Non-perturbative three-nucleon simulation using chiral lattice EFT

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E. Epelbaum, H. Krebs, D. Lee
— code contribution by S. Elhatisari —

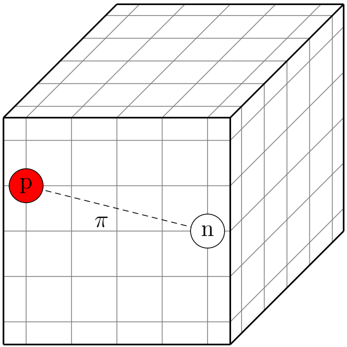
Institut für Theoretische Physik II
Ruhr-Universität Bochum

The 11th International Workshop on Chiral Dynamics

Ruhr-Universität Bochum, Germany
26-30 August 2024

Outline

Lattice definition



- work with nucleons & pions ($\neq$ lattice QCD)

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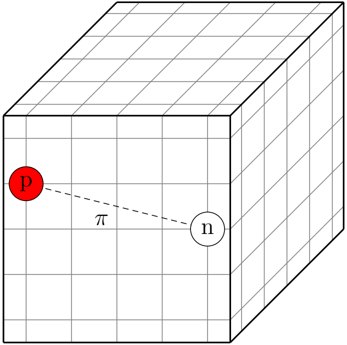

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- no Monte Carlo (MC) & perturbation theory for 3 nucleons **see plenary talk by D. Lee for many-body case**

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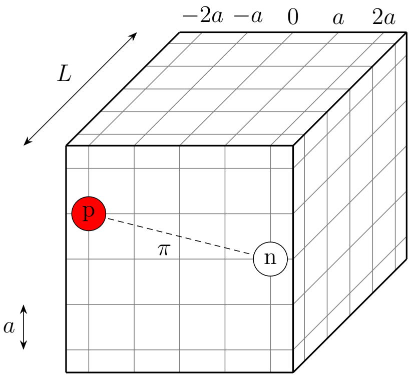

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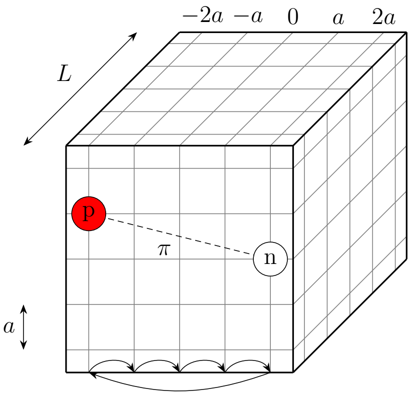

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- no Monte Carlo (MC) & perturbation theory for 3 nucleons see plenary talk by D. Lee for many-body case
- introduce lattice with length L and spacing $a = 2$ fm
- require periodic boundary conditions:
  $|\vec{r}\rangle = |\vec{r} + n_x L\vec{e}_x + n_y L\vec{e}_y + n_z L\vec{e}_z\rangle$
  $\forall n_x, n_y, n_z \in \mathbb{Z}$

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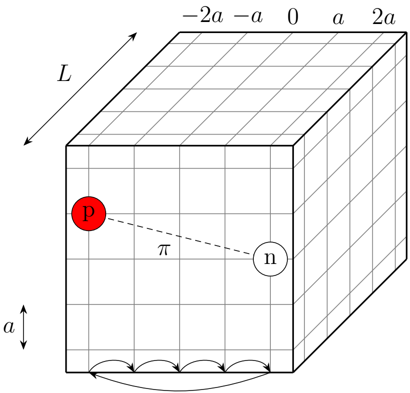

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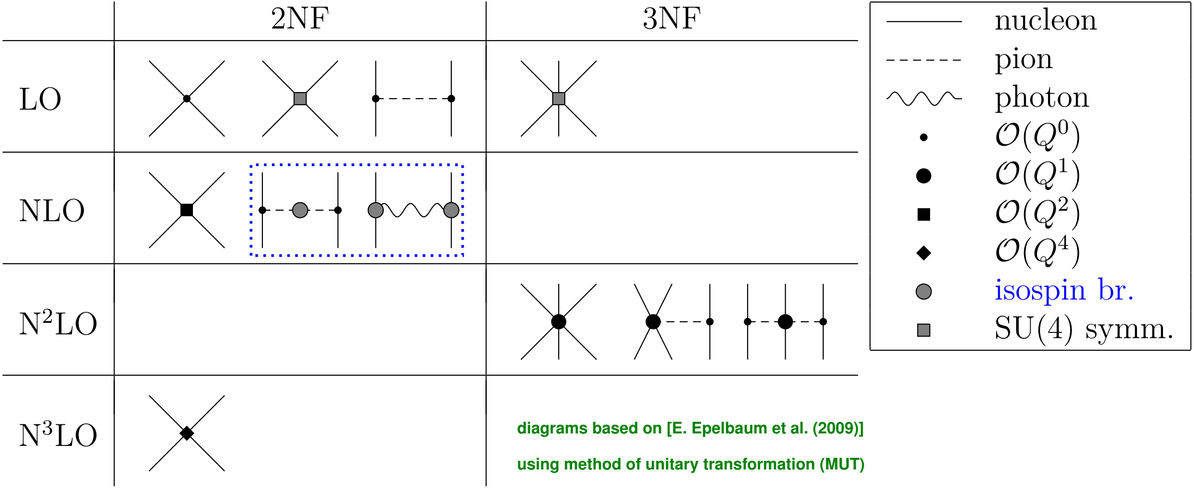
- discretize integrals and derivatives, e.g. for kinetic energy in $\hat{H}$: **[D. Lee, R. Thomson (2007)]**

improved version of

$$-\frac{\vec{\nabla}^2}{2m_{\mathrm{N}}}|\vec{r}\rangle = \frac{3}{m_{\mathrm{N}}a^2}|\vec{r}\rangle - \frac{1}{2m_{\mathrm{N}}a^2}\sum_{i=x,y,z}\Big(|\vec{r}+a\vec{e}_i\rangle + |\vec{r}-a\vec{e}_i\rangle\Big)$$

Chiral expansion of nuclear force



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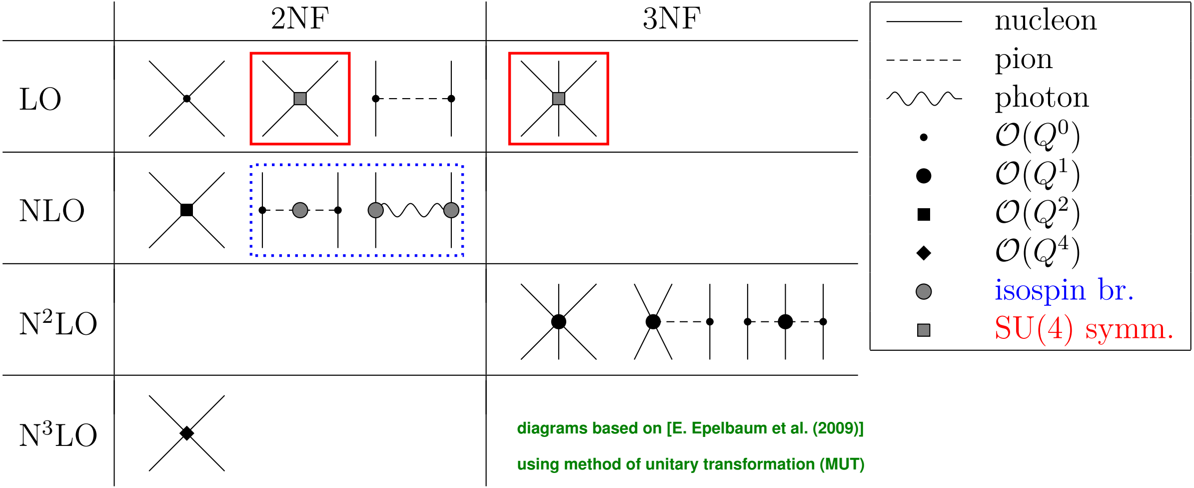

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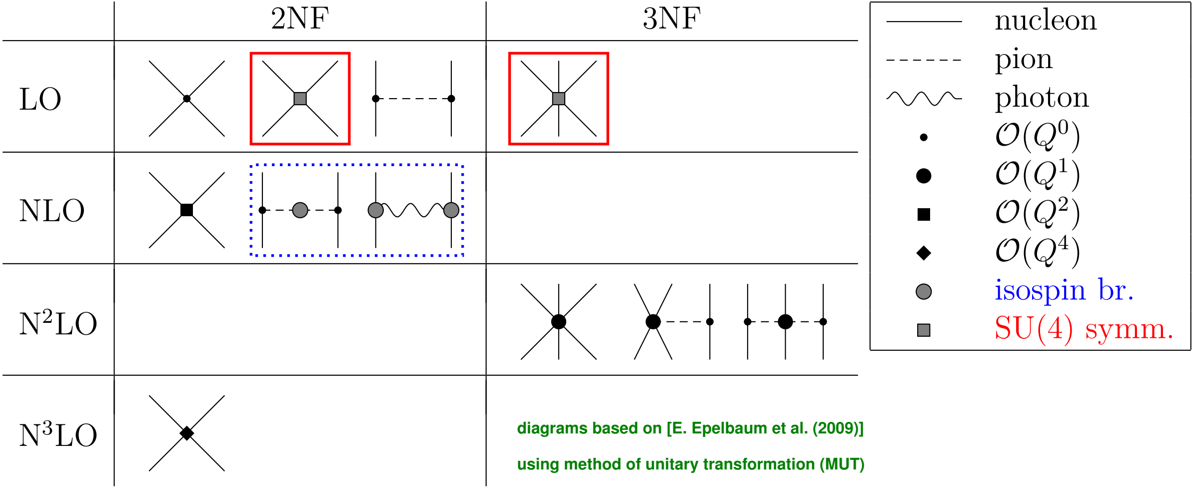

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[N. Li et al. (2018)]

no 3π and simultaneous 2π exchange (emulated by CIs)

no relativistic $1/m_{\mathrm{N}}$ corrections

Two-nucleon short-range interactions *[N. Li et al. (2018)]

$$\langle x|\hat{O}|x'\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$x = x' = 0$$

(x = 2N coordinate difference in 1D)

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$$\langle x|\hat{O}_{\mathrm{L}}|x'\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & s_{\mathrm{L}} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & s_{\mathrm{L}} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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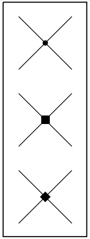
Two-nucleon short-range interactions *[N. Li et al. (2018)]

- “standard” contact interactions for different partial waves (PWs)
  - non-local smearing similar to Gaussian regulator in continuum SMS potential
    [P. Reinert et al. (2018)]



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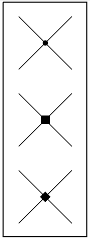

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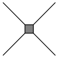
- SU(4)-invariant CI with coeff. $C_{0,2\mathrm{N}}$
  - non-local & local smearing



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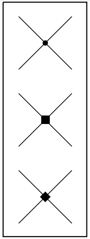

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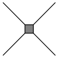

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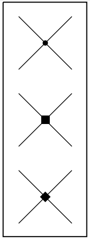

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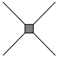

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- here*: benchmark values for s_{NL}, s_{L}, $C_{0,2\mathrm{N}}$ (x = 2N coordinate difference in 1D)
- coefficients of "standard" CIs tuned to nucleon-nucleon phase shifts *
  - PW decomposition using radial projection instead of Lüscher's formula)
  - Galilean-invariance restoration to correct deuteron binding energy for $\vec{P}_{\mathrm{tot}} \neq \vec{0}$ *

Long-range interactions

$\rightarrow$ backup slide

Uncertainty analysis

- truncation error for observable X with zero external momentum:
  $\Delta X^{\rm NLO}_{\rm trunc} = \mathcal{Q}^3 |X_{\rm NLO}|$, $\Delta X^{\rm N3LO}_{\rm trunc} = \max\{\mathcal{Q}^5 |X_{\rm NLO}|, \mathcal{Q}^2 |X_{\rm NLO} - X_{\rm N3LO}|\}$
  Epelbaum-Krebs-Meißner approach [EKM (2015a)] [EKM (2015b)] [N. Li et al. (2018)]
  - use N^{3}LO without 3NF as NLO
  - estimate $\mathcal{Q} = M_\pi^{\rm eff}/\Lambda_{\rm b} = 200\ {\rm MeV}/600\ {\rm MeV} = 1/3$ **[E. Epelbaum (2019)]**

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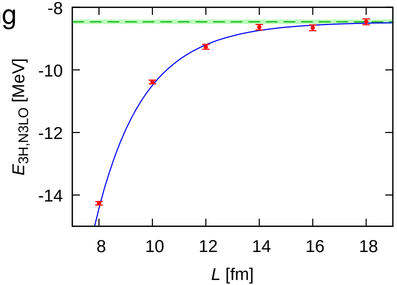
- extrapolate binding energies E to $L \to \infty$ using suitable fit function $E(L)$:
  $E(L \to \infty) = E_\infty + E_0 L^{-3/2} \exp(-L/L_0)$ **[Ulf-G. Meißner et al. (2015)]**
  - propagate truncation error from data points to extrapolated result E_∞ via statistical sampling



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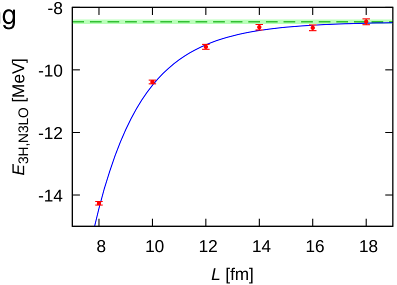
- estimate fitting error from self-determined LEC $C \pm \Delta C$ as
  $\Delta X_{\mathrm{fit}} = |X(C + \Delta C) - X(C - \Delta C)|/2$
  - add truncation error and fitting error in quadrature: $\Delta X^2_{\mathrm{tot}} = \Delta X^2_{\mathrm{trunc}} + \Delta X^2_{\mathrm{fit}}$



Binding energies

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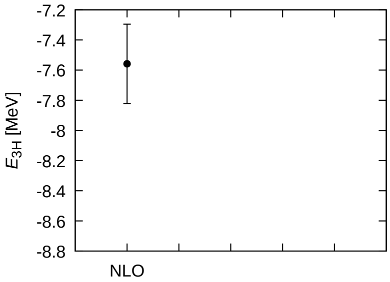

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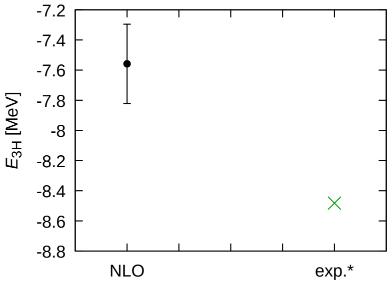

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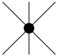
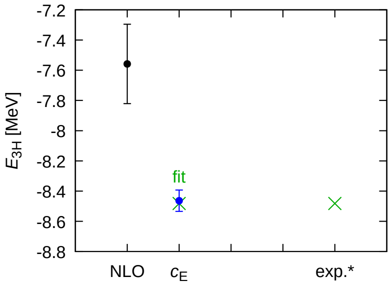
  $\Rightarrow$ three-nucleon contact interaction without smearing as in [D. Lee (2009)]


c_E



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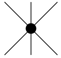
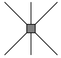


c_{E}

- $C_{0,3\mathrm{N}} = -2.42(8) \times 10^{-12}\ \mathrm{MeV}^{-5},\, c_{\mathrm{E}} = c_{\mathrm{D}} = 0$
  $\Rightarrow$ 3N version of 2N SU(4)-invariant CI with non-local & local smearing



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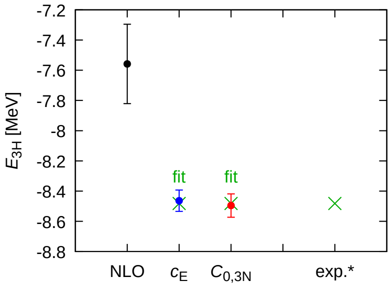

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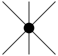

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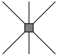

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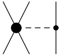
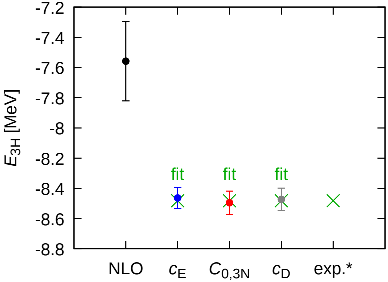


c_{D}



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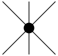

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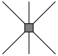

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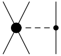
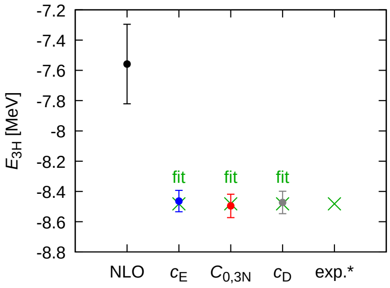
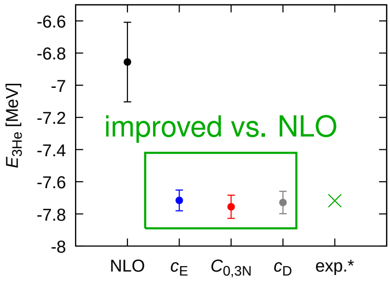


c_D



correlated $\longleftrightarrow$



*[M. Wang et al. (2017)]

Charge radii

- charge radius: **[J. Hoppe et al. (2019)] [J. Simonis et al. (2017)] [A. Ong et al. (2010)]**

$$R^2_{\text{ch,nucleus}} = \langle \psi_{\text{nucleus}} | \hat{\vec{R}}^2_{\text{point-proton}} | \psi_{\text{nucleus}} \rangle + R^2_{\text{ch,p}} + \frac{N}{Z} R^2_{\text{ch,n}} + R^2_{\text{Darwin-Foldy}}$$

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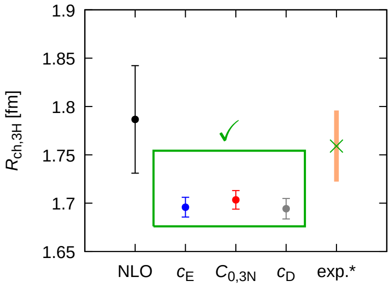
- determined ψ_{nucleus} for $L = 18$ fm using Lanczos algorithm
- R_{ch} typically a few % too small (no hard repulsive core predicted in ChEFT)



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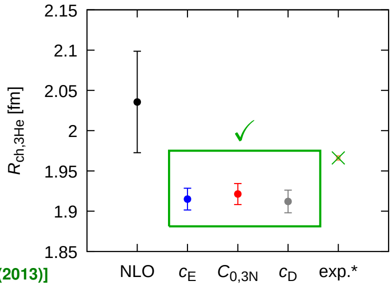

*[I. Angeli, K. P. Marinova (2013)]

Half-life of triton beta decay

- half-life: **[A. Baroni et al. (2016)] [R. Schiavilla et al. (1998)] [S. Raman et al. (1978)]**

$$t_{1/2} = \frac{1}{1+\delta_{\rm R}} \frac{K/G_{\rm V}^2}{f_{\rm V}\langle\widehat{\mathbf{F}}\rangle^2 + f_{\rm A} g_{\rm A}^2 \langle\widehat{\mathbf{GT}}\rangle^2}$$

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$$\langle \widehat{\mathbf{F}} \rangle = \sum_{n=1}^{N_{\text{nucleons}}} \langle \psi_{3\mathrm{He}} | \tau_{n,+} | \psi_{3\mathrm{H}} \rangle,$$

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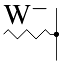

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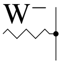

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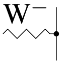

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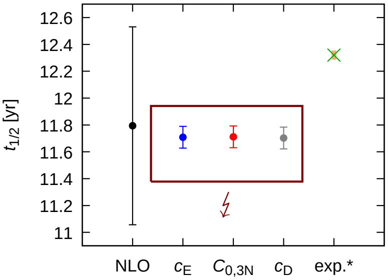

*[J. J. Simpson (1987)]

- determined $\psi_{3\text{H}}$, $\psi_{3\text{He}}$ for $L = 18$ fm using Lanczos algorithm
- half-life too small with LO current (truncation error underestimated)

Summary and outlook

- good prediction for helion binding energy and charge radii of ^{3}H, ^{3}He

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch},3\mathrm{H}}$ [fm]	$R_{\mathrm{ch},3\mathrm{He}}$ [fm]	$t_{1/2}$ [yr]
this work c_{E}-fit	$8.46(7)$ fit	$7.72(6)$	$1.6959(102)$	$1.9151(135)$	
exp. refs. on prev. slides	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$	$12.32(3)$

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  - clear improvement by 3NF at N^{3}LO compared to NLO (for fit of c_E, $C_{0,3N}$ and c_D)

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WFM pot. **radii pert.**			$1.7132(91)$	$1.9013(264)$	
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  $\Rightarrow$ consider $t_{1/2}$ (and $(\Delta t_{1/2})_\mathrm{trunc}$) for N^{2}LO current involving c_D [H. Krebs et al. (2017)]

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch},3\mathrm{H}}$ [fm]	$R_{\mathrm{ch},3\mathrm{He}}$ [fm]	$t_{1/2}$ [yr]
WFM pot. radii pert.	$8.33(2)$ fit	$7.62(2)$	$1.7132(91)$	$1.9013(264)$	$12.095(2)_{K/G_\mathrm{V}^2}$
this work c_E-fit	$8.46(7)$ fit	$7.72(6)$	$1.6959(102)$	$1.9151(135)$	$11.708(81)$
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Summary and outlook

- good prediction for helion binding energy and charge radii of ^{3}H, ^{3}He
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  $\Rightarrow$ consider $t_{1/2}$ (and $(\Delta t_{1/2})_\mathrm{trunc}$) for N^{2}LO current involving c_D [H. Krebs et al. (2017)]
- outlook: test applicability of obtained potential to
  - nucleon-deuteron phase shifts using adiabatic projection method [M. Pine et al. (2013)]
  - perturbative calculations of heavier nuclei (bound states, resonances talk by C. Wang)

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch},3\mathrm{H}}$ [fm]	$R_{\mathrm{ch},3\mathrm{He}}$ [fm]	$t_{1/2}$ [yr]
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Thank you for your attention!

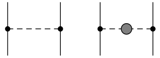
Long-range interactions

- pion propagator with Gaussian regulator: [N. Li et al. (2018)]

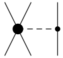
$$\frac{1}{\vec{q}^{\,2}+M_\pi^2}\exp\left(-\frac{\vec{q}^{\,2}+M_\pi^2}{\Lambda^2}\right), \qquad \Lambda = 200\ \mathrm{MeV}$$

  $\rightarrow$ reduce Monte Carlo sign problem later [S. Elhatisari et al. (2024)]

- two-nucleon 1π exchange for M_{π^0} (isospin symmetric) and M_{π^0}, $M_{\pi^\pm}$ (isospin breaking) [N. Li et al. (2018)]



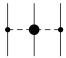
- three-nucleon 1π exchange with unsmeared CI



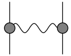
  as in [D. Lee (2009)] but not in [S. Elhatisari et al. (2024)]

  $\rightarrow$ LEC c_{D} fixed from triton binding energy

- three-nucleon double-1π exchange [D. Lee (2009)] [S. Elhatisari et al. (2024)] with LECs c_1, c_3, c_4 adjusted to πN scattering data [M. Hoferichter et al. (2015)]



- Coulomb potential with zero particle distance replaced by $a/2$



  [N. Li et al. (2018)]