Symmetries, signs, and complex actions in lattice effective field theory

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Outline

- What is lattice effective field theory?
- Chiral effective field theory for nucleons
- Computational strategies on the lattice
- Auxiliary fields, signs, and complex actions
- Phase shifts and unknown operator coefficients
- Dilute neutron matter at NLO
- How severe is the sign problem really?
- Studies of light nuclei at NNLO
- Summary, future directions, and connections

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





Leading order on lattice



Next-to-leading order on lattice



Computational strategy



Non-perturbative – Monte Carlo

"Improved LO"

Perturbative corrections

Lattice formulations

Euclidean-time transfer matrix

Free nucleons:

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

Free pions:

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

Pion-nucleon coupling:

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

... with auxiliary fields

C contact interaction:

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

 C_I contact interaction:

$$\exp\left[-\frac{1}{2}C_{I}N^{\dagger}\tau N \cdot N^{\dagger}\tau N\Delta t\right] \quad (C_{I} > 0)$$
$$= \frac{1}{\sqrt{2\pi}}\int ds_{I}\exp\left[-\frac{1}{2}s_{I}\cdot s_{I} + is_{I}\cdot N^{\dagger}\tau N\sqrt{C_{I}\Delta t}\right]$$

Euclidean-time projection 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 we can show that the determinant is positive semi-definite

Consider an eigenvector

$$\mathbf{M}\phi = \lambda\phi$$

Let us define a new vector

$$\tilde{\phi} = \tau_2 \phi^*$$

Note that

$$\mathbf{M}\tilde{\phi} = \mathbf{M}\tau_{2}\phi^{*} = \tau_{2}\tau_{2}\mathbf{M}\tau_{2}\phi^{*} = \tau_{2}\mathbf{M}^{*}\phi^{*}$$
$$= \tau_{2}\left(\mathbf{M}\phi\right)^{*} = \tau_{2}\left(\lambda\phi\right)^{*} = \lambda^{*}\tau_{2}\phi^{*} = \lambda^{*}\tilde{\phi}$$

Note also that the two vectors are orthogonal

$$\tilde{\phi}^{\dagger}\phi = \left(\tau_{2}\phi^{*}\right)^{\dagger}\phi = \phi^{T}\tau_{2}^{\dagger}\phi = \phi^{T}\tau_{2}\phi = 0$$

So complex eigenvalues come in conjugate pairs, and the real spectrum is doubly-degenerate

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

$$ilde{V}(ec{p})$$
 · 0

satisfies SU(2N) convexity bounds...

 $|\psi_{\text{init}}\rangle \rightarrow \{j \text{ flavors occupation } n_1, 2N - j \text{ flavors occupation } n_2\}$ $\langle \psi_{\text{init}} | M^{(L_t-1)}(\phi) \cdots M^{(0)}(\phi) | \psi_{\text{init}} \rangle = \det \mathbf{M}(\phi)$ $\int D\phi \ e^{-S(\phi)} \ \det \mathbf{M}(\phi)$ $S(\phi) = -\frac{\alpha_t}{2} \sum \sum \phi(\vec{n}, n_t) V^{-1}(\vec{n} - \vec{n}') \phi(\vec{n}', n_t)$ $n_{+} \vec{n} \vec{n}'$ $\mathbf{M}_{k',k}(\phi) = \langle f_{k'} | M^{(L_t-1)}(\phi) \times \cdots \times M^{(0)}(\phi) | f_k \rangle$ $\int D\phi \ e^{-S(\phi)} \ \left[\det \mathbf{M}_{n_1 \times n_1}(\phi)\right]^j \left[\det \mathbf{M}_{n_2 \times n_2}(\phi)\right]^{2N-j}$

Apply Hölder inequality

Chen, D.L. Schäfer, PRL 93 (2004) 242302; D.L., PRL 98 (2007) 182501

SU(4) convexity bounds

$$= M_{\rm LO} \qquad = M_{SU(4)} \qquad = O_{\rm observable}$$
$$= M_{\rm NLO} \qquad = M_{\rm NNLO}$$

Hybrid Monte Carlo sampling

$$Z_{n_t, \text{LO}} = \langle \psi_{\text{init}} | \boxed{(1)} \\ Z_{n_t, \text{LO}}^{\langle O \rangle} = \langle \psi_{\text{init}} | \boxed{(1)} \\ \boxed{(1)} \\ \psi_{\text{init}} \rangle \\ e^{-E_{0, \text{LO}}a_t} = \lim_{n_t \to \infty} Z_{n_t+1, \text{LO}} / Z_{n_t, \text{LO}} \\ \langle O \rangle_{0, \text{LO}} = \lim_{n_t \to \infty} Z_{n_t, \text{LO}}^{\langle O \rangle} / Z_{n_t, \text{LO}}$$

$$(1 - \Delta E_{0,\text{NLO}}a_t)e^{-E_{0,\text{LO}}a_t} = \langle M_{\text{NLO}} \rangle_{0,\text{LO}}$$

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

LO₁: Pure contact interactions

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

LO₂: Gaussian smearing $\mathcal{A}(V_{\text{LO}_2}) = Cf(\vec{q}^{\ 2}) + C_I f(\vec{q}^{\ 2}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \mathcal{A}(V^{\text{OPEP}})$

LO₃: Gaussian smearing only in even partial waves

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

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	$0 \operatorname{mod} 4$	$Y_{0,0}$
T_1	$0, 1, 3 \operatorname{mod} 4$	$\{Y_{1,0},Y_{1,1},Y_{1,-1}\}$
E	$0,2 \operatorname{mod} 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1,2,3 \operatorname{mod} 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2} - Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \operatorname{mod} 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$

LO₃: S waves

 $a = 1.97 \; {\rm fm}$

LO₃: P waves

 $a = 1.97 \; {\rm fm}$

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

1.2

1

0.8

APR CMPR v6

SP 200:

GIFPS 2008

GC 2007

2003

CMPR v8'

 $LO_3 \vdash NLO_3 \vdash$

200

∇ ♦ ₩

Δ

Close to unitarity limit result with scattering length, effective range corrections, etc.

$$\frac{E_0}{E_0^{\text{free}}} = \xi - \frac{\xi_1}{k_F a} + ck_F r_0 + \dots$$

$$\xi = 0.31(1)$$

$$\xi_1 \approx 0.8$$

$$c \approx 0.16$$

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Epelbaum, Krebs, D.L, Meißner, 0812.3653 [nucl-th]

How bad is the sign problem really?

Cost of generating new configurations

$$\sim c_1 N_{\rm neutrons} L^3 n_t + c_2 N_{\rm neutrons}^3 + \cdots$$

Sign oscillation scaling by far most significant

$$\langle \text{sign} \rangle \sim 2^{-(k_F N_{\text{neutrons}})/(400 \,\text{MeV})}$$

Current (0.05 Teraflop years) $k_F N_{\text{neutrons}} = 2000 \text{ MeV}$ 6% normal nuclear matter density for 16 neutrons

 $a = 1.97 \,\mathrm{fm}$

Near future (1 Teraflop years) $k_F N_{\text{neutrons}} = 2800 \,\text{MeV}$

15% normal nuclear matter density for 16 neutrons

 $a = 1.6 \,\mathrm{fm}$

Petascale (100 Teraflop years) $k_F N_{neutrons} = 4200 \text{ MeV}$ 15% normal nuclear matter density for 24 neutrons

 $a=1.6\,{\rm fm}$

Exascale (100 Petaflop years) $k_F N_{\text{neutrons}} = 6100 \,\text{MeV}$

50% normal nuclear matter density for 24 neutrons

 $a = 1.2 \,\mathrm{fm}$

Three-body forces at NNLO

Fit c_D and c_E to spin-1/2 nucleon-deuteron scattering and ³H binding energy

Spin-3/2 nucleon-deuteron scattering

Alpha-particle energy

Summary

- Promising but relatively new tool that combines the framework of effective field theory and computational lattice methods
- Potentially wide applications to zero and nonzero temperature simulations of cold atoms, light nuclei, neutron matter

Future directions

- Improve accuracy higher order, smaller lattice spacing, larger volume, more nucleons
- Include Coulomb effects and isospin breaking
- Compute nucleon-nucleus scattering, nucleus-nucleus scattering

Connecting lattice QCD and lattice EFT

Finite volume matching for two-nucleon states

For the same periodic volume, compute two-nucleon energies in Lattice QCD and match to two-nucleon energies Lattice EFT

Pion mass dependence?

Connecting lattice QCD and lattice EFT

Calculate g_A for the two-neutron state at finite volume

For given lattice spacing in lattice EFT, use the value of g_A obtained via Lattice QCD at the same volume to fix c_D

Connecting lattice QCD and lattice EFT

