

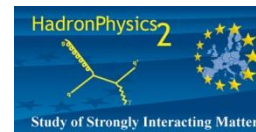
Cold atoms and nuclear physics: Lattice calculations and the question of universality

Dean Lee (NC State U. / U. Bonn)

Evgeny Epelbaum, Hans-Werner Hammer, Hermann Krebs, Ulf-G. Meißner (U. Bonn / FZ Jülich)



Recent Progress in Many-Body Theories
July 27 – 31, 2009
Ohio State University, Columbus, OH



Outline

Lattice calculations...

- Lattice effective field theory for nucleons
- Pion exchange and auxiliary fields
- Phase shifts on the lattice
- Results: Dilute neutron matter

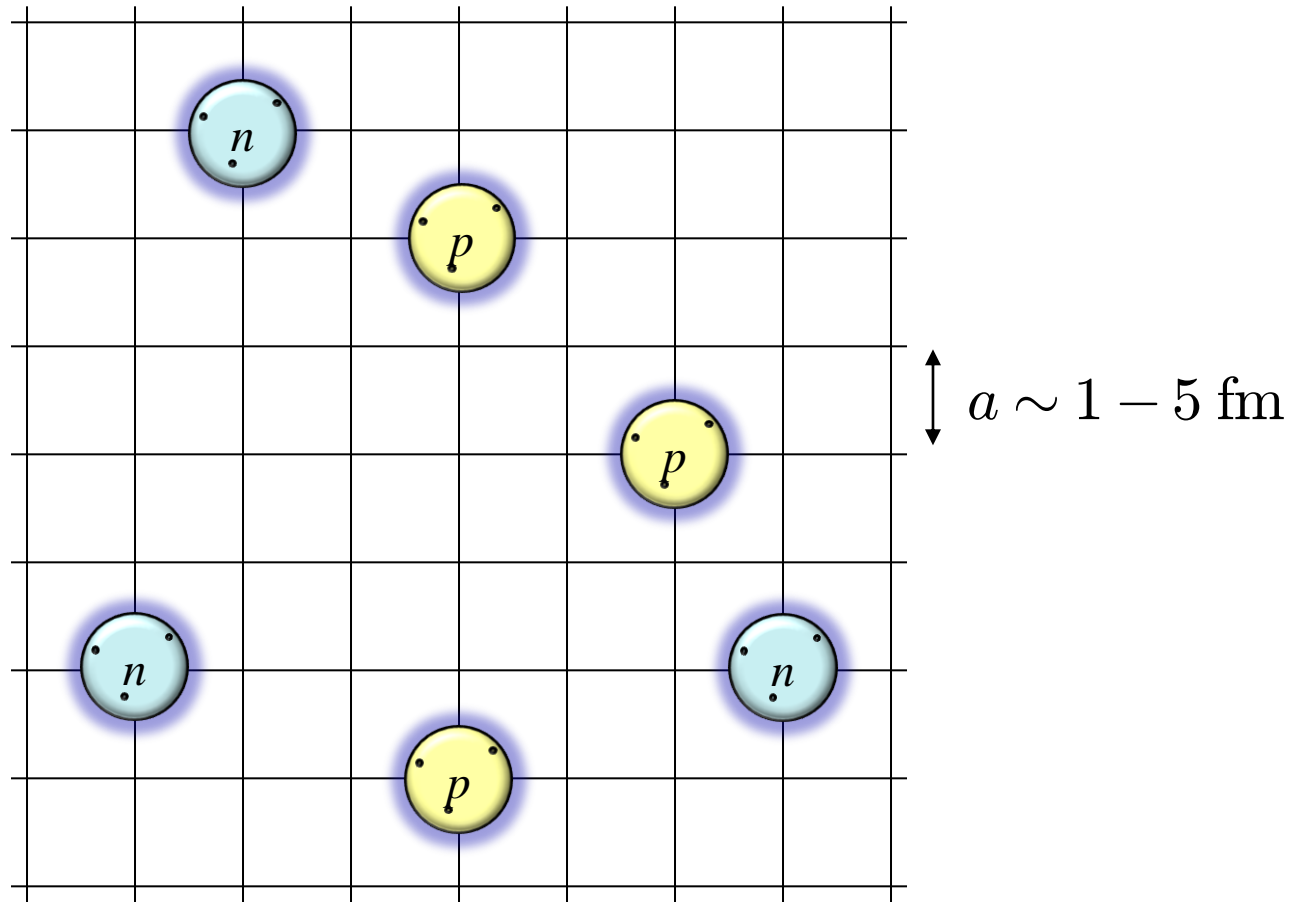
Part I

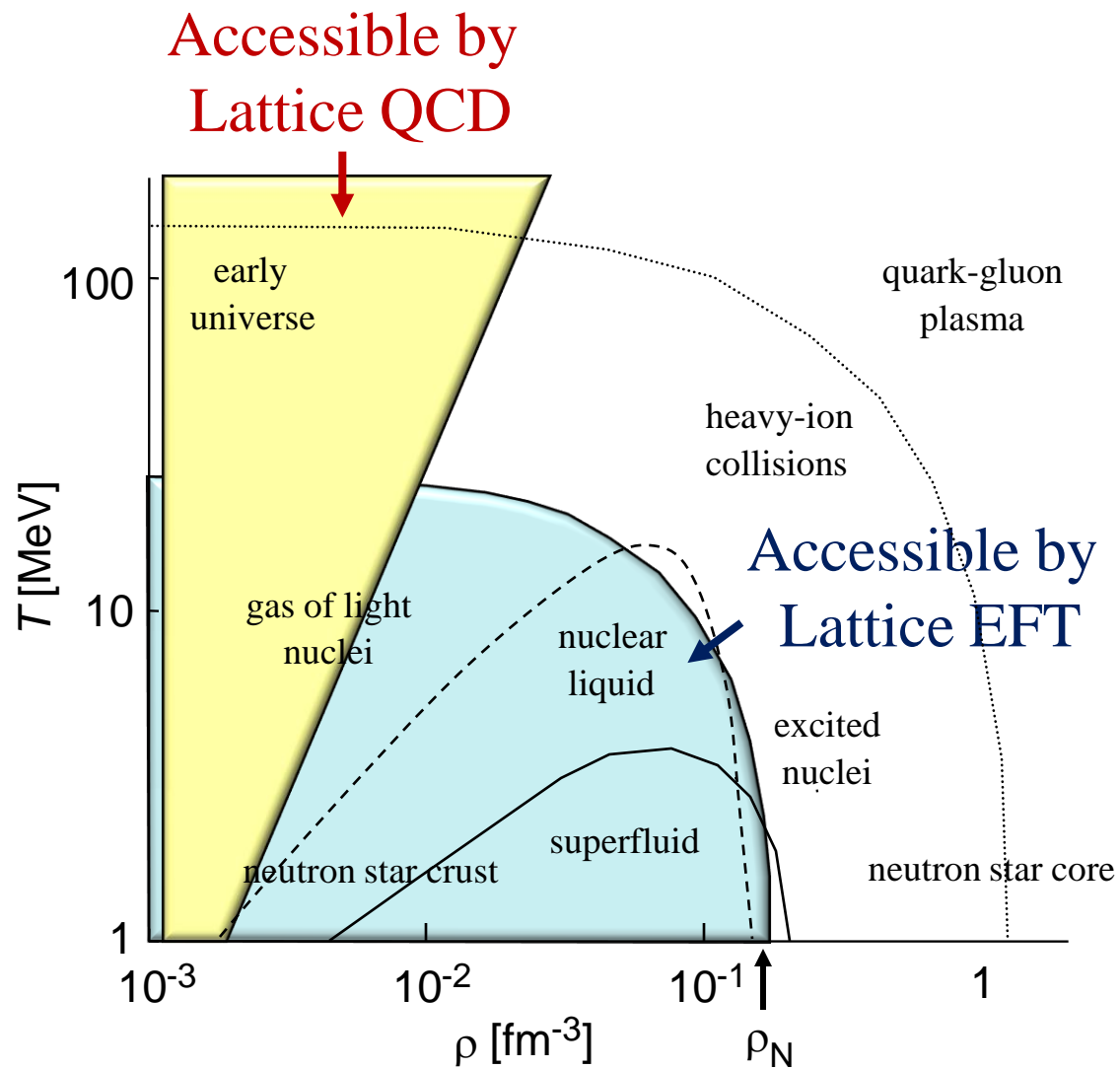
... and the question of universality

- Low-energy universality
- Universality in higher partial waves
- Effective range for general d and L
- Causality and generalized Wigner bounds

Part II

Lattice EFT for nucleons

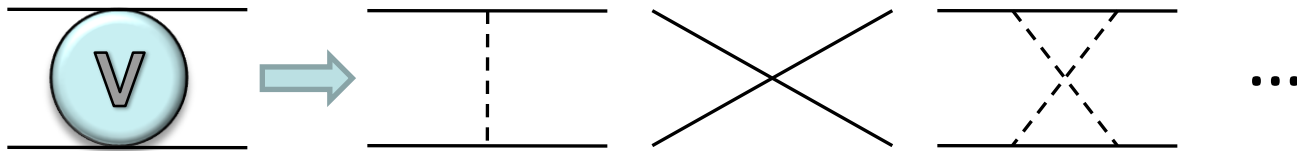




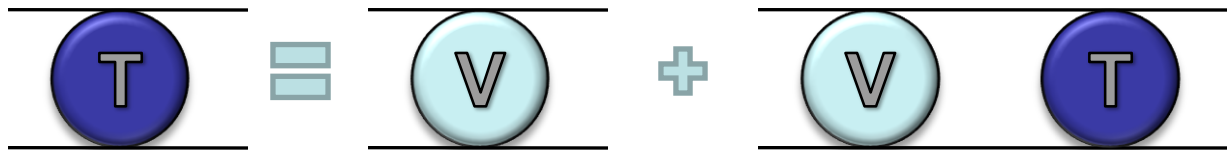
Chiral EFT for low-energy nucleons

Weinberg, PLB 251 (1990) 288; NPB 363 (1991) 3

Construct the effective potential order by order



Solve Lippmann-Schwinger equation non-perturbatively



Nuclear
Scattering Data

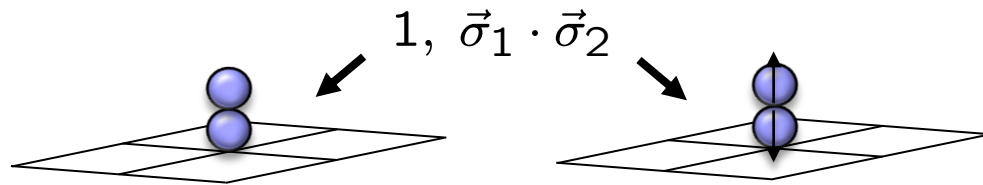
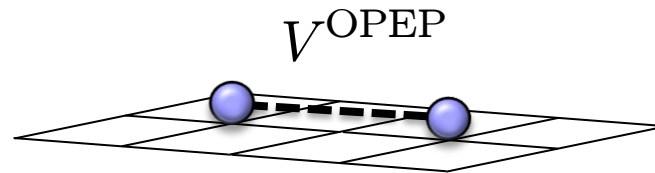
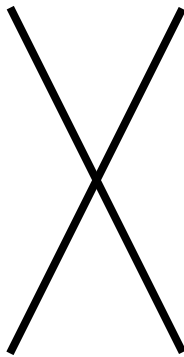
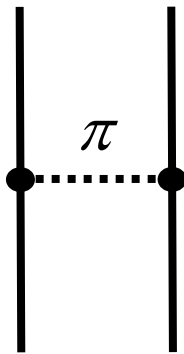


Effective
Field Theory

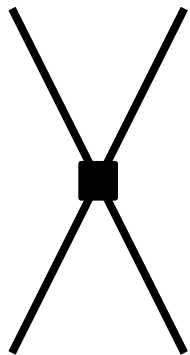
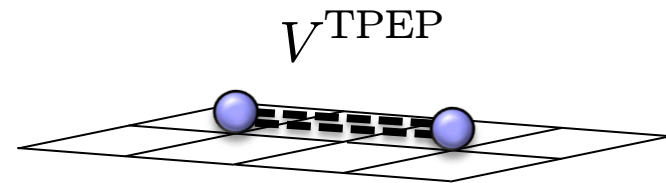
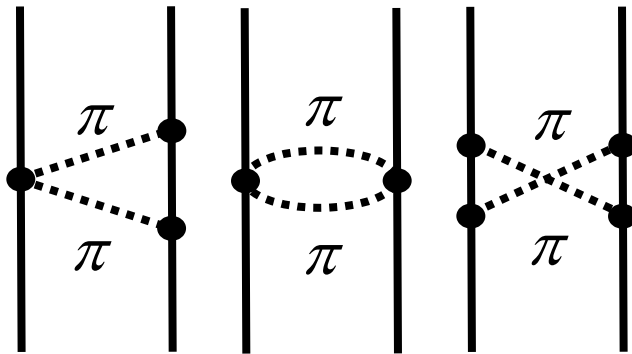
*Ordonez et al. '94; Friar & Coon '94;
Kaiser et al. '97; Epelbaum et al. '98, '03;
Kaiser '99-'01; Higa et al. '03; ...*

	2N forces	3N forces	4N forces
LO $O(Q^0)$			
NLO $O(Q^2)$			
N ² LO $O(Q^3)$			
N ³ LO $O(Q^4)$			
	+ ...	+ ...	+ ...

Leading order on lattice

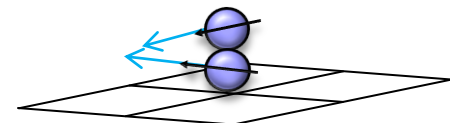
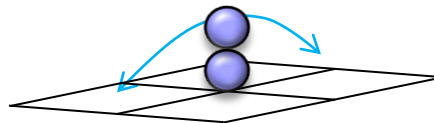


Next-to-leading order on lattice

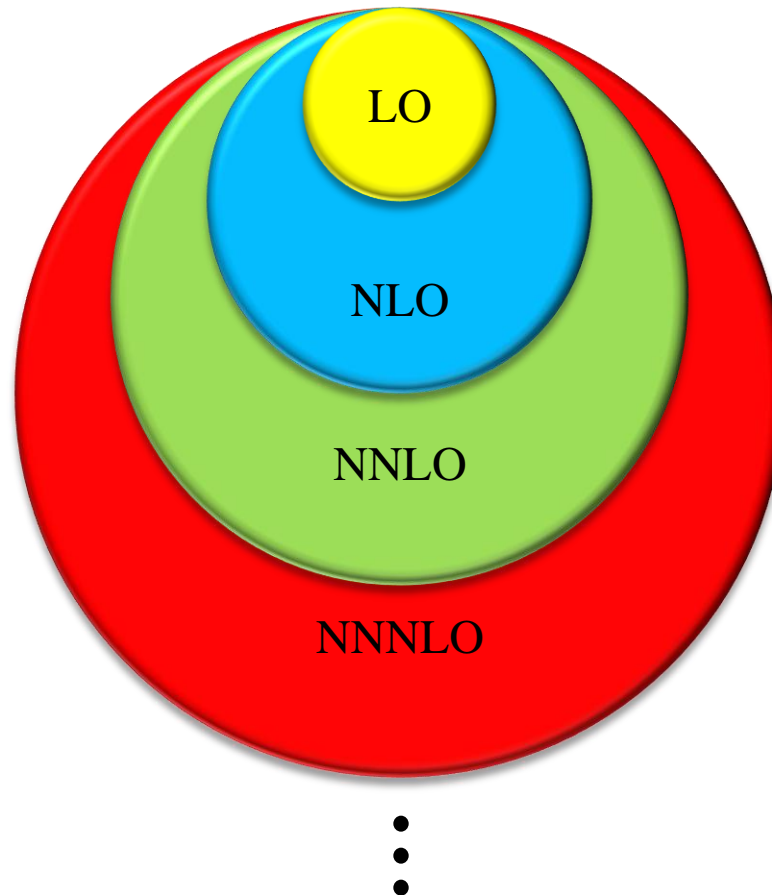


$$\vec{\nabla}_1 \cdot \vec{\nabla}_2$$

$$(\vec{\sigma}_1 \cdot \vec{\nabla}_1) (\vec{\sigma}_2 \cdot \vec{\nabla}_2) \dots$$



Computational strategy

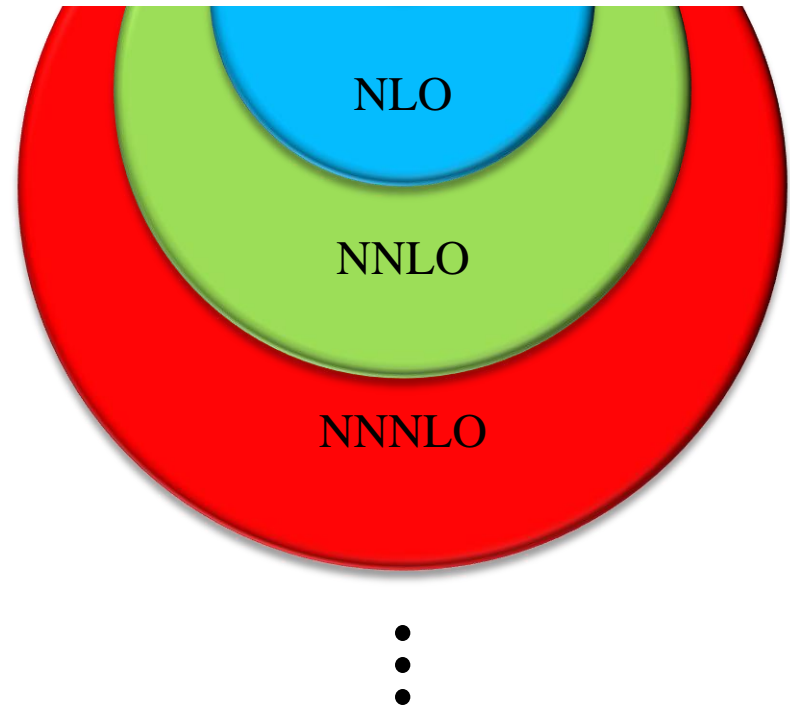


Non-perturbative – Monte Carlo



“Improved LO”

Perturbative corrections



Euclidean-time transfer matrix

Free nucleons:

$$\exp \left[\frac{1}{2m} N^\dagger \vec{\nabla}^2 N \Delta t \right]$$

Free pions:

$$\exp \left[-\frac{1}{2} (\vec{\nabla} \pi)^2 \Delta t - \frac{m_\pi^2}{2} \pi^2 \Delta t \right]$$

Pion-nucleon coupling:

$$\exp \left[-\frac{g_A}{2f_\pi} N^\dagger \boldsymbol{\tau} \vec{\sigma} N \cdot \vec{\nabla} \pi \Delta t \right]$$

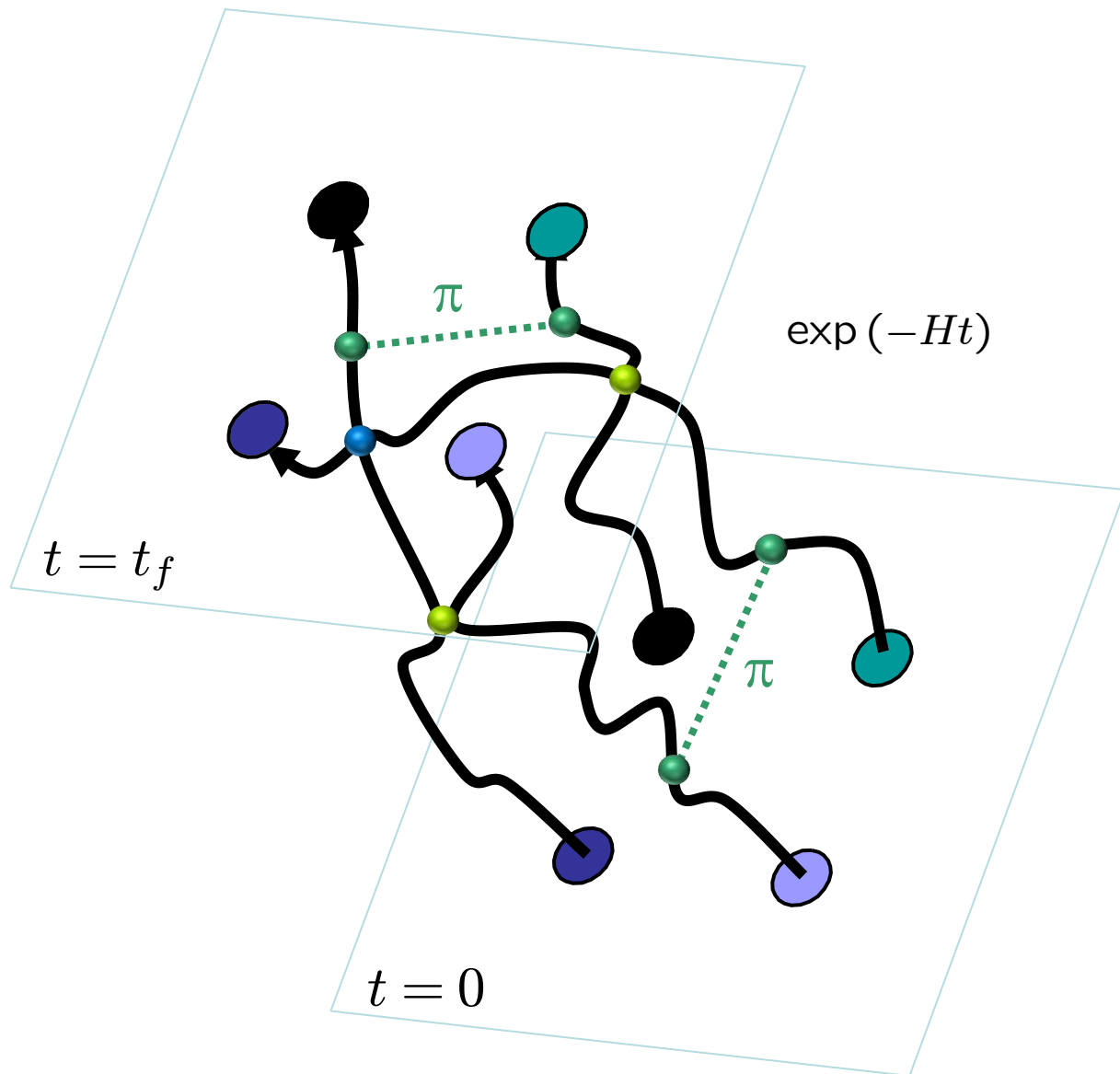
... with auxiliary fields

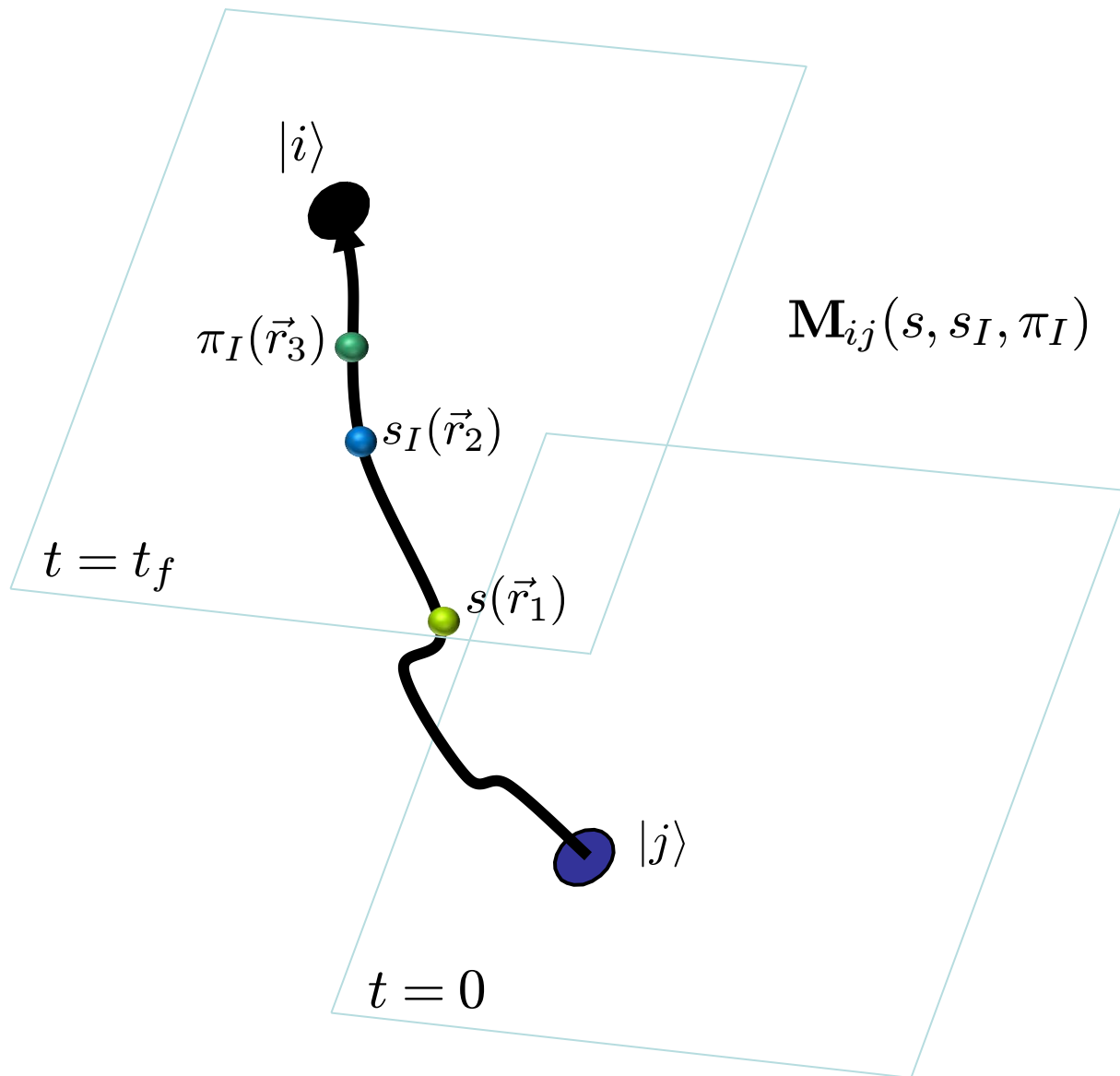
C contact interaction:

$$\begin{aligned} \exp \left[-\frac{1}{2} C N^\dagger N N^\dagger N \Delta t \right] \quad (C < 0) \\ = \frac{1}{\sqrt{2\pi}} \int ds \exp \left[-\frac{1}{2} s^2 + s N^\dagger N \sqrt{-C \Delta t} \right] \end{aligned}$$

C_I contact interaction:

$$\begin{aligned} \exp \left[-\frac{1}{2} C_I N^\dagger \boldsymbol{\tau} N \cdot N^\dagger \boldsymbol{\tau} N \Delta t \right] \quad (C_I > 0) \\ = \frac{1}{\sqrt{2\pi}} \int d\mathbf{s}_I \exp \left[-\frac{1}{2} \mathbf{s}_I \cdot \mathbf{s}_I + i \mathbf{s}_I \cdot N^\dagger \boldsymbol{\tau} N \sqrt{C_I \Delta t} \right] \end{aligned}$$





Auxiliary-field determinantal Monte Carlo

$$\langle \psi_{\text{init}} | M^{(L_t-1)}(s, s_I, \pi_I) \cdots M^{(0)}(s, s_I, \pi_I) | \psi_{\text{init}} \rangle = \det \mathbf{M}(s, s_I, \pi_I)$$

$$\mathbf{M}_{ij}(s, s_I, \pi_I) = \langle \vec{p}_i | M^{(L_t-1)}(s, s_I, \pi_I) \cdots M^{(0)}(s, s_I, \pi_I) | \vec{p}_j \rangle$$

For A nucleons, the matrix is A by A .

For the leading-order calculation, if there is no pion coupling and the quantum state is an isospin singlet then

$$\tau_2 \mathbf{M} \tau_2 = \mathbf{M}^*$$

This shows the determinant is real. Actually can show the determinant is positive semi-definite.

With nonzero pion coupling the determinant is real for a spin-singlet isospin-singlet quantum state

$$\sigma_2 \tau_2 \mathbf{M} \sigma_2 \tau_2 = \mathbf{M}^*$$

but the determinant can be both positive and negative

Some comments about Wigner's approximate SU(4) symmetry...

Theorem: Any fermionic theory with SU(2N) symmetry and two-body potential with negative semi-definite Fourier transform $\tilde{V}(\vec{p}) \leq 0$ obeys SU(2N) convexity bounds (see next slide)

Corollary: It can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;

D.L., PRL 98 (2007) 182501

Schematic of projection calculations

$$\begin{array}{l}
 \boxed{} = M_{\text{LO}} \quad \boxed{} = M_{SU(4)} \quad \boxed{} = O_{\text{observable}} \\
 \boxed{} = M_{\text{NLO}} \quad \boxed{} = M_{\text{NNLO}}
 \end{array}$$

Hybrid Monte Carlo sampling

$$Z_{n_t, \text{LO}} = \langle \psi_{\text{init}} | \boxed{} \boxed{} \boxed{} | \psi_{\text{init}} \rangle$$

$$Z_{n_t, \text{LO}}^{\langle O \rangle} = \langle \psi_{\text{init}} | \boxed{} \boxed{} \boxed{} \boxed{} \boxed{} | \psi_{\text{init}} \rangle$$

$$e^{-E_{0, \text{LO}} a_t} = \lim_{n_t \rightarrow \infty} Z_{n_t+1, \text{LO}} / Z_{n_t, \text{LO}}$$

$$\langle O \rangle_{0, \text{LO}} = \lim_{n_t \rightarrow \infty} Z_{n_t, \text{LO}}^{\langle O \rangle} / Z_{n_t, \text{LO}}$$

$$Z_{n_t, \text{NLO}} = \langle \psi_{\text{init}} | \left[\text{black bars} \right] \left[\text{blue bars} \right] \left[\text{black bars} \right] | \psi_{\text{init}} \rangle$$



$$Z_{n_t, \text{NLO}}^{\langle O \rangle} = \langle \psi_{\text{init}} | \left[\text{black bars} \right] \left[\text{blue bars} \right] \left[\text{yellow bar} \right] \left[\text{blue bars} \right] \left[\text{black bars} \right] | \psi_{\text{init}} \rangle$$



$$\langle O \rangle_{0, \text{NLO}} = \lim_{n_t \rightarrow \infty} Z_{n_t, \text{NLO}}^{\langle O \rangle} / Z_{n_t, \text{NLO}}$$

LO₁: Pure contact interactions

$$\mathcal{A}(V_{\text{LO}_1}) = C + C_I \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \mathcal{A}(V^{\text{OPEP}})$$

LO₂: Gaussian smearing

$$\mathcal{A}(V_{\text{LO}_2}) = C f(\vec{q}^2) + C_I f(\vec{q}^2) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \mathcal{A}(V^{\text{OPEP}})$$

LO₃: Gaussian smearing only in even partial waves

$$\begin{aligned} \mathcal{A}(V_{\text{LO}_3}) = & C_{1S0} f(\vec{q}^2) \left(\frac{1}{4} - \frac{1}{4} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \left(\frac{3}{4} + \frac{1}{4} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \\ & + C_{3S1} f(\vec{q}^2) \left(\frac{3}{4} + \frac{1}{4} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \left(\frac{1}{4} - \frac{1}{4} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \\ & + \mathcal{A}(V^{\text{OPEP}}) \end{aligned}$$

Physical
scattering data

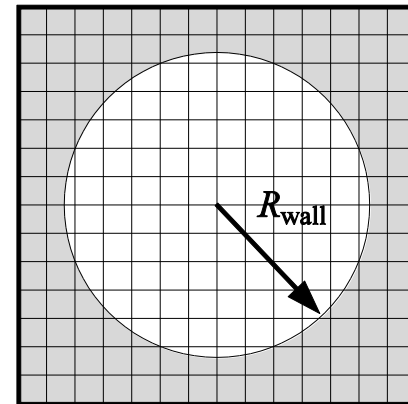


Unknown operator
coefficients

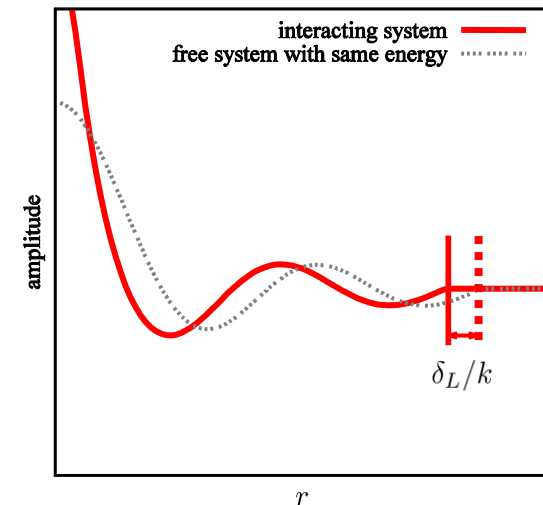
Spherical wall method

*Borasoy, Epelbaum, Krebs, D.L., Meißner,
EPJA 34 (2007) 185*

Spherical wall imposed in the center of
mass frame



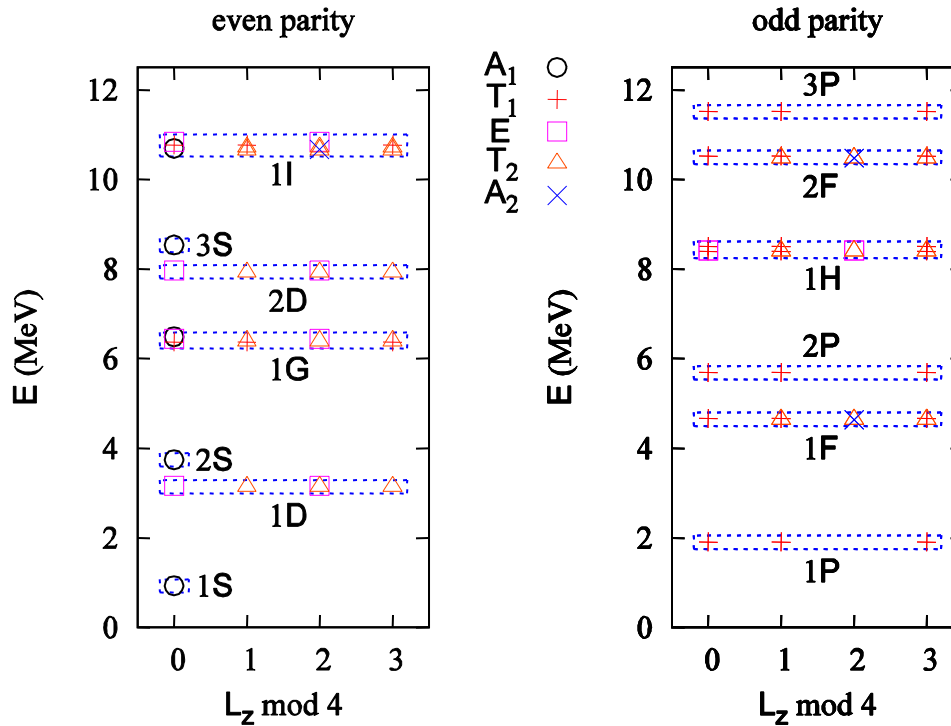
Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0, 1, 3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0, 2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1, 2, 3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



Energy levels with hard spherical wall

$$R_{\text{wall}} = 10a$$

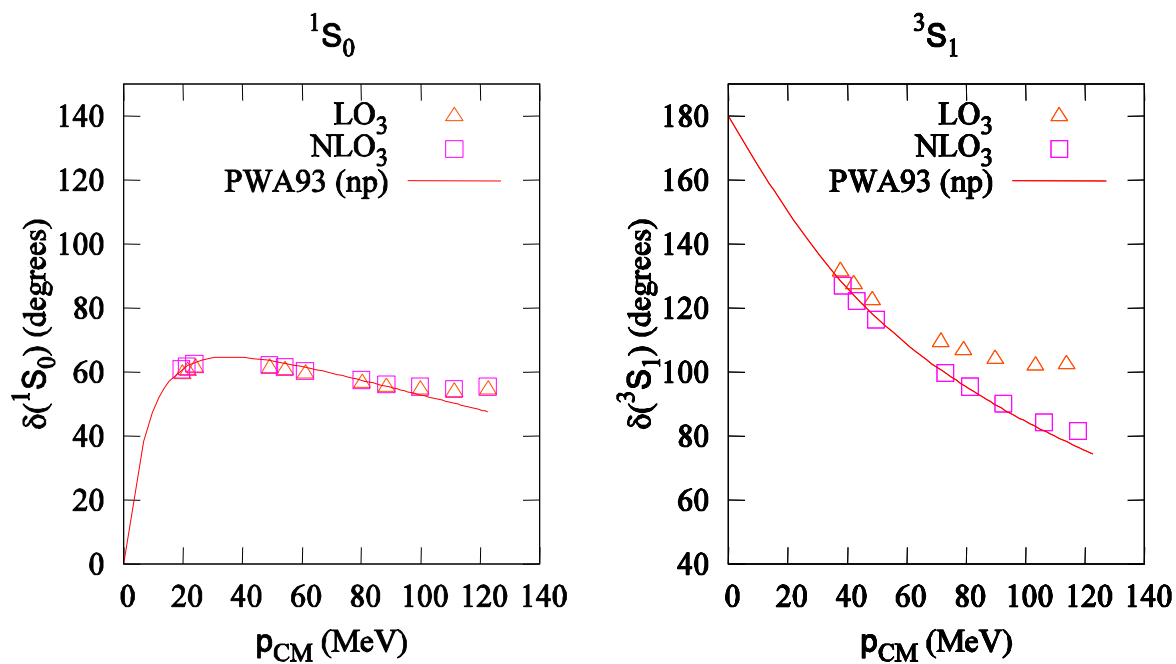
$$a = 1.97 \text{ fm}$$



Energy shift from free-particle values gives the phase shift

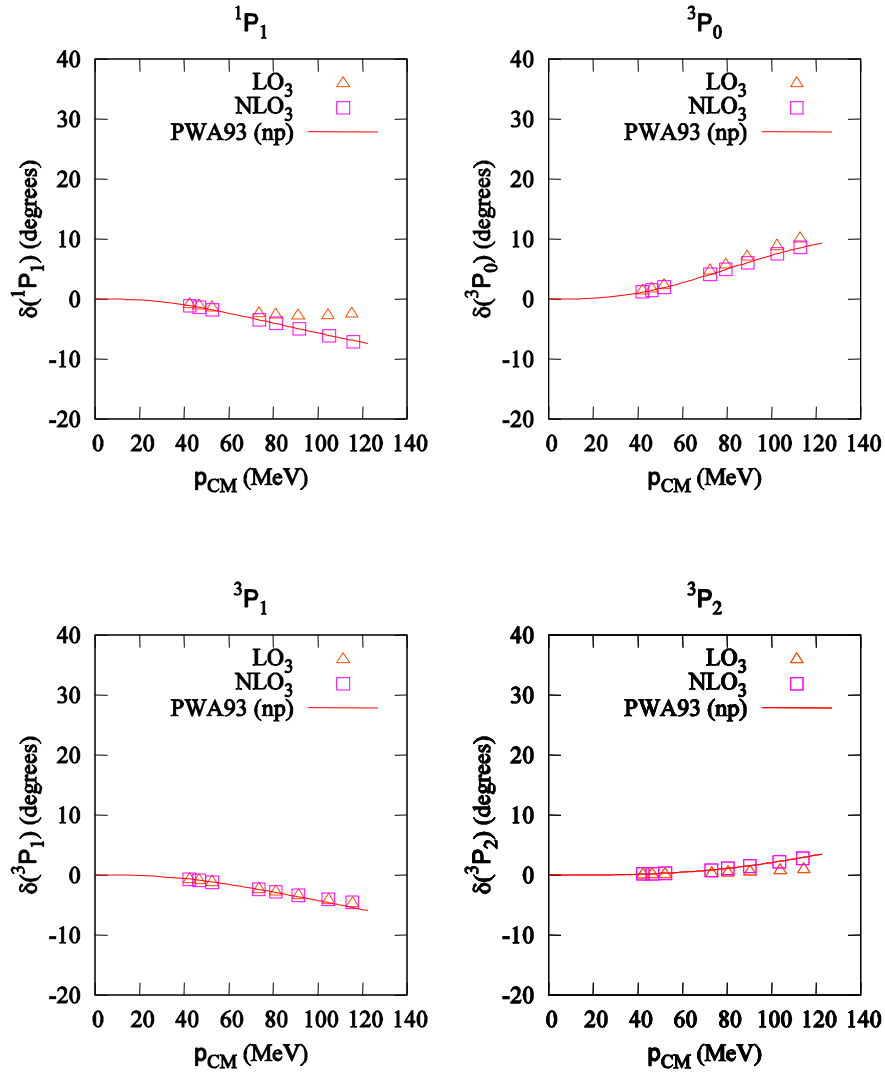
LO₃: S waves

$a = 1.97$ fm

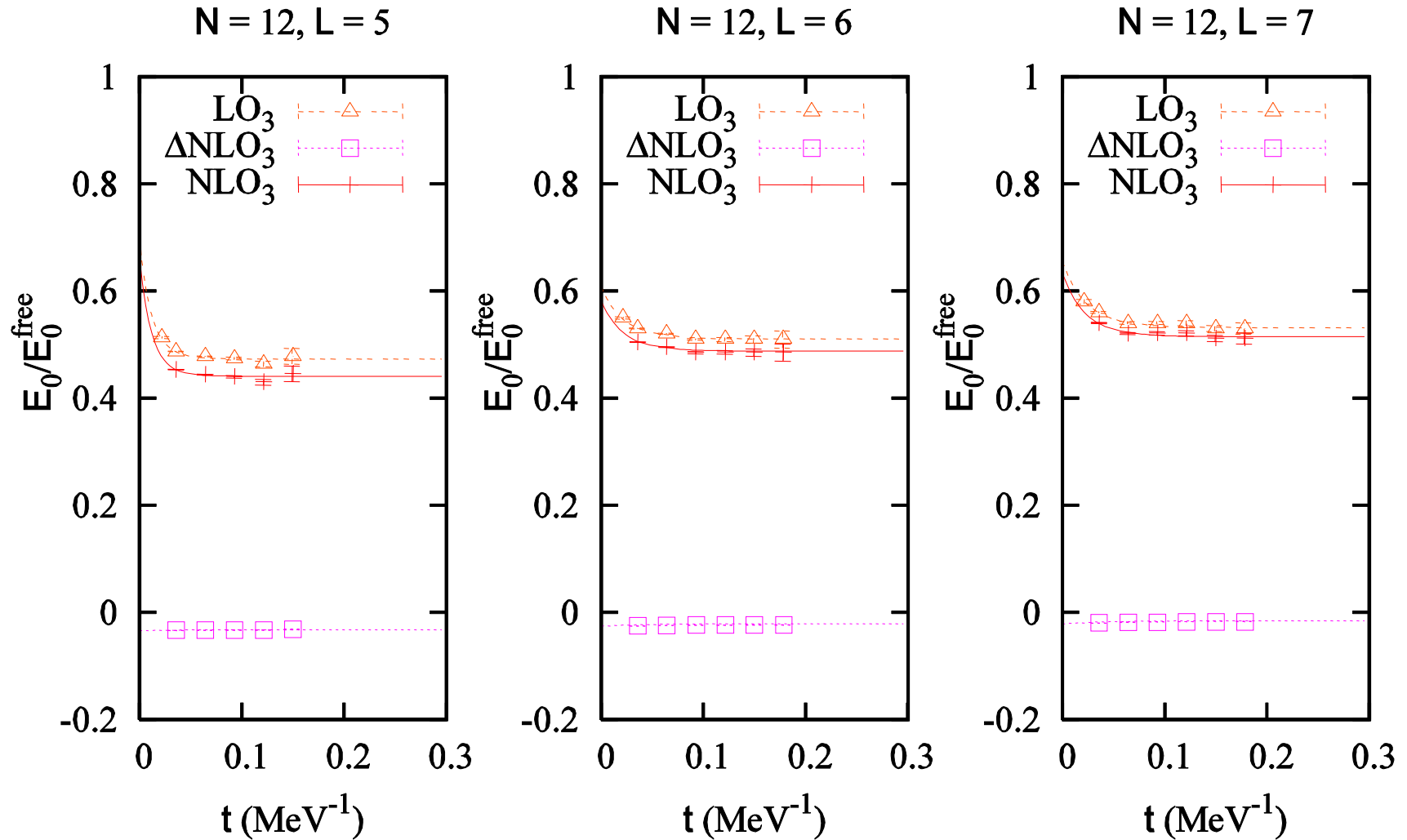


LO₃: P waves

$a = 1.97$ fm

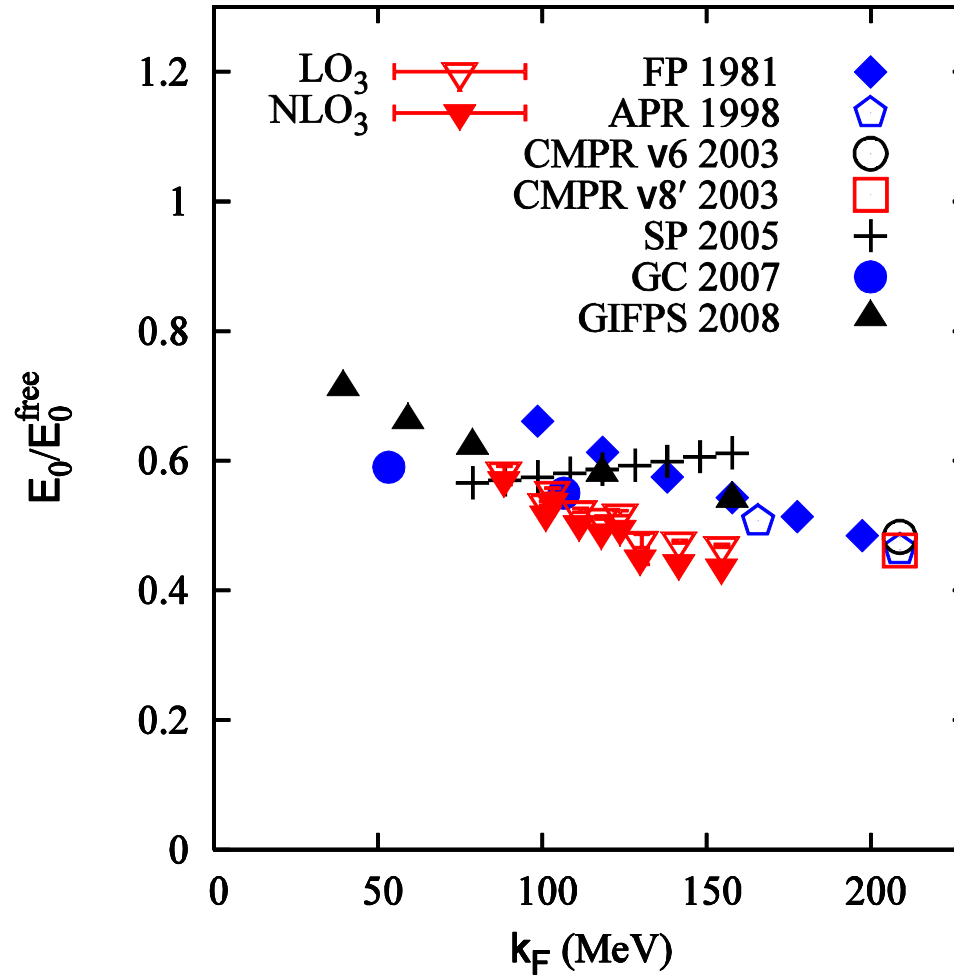


Results: Dilute neutron matter at NLO



$N = 8, 12, 16$ neutrons at $L^3 = 4^3, 5^3, 6^3, 7^3$

$a = 1.97$ fm



Epelbaum, Krebs, D.L, Meißner, 0812.3653 [nucl-th], EPJA 40 (2009) 199

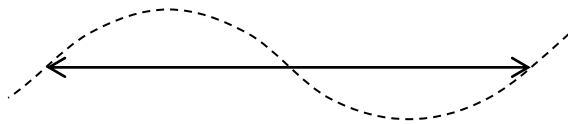
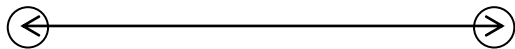
Low-energy universality

Large disparity in length scales

$$d \sim k_F^{-1} \gg R$$
$$\lambda_T \gg R$$

average separation

d



λ_T

thermal wavelength



R

range of interaction

Partial wave decomposition of the scattering amplitude

$$\psi(\vec{r}) \xrightarrow{r \rightarrow \infty} e^{i\vec{p} \cdot \vec{r}} + f(\vec{p}', \vec{p}) \frac{e^{ipr}}{r}$$

$$f(\vec{p}', \vec{p}) = \sum_{L=0}^{\infty} f_L(p) P_L(\cos \theta)$$

$$f_L(p) = \frac{-i}{2p} \left[e^{2i\delta_L(p)} - 1 \right] = \frac{1}{p [\cot \delta_L(p) - i]}$$

S-wave effective range expansion

$$f_0(p) = \frac{1}{p \cot \delta_0(p) - ip}$$

$$p \cot \delta_0(p) = -a_0^{-1} + \frac{1}{2} r_0 p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_0^{(n)} p^{2n+4}$$

Dimensional analysis: Length dimensions of coefficients

$$a_0^{-1} = [\ell]^{-1}, r_0 = [\ell], \mathcal{P}_0^{(n)} = [\ell]^{2n+3}$$

A parameter is of “natural size” if it is roughly the same order of magnitude as the interaction range raised to the corresponding length dimension.

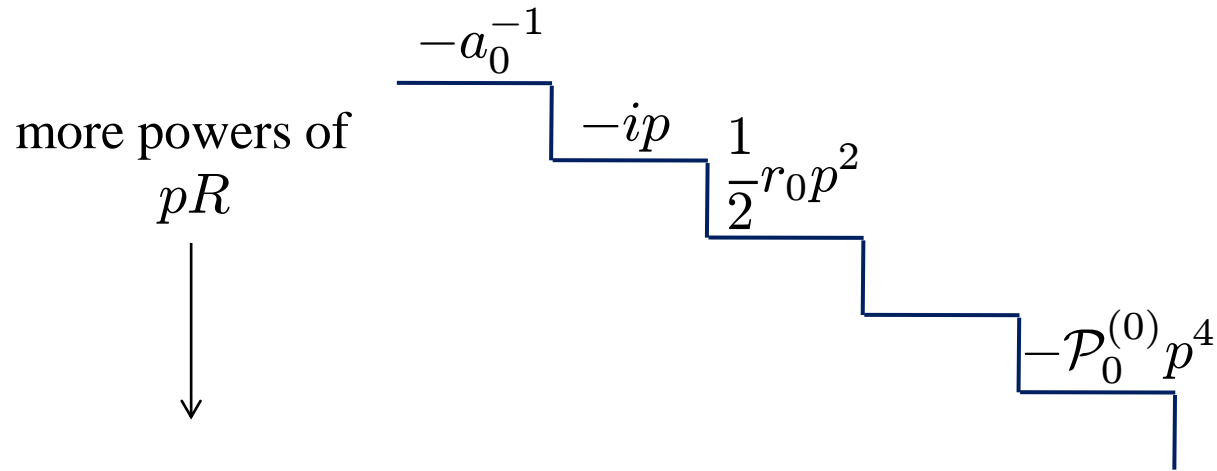
For the S-wave case,

$$a_0^{-1} \sim R^{-1}, r_0 \sim R, \mathcal{P}_0^{(n)} \sim R^{2n+3}$$

For the remainder of this talk we look for low-energy universality and consider momenta small enough such that

$$pR \ll 1$$

Assuming parameters of natural size, the terms contributing to the amplitude have a simple hierarchy



$$f_0(p) = \frac{1}{p \cot \delta_0(p) - ip}$$

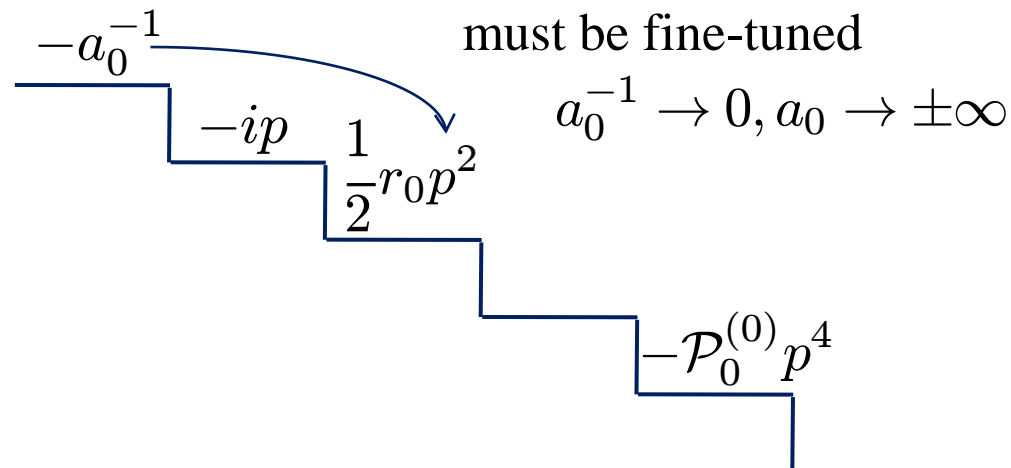
$$p \cot \delta_0(p) = -a_0^{-1} + \frac{1}{2} r_0 p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_0^{(n)} p^{2n+4}$$

Unitarity limit

At low momenta the unitarity limit is reached when the real part of the denominator in the scattering amplitude can be neglected

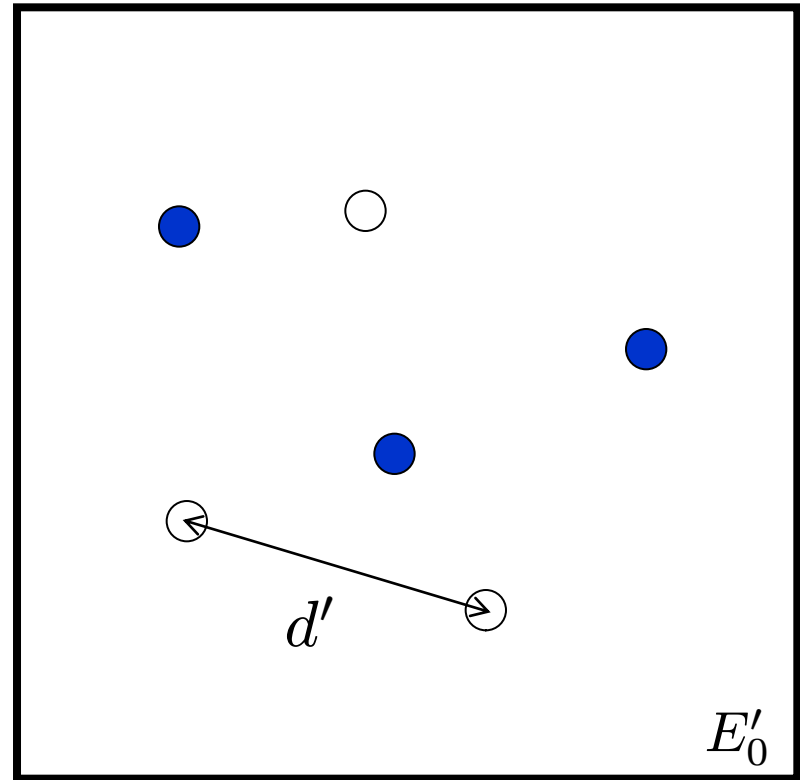
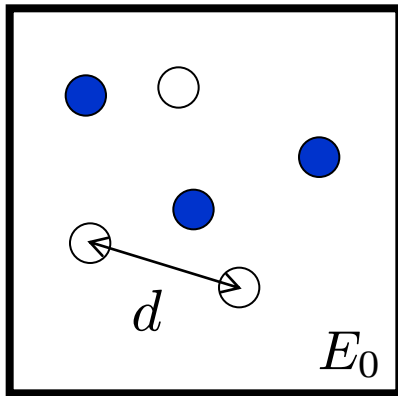
$$p \cot \delta_0(p) = \cancel{-a_0^{-1}} + \cancel{\frac{1}{2}r_0}p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \cancel{\mathcal{P}_0^{(n)}} p^{2n+4}$$

$$f_0(p) = \frac{1}{\cancel{p \cot \delta_0(p)} - ip}$$



Scale-invariant physics

$$f_0(p) \approx \frac{i}{p}$$



$$E_0 d^2 = E'_0 d'^2$$

Dilute neutrons and the unitarity limit

Neutron matter close to unitarity limit for $k_F \sim 80$ MeV

$$\frac{E_0}{A} = \xi \cdot \frac{E_0^{\text{free}}}{A} = \xi \cdot \frac{3}{5} E_F$$

ξ is a dimensionless number

$$\frac{E_0}{E_0^{\text{free}}} = \underbrace{\xi - \frac{\xi_1}{k_F a_0}}_{f(k_F a_0)} + ck_F r_0 + \dots$$

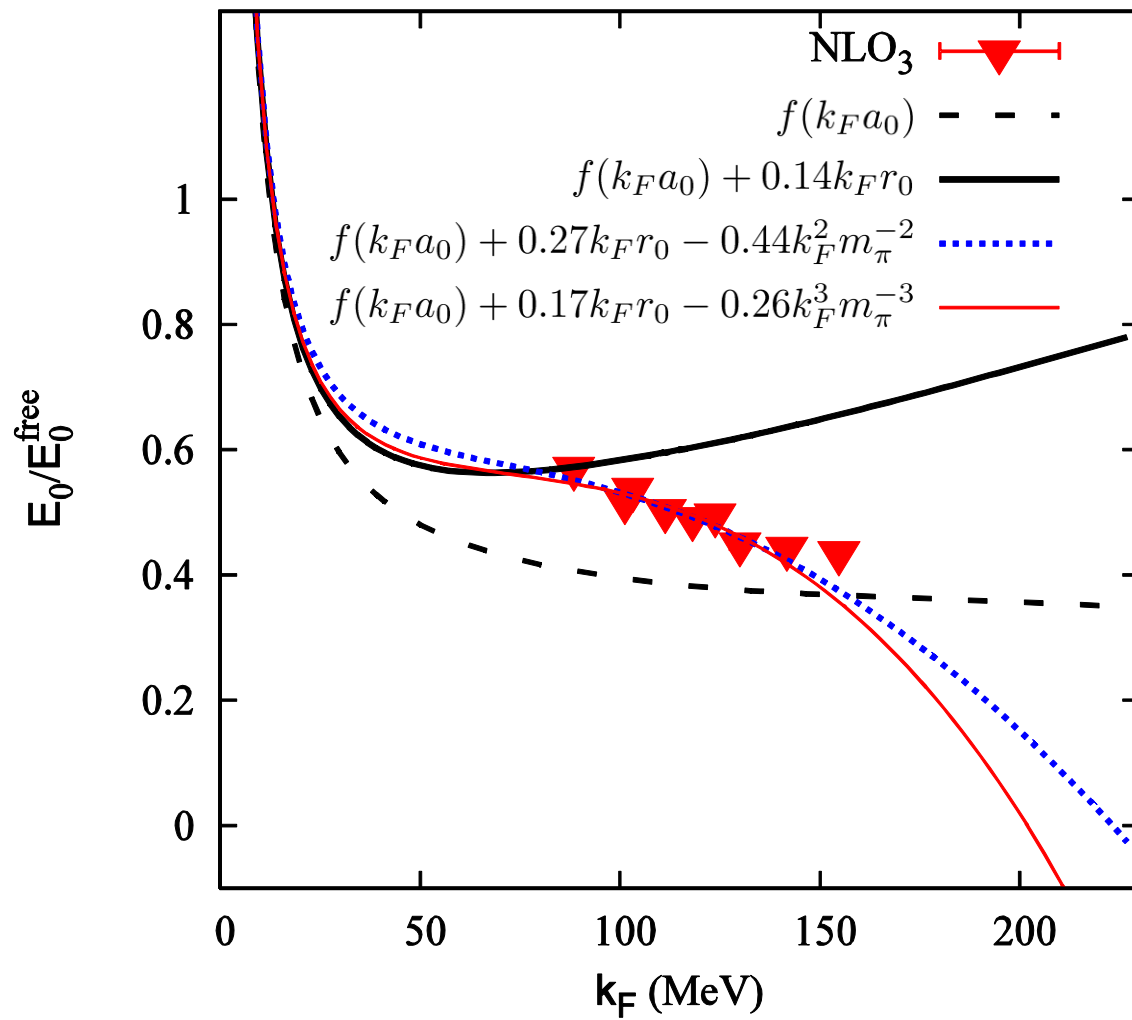
$$\xi = 0.31(1)$$

$$\xi_1 \approx 0.8$$

D.L., EPJA 35 (2009) 171;

PRC 78 (2008) 024001;

PRB 75 (2007) 134502



Universality in higher partial waves

Cold atoms: P-wave Feshbach experiments

Regal, PRL 90 (2003) 053201, ...

Nuclear physics: P-wave alpha-neutron interactions in halo nuclei

For higher partial waves the effective range expansion is

$$f_L(p) = \frac{-i}{2p} \left[e^{2i\delta_L(p)} - 1 \right] = \frac{1}{p [\cot \delta_L(p) - i]}$$
$$= \frac{p^{2L}}{p^{2L+1} \cot \delta_L(p) - ip^{2L+1}}$$

$$p^{2L+1} \cot \delta_L(p) = -a_L^{-1} + \frac{1}{2} r_L p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_L^{(n)} p^{2n+4}$$

For P-waves we have*

$$f_1(p) = \frac{p^2}{p^3 \cot \delta_1(p) - ip^3}$$
$$p^3 \cot \delta_1(p) = -a_1^{-1} + \frac{1}{2}r_1 p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_1^{(n)} p^{2n+4}$$

Dimensional analysis: Length dimensions of coefficients

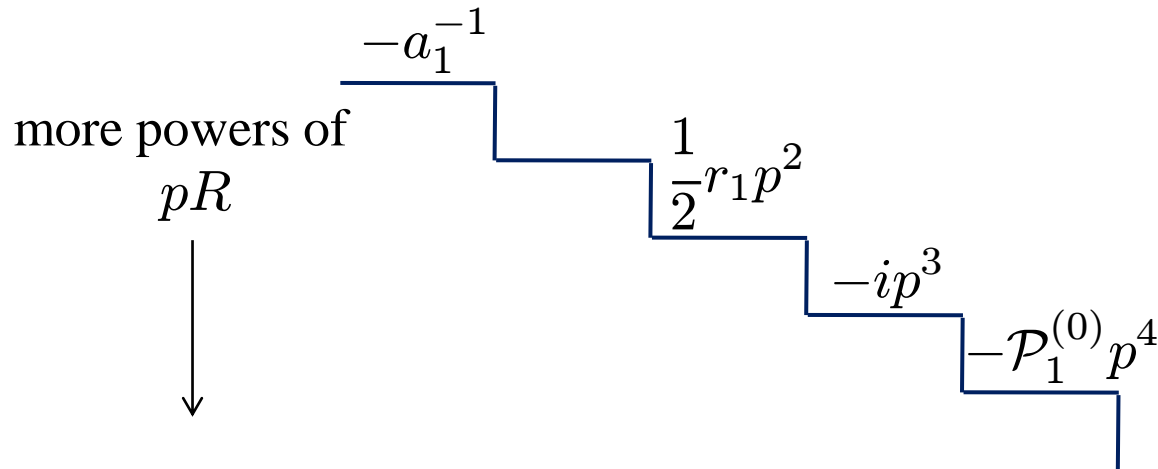
$$a_1^{-1} = [\ell]^{-3}, \quad r_1 = [\ell]^{-1}, \quad \mathcal{P}_1^{(n)} = [\ell]^{2n+1}$$

We again start with the case where the coefficients are of natural size

*caveat for van der Waals interactions in alkali atoms
Gao, PRA (1998) 1728

$$a_1^{-1} \sim R^{-3}, \quad r_1 \sim R^{-1}, \quad \mathcal{P}_1^{(n)} \sim R^{2n+1}$$

For natural size parameter, the P-wave low-momentum hierarchy is



$$f_1(p) = \frac{p^2}{p^3 \cot \delta_1(p) - ip^3}$$

$$p^3 \cot \delta_1(p) = -a_1^{-1} + \frac{1}{2}r_1 p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_1^{(n)} p^{2n+4}$$

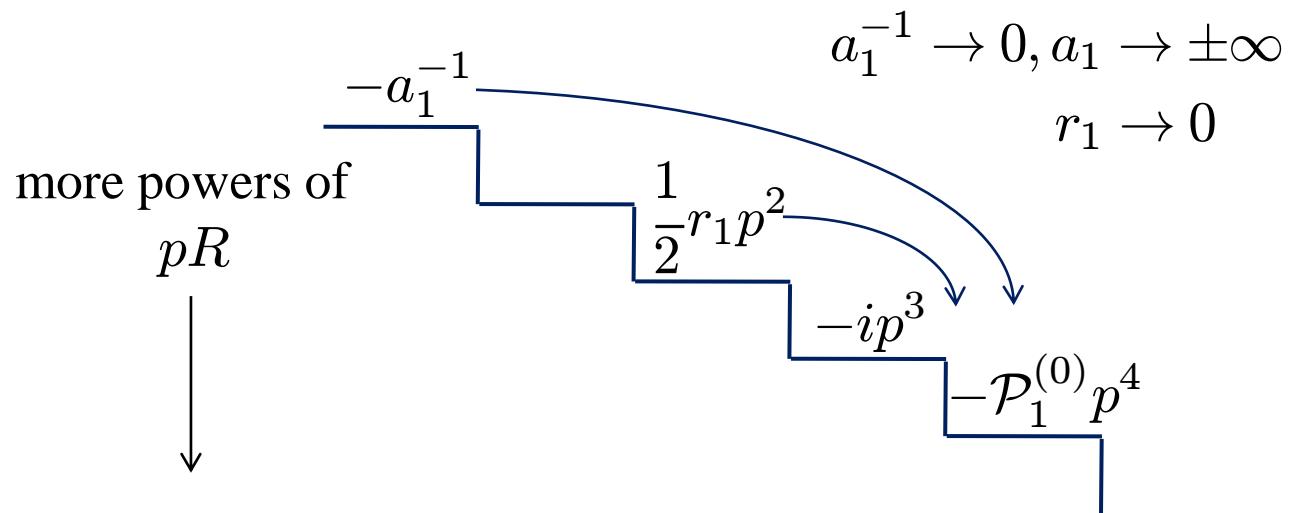
Unitarity limit for P-waves?

As in the S-wave case we look for an analogy to the unitarity limit where the real part of the denominator in the scattering amplitude can be neglected

$$p^3 \cot \delta_1(p) = \cancel{a_1}^{-1} + \cancel{\frac{1}{2}r_1} p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \cancel{\mathcal{P}_1^{(n)}} p^{2n+4}$$
$$f_1(p) = \frac{p^2}{\cancel{p^3 \cot \delta_1(p)} - ip^3}$$

This is equivalent to fine-tuning all coefficients in the effective range expansion with negative length dimensions

A first guess might be...



Effective range integral formula

Generalization of result of Bethe (1949)

$$r_L = -\frac{\Gamma(L - \frac{1}{2})\Gamma(L + \frac{1}{2})2^{2L}}{\pi R^{2L-1}} - \frac{2}{2L+1} \frac{R^2}{a_L} + \frac{\pi}{\Gamma(L + \frac{3}{2})\Gamma(L + \frac{5}{2})2^{2L+2}} \frac{R^{2L+3}}{a_L^2} - 2 \lim_{p \rightarrow 0} p^{2L} \int_0^R \left[u_L^{(p)}(r) \right]^2 dr$$

Hammer, D.L., 0907.1763 [nucl-th]

The wavefunction normalization is chosen so that for $r \geq R$

$$u_L^{(p)}(r) = \frac{pr \cos \delta_L(p) \cdot j_L(pr) - pr \sin \delta_L(p) \cdot y_L(pr)}{\sin \delta_L(p)}$$

Since the integral term is less or equal to zero,

$$r_L \leq -\frac{\Gamma(L - \frac{1}{2})\Gamma(L + \frac{1}{2})2^{2L}}{\pi R^{2L-1}} - \frac{2}{2L + 1} \frac{R^2}{a_L} + \frac{\pi}{\Gamma(L + \frac{3}{2})\Gamma(L + \frac{5}{2})2^{2L+2}} \frac{R^{2L+3}}{a_L^2}$$

If we fine-tune a_L^{-1} to be unnaturally small

$$|a_L^{-1}| \ll R^{-2L-1}$$

then

$$r_L \leq -\frac{\Gamma(L - \frac{1}{2})\Gamma(L + \frac{1}{2})2^{2L}}{\pi R^{2L-1}}$$



S-wave case was derived by Phillips and Cohen

$$r_0 \leq 2R$$

Cohen, Phillips, PLB390 (1997) 7

The upper bound for $L \geq 1$ is much more severe. Cannot fine-tune to zero.

negative coefficient for $L \geq 1$


$$r_L \leq - \frac{\Gamma(L - \frac{1}{2})\Gamma(L + \frac{1}{2})2^{2L}}{\pi R^{2L-1}}$$


negative power of R for $L \geq 1$

Hammer, D.L., 0907.1763 [nucl-th]

For $L \geq 1$, we conclude that r_L must be negative and natural size

This upper bound is related to the causality bound derived by Wigner (1954). Here is the heuristic argument...

Consider a wavepacket that is sharply peaked in momentum space

$$f(r) = \frac{1}{\sqrt{2\pi}} \int dp e^{ipr} \tilde{f}(p)$$
$$\tilde{f}(p) \approx c\delta(p - \bar{p})$$

Consider what happens when multiplying by a momentum-dependent phase shift

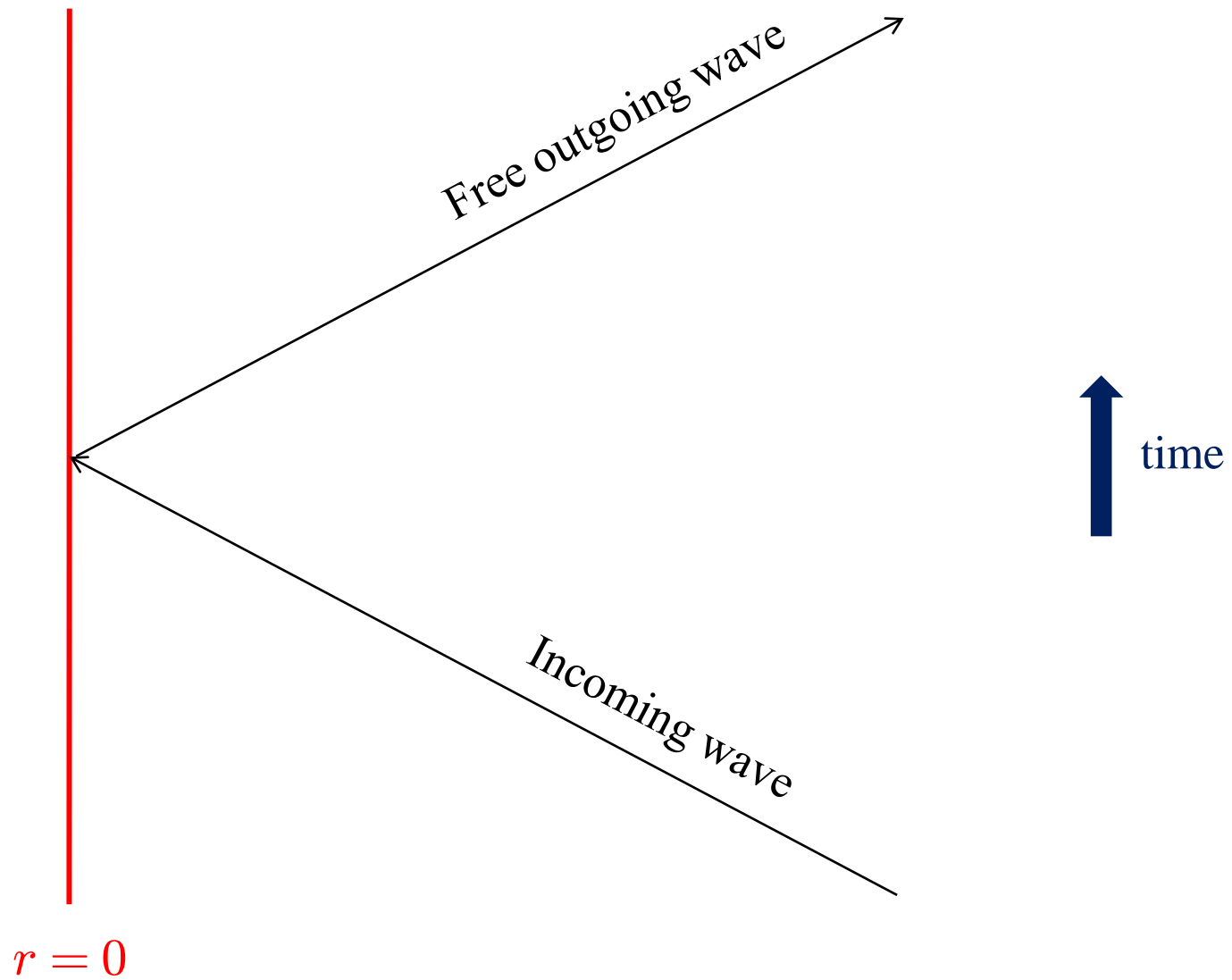
$$\tilde{g}(p) = e^{2i\delta(p)} \tilde{f}(p)$$

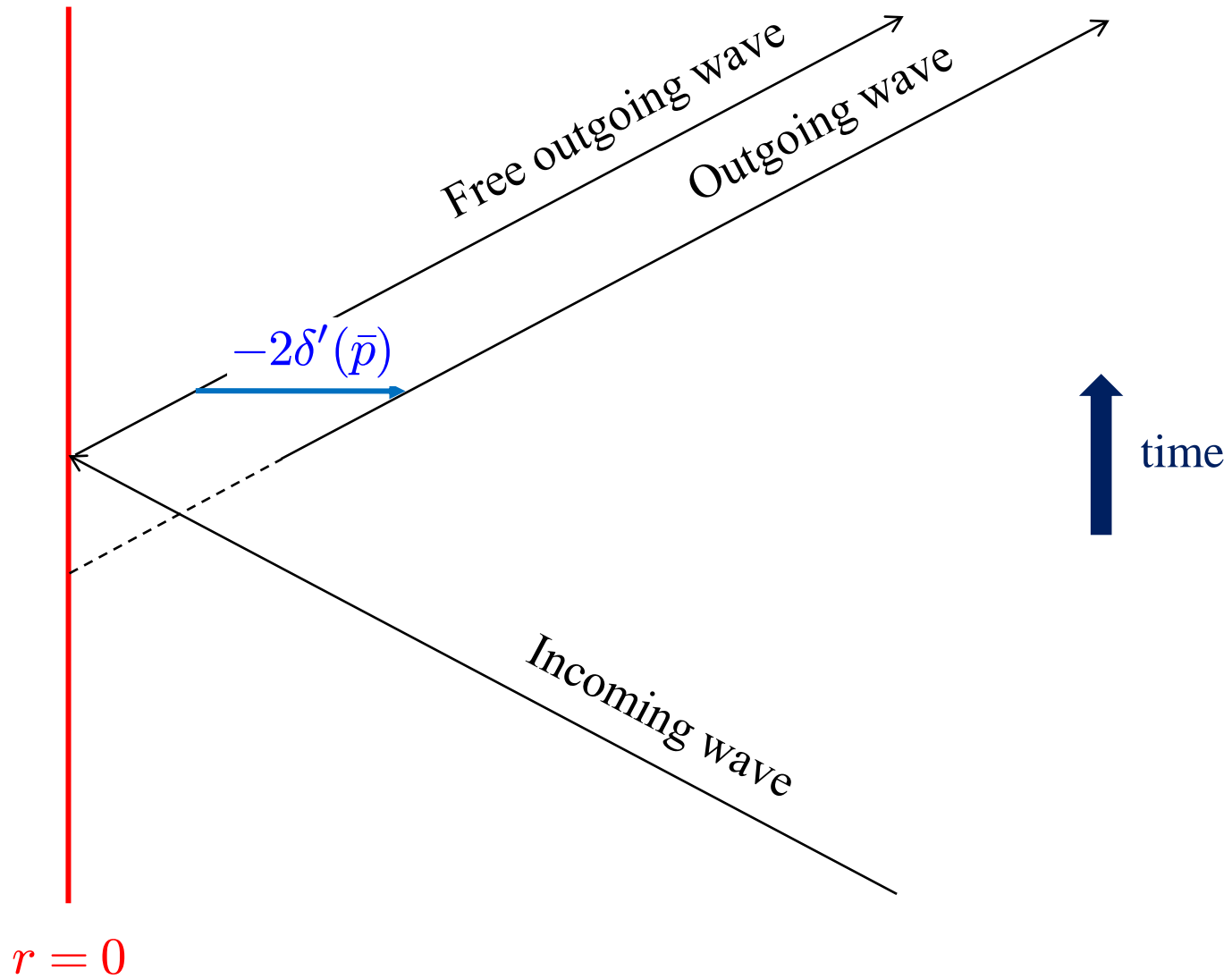
We perform the inverse Fourier transform

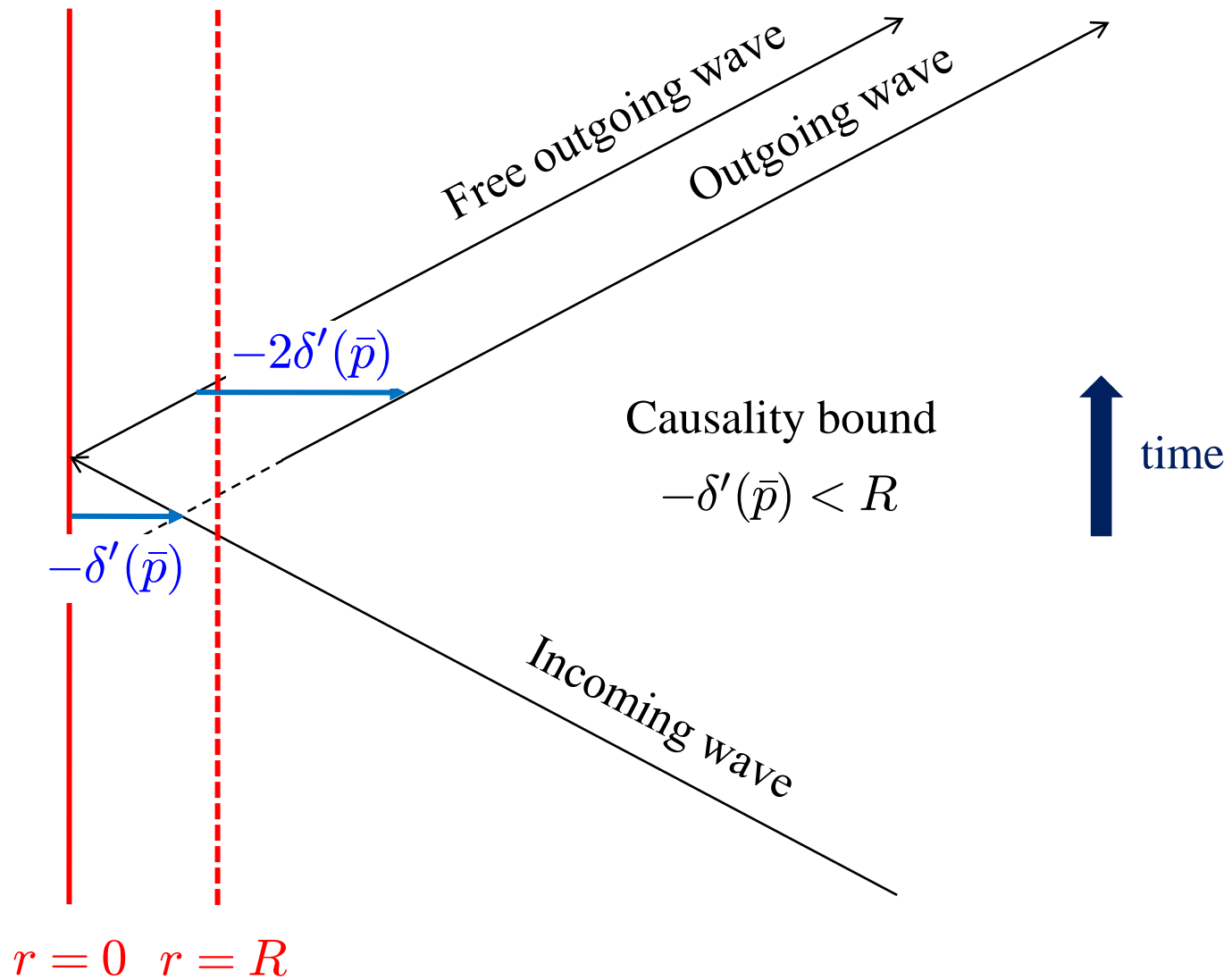
$$\begin{aligned} g(r) &= \frac{1}{\sqrt{2\pi}} \int dp e^{ipr} \tilde{g}(p) \\ &\approx e^{2i\delta(\bar{p})} e^{-2i\delta'(\bar{p})\bar{p}} f[r + 2\delta'(\bar{p})] \end{aligned}$$

There is an overall phase multiplication and the packet is translated backward in space an amount proportional to the derivative of the phase shift with respect to momentum.

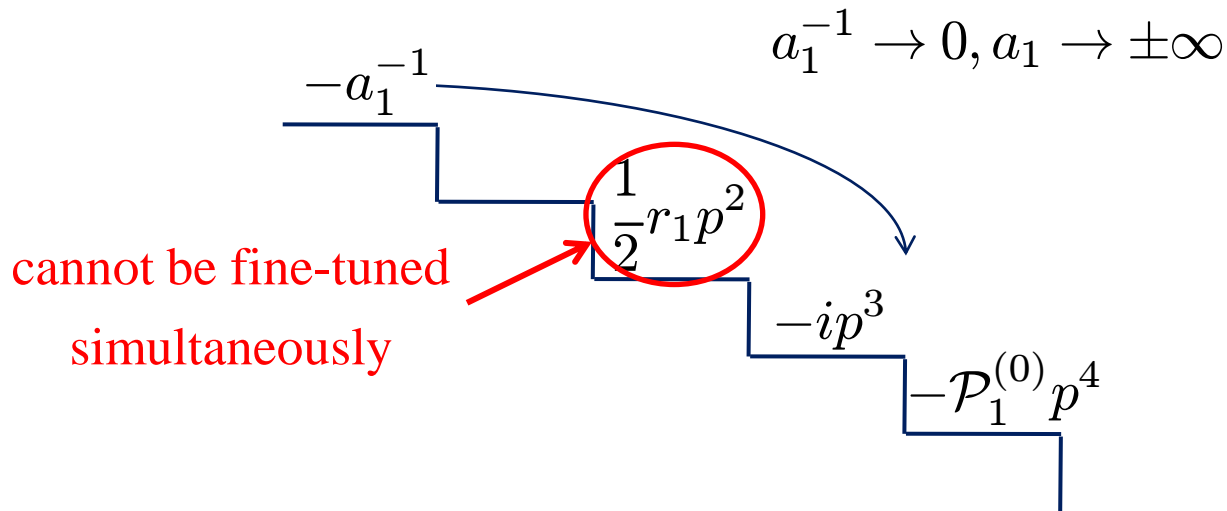
Similar relation for time delay and the derivative of the phase shift with respect to energy.







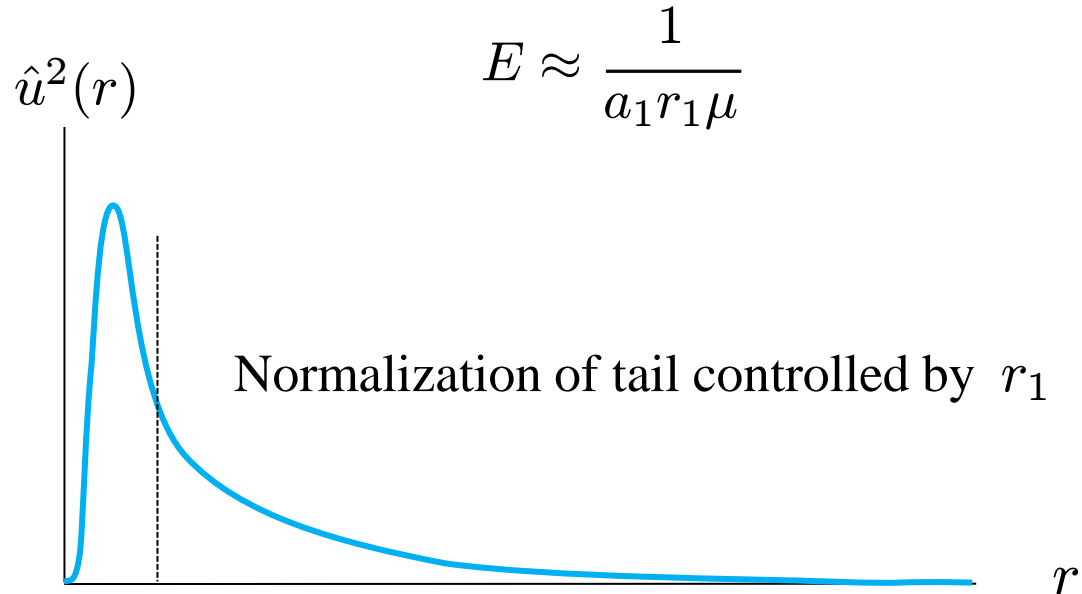
Universality for P-waves



$$f_1(p) = \frac{p^2}{p^3 \cot \delta_1(p) - ip^3}$$

$$p^3 \cot \delta_1(p) = -a_1^{-1} + \frac{1}{2} r_1 p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_1^{(n)} p^{2n+4}$$

Shallow P-wave bound state



In the limit of zero binding energy

$$P_{>}(r) \rightarrow \frac{2}{-r_1 r} \quad r \geq R$$

Generalization to arbitrary dimension

Radial Schrödinger equation

$$u_{L,d}(r) = r^{(d-1)/2} R_{L,d}(r)$$

$$-u''_{L,d}(r) + \left[\frac{\left(L + \frac{d-1}{2}\right) \left(L + \frac{d-3}{2}\right)}{r^2} + 2\mu V(r) \right] u_{L,d}(r) = 2\mu E \cdot u_{L,d}(r)$$

Partial wave scattering amplitude

$$f_{L,d}(p) \propto \frac{p^{2L}}{p^{2L+d-2} \cot \delta_{L,d}(p) - ip^{2L+d-2}}$$

Effective range expansion

even d only

$$p^{2L+d-2} \left[\cot \delta_{L,d}(p) - \delta_{d \bmod 2,0} \frac{2}{\pi} \log(p\rho_{L,d}) \right]$$
$$= -a_{L,d}^{-1} + \frac{1}{2} r_{L,d} p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} \mathcal{P}_{L,d}^{(n)} p^{2n+4}$$

Dimensional analysis:

$$a_L^{-1} = [\ell]^{2-2L-d}, \quad r_L = [\ell]^{4-2L-d}, \quad \mathcal{P}_L^{(n)} = [\ell]^{6+2n-2L-d}$$

Depends on the combination $2L + d$

$2L + d \leq 2$ Although the interactions can be non-perturbative (*i.e.*, *perturbative expansion in scattering parameter breaks down*), the interactions remain weak at low energies.
Only trivial fixed point.

$2L + d = 3$ The unitarity limit reachable – non-trivial fixed point.

$2L + d \geq 4$ Causality prevents reaching the non-trivial fixed point with finite-range interactions. Effective range emerges as a second relevant parameter that cannot be fine-tuned.

Summary

Lattice EFT – relatively new and promising tool that combines framework of effective field theory and computational lattice methods

Applications to zero and nonzero temperature simulations of light nuclei, neutron matter, cold atoms, etc.

Currently working on light nuclei at NNLO, including Coulomb corrections, isospin-symmetry breaking, storing lattice configurations for correlation functions, scattering, transitions, etc.

Part I

Causal wave propagation has significant consequences for low-energy universality

Part II

For higher partial waves in the zero-energy resonance limit, a second dimensionful parameter appears that cannot be fine-tuned to zero. This second parameter is the effective range.

Effective range expansion: van der Waals

For P-waves cannot in general define an effective range parameter

$$p^3 \cot \delta_1(p) = -a_1^{-1} + \boxed{c_{1,1}p} + \frac{1}{2}r_1p^2 + \dots$$

However in the zero-energy resonance limit where the scattering parameter is infinite

$$a_1^{-1} \rightarrow 0 \implies c_{1,1} \rightarrow 0$$