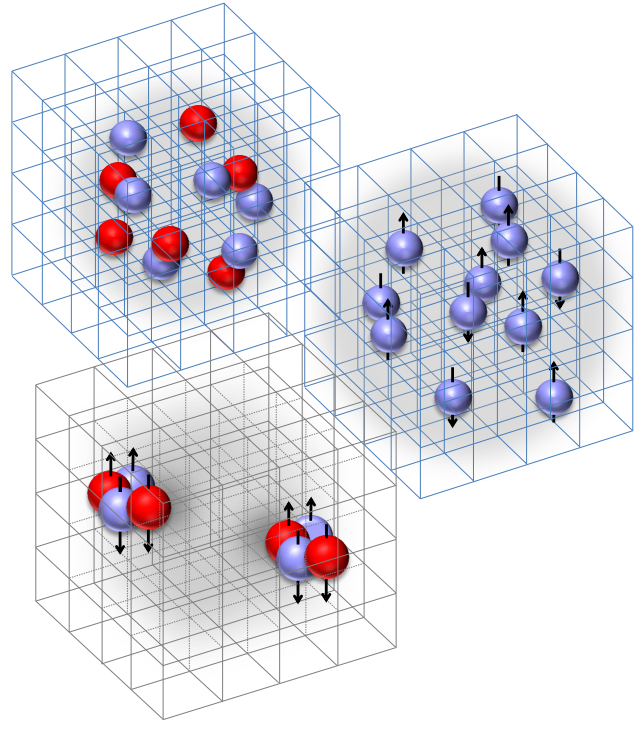


# How to put nucleons, pions, and short-range interactions on a finite lattice

How do we turn a continuum nuclear interaction into something that can be represented and calculated on a finite spatial lattice?

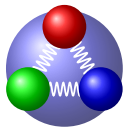
- Why chiral EFT?
  - why chiral EFT is appropriate for low-energy nuclear physics;
  - the relevant degrees of freedom and expansion scales;
- Why put it on a lattice?
  - understand lattice spacings as regulators;
- One free particle on a lattice
- Two-body contact interaction
- Spin, isospin and pions
- From Hamiltonian to transfer matrix
- First numerical exercise

# From Chiral EFT to a Spatial Lattice

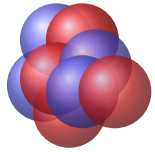
continuum nuclear physics $\longrightarrow$ regulated lattice Hamiltonian

# Why chiral EFT?

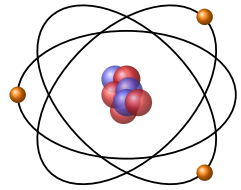
Quarks
$< 10^{-16}$



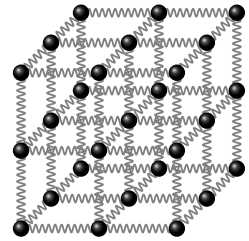
Nucleons
$\sim 10^{-13}$



Nucleus
$\sim 10^{-12}$



Atoms
$\sim 10^{-8}$ cm



Matter

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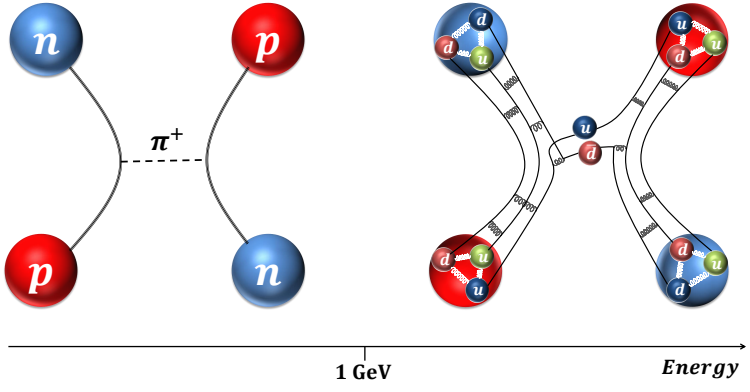
- Quantum chromodynamics (QCD) describes the strong forces by confining quarks (and gluons) into baryons and mesons.
- At low energy: $N = (p, n)$, $\pi = (\pi^+, \pi^0, \pi^-)$
- Translating QCD directly into nuclear forces:




"separation of scales"

$\Lambda_\chi$ : chiral symmetry-breakdown scale

$m_u, m_d, m_s \to 0$ chiral limit

S. Weinberg, *Phys. Lett. B* 251 (1990) 288, *Nucl. Phys.* B363 (1991) 3, *Phys. Lett. B* 295 (1992) 114.

- Effective theories provide the solution to bridge the gap between QCD and the nuclear interactions

# Chiral EFT for nucleons: nuclear forces

Chiral effective field theory organizes the nuclear interactions as an expansion in powers of momenta and other low energy scales such as the pion mass ($Q/\Lambda_\chi$).

- Short distances are not resolved explicitly; they are encoded in contact operators.
- Long-range physics: pion exchange.
- Many-body physics: three- and higher-nucleon forces.

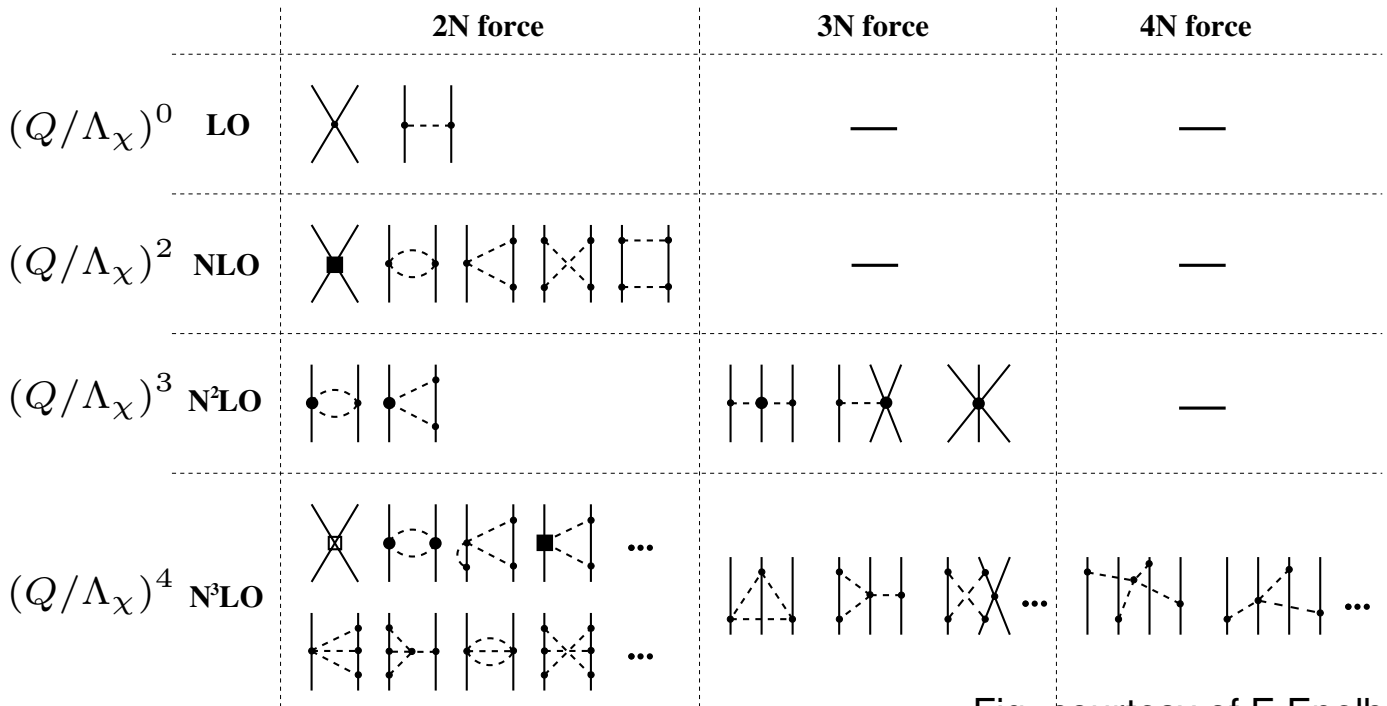
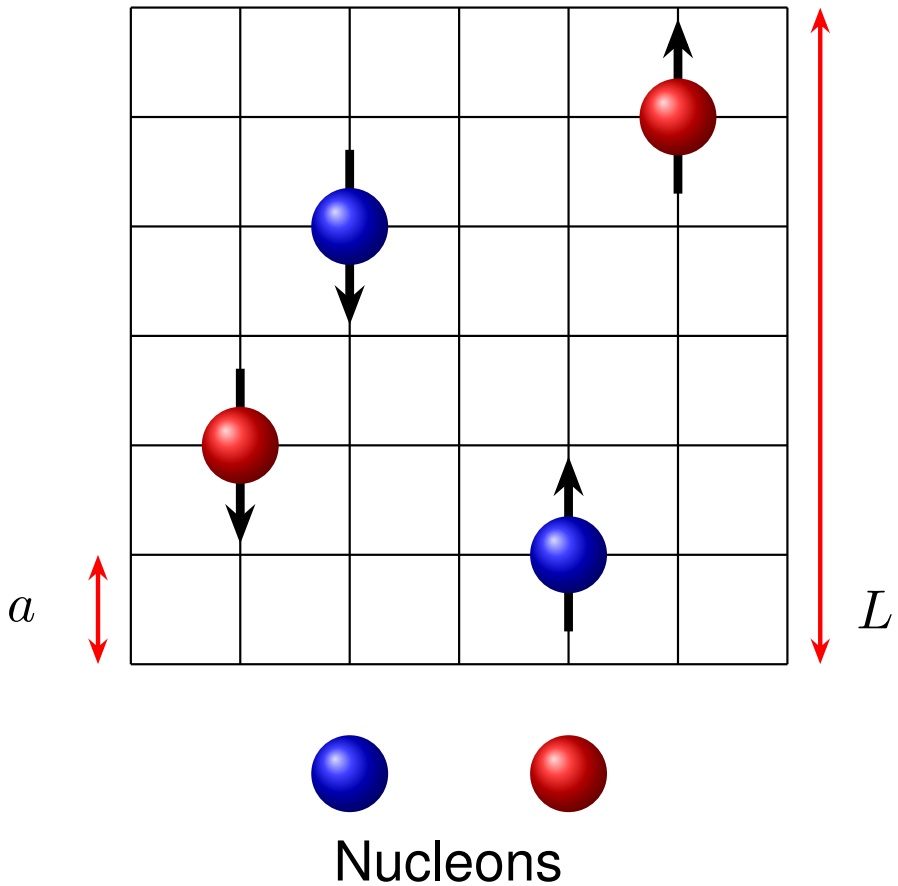



Fig. courtesy of E.Epelbaum

Ordonez et al. '94; Friar & Coon '94; Kaiser et al. '97; Epelbaum et al. '98,'03,'05,'15; Kaiser '99-'01; Higa et al. '03; ...

# Lattice effective field theory: Why a lattice?

- Lattice effective field theory is a powerful numerical method formulated in the framework of chiral effective field theory.
- Lattice EFT is a regulated EFT, not merely a numerical grid method.




$\mathbf{x} = a\,\mathbf{n}, \quad \mathbf{n} = (n_x, n_y, n_z)$

$p_{\max} = \pi/a$

UV regulator: $\Lambda \sim \pi/a$

finite volume: $L_{phys} = L\,a$

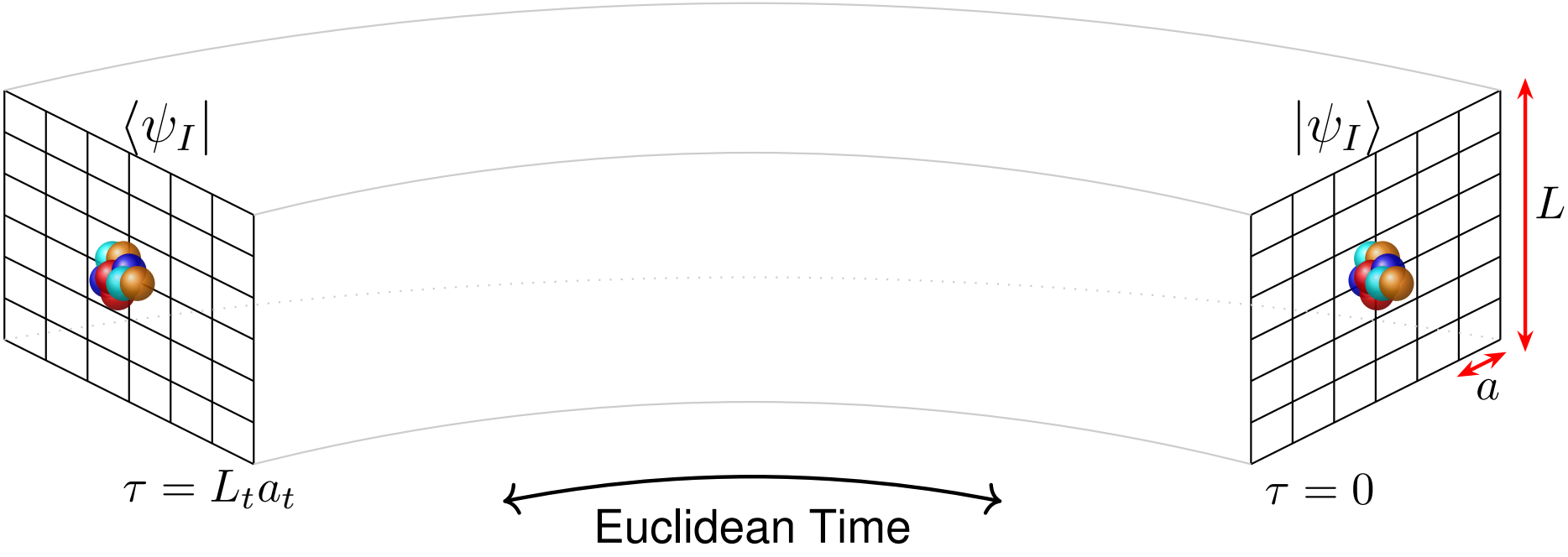
finite-dimensional Hilbert space

direct access to exact diagonalization and Monte Carlo

Lee, Prog.Part.Nucl.Phys. 63 (2009) 117-154

Laehde and Meißner, Lect. Notes Phys. 957 (2019), 1-396 Springer.

# Lattice effective field theory: Why a lattice?




- $a$ spatial lattice spacing
- $L$ number of lattice sites
- $a_t$ Euclidean time spacing

changing $a$ or $a_t$ changes the regulated theory.

**One particle in the continuum:** For a relativistic particle,

$$E(p) = \sqrt{p^2 + m^2} = m + \frac{p^2}{2m} + \mathcal{O}\left(\frac{p^4}{m^3}\right).$$

In nonrelativistic quantum mechanics we are interested in the small energy above the rest energy, $m$. So, for $p \ll m$

$$E(p) \approx m + \frac{p^2}{2m}.$$

Single particle Hamiltonian (non-relativistic kinetic energy), $\hat{h}_{\text{free}} = \dfrac{\hat{p}^2}{2m}$.

Then, we introduce the second quantization $|p\rangle = a_p^\dagger |0\rangle$, $\hat{h}_{\text{free}}|p\rangle = \dfrac{\hat{p}^2}{2m}|p\rangle$.

Therefore the free Hamiltonian for an arbitrary number of particles is

$$H_{\text{free}} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p \qquad \Longrightarrow \qquad H_{\text{free}}\,|p\rangle = \frac{p^2}{2m}\, a_p^\dagger |0\rangle.$$

This is the energy of one momentum eigenstate. In second quantization we simply sum this kinetic energy over all occupied momentum modes.

**The free Hamiltonian in coordinate space:** Now define the field operator in a periodic box of physical length $L\,a$:

$$\psi(x) = \frac{1}{\sqrt{L\,a}} \sum_p e^{ipx} a_p, \qquad \psi^\dagger(x) = \frac{1}{\sqrt{L\,a}} \sum_p e^{-ipx} a_p^\dagger.$$

Then explicitly,

$$-\frac{1}{2m} \int_0^{L\,a} dx\, \psi^\dagger(x) \frac{\partial^2}{\partial x^2} \psi(x) = \frac{1}{L\,a} \sum_{p,p'} \frac{p^2}{2m} a_{p'}^\dagger a_p \int_0^{L\,a} dx\, e^{i(p-p')x} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p.$$

Therefore,

$$\boxed{-\frac{1}{2m} \int_0^{L\,a} dx\, \psi^\dagger(x) \frac{\partial^2}{\partial x^2} \psi(x) \;=\; H_{\text{free}}}$$

Since we work in a periodic box, we can integrate by parts:

$$\boxed{H_{\text{free}} = \frac{1}{2m} \int_0^{L\,a} dx \left(\frac{\partial \psi^\dagger}{\partial x}\right)\left(\frac{\partial \psi}{\partial x}\right)}$$

The boundary term vanishes because the fields are periodic.

# Lattice effective field theory

**From the continuum to the spatial lattice:**

$$\text{Let} \qquad x_n = na, \qquad n = 0, \ldots, L-1,$$

Define dimensionless lattice operators by

$$a_n = \sqrt{a}\,\psi(x_n), \qquad \text{so that for fermions,} \qquad \{a_n, a_{n'}^\dagger\} = \delta_{nn'}.$$

Then discretize the derivative:

$$\left.\frac{\partial\psi(x)}{\partial x}\right|_{x=x_n} \longrightarrow \frac{a_{n+1} - a_n}{a^{3/2}}.$$

Using the continuum form,

$$H_{\text{free}} = \frac{1}{2m}\int dx\,(\partial_x\psi^\dagger)(\partial_x\psi),$$

we obtain

$$\boxed{H_{\text{free}}^{\text{lat}} = \frac{1}{2ma^2}\sum_n \left(a_{n+1}^\dagger - a_n^\dagger\right)(a_{n+1} - a_n) = \frac{1}{2ma^2}\sum_n \left[2a_n^\dagger a_n - a_{n+1}^\dagger a_n - a_n^\dagger a_{n+1}\right]}.$$

$\underbrace{a_{n+1}^\dagger a_n}_{n\to n+1}$ $\underbrace{a_n^\dagger a_{n+1}}_{n+1\to n}$ as **forward and backward hopping.**

**Free-particle spectrum on the lattice:** With the periodic boundary conditions already imposed ($a_{n+L} = a_n$), a momentum eigenstate is

$$\boxed{|p\rangle = \frac{1}{\sqrt{L}} \sum_{n=0}^{L-1} e^{ipna}\, a_n^\dagger |0\rangle}$$

The corresponding one-particle wavefunction on the lattice is

$$\phi_p(n) \equiv \langle n|p\rangle = \frac{1}{\sqrt{L}} e^{ipna}.$$

Periodicity quantizes the allowed momenta:

$$\phi_p(n+L) = \phi_p(n) \implies e^{ip(n+L)a} = e^{ipna} \implies e^{ipLa} = 1 \implies \boxed{p_k = \frac{2\pi k}{La}}.$$

For even $L$, choose

$$k = -\frac{L}{2}, \ldots, \frac{L}{2} - 1 \qquad \longrightarrow \qquad -\frac{\pi}{a} \le p < \frac{\pi}{a}.$$

This is the **first Brillouin zone**, and it connects directly to

$$p_{\max} \sim \frac{\pi}{a}.$$

## Free-particle spectrum: from hopping to the dispersion relation

For nearest-neighbor hopping in one dimension,

$$\boxed{H_{\text{free}}^{\text{lat}} = \frac{1}{2ma^2}\sum_n \left[2a_n^\dagger a_n - a_n^\dagger a_{n+1} - a_n^\dagger a_{n-1}\right].}$$

In the one-particle basis $\quad |n\rangle = a_n^\dagger|0\rangle,$

this is simply an $L \times L$ periodic matrix $\quad \boxed{H_{nn'} = \frac{1}{ma^2}\left[\delta_{nn'} - \frac{1}{2}\left(\delta_{n',n+1} + \delta_{n',n-1}\right)\right]}$

Because the Hamiltonian is translationally invariant, its eigenstates are plane waves,

$$|p_k\rangle = \frac{1}{\sqrt{L}}\sum_{n=0}^{L-1} e^{ip_k na}|n\rangle, \qquad \boxed{p_k = \frac{2\pi k}{La}.}$$

Acting with $H_{\text{free}}^{\text{lat}}$ $\quad H_{\text{free}}^{\text{lat}}|p\rangle = \frac{1}{2ma^2}\left[2 - e^{ipa} - e^{-ipa}\right]|p\rangle = \boxed{\frac{1-\cos(pa)}{ma^2}}|p\rangle.$

Therefore $\quad \boxed{E_{\text{lat}}(p) = \frac{1-\cos(pa)}{ma^2}.}$

## Finite lattice spacing modifies the free-particle dispersion

For nearest-neighbor hopping $$E_{\rm lat}(p) = \frac{1-\cos(pa)}{ma^2}.$$

Expanding for $pa \ll 1$ $$E_{\rm lat}(p) = \boxed{\frac{p^2}{2m} - \frac{a^2p^4}{24m} + \mathcal{O}(a^4p^6).}$$

Thus $$a \to 0 \quad \Longrightarrow \quad E_{\rm lat}(p) \to \frac{p^2}{2m}.$$

**Finite $a$ changes the dispersion relation: the difference from $p^2/(2m)$ is a lattice artifact.**

$$\boxed{\Delta E(p) = E_{\rm lat}(p) - E_{\rm cont}(p) = -\frac{a^2p^4}{24m} + \cdots.} \quad \Longrightarrow \quad \boxed{\frac{\Delta E}{E_{\rm cont}} = -\frac{(pa)^2}{12} + \cdots.}$$

---

Everything generalizes immediately to three dimensions,

$$\boxed{E_{\rm lat}(\mathbf{p}) = \frac{1}{ma^2}\sum_{l=1}^{3}[1-\cos(p_l a)] = \frac{\mathbf{p}^2}{2m} + \mathcal{O}(a^2p^4).}$$

## Improved kinetic energy: cancel the finite-$a$ errors

Can we make the lattice dispersion follow $p^2/(2m)$ more accurately **without decreasing the lattice spacing**? Allow hopping over several lattice spacings,

$$H_{\text{free}} = \frac{1}{ma^2} \sum_n \left[ \omega_0 a_n^\dagger a_n - \frac{1}{2} \sum_{r=1}^{R} \omega_r \left( a_n^\dagger a_{n+r} + a_n^\dagger a_{n-r} \right) \right].$$

The plane waves remain eigenstates, with

$$E_{\text{lat}}(p) = \frac{1}{ma^2} \left[ \omega_0 - \sum_{r=1}^{R} \omega_r \cos(rpa) \right].$$

| | $\omega_0$ | $\omega_1$ | $\omega_2$ | $\omega_3$ | leading error |
|---|---|---|---|---|---|
| nearest neighbor | $1$ | $1$ | $0$ | $0$ | $\mathcal{O}(a^2p^4)$ |
| $\mathcal{O}(a^2)$ improved | $\frac{5}{4}$ | $\frac{4}{3}$ | $-\frac{1}{12}$ | $0$ | $\mathcal{O}(a^4p^6)$ |
| $\mathcal{O}(a^4)$ improved | $\frac{49}{36}$ | $\frac{3}{2}$ | $-\frac{3}{20}$ | $\frac{1}{90}$ | $\mathcal{O}(a^6p^8)$ |

longer-range hopping $\implies$ smaller lattice artifacts.

# From one particle to many particles (interactions)

We now return to three spatial dimensions and add the simplest interaction. Start in the continuum,

$$H = H_{\rm free} + H_{\rm int} \implies H_{\rm int} = \frac{C_0}{2}\int dx^3 : \rho^2(\mathbf{x}) : \implies \rho(\mathbf{x}) = \sum_\alpha a^\dagger_\alpha(\mathbf{x})\, a_\alpha(\mathbf{x}).$$

$\alpha$ denotes the internal spin/isospin state. The lattice connection explicitly,

$$a_\alpha(\mathbf{n}) = a^{3/2}\,\psi_\alpha(\mathbf{x}), \qquad \text{and} \qquad \int dx^3 \to a^3 \sum_{\mathbf{n}}$$

and the dimensionless local density $\rho(\mathbf{n}) = \sum_\alpha a^\dagger_\alpha(\mathbf{n})\, a_\alpha(\mathbf{n}).$

$$H^{\rm phys}_{\rm int} = \frac{C_0}{2a^3}\sum_{\mathbf{n}} : \rho^2(\mathbf{n}) : \implies H^{\rm lat}_{\rm int} = a\, H^{\rm phys}_{\rm int} \implies H^{\rm lat}_{\rm int} = \frac{C_0^{\rm lat}}{2}\sum_{\mathbf{n}} : \rho^2(\mathbf{n}) :$$

where $C_0 = a^2\, C_0^{\rm lat}$.

What does $: \rho^2 :$ actually mean?
What exactly is $C_0^{\rm lat}$?

# From one particle to many particles

**What does** $:\rho^2:$ **actually mean:** For fermions at one lattice site,

$$\rho(\mathbf{n}) = \sum_\alpha a_\alpha^\dagger(\mathbf{n})\, a_\alpha(\mathbf{n}) = \sum_\alpha n_\alpha \quad \Longrightarrow \quad \text{For a fermionic mode} \quad n_\alpha^2 = n_\alpha$$

Now square the total density:

$$\rho^2 = \left(\sum_\alpha n_\alpha\right)^2 = \sum_\alpha n_\alpha^2 + \sum_{\alpha\neq\beta} n_\alpha n_\beta = \rho + \sum_{\alpha\neq\beta} n_\alpha n_\beta$$

Normal ordering $(::)$ removes precisely such one-body contraction (self-interaction)

$$:\rho^2(\mathbf{n}) := \rho^2(\mathbf{n}) - \rho(\mathbf{n}) = \rho(\mathbf{n})\,[\rho(\mathbf{n}) - 1] = \sum_{\alpha\neq\beta} n_\alpha n_\beta = 2\sum_{\alpha<\beta} n_\alpha n_\beta$$

$$\Longrightarrow \qquad \frac{1}{2} :\rho^2(\mathbf{n}) := \sum_{\alpha<\beta} n_\alpha n_\beta$$

counts the number of distinct pairs occupying that lattice site.

**For the simplest two-component system:** $\alpha = \uparrow, \downarrow$,

$$\frac{1}{2} :\rho^2(\mathbf{n}) := \rho_\uparrow(\mathbf{n})\rho_\downarrow(\mathbf{n})$$

# From one particle to many particles

The coupling $C_0 = a^2\, C_0^{\rm lat}$ is not physical by itself, and it depends

$$a, \quad \Lambda \sim \pi/a \quad \text{regularization scheme.}$$

**Why must the contact coupling be fitted?:** The two-body scattering equation is,

$$T(E) = V + V\, G_0(E) T(E).$$

For a momentum-independent contact interaction, $V = C_0$, so formally,

$$T(E) = \frac{C_0}{1 - C_0\, G_0(E)} = \frac{1}{C_0^{-1} - G_0(E)}.$$

On the lattice $$G_0(E) \sim \sum_{\mathbf{q}\in BZ} \frac{1}{E - 2E_{\rm lat}(\mathbf{q}) + i\epsilon}.$$

But the allowed momentum region depends on, $|q_i| \leq \frac{\pi}{a}$, therefore changing $a$ changes $G_0$, and consequently the coupling must change,

$$C_0 \to C_0(a)$$

The physical quantity is not $C_0$. Physical quantities are $\boxed{a_s, r_s, E_B, \delta_l(p)}$.

# Exact Few-Body Calculations on the Lattice

$$\boxed{H|\Psi_n\rangle = E_n|\Psi_n\rangle}$$

basis $\rightarrow H_{\text{kin}} \rightarrow V \rightarrow$ symmetries $\rightarrow E_n$

# Exact few-body calculations on the lattice

We have learned how to construct a lattice Hamiltonian.

Now we ask new questions:

How to determine its coupling constant?

Given a few-body lattice Hamiltonian, how do we solve it exactly?

The central idea is simple:

$H|\Psi_n\rangle = E_n|\Psi_n\rangle \quad \longrightarrow \quad$ finite-dimensional matrix eigenvalue problem.

basis $\rightarrow H_{\text{kin}} \rightarrow V \rightarrow$ symmetry projection $\rightarrow$ `eigs` $\rightarrow E_n$

# Exact few-body calculations on the lattice

We consider two-component fermion $\uparrow, \downarrow$
with masses $m_\uparrow$, $m_\downarrow$.
Only particles with unlike species interact
through an $S$-wave contact interaction.

$$\Longrightarrow \boxed{H_A = \sum_{i=1}^{A} T_i + C_0 \sum_{\substack{i<j \\ \text{unlike species}}} \delta_{\mathbf{r}_i,\mathbf{r}_j}.}$$

```
main_01_tune_dimer.m
main_02_dimer_fermion.m
main_03_dimer_dimer.m
```


Wu, SE, Meissner, Shen, Geng, *Phys. Rev. Lett.* 136 (2026) 14, 142502
SE, *Turk. J. Phys.* 42 (2018) 6, 631-640
SE, Katterjohn Lee, Meissner, Rupak, *Phys. Lett. B* 768 (2017) 337-344
SE, Lee *Phys. Rev. C* 90 (2014) 6, 064001


**Step 1**

$A = 2$

Fit the two-body coupling constant:

$E_2(C_0) = -B_2.$

$C_0$ is determined

**Step 2**

$A = 3$

Solve the dimer-fermion system:

$\uparrow\uparrow\downarrow$ .

$N_{\text{basis}} = L^6$

**Step 3**

$A = 4$

Solve the dimer-dimer system:

$\uparrow\uparrow\downarrow\downarrow$ .

$N_{\text{basis}} = L^9$

two-body calibration $\rightarrow$ three-body spectrum $\rightarrow$ four-body spectrum.

# Construct the relative-coordinate basis

For $A$ particles on a cubic lattice, a naive coordinate basis has $L^{3A}$ states.

But translational invariance allows us to remove the center-of-mass coordinate.

Choose particle $A$ as the reference particle and define

$$\mathbf{r}_i = \mathbf{x}_i - \mathbf{x}_A, \qquad i = 1, \ldots, A-1.$$

Then only $A-1$ relative coordinates are stored $\quad N_{\text{basis}} = L^{3(A-1)}.$

The function `relative_coordinates.m` implements

$$\mathbf{r}_i = \mathbf{x}_i - \mathbf{x}_A.$$

```
function [idx, coord] = relative_coordinates(L, nA, ndim)

N = L^(ndim*(nA-1));
idx = (0:N-1)';

coord = cell(nA,ndim);

for a = 1:nA
    for d = 1:ndim
        power = ndim*(a-1) + (d-1);
        coord{a,d} = mod(floor(idx/L^power),L);
    end
end

% For a = nA the powers are beyond the stored basis digits,
% hence coord{nA,d}=0 automatically:
% particle A is the reference particle.
end
```

# The kinetic term on a periodic lattice

For one particle, the lattice kinetic energy is represented by a finite difference operator,

$$T = \frac{1}{2ma^2} \sum_{\mathbf{n}} \left[ 2\omega_0 \, a^\dagger_{\mathbf{n}} a_{\mathbf{n}} - \sum_{k=1}^{n_k} \sum_{\alpha=x,y,z} \omega_k \left( a^\dagger_{\mathbf{n}} a_{\mathbf{n}+k\hat{\alpha}} + a^\dagger_n a_{\mathbf{n}-k\hat{\alpha}} \right) \right],$$

The code uses improved finite-difference coefficients,

$$w_k = \begin{cases} (-1)^{k+1} \dfrac{2\,(n_k!)^2}{k^2\,(n_k+k)!\,(n_k-k)!}, & k \neq 0 \\ \sum_{k=1}^{n_k} w_k, & k = 0\,. \end{cases}$$

---

The first $A-1$ particles are easy: $\mathbf{r}_i = \mathbf{x}_i - \mathbf{x}_A$.

If particle $i < A$ hops: $\mathbf{x}_i \to \mathbf{x}_i + k\hat{e}_d \implies \boxed{\mathbf{r}_i \to \mathbf{r}_i + k\hat{e}_d.}$

---

If the reference particle ($A$) hops $\implies \mathbf{x}_A \to \mathbf{x}_A + k\hat{e}_d,$

every relative coordinate changes $\implies \boxed{\mathbf{r}_i = \mathbf{x}_i - \mathbf{x}_A \to \mathbf{r}_i - k\hat{e}_d, \qquad i = 1, \ldots, A-1}$

# Improved kinetic-term coefficients

The coefficients are generated directly in `build_kinetic_relative.m`:

```
w  = zeros(1,iKine);
w0 = 0.0;

for k = 1:iKine
    w(k) = (-1)^(k+1) * 2*factorial(iKine)^2 / ...
           (k^2*factorial(iKine+k)*factorial(iKine-
      k));
    w0 = w0 + w(k);
end
```

The diagonal kinetic-energy contribution from each particle is

```
for a = 1:nA
    diagonal = (2*ndim*w0)/(2*mbar(a))*cutoff;
    Hkin = Hkin + spdiags(diagonal*ones(N,1),0,N,N)
       ;
end
```

$$m_{\mathrm{bar}} = m\,a$$

```
cutoff = 1/a
```

is the factor defining the energy units in the code.

This is the most important part of `build_kinetic_relative.m`.

```
% Hopping of the reference particle A.
% If x_A -> x_A + k e_d,
% each r_i=x_i-x_A shifts by -k e_d.

a = nA;

for d = 1:ndim
  for k = 1:iKine
    idx_p = idx;
    idx_m = idx;

    for i = 1:nA-1
      base = L^(ndim*(i-1)+(d-1));

      idx_p = idx_p - coord{i,d}*base ...
                    + mod(coord{i,d}-k,L)*base;

      idx_m = idx_m - coord{i,d}*base ...
                    + mod(coord{i,d}+k,L)*base;
    end

    hop = -w(k)/(2*mbar(a))*cutoff;

    Hkin = Hkin ...
       + sparse(idx+1,idx_p+1,hop*ones(N,1),N,N)
      ...
       + sparse(idx+1,idx_m+1,hop*ones(N,1),N,N);
  end
end
```

# The zero-range contact interaction

The interaction is local and acts only when two unlike particles occupy the same lattice site.

For one pair $(i, j)$ $\boxed{V_{ij} = C_0 \ \delta_{\mathbf{r}_i, \mathbf{r}_j}.}$

For a set of interacting unlike pairs,

$$\boxed{V = C_0 \sum_{(i,j)\in\mathcal{P}} \delta_{\mathbf{r}_i, \mathbf{r}_j}.}$$

Examples:

$$\begin{aligned} \uparrow\downarrow: &\quad \mathcal{P} = \{(1,2)\}, \\ \uparrow\uparrow\downarrow: &\quad \mathcal{P} = \{(1,3),(2,3)\}, \\ \uparrow\uparrow\downarrow\downarrow: &\quad \mathcal{P} = \{(1,3),(1,4),(2,3),(2,4)\}. \end{aligned}$$

The function `build_contact_relative.m` tests whether two particles are at the same lattice point.

```
V = sparse(N,N);

for ip = 1:size(pairs,1)
    i = pairs(ip,1);
    j = pairs(ip,2);

    same_site = true(N,1);

    for d = 1:ndim
        same_site = same_site & ...
            (coord{i,d} == coord{j,d});
    end

    V = V + spdiags( ...
        c0*cutoff*double(same_site),0,N,N);
end
```

# Tune the two-body coupling

Before solving three- and four-body systems, we determine the coupling $C_0$ from one two-body observable.

$$H_2(C_0) = T_1 + T_2 + C_0\,\delta_{\mathbf{r}_1,\mathbf{r}_2}\,.$$

We choose a target dimer binding energy,

$$E_2(C_0) = -B_2.$$

---

physical input

$\Downarrow$

$C_0$

$\Downarrow$

few-body Hamiltonian

The main program is `main_01_tune_dimer.m`.

```
m_up   = 939.0;      % MeV
m_down = 939.0;      % MeV

Btarget = 2.2246;       % desired dimer binding
      energy
L2 = 30;              % two-body box

masses2 = [m_up m_down];

c0 = tune_dimer_contact( ...
    L2,cutoff,masses2,Btarget,iKine,ndim);

E2 = lowest_two_body_energy( ...
    L2,cutoff,masses2,c0,iKine,ndim);
```

The fitting routine minimizes

$$\chi^2(C_0) = \left[E_2(C_0) + B_2\right]^2.$$

```
objective = @(c) dimer_chi2(c,Hkin,Vunit,Btarget,
      optsE);
c0 = fminsearch(objective,-0.25,optsFit);
```

# The dimer-fermion system

Now use the same fitted interaction in the three-body system

$$\boxed{\uparrow\uparrow\downarrow\,.}$$

Particles $1$ and $2$ are identical $\uparrow$ fermions, while particle $3$ is a $\downarrow$ fermion.

Only unlike pairs interact:

$$\boxed{\mathcal{P} = \{(1,3),(2,3)\}.}$$

The Hamiltonian is

$$\boxed{H_3 = T_1 + T_2 + T_3 + C_0\,\left(\delta_{\mathbf{r}_1,\mathbf{r}_3} + \delta_{\mathbf{r}_2,\mathbf{r}_3}\right).}$$

After removing the center of mass,

$$\boxed{N_{\text{basis}} = L^6.}$$

The main program is `main_02_dimer_fermion.m`.

```
L = 5;
nA = 3;
numeigs = 4;

masses = [m_up m_up m_down];
pairs  = [1 3; 2 3];

Hkin = build_kinetic_relative( ...
    L,cutoff,masses,iKine,ndim);

V = build_contact_relative( ...
    L,cutoff,nA,pairs,c0,ndim);

H = Hkin + V;

Nbasis = size(H,1);
```

$$\boxed{L = 5 \quad \Rightarrow \quad N_{\text{basis}} = 5^6 = 15625.}$$

# The dimer-fermion system

Define an operator $P$, with desired eigenvalue, $P|\Psi\rangle = s|\Psi\rangle = \pm|\Psi\rangle$.

Particles $1$ and $2$ are identical fermions; instead of explicitly constructing a smaller antisymmetric basis, the code uses a symmetry penalty.

$$\boxed{H = H_3 + \lambda(1 + P_{12})}$$

If $P_{12}|\Psi\rangle = -|\Psi\rangle$, then the penalty vanishes.

If $P_{12}|\Psi\rangle = +|\Psi\rangle$, the state is shifted upward by $2\lambda$.

We also separate the spectrum by parity,

$$\boxed{\Pi|\Psi\rangle = \pm|\Psi\rangle.}$$

$$\boxed{H = H_3 + \lambda(1 + P_{12}) + \lambda(1 + \Pi)}$$

The exchange and parity maps are constructed as index maps.

```
P12  = permutation_map_relative(L,nA,[2 1 3],ndim);
Pinv = parity_map_relative(L,nA,ndim);
lambda = 100.0;
for parity = [-1 +1]
    maps    = {P12, Pinv};
    desired = [-1, parity];

    Hfun = @(x) apply_symmetry_penalty( ...
        x,H,maps,desired,lambda);

    [~,D] = eigs( ...
        Hfun,Nbasis,numeigs,'smallestreal',opts);
end
```

The eigensolver only needs matrix-vector products. Therefore the penalty is applied directly to a vector:

```
function y = apply_symmetry_penalty( ...
    x,H,maps,eigenvalues,lambda)

y = H*x;
for k = 1:length(maps)
    Pindex = maps{k};
    s = eigenvalues(k);

    y = y + lambda*(x - s*x(Pindex));
end
```

# The dimer-dimer system

Now move to four particles,

$$\boxed{\uparrow\uparrow\downarrow\downarrow\,.}$$

Particles $1, 2$ are identical $\uparrow$ fermions, and particles $3, 4$ are identical $\downarrow$ fermions.

Only unlike particles interact:

$$\boxed{\mathcal{P} = \{(1,3),(1,4),(2,3),(2,4)\}.}$$

The Hamiltonian is

$$\boxed{H_4 = \sum_{i=1}^{4} T_i + C_0\ (\delta_{13} + \delta_{14} + \delta_{23} + \delta_{24})\,.}$$

After removing the center of mass,

$$\boxed{N_{\text{basis}} = L^9.}$$

The main program is `main_03_dimer_dimer.m`.

```
L = 3;
nA = 4;
numeigs = 4;

masses = [m_up m_up m_down m_down];

pairs = [1 3;
         1 4;
         2 3;
         2 4];

Hkin = build_kinetic_relative( ...
    L,cutoff,masses,iKine,ndim);

V = build_contact_relative( ...
    L,cutoff,nA,pairs,c0,ndim);

H = Hkin + V;

Nbasis = size(H,1);
```

$$\boxed{L = 3 \quad \Rightarrow \quad N_{\text{basis}} = 3^9 = 19683.}$$

# The dimer-dimer system

There are now two independent exchange symmetries.

For the identical $\uparrow$ fermions,

$$\boxed{P_{12}|\Psi\rangle = -|\Psi\rangle.}$$

For the identical $\downarrow$ fermions,

$$\boxed{P_{34}|\Psi\rangle = -|\Psi\rangle.}$$

For the example in the code, we also choose even parity,

$$\boxed{\Pi|\Psi\rangle = +|\Psi\rangle.}$$

$$\boxed{H = H_4 + \lambda(1 + P_{12}) + \lambda(1 + P_{34}) + \lambda(1 - \Pi).}$$

The symmetry maps are again simple index maps.

```
P12 = permutation_map_relative(L,nA,[2 1 3 4],
      ndim);
P34 = permutation_map_relative(L,nA,[1 2 4 3],
      ndim);

Pinv = parity_map_relative(L,nA,ndim);

maps    = {P12, P34, Pinv};
desired = [-1, -1, +1];

lambda = 100.0;

Hfun = @(x) apply_symmetry_penalty( ...
    x,H,maps,desired,lambda);

[~,D] = eigs( ...
    Hfun,Nbasis,numeigs,'smallestreal',opts);
```

$$\boxed{P_{12} = -1, \qquad P_{34} = -1, \qquad \Pi = +1.}$$

Only states satisfying all desired symmetry conditions remain in the low-energy spectrum.

# Exact diagonalization: What is exact and What is not?

The calculation solves exactly

$$H_L|\Psi_n^{(L)}\rangle = E_n^{(L)}|\Psi_n^{(L)}\rangle$$

for the chosen finite lattice Hamiltonian.

What is exact?

$E_n^{(L)}$ and $\Psi_n^{(L)}$ of the finite sparse matrix.

What is still approximate?

finite volume $L$,
finite lattice spacing $a$,
chosen regulator and interaction,
limited number of computed eigenstates.

After removing the center of mass,

$$N_{\text{basis}} = L^{3(A-1)}.$$

For a modest lattice $L = 5$,

$$A = 2: \quad 5^3 = 125,$$
$$A = 3: \quad 5^6 = 15625,$$
$$A = 4: \quad 5^9 = 1{,}953{,}125.$$

The Hilbert space grows exponentially with particle number.

As $A$ increases exact diagonalization rapidly becomes impossible.

Exact few-body calculations teach us how the Hamiltonian works. For larger nuclei, we need transfer matrices, Euclidean-time projection, auxiliary fields, and Monte Carlo sampling.

# Transition to realistic nuclear lattice EFT

The two-component fermion examples teach the essential numerical structure.

For realistic nuclear systems, we keep the same computational logic but replace the simple contact Hamiltonian by a nuclear lattice EFT Hamiltonian,

$$\boxed{H = H_{\text{kin}}^{\text{imp}} + V_{NN} + V_{3N} + \cdots .}$$

The basis now includes spin and isospin degrees of freedom, and the interactions include

$$\boxed{\text{contact interactions} + \text{pion exchange} + \text{three-nucleon forces} + \cdots .}$$

But the conceptual chain remains the same:

$$\boxed{\text{basis} \rightarrow H \rightarrow \text{symmetries} \rightarrow \text{low-energy spectrum.}}$$

# EXERCISES: Two-body bound state on the lattice

**Exercise 1:** Consider two distinguishable particles of equal mass $m$ interacting in the $S$ wave. Take an attractive interaction with the zero-range limit and show that

$$\boxed{\kappa = \frac{1}{a_s}}.$$

**Exercise 2:** Consider a cubic lattice with $L$ sites in each direction and spatial lattice spacing $a$. The physical box size is $L_{\rm phys} = La$, and the allowed momenta are $q_i = 2\pi n_i/La$, $n_i = 0, 1, \ldots, L-1$. For nearest-neighbor hopping, the single-particle lattice dispersion is

$$\varepsilon_{\rm lat}(\mathbf{q}) = \frac{1}{ma^2} \sum_{i=1}^{3} \left[1 - \cos(q_i a)\right].$$

The two particles, labelled $\uparrow$ and $\downarrow$, interact through an attractive on-site interaction

$$H_{\rm int} = U \sum_{\mathbf{n}} n_\uparrow(\mathbf{n}) n_\downarrow(\mathbf{n}), \qquad U < 0.$$

For a bound state $E = -B < 0$, show that this becomes

$$\boxed{\frac{1}{U} = -\frac{1}{L^3} \sum_{\mathbf{q}} \frac{1}{B + 2\varepsilon_{\rm lat}(\mathbf{q})}}.$$

# EXERCISES: Two-body bound state on the lattice

**Exercise 3:** Introduce the dimensionless variables

$$\mathbf{k} = a\mathbf{q}, \qquad g = ma^2U, \qquad b = ma^2B.$$

If $C_0$ is the continuum contact coefficient,

$$U = \frac{C_0}{a^3}, \qquad C_0^{\rm lat} = \frac{C_0}{a^2} = aU, \qquad m_{\rm lat} = ma, \qquad \Longrightarrow \qquad \boxed{g = m_{\rm lat} C_0^{\rm lat}}.$$

Show that the exact finite-volume equation can be written as

$$\boxed{\frac{1}{g} = -\frac{1}{L^3}\sum_{\mathbf{k}} \frac{1}{b + 2\sum_{i=1}^{3}[1-\cos k_i]}}.$$

and in the infinite-volume limit can be written as

$$\boxed{\frac{1}{g} = -J(b) = -\int_{-\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \frac{1}{b + 2\sum_{i=1}^{3}[1-\cos k_i]}}.$$

# EXERCISES: Two-body bound state on the lattice

**Exercise 4:** For the on-site interaction, sum the geometric series for repeated two-body scattering and show that the lattice two-body $T$ matrix has the form

$$T(E) = \frac{1}{U^{-1} - G_0(E)}.$$

Evaluate the zero-energy loop and show that

$$G_0(0) = -ma^2 J(0).$$

**Exercise 5:** Use the continuum threshold relation $\mathcal{T}(0) = 4\pi a_s/m$, and the fact that the continuum-normalized contact amplitude is $\mathcal{T} = a^3 T$ to derive

$$\boxed{\frac{a}{4\pi a_s} = \frac{1}{g} + J(0)}.$$

**Exercise 6:** Numerically evaluate $J(0)$. Hence determine the critical coupling $g_c$ for which $a_s$ diverges. Show that

$$\boxed{g_c = -\frac{1}{J(0)}}.$$

Interpret this point physically.

# EXERCISES: Two-body bound state on the lattice

**Exercise 7:** Combine the continuum result $\kappa = 1/a_s$ with the matching relation above and show that

$$\boxed{\kappa a = \frac{a}{a_s} = 4\pi \left[ \frac{1}{g} + J(0) \right]}.$$

Show also that the exact continuum benchmark in dimensionless units is simply

$$\boxed{b_{\text{cont}} = (\kappa a)^2}.$$

# Two-body bound state on the lattice

**Exercise 8 (Numerical work):** A minimal working Python program, `two_body_contact_starter.py`, is provided. It constructs the relative-coordinate Hamiltonian for $m = a = 1$ and computes the lowest eigenvalue using sparse diagonalization.
For $m = a = 1$, the scaled relative-coordinate Hamiltonian is

$$H_{\mathbf{r},\mathbf{r}} = 6 + g\,\delta_{\mathbf{r},\mathbf{0}},$$
$$H_{\mathbf{r},\mathbf{r}\pm\hat{\mathbf{e}}_\mathbf{i}} = -1,$$

with periodic boundary conditions.

A) Run the supplied code for $L = 10$ and $g = -5$. Record the numerical ground-state energy.

B) Add a function that solves the exact finite-volume equation from Exe. 3. Compare the exact result with the sparse-matrix diagonalization. Quote the absolute difference.

C) Study finite-volume convergence for $L = 4, 6, 8, 10, 12, 16, 20$ at fixed $g = -5$. Determine the infinite-volume lattice binding energy and plot

$$\frac{B_L}{B_\infty^{\mathrm{lat}}} - 1$$

versus $L$.

# EXERCISES: From one particle to many particles

**Exercise 9 (Numerical work):**

D) Evaluate $J(0)$ numerically and determine $g_c$.

E) For several couplings more attractive than $g_c$, for example

$$g = -4.0, -4.2, -4.5, -5, -8, -12, -20,$$

calculate

$$\frac{a_s}{a}, \qquad \kappa a, \qquad b_{\text{cont}}, \qquad b_{\text{lat}}.$$

Plot

$$\boxed{\frac{B_{\text{lat}}}{B_{\text{cont}}} \quad \text{versus} \quad \kappa a}.$$

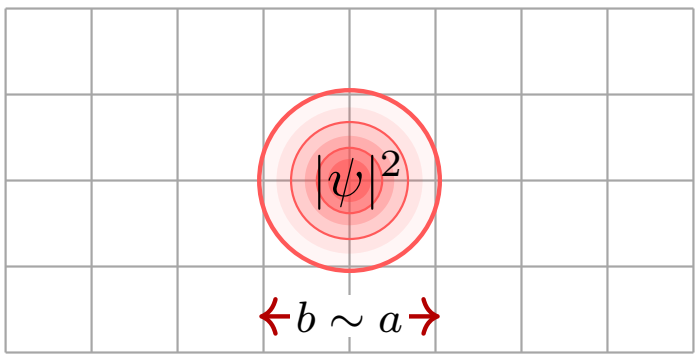
Answer the following question in a short paragraph:
*What physical length scale determines when the lattice result deviates significantly from the continuum result? Why is "the coupling is too strong" not the most precise statement?*

# Why do strong point-like contacts generate lattice artifacts?

A very attractive zero-range interaction can produce a very compact bound state. The key quantity is not just the coupling itself, but the dimensionless ratio

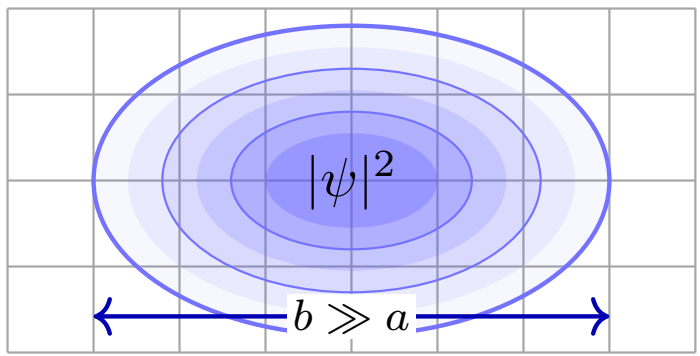
$$\kappa a, \qquad \kappa \sim \text{binding momentum}, \qquad b \sim \kappa^{-1}.$$

**Bad regime:** $\kappa a \sim 1$




The state is so compact that it probes the one-site structure of the point-like lattice contact. The UV details of the regulator become important, and lattice artifacts grow.

**Good regime:** $\kappa a \ll 1$

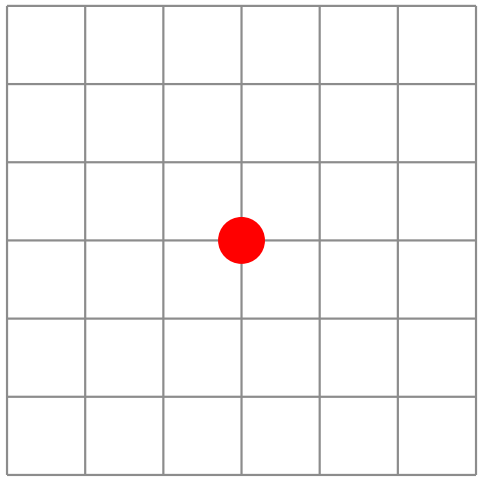



The relative bound-state probability density extends over many lattice sites. The state does **not** resolve the short-distance details of the regulator.

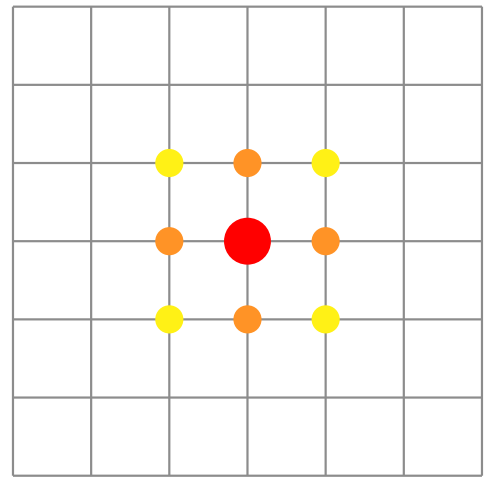
too strong coupling constant $\iff$ the physical size $\kappa^{-1} \sim a$.

# Smearing is part of the regulator

**A point-like lattice contact probes only one site.**



**Smearing distributes the short-range interaction over neighboring sites.**



**Non-local smearing:** $$a_{s,i}^{s_{\rm NL}}(\mathbf{n}) = a_{s,i}(\mathbf{n}) + s_{\rm NL} \sum_{|\mathbf{n}'|=1} a_{s,i}(\mathbf{n}+\mathbf{n}') + \cdots$$

**Local smearing:** $$\rho^{s_{\rm L}}(\mathbf{n}) = \rho(\mathbf{n}) + s_{\rm L} \sum_{|\mathbf{n}'|=1} \rho(\mathbf{n}+\mathbf{n}') + \cdots .$$

Its purpose is not simply “numerical smoothing.” It changes the regulator and can improve the effective-range behavior and reduce lattice artifacts.

If the regulator/smearing changes, the LECs must be refitted.

# Local vs. non-local smearing: a momentum-space interpretation

**Local smearing**

Smear the *local density* entering the interaction:

$$\rho^{s_{\mathrm{L}}}(\mathbf{n}) = \rho(\mathbf{n}) + s_{\mathrm{L}} \sum_{|\boldsymbol{\delta}|=1} \rho(\mathbf{n}+\boldsymbol{\delta}) + \cdots .$$

After Fourier transform,

$$\boxed{\rho^{s_{\mathrm{L}}}(\mathbf{q}) = f_{\mathrm{L}}(\mathbf{q})\,\rho(\mathbf{q}),}$$

with $f_{\mathrm{L}}(\mathbf{q}) = 1 + 2s_{\mathrm{L}} \sum_{i=1}^{3} \cos(q_i a) + \cdots .$

Therefore the interaction depends on the **momentum transfer**

$$\boxed{V_{\mathrm{L}}(\mathbf{p}', \mathbf{p}) = V_{\mathrm{L}}(\mathbf{q}), \qquad \mathbf{q} = \mathbf{p}' - \mathbf{p}.}$$

$$\boxed{\text{local} \implies \text{depends only on } \mathbf{q}}$$

**Non-local smearing**

Smear the *single-particle field* itself:

$$a^{s_{\mathrm{NL}}}(\mathbf{n}) = a(\mathbf{n}) + s_{\mathrm{NL}} \sum_{|\boldsymbol{\delta}|=1} a(\mathbf{n}+\boldsymbol{\delta}) + \cdots .$$

After Fourier transform,

$$\boxed{a^{s_{\mathrm{NL}}}(\mathbf{p}) = f_{\mathrm{NL}}(\mathbf{p})\,a(\mathbf{p}),}$$

with $f_{\mathrm{NL}}(\mathbf{p}) = 1 + 2s_{\mathrm{NL}} \sum_{i=1}^{3} \cos(p_i a) + \cdots .$

So the interaction depends separately on **incoming and outgoing momenta**.

$$\boxed{V_{\mathrm{NL}}(\mathbf{p}', \mathbf{p}) \sim f_{\mathrm{NL}}(\mathbf{p}')\, V\, f_{\mathrm{NL}}(\mathbf{p}).}$$

$$\boxed{\text{non-local} \implies \text{depends separately on } \mathbf{p}, \mathbf{p}'}$$

# From a Toy Interaction to Realistic Nuclear Lattice EFT

---

$$\uparrow, \downarrow \quad \longrightarrow \quad p\uparrow,\ p\downarrow,\ n\uparrow,\ n\downarrow$$

contact interaction $\longrightarrow$ spin $+$ isospin $+$ pion exchange

# Realistic nuclear lattice EFT

**Nucleons have spin and isospin:** Introduce occupation-number language:

$$a^\dagger_{s,i}(\mathbf{n}), \qquad s = \uparrow, \downarrow, \qquad i = p, n.$$

At every lattice site $\mathbf{n}$, a nucleon can occupy four internal states,

$$\boxed{p\uparrow, \qquad p\downarrow, \qquad n\uparrow, \qquad n\downarrow\,.}$$

$$\rho(\mathbf{n}) = \sum_{s,i} a^\dagger_{s,i}(\mathbf{n})\, a_{s,i}(\mathbf{n}) \quad \Longrightarrow \quad \text{“how many nucleons?”}$$

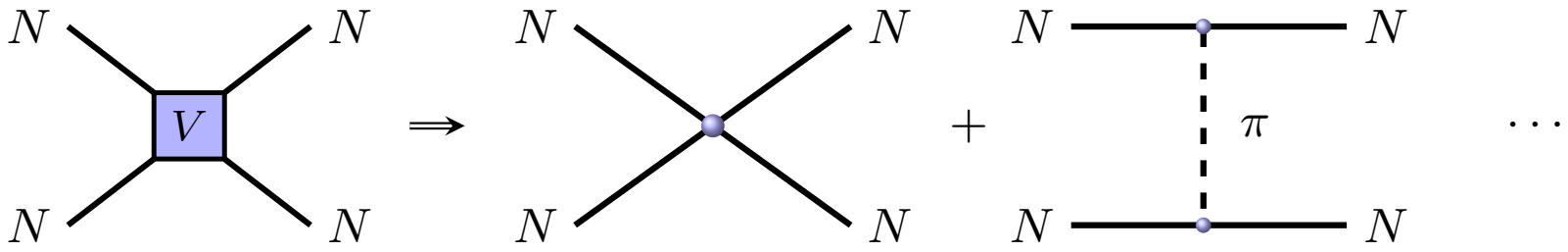
$$\rho_S(\mathbf{n}) = \sum_{s,s',i} a^\dagger_{s,i}(\mathbf{n})\, [\sigma_S]_{s,s'}\, a_{s',i}(\mathbf{n}) \quad \Longrightarrow \quad \text{“how are the spins oriented?”}$$

$$\rho_I(\mathbf{n}) = \sum_{s,i,i'} a^\dagger_{s,i}(\mathbf{n})\, [\tau_I]_{i,i'}\, a_{s,i'}(\mathbf{n}) \quad \Longrightarrow \quad \text{“proton or neutron?”}$$

$$\rho_{S,I}(\mathbf{n}) = \sum_{s,s',i,i'} a^\dagger_{s,i}(\mathbf{n})\, [\sigma_S]_{s,s'}\, [\tau_I]_{i,i'}\, a_{s',i'}(\mathbf{n}) \quad \Longrightarrow \quad \text{“how are spin and isospin correlated?”}$$

These densities are the building blocks from which the nuclear interaction is constructed.

# Realistic nuclear lattice EFT




**The LO nuclear contact interaction:** At LO there are no derivatives in the short-range interaction. Therefore the contact is momentum independent and zero range,

$$V_{\text{contact}}^{\text{LO}} \sim \delta^{(3)}(\mathbf{r}).$$

What scalar operators can act on the spin and isospin of two nucleons?

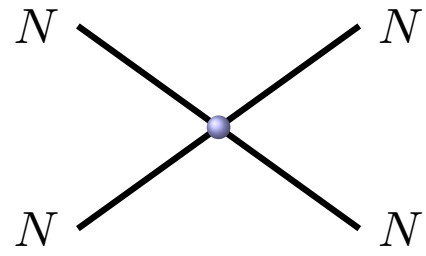
$$1, \qquad \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, \qquad \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2, \qquad (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2).$$

---

These are natural **scalar operator structures**, but are they four independent physical contact interactions?

Pauli principle $\Longrightarrow$ only two independent LO $NN$ contact channels.

**The LO nuclear contact channels:**




A nonderivative contact acts in $\ell = 0$, so the spatial wave function is symmetric:

$$(-1)^{\ell} = +1.$$

The total two-nucleon wave function must be antisymmetric $\Longrightarrow$ the spin-isospin part must be antisymmetric.

Only two possibilities survive:

$$\boxed{S = 0, \quad I = 1} \Longleftrightarrow {}^1S_0 \qquad \boxed{S = 1, \quad I = 0} \Longleftrightarrow {}^3S_1$$

There are consequently only two independent numbers that the LO contact interaction needs to specify:

$$\boxed{C_{^1S_0}} \qquad \boxed{C_{^3S_1}}$$

Everything else is simply a choice of operator basis for representing these two numbers.

**The LO nuclear contact channels:** $\{1, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\}$ basis

At LO the momentum-independent $NN$ contact interaction can be written

$$\boxed{V_{\text{contact}}^{\text{LO}} = C + C_I \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2}$$

$^1S_0 \, (I = 1)$

$\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = +1$

$$\boxed{C_{^1S_0} = C + C_I .}$$

$^3S_1 \, (I = 0)$

$\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = -3$

$$\boxed{C_{^3S_1} = C - 3C_I .}$$

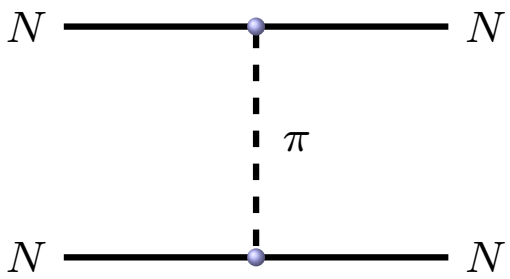
Thus $C$ and $C_I$ are simply another parametrization of the two S-wave couplings.

Conversely,

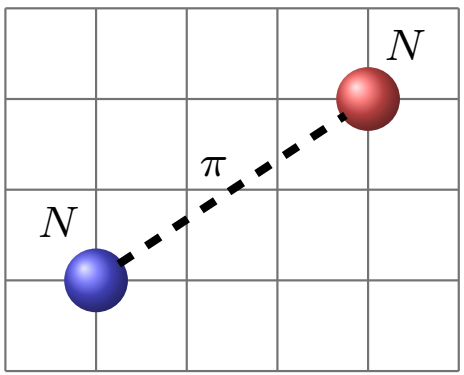
$$C = \frac{3C_{^1S_0} + C_{^3S_1}}{4}, \qquad C_I = \frac{C_{^1S_0} - C_{^3S_1}}{4}.$$

## Long-range physics: one-pion exchange

**Continuum picture**




**On the spatial lattice**




$V_{\rm OPE}$

$$\mathbf{q} = \mathbf{p}' - \mathbf{p}.$$

At LO

$$V_{\rm OPE}(\mathbf{q}) = -\frac{g_A^2}{4f_\pi^2}\,\frac{(\boldsymbol{\sigma}_1\cdot\mathbf{q})(\boldsymbol{\sigma}_2\cdot\mathbf{q})}{\mathbf{q}^2+m_\pi^2}\,(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2).$$

$\dfrac{1}{\mathbf{q}^2+m_\pi^2}$ pion propagator

$(\boldsymbol{\sigma}_1\cdot\mathbf{q})$ and $(\boldsymbol{\sigma}_2\cdot\mathbf{q})$ derivative $\pi N$ couplings

$\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2$ isospin structure

pion exchange $\Longrightarrow$ finite-range, spin- and isospin-dependent force.

# The chiral lattice Hamiltonian

At leading order,

$$\boxed{H_{\text{LO}} = H_{\text{free}}^{\text{lat}} + V_{\text{contact}}^{\text{LO}} + V_{\text{OPE}}^{\text{lat}}.}$$

At higher orders we add

derivative $NN$ contacts,
two-pion exchange,
three-nucleon forces,
Coulomb and isospin-breaking terms, . . .

$$\boxed{\text{operator basis} + \text{regulator} + \text{fitted LECs} = \text{a specified lattice interaction.}}$$