Nuclear Green's function Monte Carlo with chiral forces

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with
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Physics of exotic nuclei: Theoretical advances and challenges

Outline

1. Motivation
   - *Ab-initio* calculations for nuclei
   - Nuclear interactions
     - Phenomenology
     - Chiral Effective Field Theory
2. Results
   - $A \leq 4$ binding energies
   - $A \leq 4$ radii
   - Perturbative calculations
   - Distributions
3. Conclusion
   - Summary
   - Future work
   - Acknowledgments

Nuclear structure methods: solving the many-body Schrödinger equation

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle .$$

Looks innocent, but "Nuclear physics is hard!"
$2^A\binom{A}{Z}$ coupled differential equations in $3A-3$ variables.
^{12}C:$\rightarrow$3 784 704 equations in 33 variables.

Green's function Monte Carlo (GFMC): propagate in imaginary time to project out the ground state.

$$\left|\Psi(t)\right\rangle = e^{-(H-E_T)t}\left|\Psi_T\right\rangle \Rightarrow \lim_{t\to\infty}\left|\Psi(t)\right\rangle \propto \left|\Psi_0\right\rangle .$$

The trial wave function is a symmetrized product of correlation operators acting on a Jastrow wave function.

Trial Wave Function

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+U_{ij})\right]|\Psi_J\rangle \,,$$

$$U_{ij} = \sum_{p=2}^{m} u_p(r_{ij})\,O^p_{ij}, \;\; |\Psi_J\rangle = \prod_{i<j} f_c(r_{ij})\,|\Phi_A\rangle \,,$$

$$|\Phi_4\rangle = \mathcal{A}\,|p\!\uparrow p\!\downarrow n\!\uparrow n\!\downarrow\rangle \,,$$

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+u_\sigma(r_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + u_{t\tau}(r_{ij})S_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)\right]\prod_{i<j} f_c(r_{ij})\,|\Phi_4\rangle$$

The wave function is imperfect: $\Psi_T = c_0\Psi_0 + \sum_{i\neq 0} c_i\Psi_i$.

Propagate in imaginary time to project out the ground state Ψ_0:

$$\Psi(t) = e^{-(H-E_T)t}\Psi_T = e^{-(E_0-E_T)t}\left[c_0\Psi_0 + \sum_{i\neq 0} c_i e^{-(E_i-E_0)t}\Psi_i\right]$$

$$\Rightarrow \lim_{t\to\infty}\Psi(t) \propto \Psi_0.$$

A cartoon

$$H = \frac{p_x^2}{2m} + V(x),\ \ V = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

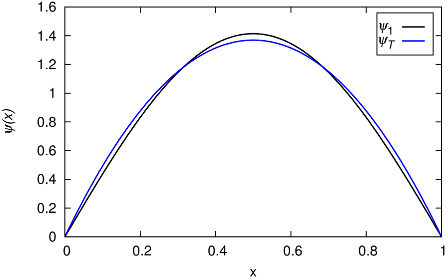
$$\hbar = m = L = 1$$

Solution

$$\psi_n(x) = \sqrt{2}\sin(n\pi x),\ \ E_n = \frac{n^2\pi^2}{2}.$$

"Trial wave function."

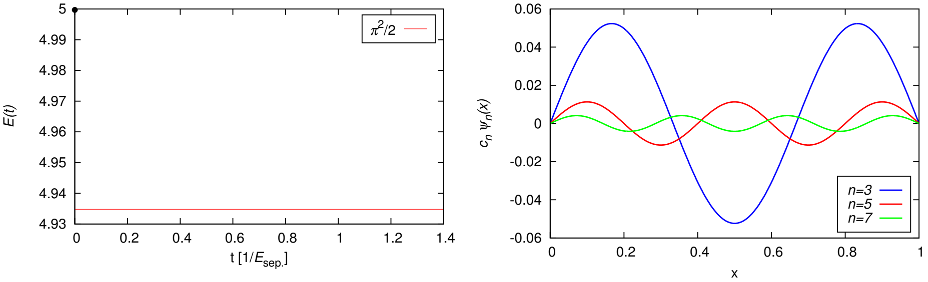
$$\psi_T(x) = -\sqrt{30}\left[\left(x - \frac{1}{2}\right)^2 - \frac{1}{4}\right].$$



A cartoon

$$E(t) = \frac{\langle \psi_T | H e^{-(H-E_1)t} | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_1)t} | \psi_T \rangle}, \qquad \psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

$$t = 0.0(1/E_{\text{sep.}})$$



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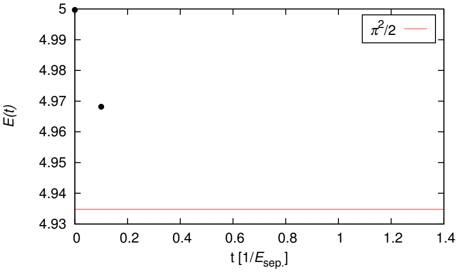

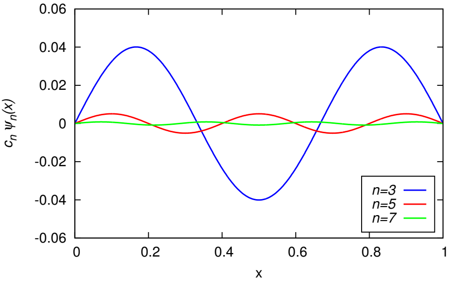

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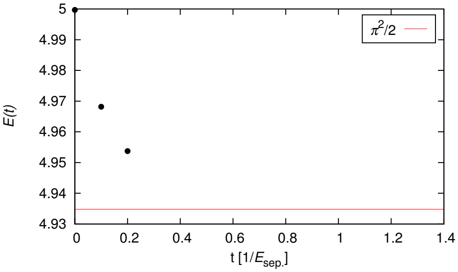

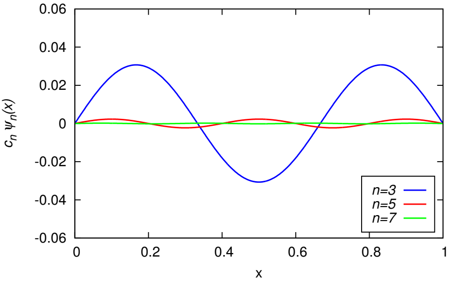

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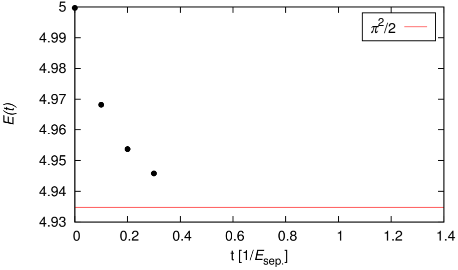

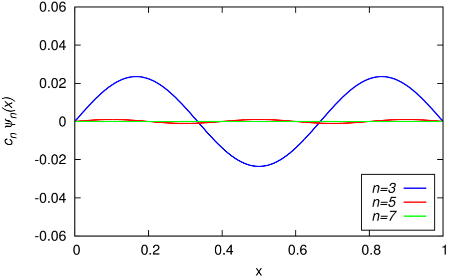

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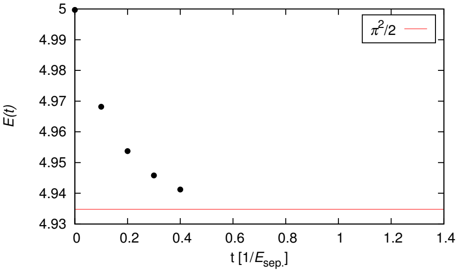

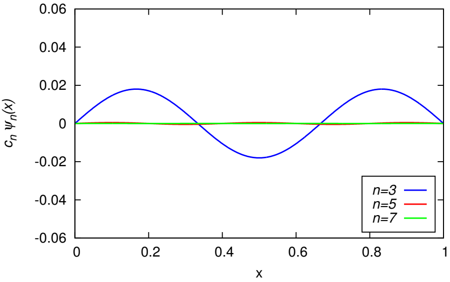

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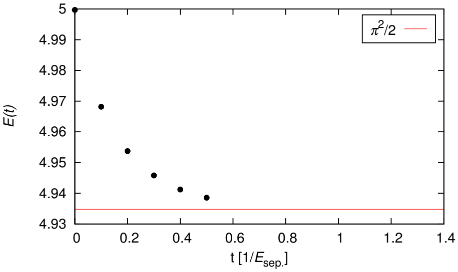

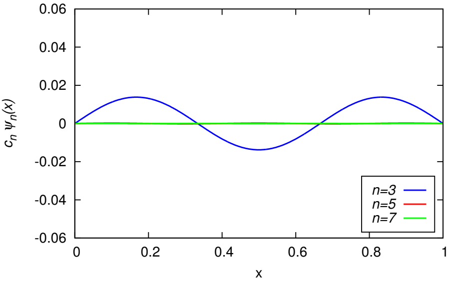

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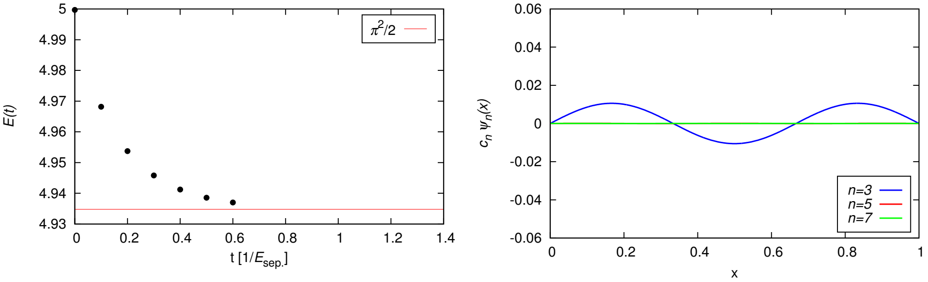

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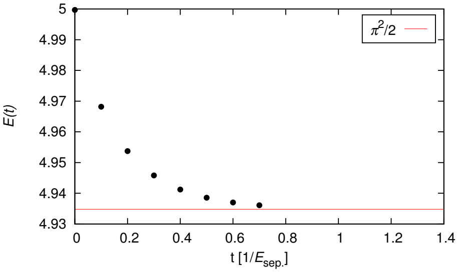

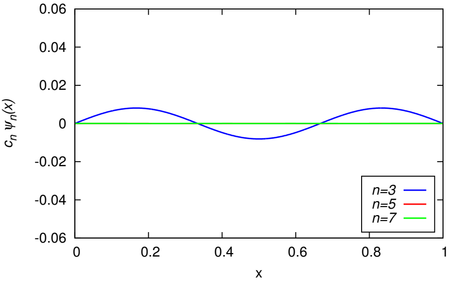

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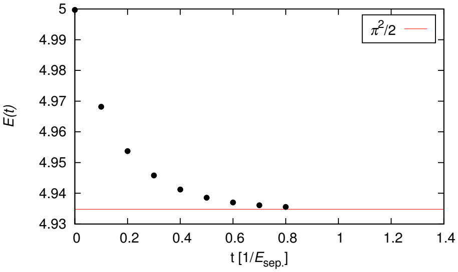
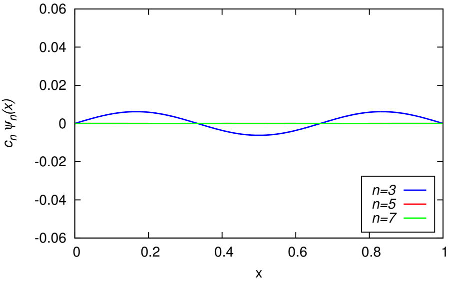
$$t = 0.8(1/E_{\text{sep.}})$$





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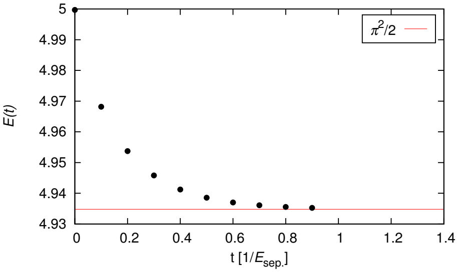
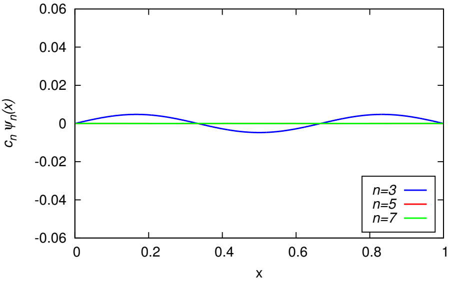
$$t = 0.9(1/E_{\text{sep.}})$$





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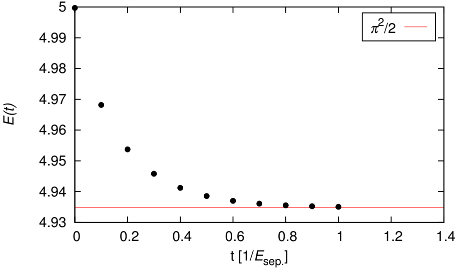

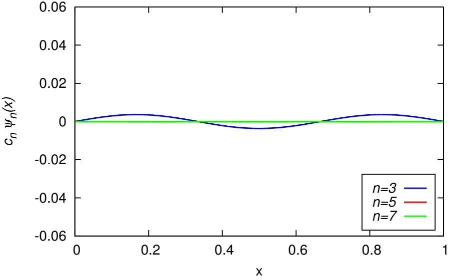

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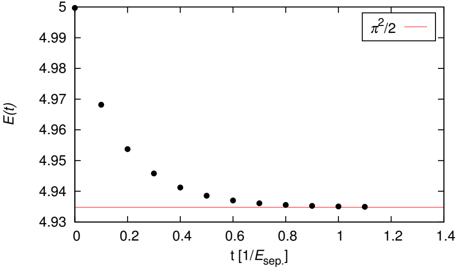

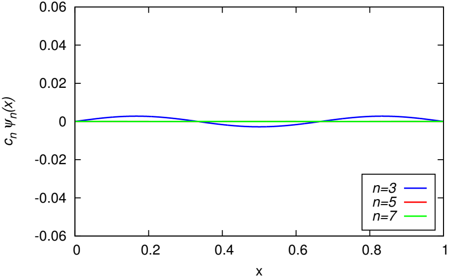

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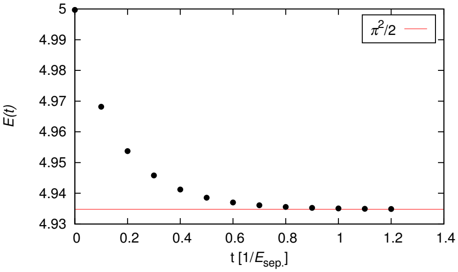

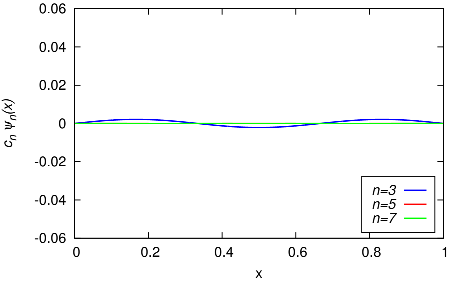

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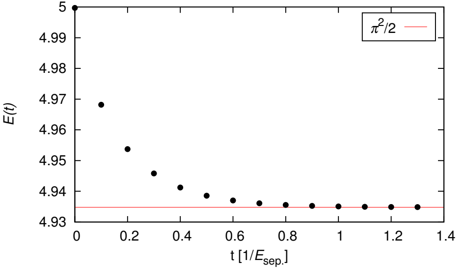

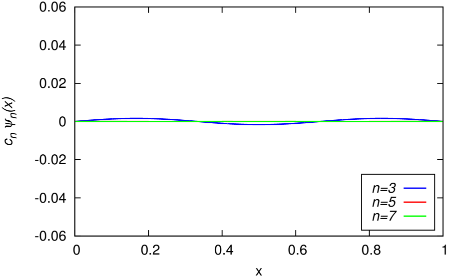

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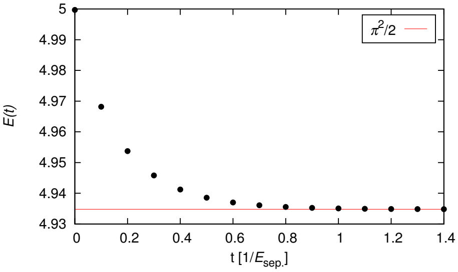

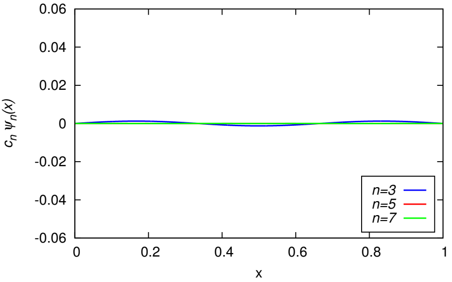

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Limitations

A so-called "walker" consists of the $3A$ positions and $2^A\binom{A}{Z}$ spin-isospin states (in the charge basis).

^{12}C:$\rightarrow$Remember 3 784 704 spin-isospin states!

However: Recall Stefano's talk.

We can calculate "mixed estimates": $\frac{\langle\Psi(t)|O|\Psi_T\rangle}{\langle\Psi(t)|\Psi_T\rangle}$

$$\langle O(t)\rangle = \frac{\langle\Psi(t)|O|\Psi(t)\rangle}{\langle\Psi(t)|\Psi(t)\rangle} \approx \langle O(t)\rangle_{\text{Mixed}} + [\langle O(t)\rangle_{\text{Mixed}} - \langle O\rangle_T].$$

However

For ground-state energies, $O = H$, and $[H, G] = 0$:

$$\langle H \rangle_{\text{Mixed}} = \frac{\langle \Psi_T | e^{-(H-E_T)t/2} H e^{-(H-E_T)t/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)t/2} e^{-(H-E_T)t/2} | \Psi_T \rangle}, \qquad \lim_{t \to \infty} \langle H \rangle_{\text{Mixed}} = E_0.$$

Motivation

Nuclear interactions - The Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \cdots$$

The focus of this talk is on the two-body interaction. Until recently, there were two broad choices for v_{ij}.

- Local, real-space, phenomenological: Argonne's v_{18}[1] - informed by theory, phenomenology, and experiment (well tested and very successful).
- Non-local, momentum-space, effective field theory (EFT): N^3LO[2] - informed by chiral EFT and experiment (well liked and often used in basis-set methods, such as the no-core shell model).

[1] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[2] e.g. D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (2003)

Motivation

Nuclear interactions - Argonne's v_{18}

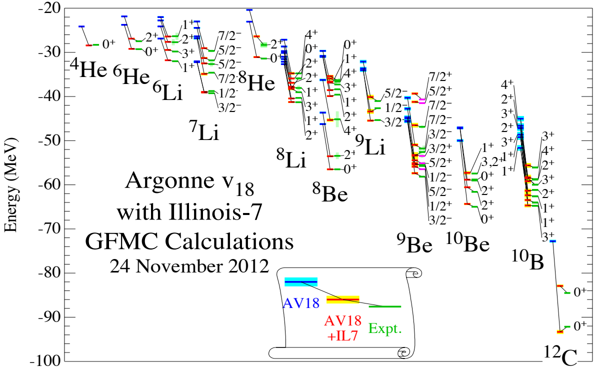
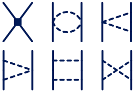
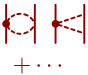
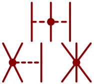
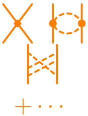


Figure 1 : Many excellent results using Green's function Monte Carlo (GFMC) and phenomenological potentials. From http://www.phy.anl.gov/theory.

This is great! But... Until recently the nucleon-nucleon potentials used have been restricted to the phenomenological Argonne-Urbana/Illinois family of interactions.

Motivation

Nuclear interactions - Chiral EFT

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$		

- Chiral EFT is an expansion in powers of Q/Λ_b.
  $Q \sim m_\pi \sim 100$ MeV;
  $\Lambda_b \sim 800$ MeV.
- Long-range physics: given explicitly (no parameters to fit) by pion-exchanges.
- Short-range physics: parametrized through contact interactions with low-energy constants (LECs) fit to low-energy data.
- Many-body forces enter systematically and are related via the same LECs.

Motivation

Nuclear interactions - Chiral EFT

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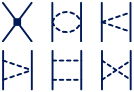
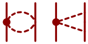
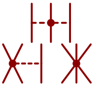
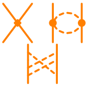
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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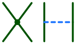
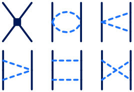
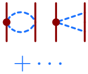
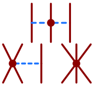
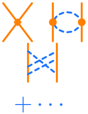
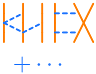
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$		

- Chiral EFT is an expansion in powers of Q/Λ_b.
  $Q \sim m_\pi \sim 100$ MeV;
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- Short-range physics: parametrized through contact interactions with low-energy constants (LECs) fit to low-energy data.
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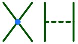
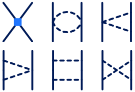
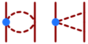
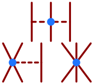
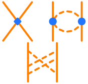
Motivation

Nuclear interactions - Chiral EFT

		NN	NNN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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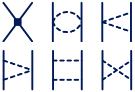
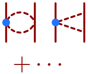
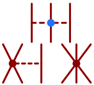
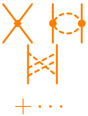
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		
N^3LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$		

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Nuclear interactions - Chiral EFT

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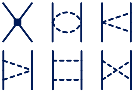
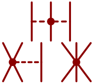
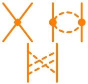
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
$\mathrm{N^2LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
$\mathrm{N^3LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

Local construction possible up to $\mathrm{N^2LO}$.

- Regulator:
  ~~$f(p,p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$~~ $\rightarrow$
  $f_{\mathrm{long}}(r) = 1 - e^{-(r/R_0)^4}$.
- Choose contacts $\propto \mathbf{q}$.
- Long-range potential:
  $V(r) \supset V_C(r) + V_S(r)\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$,
  $V_C(r) \propto \int_{2m_\pi}^{\tilde{\Lambda}} d\mu \mu e^{-\mu r} \rho_C(\mu)$,
  etc. SFR cutoff.

Local chiral EFT potential ∼ a v_7 potential

$$v_{ij} = \sum_{p=1}^{7} v_p(r_{ij}) O^p_{ij} + \sum_{p=15}^{18} v_p(r_{ij}) O^p_{ij}.$$

Charge-independent operators

$$O_{ij}^{p=1,14} = \left[1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}, \mathbf{L}\cdot\mathbf{S}, \mathbf{L}^2, \mathbf{L}^2(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j), (\mathbf{L}\cdot\mathbf{S})^2\right] \otimes \left[1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\right].$$

Charge-independence-breaking operators

$$O_{ij}^{p=15,18} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes T_{ij}, \text{ and } (\tau_{zi} + \tau_{zj}).$$

Tensor operators

$$S_{ij} = 3(\boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij})(\boldsymbol{\sigma}_j \cdot \hat{\mathbf{r}}_{ij}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,\ T_{ij} = 3\tau_{zi}\tau_{zj} - \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

Motivation

Nuclear interactions - Chiral EFT

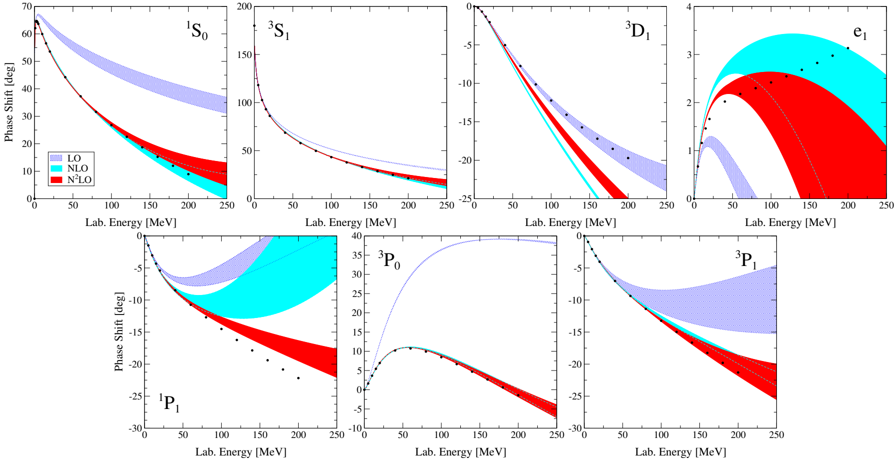


Figure 2 : Phase shifts for the *np* potential. From A. Gezerlis et al. (2014) arXiv:1406.0454 [nucl-th]

Results

$A = 3$ binding energies - $\langle H \rangle$

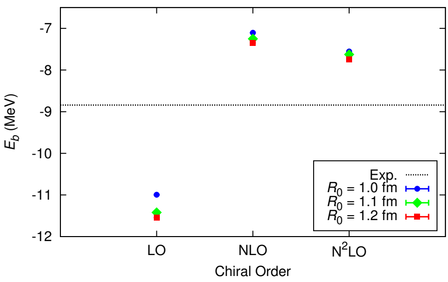


Figure 3 : ^{3}H binding energy at different chiral orders and cutoff values.

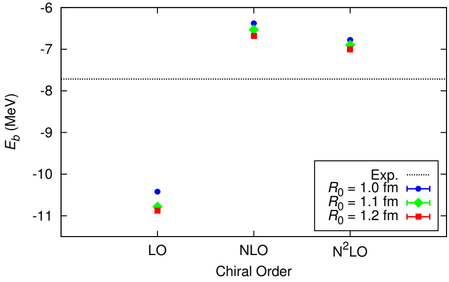


Figure 4 : ^{3}He binding energy at different chiral orders and cutoff values.

Results

^{4}He binding energies - $\langle H \rangle$

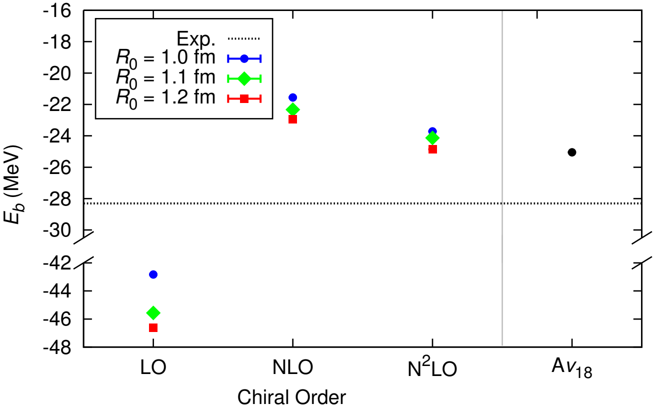


Figure 5 : ^{4}He binding energy at different chiral orders and cutoff values.

Results

^{4}He binding energies - $\langle H \rangle$

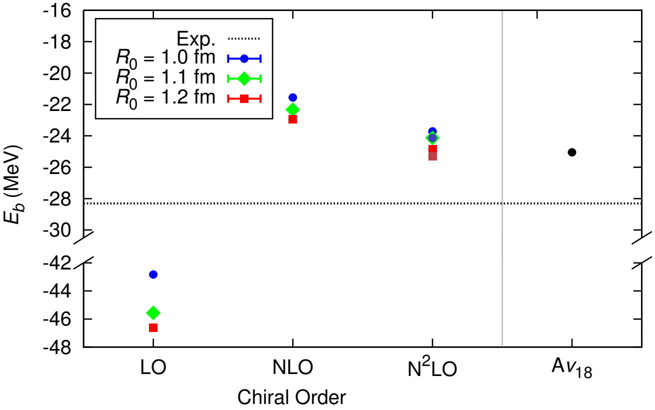


Figure 5 : ^{4}He binding energy at different chiral orders and cutoff values. SFR dependence weak.

Results

$A = 3$ radii - $r^2_{\text{pt.}} = r^2_{\text{ch.}} - r^2_p - \frac{N}{Z} r^2_n$

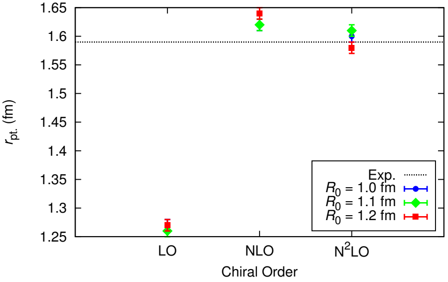


Figure 6 : ^{3}H radii at different chiral orders and cutoff values.

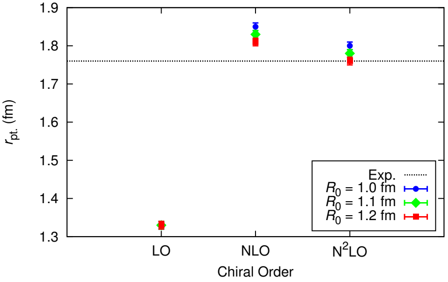


Figure 7 : ^{3}He radii at different chiral orders and cutoff values.

Results

^{4}He radii - $r^2_{\text{pt.}} = r^2_{\text{ch.}} - r^2_p - \frac{N}{Z} r^2_n$

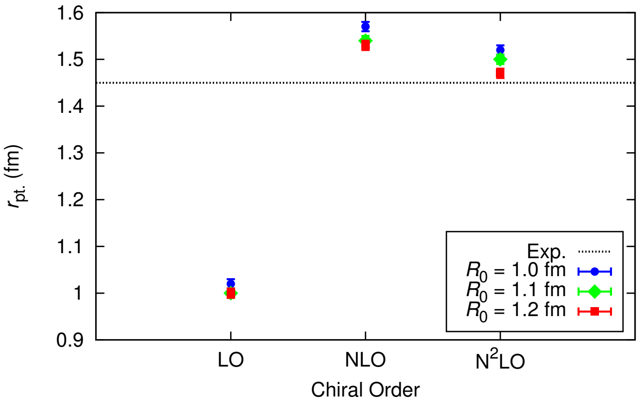


Figure 8 : ^{4}He radii at different chiral orders and cutoff values.

Results

^{4}He perturbation - $\langle \Psi_{\rm NLO} | H_{\rm N^2LO} | \Psi_{\rm NLO} \rangle$

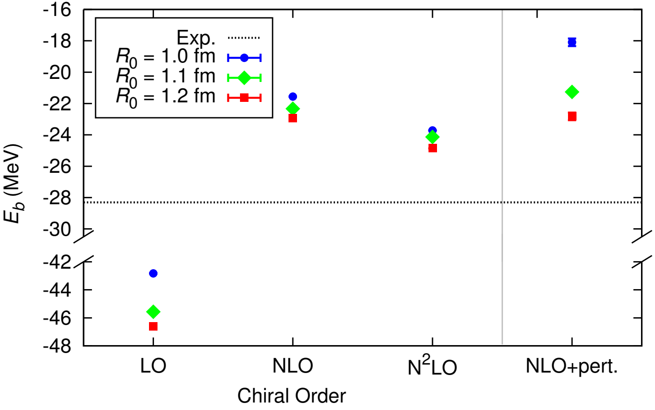


Figure 9 : ^{4}He binding energy at different chiral orders and cutoff values plus a first-order perturbative calculation of $\langle H_{\rm N^2LO} \rangle$.

Hints from the deuteron.

- Write $H \rightarrow \langle k' J M_J L' S | H | k J M_J L S \rangle$.
- Diagonalize$\rightarrow \{\psi_D^{(i)}(r)\}$.
- Second- and third-order perturbation calculations possible.

Table 1 : Perturbation calculations for ^{2}H with different cutoff values for R_0.

Calculation	E_b (MeV)		
	$R_0 = 1.0$ fm	$R_0 = 1.1$ fm	$R_0 = 1.2$ fm
$E^{(0)}_{0\,(\mathrm{NLO})}$	-2.15	-2.16	-2.16
$E^{(0)}_{0\,(\mathrm{NLO})} + V^{(1)}_{\mathrm{pert.}}$	-1.44	-1.80	-1.90
$E^{(0)}_{0\,(\mathrm{NLO})} + V^{(2)}_{\mathrm{pert.}}$	-2.11	-2.17	-2.18
$E^{(0)}_{0\,(\mathrm{NLO})} + V^{(3)}_{\mathrm{pert.}}$	-2.13	-2.18	-2.19
$E^{(0)}_{0\,(\mathrm{N^2LO})}$	-2.21	-2.21	-2.20

Proton distribution: $\rho_{1,p}(r) = \frac{1}{4\pi r^2}\langle\Psi|\sum_i \frac{1+\tau_z(i)}{2}\delta(r - |\mathbf{r}_i - \mathbf{R}_{\text{c.m.}}|)|\Psi\rangle.$

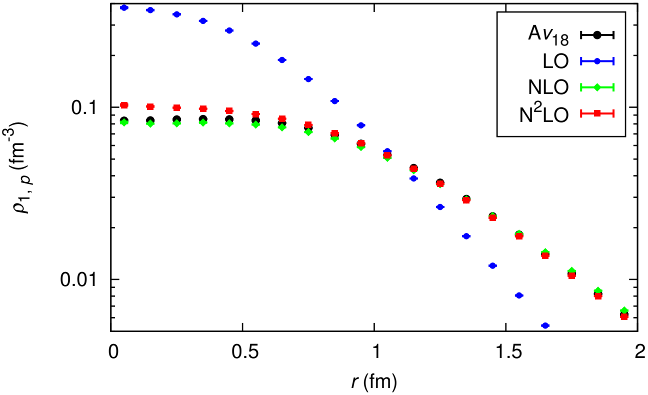


Figure 10 : ^{4}He proton distribution at different chiral orders.

Results

Distributions - ^{4}He

Two-body $T = 1$ distribution:

$$\rho_2^{(T=1)}(r) = \frac{1}{4\pi r^2}\langle\Psi|\sum_{i<j}\frac{3+\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j}{4}\delta(r-|\mathbf{r}_{ij}|)|\Psi\rangle.$$

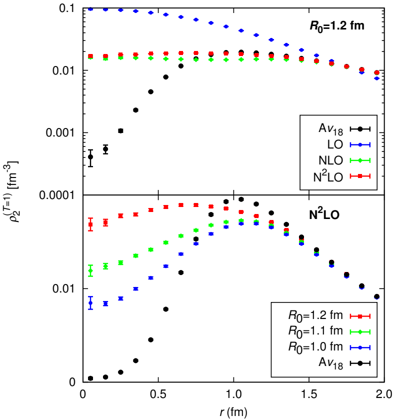


Figure 11 : ^{4}He two-body $T = 1$ distributions.

Coulomb Sum Rule: $S_L(q) = 1 + \rho_{LL}(q) - Z|F_L(q)|^2$;

$$\rho_{LL}(q) \propto \int d^3 r j_0(qr) \rho_2^{(T=1)}(r).$$

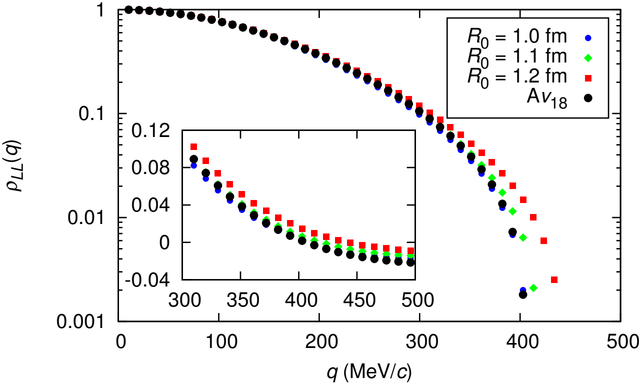


Figure 12 : (PRELIMINARY) Fourier transform of the two-body distributions.

Conclusion

Summary

- Nuclear structure calculations probe nuclear Hamiltonians.
  - Phenomenological potentials have been very successful but are perhaps unsatisfactory.
  - Chiral EFT potentials have a more direct connection to QCD, but until now, have been non-local.
- GFMC calculations of light nuclei are now possible with chiral EFT interactions.
- Binding energies at N^2LO are reasonably similar to results for two-body-only phenomenological potentials.
- Radii show expected trends.
- The softest of the potentials with $R_0 = 1.2$ fm is more perturbative in the difference between N^2LO and NLO.
- The high-momentum (short-range) behavior of chiral EFT interactions is distinct from the phenomenological interactions.

- Include 3-nucleon force which appears at N^2LO.
- Include 2-nucleon force at N^3LO (which will be non-local).
- Extend to larger nuclei with $4 < A \leq 12$.
- Second-order perturbation calculation in GFMC.
- Study of, for example, Coulomb sum rule to probe possible consequences of different short-range behavior.

Status.
Include 3-nucleon force which appears at N^2LO. (Work in progress with Ingo Tews of Darmstadt). Plan:

- Include the spin-isospin structures coming from chiral EFT. Done at the VMC level.
- Fit c_D and c_E.
- Calculate larger nuclei and light reactions.
- Work with Stefano to include these forces in AFDMC calculations of neutron matter (and nuclei).

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NUCLEI

Nuclear Computational Low-Energy Initiative