Quantum Monte Carlo calculations of pions and nucleons

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Why add pions?

- In nuclear structure calculations pions are often (usually) integrated out and replaced by an instantaneous interaction.
- Here we want to include the pion degrees of freedom.
  - Test the instantaneous approximation.
  - Obtain the induced three-body interactions, (and add Delta degrees of freedom later)
  - Study pion-nucleon scattering.
  - Simplify calculation of currents.
  - Possibility to lead to simplifed calculations (like 3-body).
- Develop low variance methods to add relativistic boson fields to world line nucleon simulations.

Keeping pions

- Known for many decades that pions mainly have an axial-vector coupling to nuclei.
- This is an $i\gamma^5$ coupling which for nonrelativistic nucleons becomes for a nucleon at position $\boldsymbol{r}$,

$$[\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}][\boldsymbol{\tau} \cdot \boldsymbol{\pi}(\boldsymbol{r})]$$

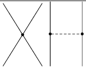
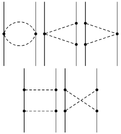
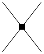
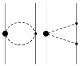
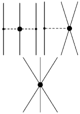
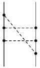
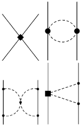
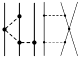
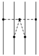
- More modern formalism uses chiral effective field theory.
- Here we expand, keep nonrelativistic nucleons, keep quadratic terms in pion fields.

Lagrangian density

$$
\begin{aligned}
\mathcal{L}_0 = {} & \frac{1}{2}\partial_\mu \pi_i \partial^\mu \pi_i - \frac{1}{2} m_\pi^2 \pi_i \pi_i + N^\dagger \Big[i\partial_0 + \frac{\nabla^2}{2M_0} \\
& - \frac{1}{4f_\pi^2}\epsilon_{ijk}\tau_i \pi_j \partial_0 \pi_k - \frac{g_A}{2f_\pi}\tau_i \sigma^j \partial_j \pi_i - M_0 \Big] N \\
& - \frac{1}{2} C_S (N^\dagger N)(N^\dagger N) - \frac{1}{2} C_T (N^\dagger \sigma_i N)(N^\dagger \sigma_i N)\,,
\end{aligned}
$$

m_π is the pion mass, M_0 is the bare nucleon mass, $f_\pi = 92$ MeV is the pion decay constant, $g_A = 1.26$ is the nucleon axial-vector coupling constant, C_S and C_T are low-energy constants, and $i = x, y, z$.

Comparison to chiral effective field theory nucleon potentials

	2N Force		3N Force		4N Force	
	Present	Not Present	Present	Not Present	Present	Not Present
LO						
NLO						
N2LO						
N3LO						

Avoiding a real-space lattice

- We could use a real-space lattice to define the pion field theory.
- One goal is to see the changes that pions make on our Green's function Monte Carlo or Auxiliary field diffusion Monte Carlo results.
- Since our nucleons move in the continuum, we would prefer to avoid a real-space lattice for pions.
- Defining and calculating the field theory in free space is possible, but it is simpler to calcuate in a periodic box.
- We transform to field oscillators ($\sim$ momentum states in the periodic box).

Pion mode amplitudes

- Take cubic box of side L

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \text{ with } n_i = 0, \pm 1, \pm 2, \dots$$

- Expand in plane waves.
  $\Pi_i(\boldsymbol{x})$ is the momentum conjugate to $\pi(\boldsymbol{x})$.

$$\pi_i(\boldsymbol{x}) = \frac{1}{\sqrt{L^3}} \sum_{\boldsymbol{k}} \pi_{i\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}},$$

$$\Pi_i(\boldsymbol{x}) = \frac{1}{\sqrt{L^3}} \sum_{\boldsymbol{k}} \Pi_{i\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}.$$

Standing wave states

- To have real amplitudes we write sine and cosine amplitudes

$$\pi^c_{i\boldsymbol{k}} = \frac{1}{\sqrt{2}}(\pi_{i\boldsymbol{k}} + \pi_{i-\boldsymbol{k}}),$$
$$\pi^s_{i\boldsymbol{k}} = \frac{i}{\sqrt{2}}(\pi_{i\boldsymbol{k}} - \pi_{i-\boldsymbol{k}}),$$

- If we include $\boldsymbol{k}$ we do not include $-\boldsymbol{k}$.
  For $k = 0$ we have $\pi^c_{i0} = \pi_{i0}/\sqrt{2}$ and $\pi^s_{i0} = 0$.
- Our pion canonical variables are:

$$\pi_i(\boldsymbol{x}) = \sqrt{\frac{2}{L^3}}\sum_{\boldsymbol{k}}{}' [\pi^c_{i\boldsymbol{k}} \cos(\boldsymbol{k}\cdot\boldsymbol{x}) + \pi^s_{i\boldsymbol{k}} \sin(\boldsymbol{k}\cdot\boldsymbol{x})],$$
$$\Pi_i(\boldsymbol{x}) = \sqrt{\frac{2}{L^3}}\sum_{\boldsymbol{k}}{}' [\Pi^c_{i\boldsymbol{k}} \cos(\boldsymbol{k}\cdot\boldsymbol{x}) + \Pi^s_{i\boldsymbol{k}} \sin(\boldsymbol{k}\cdot\boldsymbol{x})]\,,$$

Hamiltonian

$$
\begin{aligned}
H &= H_N + H_{\pi\pi} + H_{AV} + H_{WT}, \\
H_N &= \sum_{i=1}^{A} \left[\frac{P_i^2}{2M_P} + M_P + \beta_K P_i^2 + \delta M \right] + \sum_{i<j}^{A} \delta_{k_c}(\boldsymbol{r}_i - \boldsymbol{r}_j)[C_S + C_T \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j], \\
H_{\pi\pi} &= \frac{1}{2} \sum_{\boldsymbol{k}}{}' \left[|\boldsymbol{\Pi}_{\boldsymbol{k}}^c|^2 + \omega_{\boldsymbol{k}}^2 |\boldsymbol{\pi}_{\boldsymbol{k}}^c|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^s|^2 + \omega_{\boldsymbol{k}}^2 |\boldsymbol{\pi}_{\boldsymbol{k}}^s|^2 \right], \\
H_{AV} &= \sum_{i=1}^{A} \frac{g_A}{2f_\pi} \sqrt{\frac{2}{L^3}} \sum_{\boldsymbol{k}}{}' \left\{ \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \left[\boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^s \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i) \; - \; \boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^c \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i) \right] \right\}, \\
H_{WT} &= \sum_{i=1}^{A} \frac{1}{2f_\pi^2 L^3} \boldsymbol{\tau}_i \cdot \left[\sum_{\boldsymbol{k}}{}' \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i) \boldsymbol{\pi}_{\boldsymbol{k}}^c \times \sum_{\boldsymbol{q}}{}' \cos(\boldsymbol{q} \cdot \boldsymbol{r}_i) \boldsymbol{\Pi}_{\boldsymbol{q}}^c \right. \\
&+ \sum_{\boldsymbol{k}}{}' \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i) \boldsymbol{\pi}_{\boldsymbol{k}}^c \times \sum_{\boldsymbol{q}}{}' \sin(\boldsymbol{q} \cdot \boldsymbol{r}_i) \boldsymbol{\Pi}_{\boldsymbol{q}}^s \\
&+ \sum_{\boldsymbol{k}}{}' \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i) \boldsymbol{\pi}_{\boldsymbol{k}}^s \times \sum_{\boldsymbol{q}}{}' \cos(\boldsymbol{q} \cdot \boldsymbol{r}_i) \boldsymbol{\Pi}_{\boldsymbol{q}}^c \\
&+ \left. \sum_{\boldsymbol{k}}{}' \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i) \boldsymbol{\pi}_{\boldsymbol{k}}^s \times \sum_{\boldsymbol{q}}{}' \sin(\boldsymbol{q} \cdot \boldsymbol{r}_i) \boldsymbol{\Pi}_{\boldsymbol{q}}^s \right],
\end{aligned}
$$

Cutoff

$\delta_{k_c}(\boldsymbol{r}_i - \boldsymbol{r}_j)$ is a smeared out delta function for the contact term, which we take to be consistent with the cutoff employed for the pion modes,

$$\delta_{k_c}(\boldsymbol{r}) = \frac{1}{L^3}\left(1 + 2{\sum_{\boldsymbol{k}}}' \cos(\boldsymbol{k}\cdot\boldsymbol{r})\right).$$

We report the cutoff in terms of the maximum ω_k calculated by $\omega_c^s = \sqrt{k_c^2 + m_\pi^2}$, where

$$\frac{4\pi k_c^3}{3} = \left(\frac{2\pi}{L}\right)^3 N_{\boldsymbol{k}},$$

$N_{\boldsymbol{k}}$ being the number of $\boldsymbol{k}$ vectors in the unprimed sums.
Other choices for the cutoff/form factor should/could be explored.
Other choices will not change the implementation.

Monte Carlo ingredients

- For Green's function Monte Carlo or Auxiliary field diffusion Monte Carlo, we know the recipe.
- We choose our basis, the eigenstates of the nucleon positions and spin/isospins and pion mode amplitudes.
- We would like an initial trial/importance function, $\langle RS\Pi|\Psi_T\rangle$.
- We need the usual propagators – pions are equivalent to nonrelativistic harmonic oscillators, nucleons are nonrelativistic.
- Since pions are bosons, the sign/phase problem is the same as for the case without pions.

Trial wave function

- We assume the pion motion is significantly faster than the nucleons, and use a Born-Oppenheimer approximation with fixed nucleons to construct the trial function.
- Keeping just the axial vector terms, we write

$$\boldsymbol{B}_{\boldsymbol{k}}^{c} \equiv \sqrt{\frac{2}{L^3}}\frac{g_A}{f_\pi}\sum_{i=1}^{A}\boldsymbol{\tau}_i \sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\sigma}_i\cdot\boldsymbol{k},$$

$$\boldsymbol{B}_{\boldsymbol{k}}^{s} \equiv -\sqrt{\frac{2}{L^3}}\frac{g_A}{f_\pi}\sum_{i=1}^{A}\boldsymbol{\tau}_i \cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\sigma}_i\cdot\boldsymbol{k},$$

- Complete the square

$$\begin{aligned} H_{\pi\pi} + H_{AV} &= \frac{1}{2}{\sum_{\boldsymbol{k}}}' \Big[|\boldsymbol{\Pi}_{\boldsymbol{k}}^{c}|^2 + \omega_{\boldsymbol{k}}^2|\tilde{\pi}_{\boldsymbol{k}}^{c}|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^{s}|^2 + \omega_{\boldsymbol{k}}^2|\tilde{\pi}_{\boldsymbol{k}}^{s}|^2 \\ &\quad - \frac{1}{4\omega_k^2}\left(\left|\boldsymbol{B}_{\boldsymbol{k}}^{c}\right|^2 + \left|\boldsymbol{B}_{\boldsymbol{k}}^{s}\right|^2\right)\Big] \end{aligned} \quad (1)$$

with $\tilde{\pi}_{\boldsymbol{k}}^{c,s} \equiv \pi_{i\boldsymbol{k}}^{c,s} - \boldsymbol{B}_{\boldsymbol{k}}^{c,s}/2\omega_k^2$.

Trial wave function

- The $\tilde{\pi}_{\boldsymbol{k}}^{c,s}$ operators do not commute because of the nucleon spin-isospin operators contained in $\boldsymbol{B}_{\boldsymbol{k}}^{c,s}$.
- We construct the trial function ignoring these commutators

$$\langle RS\Pi|\Psi_T\rangle = \langle RS\Pi| \exp\left[-\sum_{\boldsymbol{k}}{}' \frac{\omega_k}{2}(|\tilde{\pi}_{\boldsymbol{k}}^{c}|^2 + |\tilde{\pi}_{\boldsymbol{k}}^{s}|^2)\right]|\Phi\rangle \,. \qquad (2)$$

where $|\Phi\rangle$ is an A nucleon model state.

Trial wave function

In terms of the original pion coordinates:

$$\langle RS\Pi|\Psi_T\rangle = \langle RS\Pi| \exp\left\{ -\sum_{\boldsymbol{k}}{}' \left[\frac{\omega_k}{2}(|\boldsymbol{\pi}^c_{\boldsymbol{k}}|^2 + |\boldsymbol{\pi}^s_{\boldsymbol{k}}|^2) \right.\right.$$

$$- \frac{\alpha_k}{2\omega_k}\left(\boldsymbol{\pi}^c_{\boldsymbol{k}} \cdot \boldsymbol{B}^c_{\boldsymbol{k}} + \boldsymbol{\pi}^s_{\boldsymbol{k}} \cdot \boldsymbol{B}^s_{\boldsymbol{k}}\right)$$

$$\left.\left. + \frac{1}{4}\omega_k \alpha_k^2 G_k^2 \sum_{i<j}^{A} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \boldsymbol{\sigma}_j \cdot \boldsymbol{k} \cos(\boldsymbol{k} \cdot \boldsymbol{r}_{ij}) \right] \right\} |\Phi\rangle \,.$$

where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$,

$$G_k = \frac{1}{\omega_k^2} \frac{g_A}{f_\pi} \sqrt{\frac{2}{L^3}}\,, \tag{3}$$

We have include variational parameters α_k, which rescale the coupling for different momenta.

Nucleon model state

- For 1 particle, the nucleon model state is simply one of the four $|p\uparrow\rangle$, $|p\downarrow\rangle$, $|n\uparrow\rangle$, $|n\downarrow\rangle$.
- For s-wave nuclei, we solve 2-body equation for the short range interaction with appropriate boundary conditions for the binding energy.
- In general we plan to use either standard GFMC or AFDMC type trial functions for the nuclear model states.

Variational calculations

$$E_0 \geq \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

- These calculations go through exactly as standard nuclear physics calculations.
  - We have an extra a set of boson field amplitudes (i.e. harmonic oscillators) to diffuse.
  - Nucleon charge is not conserved (e.g. proton can emit a π^+ to become a neutron)
  - So GFMC calculations with full spin/isospin sums scale like 4^A (For $Z = A/2$ nucleon charge conservation gives $\frac{A!}{(A/2)!^2} 2^A \simeq 4^A \sqrt{\frac{2}{\pi A}}$ states.)

Variational calculations

- For calculations with spin/isospin sums (like GFMC) we sample the pion mode amplitudes Π and the nucleon positions R from

$$\frac{\sum_S \langle \Psi_T | \Pi R S \rangle \langle \Pi R S | \Psi_T \rangle}{\int d\Pi \int dR \sum_S \langle \Psi_T | \Pi R S \rangle \langle \Pi R S | \Psi_T \rangle}$$

- And evaluate

$$\frac{\sum_S \langle \Psi_T | H | \Pi R S \rangle}{\sum_S \langle \Psi_T | \Pi R S \rangle}$$

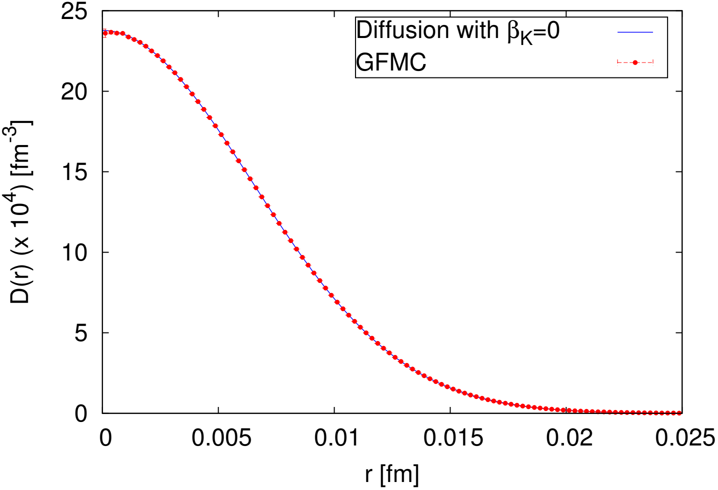
- Here we look at light nuclei and use spin/isospin sums. Later, we can use Auxiliary field diffusion Monte Carlo to sample spin/isospin.
- Use linear method to optimize parameters.

GFMC Notes

- The propagator has the same form as other real-space methods.
- We use GFMC method with Trotter breakup for nucleon propagators (with importance sampling).
- We sample the exact Harmonic oscillator propagators for the pion mode amplitudes (with importance sampling).
- Using the exact harmonic oscillator propagators allows us to use time steps set by the nucleon time scales rather than the pion energies.
- We use forward walking to calculate expectation values of operators that do not commute with H.

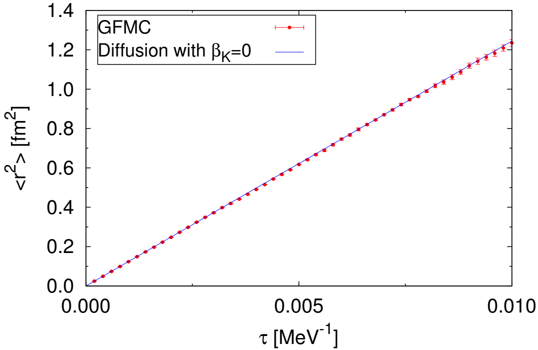
1-nucleon renormalization

Short time density-density correlation:



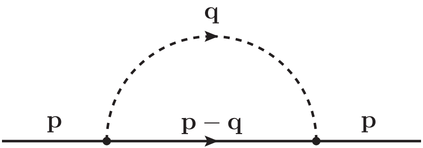
1-nucleon renormalization

Nucleon diffusion:



We take kinetic mass counter term to be zero.
(The correction at lowest order perturbation theory is small too.)

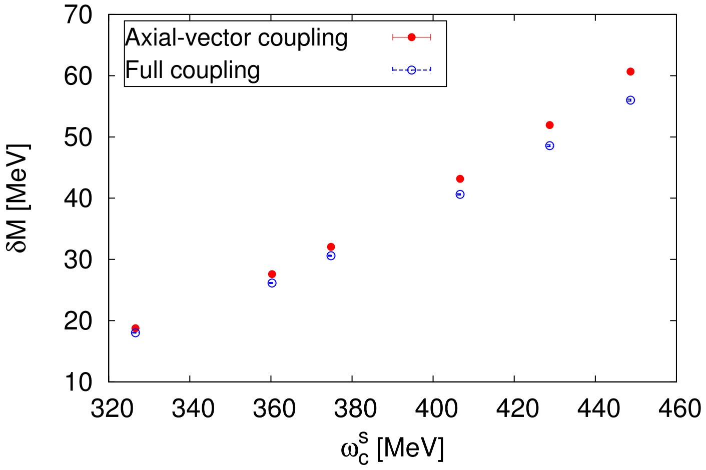
Lowest-order diagram



$$\Sigma(E, \boldsymbol{p}) = \frac{3}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \frac{1}{L^3}\sum_{\boldsymbol{q}} \frac{1}{\omega_q}$$

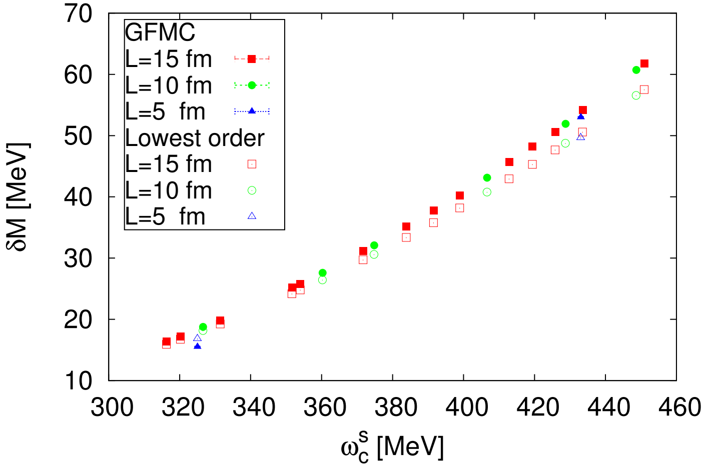
$$\times \frac{q^2}{E - \left(\frac{1}{2M_P} + \beta_K\right)|\boldsymbol{p} - \boldsymbol{q}|^2 - M_P - \delta M - \omega_q}.$$

Rest mass, $L = 10$fm



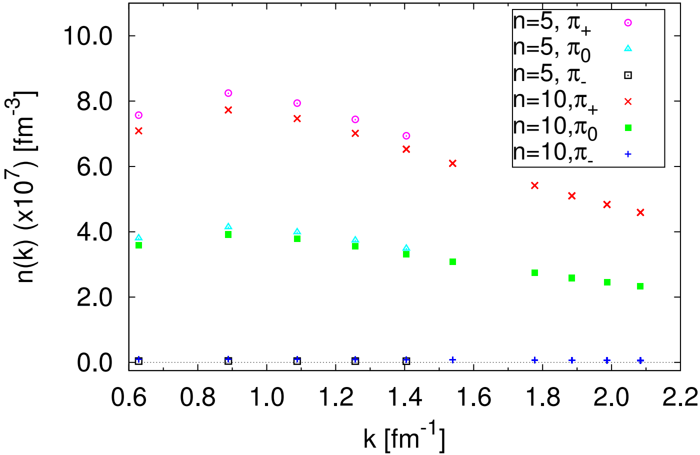
Rest mass

Both without Weinberg Tomazawa interaction:



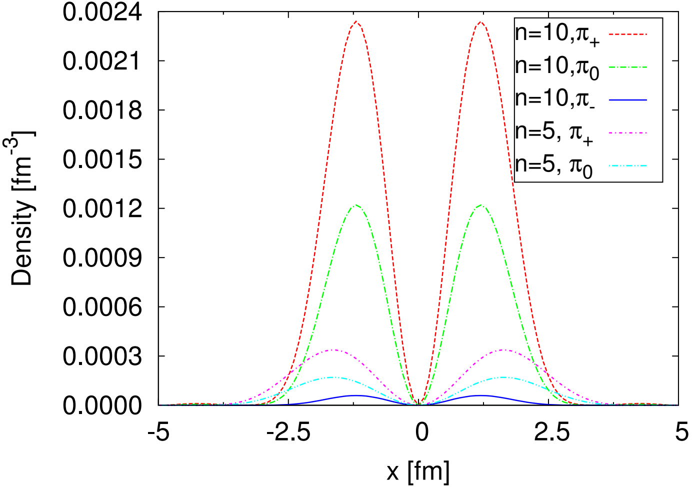
Pion momentum distribution

Single proton in box, *n* is number of *k*-shells.



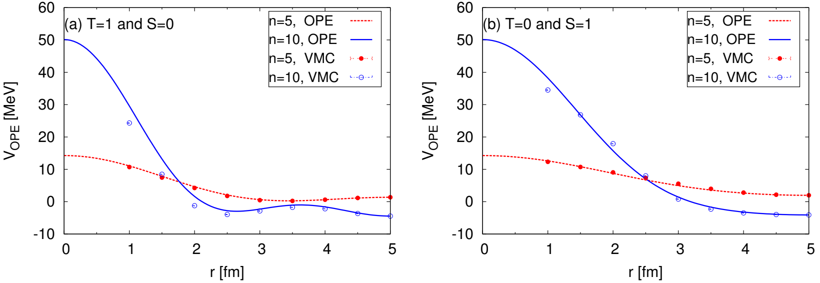
Pion density around nucleon (sort of)

$n = 5$ is a cutoff $\omega_c \simeq 327$ MeV, and $n = 10$ is $\omega_c \simeq 449$ MeV.



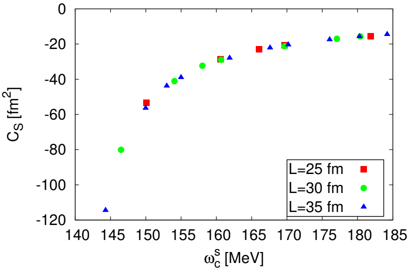
One-pion exchange

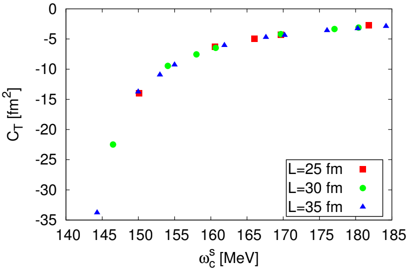
Comparison of instantaneous OPE in box to calculation with infinite mass nuclei:



Low energy constant fits

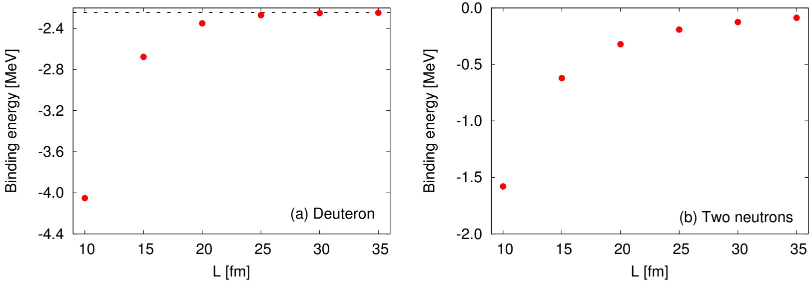
For simplicity/expediency we fit to results for Argonne $v6'$ and $v8'$ in a periodic box using a Lanczos solver, rather than Lüscher method and experiment.





Deuteron and 2 neutrons in box

Deuteron and 2 neutrons in box:



Conclusion – Future

- We have shown that calculating with relativistic pion fields and continuum nuclei is straightforward.
- This formalism seems to have the same sort of phase/sign problem as that for nucleons alone.
- Pions are relatively cheap, and are bosons. Currents should be easier. Adding Deltas may make 3-body interactions simpler.
- We have shown how to calculate the needed counter terms and low-energy constants.
- We are working on larger systems now.