Latest Results from Nuclear Lattice Effective Field Theory

Nuclear Lattice EFT Collaboration

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See also talk by Timo Lähde – June 25















Outline

What is lattice effective field theory?

Carbon-12 spectrum and the Hoyle state

Ab initio lattice calculations up to A = 28

Oxygen-16 structure and spectrum

Properties of neutron matter

Scattering and reactions on the lattice

Summary and future directions

Lattice quantum chromodynamics



Lattice effective field theory





Low energy nucleons: Chiral effective field theory

Construct the effective potential order by order





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	$2 \operatorname{mod} 4$	$\frac{Y_{3,2} - Y_{3,-2}}{\sqrt{2}}$





Improved leading order action (LO₃):

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

$$\mathcal{A}(V^{\text{OPEP}}) = -\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\vec{q}\cdot\vec{\sigma}_1)(\vec{q}\cdot\vec{\sigma}_2)}{q^2 + m_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$



a = 1.97 fm





 $\delta(^{3}P_{1})$ (degrees)





Three nucleon forces

Two unknown coefficients at NNLO from three-nucleon forces. Determine c_D and c_E using ³H binding energy and the weak axial current at low cutoff momentum.



Neutrons and protons: Isospin breaking and Coulomb

Isospin-breaking and power counting [*Friar*, *van Kolck*, *PRC* 60 (1999) 034006; Walzl, Meißner, Epelbaum NPA 693 (2001) 663; Friar, van Kolck, Payne, Coon, PRC 68 (2003) 024003; Epelbaum, Meißner, PRC72 (2005) 044001...]

Pion mass difference



Coulomb potential







Triton and Helium-3





Euclidean time projection



Auxiliary field transformation

We can write exponentials of the interaction using a Gaussian integral identity

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.

We introduce sixteen auxiliary fields

$$sN^{\dagger}N, \ i\vec{s}_{S}\cdot N^{\dagger}\vec{\sigma}N, \ is_{I}\cdot N^{\dagger}\boldsymbol{\tau}N, \ \vec{s}_{SI}\cdot N^{\dagger}\vec{\sigma}\boldsymbol{\tau}N$$



Spectral convexity, pairing, and clustering

Theorem:

Any fermionic theory with SU(2N) symmetry and two-body potential with negative semi-definite Fourier transform obeys SU(2N) convexity bounds.



Corollary:

System can be simulated without sign oscillations

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

There are 2N species of fermions. We calculate the path integral using projection Monte Carlo with one auxiliary field coupled to the total particle density.

The path integral is

$$\int D\phi \ e^{-S(\phi)} \det \mathbf{G}(\phi)$$

where the auxiliary field has a quadratic action of the form

$$S(\phi) = -\frac{\alpha_t}{2} \sum_{n_t} \sum_{\vec{n},\vec{n}'} \phi(\vec{n},n_t) V^{-1}(\vec{n}-\vec{n}')\phi(\vec{n}',n_t)$$

inverse of potential

We choose the sector with K + 1 particles for species 1 to j, and K particles for species j + 1 to 2N.



The auxiliary field is coupled to the total particle density. The total particle density is an operator which diagonal in particle species. Therefore the matrix has the following block diagonal structure...



The path integral is then

$$Z_{j,K+1;2N-j,K} = \int D\phi \ e^{-S(\phi)} \left[\det \mathbf{M}_{(K+1)\times(K+1)}(\phi) \right]^{j} \left[\det \mathbf{M}_{K\times K}(\phi) \right]^{2N-j}$$

The Hölder inequality states that for any positive p, q satisfying

$$1/p + 1/q = 1$$

we have

$$\int dx \ |f(x)g(x)| \le \left[\int dx \ |f(x)|^p \right]^{1/p} \times \left[\int dx \ |g(x)|^q \right]^{1/q}$$

Application of the Hölder inequality leads to the spectral convexity theorem



SU(4) convexity bounds



Schematic of lattice Monte Carlo calculation

$$= M_{\rm LO} = M_{\rm approx} = O_{\rm observable}$$
$$= M_{\rm NLO} = M_{\rm NNLO}$$

Hybrid Monte Carlo sampling

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

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

Particle clustering included automatically











Carbon-12 spectrum and the Hoyle state



See also talk by Timo Lähde – June 25



Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501 Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 (2012) 252501

Ground state of Carbon-12

 $L = 11.8 \,\mathrm{fm}$

$LO^*(O(Q^0))$	-96(2) MeV
NLO $(O(Q^2))$	-77(3) MeV
NNLO $(O(Q^3))$	-92(3) MeV
Experiment	-92.2 MeV

*contains some interactions promoted from NLO

Simulations using general initial/final state wavefunctions



$$\bigwedge_{j=1,\cdots,A} |\psi_j(\vec{n})\rangle$$

Construct states with well-defined momentum using all possible translations.

$$L^{-3/2} \sum_{\vec{m}} e^{i\vec{P}\cdot\vec{m}} \bigwedge_{j=1,\cdots,A} |\psi_j(\vec{n}-\vec{m})\rangle$$

Shell model wavefunctions

$$\psi_j(\vec{n}) = \exp(-c\vec{n}^2)$$

$$\psi'_j(\vec{n}) = n_x \exp(-c\vec{n}^2)$$

$$\psi''_j(\vec{n}) = n_y \exp(-c\vec{n}^2)$$

$$\psi'''_j(\vec{n}) = n_z \exp(-c\vec{n}^2)$$

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Alpha cluster wavefunctions

$$\psi_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m})^2]$$

$$\psi'_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}')^2]$$

$$\psi''_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}'')^2]$$

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Shell model wavefunctions by themselves do not have enough local four nucleon correlations,

 $< (N^{\dagger}N)^4 >$

Needs to develop the four nucleon correlations via Euclidean time projection.

But can reproduce same results starting directly from alpha cluster wavefunctions [Δ and Λ in plots on next slide].



Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)

Structure of ground state and first 2+

Strong overlap with compact triangle configuration





b = 1.97 fm

Structure of Hoyle state and second 2+

Strong overlap with bent arm configuration



24 rotational orientations

b = 1.97 fm

Excited state spectrum of carbon-12 (even parity)

	2^+_1	0_{2}^{+}	2^+_2
$LO^*(O(Q^0))$	-94(2) MeV	-89(2) MeV	-88(2) MeV
NLO $(O(Q^2))$	-74(3) MeV	-72(3) MeV	-70(3) MeV
NNLO $(O(Q^3))$	-89(3) MeV	-85(3) MeV	-83(3) MeV
Experiment	–87.72 MeV	–84.51 MeV	-82.6(1) MeV (A,B) -81.1(3) MeV (C) -82.13(11) MeV (D)

*contains some interactions promoted from NLO

- *A Freer et al.*, *PRC* 80 (2009) 041303
- *B*-Zimmerman et al., *PRC* 84 (2011) 027304
- C-Hyldegaard et al., PRC 81 (2010) 024303

D-Itoh et al., PRC 84 (2011) 054308

Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)

Preliminary: *Ab initio* lattice calculations up to A = 28



Preliminary: *Ab initio* lattice calculations up to A = 28





Preliminary: Oxygen-16 structure and spectrum



<u>Tetrahedral cluster structure of first 0⁺ and 3⁻</u>



8 rotational orientations

b = 1.97 fm

Finding the second 0⁺ state



Cluster structure of second 0⁺ state and first 2⁺ state



6 rotational orientations

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

Low-lying spectrum of Oxygen-16



Preliminary: Properties of neutron matter

Neutron Star





Energy per neutron in the ground state



Figure adapted from Tews, et al., PRL 110 (2013) 032504

Energy per neutron in the ground state



Figure adapted from Gezerlis, et al., arXiv: 1303.6243

Preliminary: Scattering and reactions on the lattice

Projected adiabatic matrix method



Using cluster wavefunctions for initial continuum scattering states

$$|\vec{R}>$$

Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time

$$|\vec{R}>_t = e^{-Ht}|\vec{R}>$$

$$\vec{R}>_t =$$

Construct a norm matrix and matrix of expectation values

$$\langle N \rangle_{t} = {}_{t} \langle \vec{R}' | \vec{R} \rangle_{t} =$$

$$\langle \vec{R}' | \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} | \vec{R} \rangle_{t} =$$

$$\langle \vec{R}' | \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} | \vec{R} \rangle_{t} =$$

$$\langle \vec{R}' | \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} \boxed{\qquad} | \vec{R} \rangle_{t} =$$

Compute the projected adiabatic matrix

$$< O >_{\text{adiab}} = < N >_t^{-1/2} < O >_t < N >_t^{-1/2}$$

Projected adiabatic Hamiltonian is now an effective two-body Hamiltonian. Similar in spirit to no-core shell model with resonating group method.

But some differences. Distortion of the nucleus wavefunctions is automatic due to projection in Euclidean time.



Example: Quartet neutron-deuteron scattering



Pine, D.L., Rupak, work in progress

Quartet neutron-deuteron scattering (pionless EFT at LO)



Pine, D.L., Rupak, work in progress

Use coupled channels for capture reactions and break up processes.

Lattice Green's function methods for radiative capture tested for $n + p \rightarrow d + \gamma$ in pionless effective field theory at leading order.

Elastic scattering amplitude (${}^{1}S_{0}$ and ${}^{3}S_{1}$)



M1 radiative capture amplitude



Rupak, D.L., arXiv:1302.4158 [nucl-th], PRL in press

<u>M1 transition amplitude $n + p \rightarrow d + \gamma$ </u>



Rupak, D.L., arXiv:1302.4158 [nucl-th], PRL in press

Summary

A golden age for nuclear theory from first principles. Big science discoveries being made and many more around the corner.

Lattice effective field theory is a relatively new and promising tool that combines the framework of effective field theory and computational lattice methods. May play a significant role in the future of *ab initio* nuclear theory.

Topics to be addressed in the near future...

Different lattice spacings, $N \neq Z$ and odd nuclei, nucleus-nucleus scattering and reactions, calculation with interactions at N3LO, clustering in heavier nuclei, transition from S-wave to P-wave pairing in superfluid neutron matter, etc.