Description of light nuclei in a pionless effective field theory using the stochastic variational method

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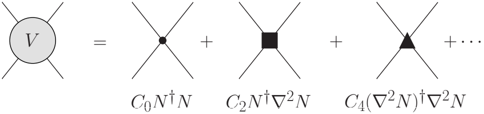
Effective Field Theories

Effective Field Theory:

- low-energy theory of some "fundamental" theory
- external momenta much smaller than some high-energy scale: $p \ll M_{\text{hep}}$
- the S-matrix calculated in an EFT is an expansion in the powers of $Q = p/M_{\text{hep}}$
- the degrees of freedom (DOFs) $\neq$ those of the underlying theory
- fundamental symmetries constrain the dynamics of the EFTs
- a finite number of parameters (LECs) arises at each order; their values are found by matching with the fundamental theory or from experiment
- counting rules tell what order is to be assigned to a particular graph

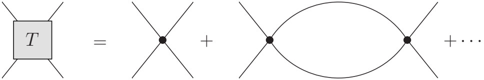
Pionless Nuclear EFT

- high momentum scale $\simeq m_\pi$: $p \lesssim m_\pi$, $E \lesssim 20$ MeV for NN
- contact interactions (with derivatives) $\Longrightarrow$ delta-functions



Weinberg (1990), Kaplan, Savage, Wise (1998), Kong, Ravndal (1999), ...
Beane, Bertulani, Cohen, Hammer, Higa, Gelman, van Kolck, Phillips, Rupak, ...
reviews — Bedaque, van Kolck (2002), Epelbaum (2006)

- loops divergent (couple to arbitrary high momenta)



- need to regularize and renormalize

- can be done along quantum field theory lines (order-by-order)
- or use a formfactor and solve the Schrödinger equation Kirscher (2009)

— potential iterated to all orders, one has to make sure higher order corrections are small!

Aims

- build a potential model based on a pionless EFT (similar to Kirscher (2009))
- calculate *NN* phase shifts, *NN*, *NNN*, and *NNNN* binding energies

- potential model gives wave functions that can be used to calculate other observables (e.g., charge radii)

- study correlations between (some of) these observables
- investigate the regulator (cutoff) dependence and the related limitations of the approach

- we work at NNLO; the expansion parameter $Q \simeq 1/3$, hence the expected accuracy is $\sim Q^3 = 3\%$
- we can expect that denser systems are harder to describe (e.g., ^{4}He vs. ^{3}H or ^{3}He)

- we can also expect that short cutoffs can cause a lot of trouble Scaldeferri (1996), Phillips (1996)

NN interactions

- counting for systems with large *S*-wave scattering lengths
- terms up to p^2:

$$V_{ij} = \overbrace{C_1 + C_2\, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j}^{LO\,(Q^{-1})} + \overbrace{D_1 q^2 + D_2 k^2 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \left(D_3 q^2 + D_4 k^2\right)}^{NLO\,(Q^0)} + \cancel{\frac{1}{2} D_5 \left(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j\right) \cdot \boldsymbol{q} \times \boldsymbol{k}} \\ + \underbrace{D_6 (\boldsymbol{q} \cdot \boldsymbol{\sigma}_i)(\boldsymbol{q} \cdot \boldsymbol{\sigma}_j)}_{NNLO\,(Q^1)} + \cancel{D_7 (\boldsymbol{k} \cdot \boldsymbol{\sigma}_i)(\boldsymbol{k} \cdot \boldsymbol{\sigma}_j)}\,, \tag{1}$$

$\boldsymbol{q} = \boldsymbol{p}_i - \boldsymbol{p}_i'$, $\boldsymbol{k} = (\boldsymbol{p}_i + \boldsymbol{p}_i')/2$.

- *r*-space:

$$V_{ij} = G(r,\sigma)\left(A_1 + A_2 \boldsymbol{\tau_i} \cdot \boldsymbol{\tau_j}\right) + r^2 G(r,\sigma)\left(A_3 + A_4 \boldsymbol{\tau_i} \cdot \boldsymbol{\tau_j}\right) + \left\{\nabla^2, G(r,\sigma)\right\}\left(A_5 + A_6 \boldsymbol{\tau_i} \cdot \boldsymbol{\tau_j}\right) \\ + G(r,\sigma) A_7 \left(1 - \boldsymbol{\tau_i} \cdot \boldsymbol{\tau_j}\right)\left[3(\hat{\boldsymbol{r}} \cdot \boldsymbol{\sigma}_i)(\hat{\boldsymbol{r}} \cdot \boldsymbol{\sigma}_j) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right]\,, \tag{2}$$

$G(r,\sigma) = \exp\left(-\frac{1}{2}\frac{r^2}{\sigma^2}\right)$ with $r = |\boldsymbol{r}| \equiv \left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|$, and A_i are linear combinations of C_i and D_i.

- include the Coulomb interaction

$$V^{\mathrm{C}}_{pp} = \frac{\alpha_{\mathrm{em}}}{r} \tag{3}$$

NNN interactions

- at LO (Q^{-1}), there is only one *NNN* contact interaction Bedaque (2002), Epelbaum (2002); we choose

$$V_{ijk}^{\mathrm{LO}} = E_1 \qquad (4)$$

- NLO (Q^0) terms take into account the dependence on *NN* scattering lenghts; absorbed in the LO piece
- terms up to p^2 Girlanda (2011):

$$V_{ijk} = \overbrace{q_i^2 \left(F_1 + F_2 \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + F_3 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + F_4 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \right)}^{NNLO\ (Q^1)} + \cancel{\left[3(\boldsymbol{q}_i \cdot \boldsymbol{\sigma}_i)(\boldsymbol{q}_i \cdot \boldsymbol{\sigma}_j) - q_i^2 \right] (F_5 + F_6 \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)}$$
$$+ \cancel{\frac{1}{2}(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j) \cdot \boldsymbol{q}_i \times (\boldsymbol{k}_i - \boldsymbol{k}_j)(F_7 + F_8 \boldsymbol{\tau}_j \cdot \boldsymbol{\tau}_k)} + \cancel{(\boldsymbol{k}_i \cdot \boldsymbol{\sigma}_i)(\boldsymbol{k}_j \cdot \boldsymbol{\sigma}_j)(F_9 + F_{10} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)} \qquad (5)$$

- non-*S*-wave interactions are suppressed compared to the *NN* case Griesshammer (2005)
- nuclei under study — ^{3}H, ^{3}He, ^{4}He — are largely SU(4) symmetric with a space symmetric ground state, hence $F_{1...4}$ are equivalent, and we can choose

$$V_{ijk}^{\mathrm{NNLO}} = F_1 (q_i^2 + q_j^2 + q_k^2) \, . \qquad (6)$$

NNN interactions

- r-space — LO+NLO *NNN* potential:

$$V_{ijk} = \left[B_1 + B_2 \frac{1}{\sigma^2}\left(r_{ij}^2 + r_{ik}^2 + r_{jk}^2\right)\right] \exp\left(-\frac{1}{2\sigma^2}\left(r_{ij}^2 + r_{ik}^2 + r_{jk}^2\right)\right) \tag{7}$$

- CSB *NNN* force needed to renormalise the *pp* Coulomb interaction (counted as $\alpha_{\mathrm{em}} M/m_\pi$) Vanasse (2014)
- we include the Coulomb, hence we will also include the CSB *NNN* force:

$$V_{ppx}^{\mathrm{CSB}} = B_{\mathrm{CSB}} \exp\left(-\frac{1}{2\sigma^2}\left(r_{ij}^2 + r_{ik}^2 + r_{jk}^2\right)\right) \tag{8}$$

- changes the strength of the LO *NNN* interaction if any two of the interacting nucleons are protons

Strategy

- we have seven parameters $A_{1..7}$ in the *NN* potential and three parameters $B_{1,2}$, $B_{\rm CSB}$ in the *NNN* potential
- observables we want to fit at this order:
  - *NN*: $a^{pn}_{^1S_0}$, $a^{pn}_{^3S_1}$, $r^{pn}_{^1S_0}$, $r^{pn}_{^3S_1}$, ϵ_1
  - *NNN*: $E(^3\text{H})$, $E(^3\text{He})$
- *P*-wave phase shifts are of higher orders and have to be small

— constraints: Born scattering amplitude is zero at a small finite momentum $k = 0.4\ \text{fm}^{-1}$ in all *P*-waves

$$\langle \psi_1 |\, V_{I=0}\, | \psi_1 \rangle = \langle \psi_1 |\, V_{I=1}\, | \psi_1 \rangle = 0\,. \tag{9}$$

— no tensor interaction in $I = 1$ state, hence all triplet *P*-waves are the same at this order

- strategy:
  - fit *NN* potential to the *NN* data
  - take B_1 arbitrary, B_2 fit to triton energy, $B_{\rm CSB}$ fit to ^{3}He energy

— correlation lines

- investigate how the parameters of ^{4}He (and three-nucleon parameters other than energies) flow along these correlation lines
- methods:
  - two-body: Kohn Variational Method Kohn (1948), Miller, Jansen op de Haar (1987)
  - many-body: Stochastic Variational Method Varga, Suzuki (1998)

Stochastic Variational Method

- based on a stochastic trial algorithm
- can be expressed in a Gaussian basis
- easily scalable and accurate
- best for ground states — excited states need extra care

Hamiltonian of N nucleons

$$H = T + V = \sum_{i=1}^{N} \frac{p_i^2}{2M_i} + \sum_{i<j}^{N} V_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j) + \sum_{i<j<k}^{N} V_{ijk}(\boldsymbol{r}_i - \boldsymbol{r}_j, \boldsymbol{r}_k - \boldsymbol{r}_j) \tag{10}$$

Trial function

$$|\Psi_0\rangle = \sum_i c_i\, |\psi_i\rangle = \sum_i c_i \left| \psi^{\alpha_i}_{JJL_iS_i}(\mathrm{A}_i, u_i, K_i) \right\rangle \tag{11}$$

Basis functions for the system of N nucleons:

$$\left| \psi^{\alpha}_{JJ_ZLS}(\mathrm{A}, u, K) \right\rangle = \sum_{M,S_Z} C^{JJ_Z}_{LMSS_Z}\, |f_{KLM}\rangle_{\mathrm{A},u} \left| \chi^{\alpha}_{SS_Z} \right\rangle$$

$$\langle \{\boldsymbol{x}\} |\, f_{KLM}\rangle_{\mathrm{A},u} = f_{KLM}(\{\boldsymbol{x}\}, \mathrm{A}, u) = v^{2K}\, \mathbb{Y}_{LM}(\boldsymbol{v}) \exp\left(-\frac{1}{2} \mathrm{A}^{ij} \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{x}_j \right) \tag{12}$$

- $\{\boldsymbol{x}\} = \{\boldsymbol{x}_i,\ i = 1, \ldots, N-1\}$ are the Jacobi coordinates
- A is a symmetric positive-definite $(N-1) \times (N-1)$ matrix
- $\mathbb{Y}_{LM}(\boldsymbol{v}) = v^L Y_{LM}(\hat{\boldsymbol{v}})$, with $\boldsymbol{v} = \sum_i u^i \boldsymbol{x}_i$
- the "direction vector" $u = \left(u^i,\ i = 1, \ldots, N-1\right)$ encodes angular dependence of the w.f.

Stochastic Variational Method

- we look for the lowest eigenvalue E_0 of the generalised eigenvalue problem

$$\mathrm{H}^{ij} c_j = E \mathrm{N}^{ij} c_j , \quad i, j = 1, \ldots, m , \tag{13}$$

where H and N are the Hamiltonian and overlap matrices in the current basis,

$$\mathrm{H}^{ij} = \left\langle \psi_i \middle| H \middle| \psi_j \right\rangle , \quad \mathrm{N}^{ij} = \left\langle \psi_i \middle| \psi_j \right\rangle \tag{14}$$

N is not a diagonal matrix since the basis states are not orthogonal

- in a Gaussian basis with Gaussian potentials, H_{ij} and N_{ij} are easily expressed algebraically via A, A^{-1}, $\boldsymbol{v}$, and other parameters of the w.f.

$$\langle \{\boldsymbol{x}\} | \, f_{KLM} \rangle_{\mathrm{A},u} = f_{KLM}(\{\boldsymbol{x}\}, \mathrm{A}, u) = v^{2K} \mathbb{Y}_{LM}(\boldsymbol{v}) \exp\left(-\frac{1}{2} \mathrm{A}^{ij} \boldsymbol{x}_i^{\mathrm{T}} \boldsymbol{x}_j \right) \tag{15}$$

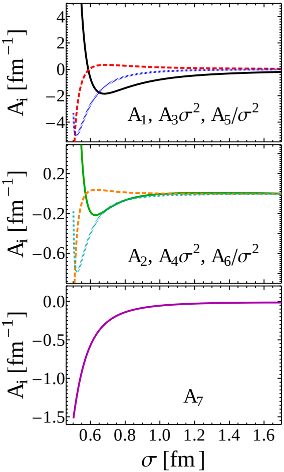
- A^{-1} positive definite — can be inverted efficiently (e.g., Cholesky decomposition)
- a single state is added — a very efficient method for solving the eigenvalue problem with $m+1$ basis states
- efficient trial strategy: adding one state after another
- can lead to very large basis sizes — basis refinement (time to time, remove states that are less useful)

- typical times on a regular PC: 0.5..2 hours for 3N, 3..18 hours for 4N
- can be parallelized

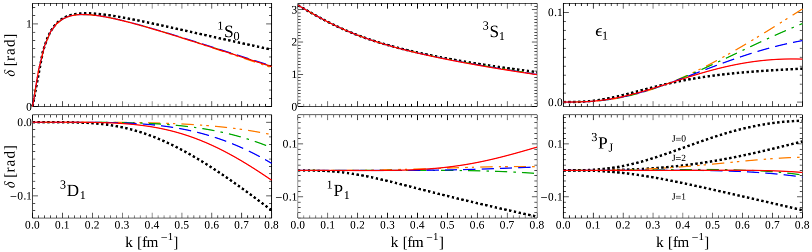
Two nucleons: *NN* potential

$$V_{ij} = G(r,\sigma)\left(A_1 + A_2\boldsymbol{\tau_i}\cdot\boldsymbol{\tau_j}\right) + r^2 G(r,\sigma)\left(A_3 + A_4\boldsymbol{\tau_i}\cdot\boldsymbol{\tau_j}\right) + \left\{\nabla^2, G(r,\sigma)\right\}\left(A_5 + A_6\boldsymbol{\tau_i}\cdot\boldsymbol{\tau_j}\right)$$
$$+ G(r,\sigma)A_7\left(1 - \boldsymbol{\tau_i}\cdot\boldsymbol{\tau_j}\right)\left[3(\hat{\boldsymbol{r}}\cdot\boldsymbol{\sigma}_i)(\hat{\boldsymbol{r}}\cdot\boldsymbol{\sigma}_j) - (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)\right] \quad (16)$$

- solve the Lippman-Schwinger equation;
- fit A_i to the data:
  $a^{pn}_{^1S_0} = -23.75$ fm, $a^{pn}_{^3S_1} = 5.42$ fm,
  $r^{pn}_{^1S_0} = 2.81$ fm, $r^{pn}_{^3S_1} = 1.76$ fm,
  $\epsilon_1 = 1.1592^\circ$ at $T_{\rm lab} = 10$ MeV
- + the *P*-wave constraints
- 5 parameters, 5 numbers to fit
- works fine at soft cutoffs
- issues expected (and seen) at short cutoffs $\sigma \lesssim 0.6$ fm



Two nucleons: phase shifts



- shown at $\sigma = 0.6, 0.8, 1.0, 1.2$ fm, in comparison with PWA93
- works well up to $T_{lab} \sim$ 20MeV
- $^3S_1$ phase shift is very well reproduced at all energies
- deuteron bound state is at the right position too

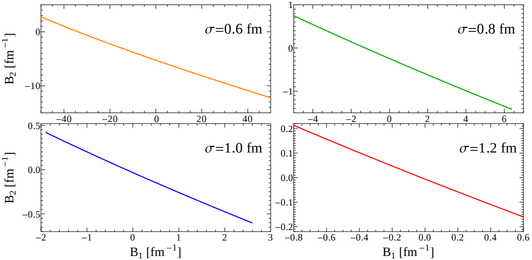
Range σ [fm]	0.6	0.8	1.0	1.2	exp.
Energy [MeV]	−2.207	−2.207	−2.204	−2.198	−2.224

- *P*-wave phase shifts are well constrained (again, hints of possible issues at $\sigma = 0.6$ fm)
- $^3D_1$ phase shift is not constrained but is small at low energies

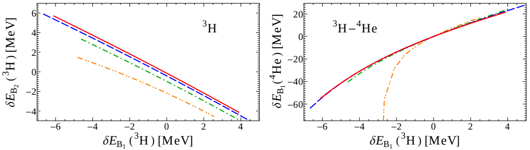
— it works well for *NN*!

Three and four nucleons: correlations

- fit B_1 and B_2 so that $E(^3\mathrm{H}) = -8.48$ MeV
- correlation lines
- ^{3}H is underbound by *NN* forces only
- different σ's:
  – very different scales of B_1 and B_2
  – yet similar LO and NLO *NNN* contributions to the g.s. energy (below)



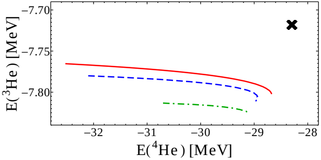
- ^{3}H – ^{4}He correlations:
  – analogy of the Tjon line
  (no CSB *NNN* forces included yet)
- $\sigma = 0.6$ fm blows up in ^{4}He:
  – gigantic LO *NNN* contribution
  – cancellation with NLO *NNN* cannot be expected to occur!

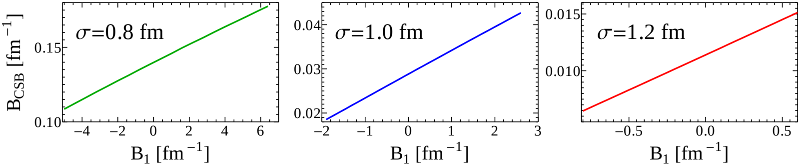


— $\sigma = 0.6$ fm is too short to work!
— we don't consider it in the following

Three and four nucleons: CSB *NNN* force

- no CSB *NNN* force included here
- both ^{3}He and ^{4}He are overbound (the former only slightly)
- fit CSB *NNN* force to reproduce $E(^3\mathrm{He}) = -7.718$ MeV
  - can be done perturbatively
- ^{4}He energy is shifted up too
  - still slightly overbound





- linear correlation between B_{CSB} and B_1
- CSB *NNN* force is very small (about 10% of the LO *NNN* force)
- ^{3}He – ^{4}He correlation picture is uninformative ($E(^3\mathrm{He})$ fixed)
- look at other observables, namely, charge radii, to identify *NNN* parameters that give close-to-physical results

Three and four nucleons: charge radii

- with the SVM wave function, it is easy to calculate charge radii:

$$F_C(q^2) = \frac{1}{Z} \langle +\boldsymbol{q}/2 |\, J^0_{\rm em}(\boldsymbol{q}) \,| -\boldsymbol{q}/2 \rangle \ , \qquad F_C(q^2) = 1 - \frac{q^2 r^2_{\rm ch}}{6} + \ldots \ ; \tag{17}$$

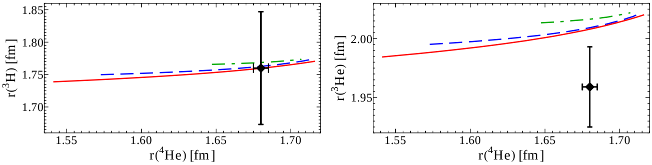
- LO (Q^{-0}) result:

$$r^2_{\rm ch} = \frac{1}{Z} \langle \Psi_0 | \sum_{j=1}^{A} \frac{1}{2} (1+\tau_3)_j \, \boldsymbol{r}^2_j \, | \Psi_0 \rangle + r^2_p + \frac{3}{4M^2} + \frac{N}{Z} r^2_n \tag{18}$$

  Z protons and $N = A - Z$ neutrons
  $r_p = 0.8751$ fm — proton charge radius, $r^2_n = -0.1161$ fm^2 — neutron charge radius squared

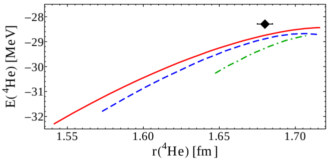
- no corrections at NLO (Q^1)
- NNLO (Q^2): relativistic corrections
  - Foldy correction; vertices and propagators recoils
  - dimensional estimate: $\delta r_{\rm ch} \sim C/M \sim 0.01$ fm
  - very small for the deuteron Chen (1999)
  - estimated by calculating vertex recoils: $\delta r_{\rm ch} \lesssim 0.003$ fm for ^{4}He, even less for ^{3}H, ^{3}He
- two-nucleon contributions start at N^{3}LO (Q^3) Valderrama (2014)

Three and four nucleons: charge radii correlations



- ^{3}H charge radius is in agreement for all *NNN* potentials
- ^{3}He charge radius is somewhat larger, in particular at the point where $r_{\rm ch}(^4\text{He}) = r_{\rm ch}^{\rm exp}(^4\text{He})$
- ^{3}He discrepancy never larger than 2 std. deviations
- cutoff dependence of 3N charge radii is very small (less than 2 % effect)

- $r_{\rm ch}(^4\text{He})$ decreases with increasing binding energy (as expected)
- the residual cutoff dependence of $E(^4\text{He})$ gives an uncertainty estimate of 0.5..1 MeV
- at the point where $r_{\rm ch}(^4\text{He}) = r_{\rm ch}^{\rm exp}(^4\text{He})$, alpha is overbound by $\sim$ 0.5 MeV
- this is about 2% of the binding energy and within the expected uncertainty



Summary and outlook

- model gives excellent agreement with experiment for $A = 3$ nuclei
- CSB *NNN* corrections are very small
- study of correlations:

— there is also a range of parameters where both $A = 3$ and $A = 4$ nuclei are in agreement

- short range cutoffs cause a lot of trouble, more so in denser nuclei, especially ^{4}He

- working on heavier nuclei (parallelization is essential)

- we used SU(4) symmetry to limit the number of NNLO *NNN* parameters

— will not in general work for heavier nuclei

— need to study scattering of nucleons by the deuteron and $A = 3$ nuclei

- combine Kohn variational method and the SVM