Computational tricks in the relativistic three-nucleon problem

W. N. Polyzou* - The University of Iowa
* Research supported by the in part by the US DOE Office of Science

May 10, 2013
Happy Birthday James!

Your leadership in moving the nuclear physics community to develop a quantitative understanding of the dynamics and structure of nuclei using national computational facilities has been both transformational and inspirational.
Collaborators

- Ch. Elster, T. Lin, H. Mohammadreza (Ohio)
- W. Glöckle (Bochum)
- J. Golak, R. Skibíński, H. Witała (Jagiellonian U)
- B. Keister (NSF)
- F. Coester, S. Veerasamy (Iowa)
Outline

- Physics motivation
- Structure relativsitic models
- Computational issues (differences with the non-relativistic three-nucleon problem).
Physics motivation

- Make realistic models of few-hadron systems that are valid at the few-GeV scale.

- Understand the role of relativistic effects on few-GeV scale scattering observables.

- Understand the role of sub-nucleon degrees of freedom at the few-GeV scale. Relevant scale: $0.2 \text{ fm} \leftrightarrow 1 \text{ GeV}$.

- Field theories strongly coupled at this scale.
Relativistic effects are non-trivial in scattering reactions below the few GeV scale

Illustrative examples

Models are constrained so (1) two-body

\[ S_{2br}(p = 0) = S_{2bnr}(p = 0) \]

and (2) three-nucleon S-matrices satisfy cluster properties

\[ S_{3b} \rightarrow S_{2b ij} \otimes I_k \]
Examples

$pd$ breakup reactions at $508\,MeV$.

Calculations from T. Lin, et. al.

Data from V. Punjabi et al.,

• solid red lines: relativistic calculation.
• dashed green lines: non-relativistic calculation.
symmetric outgoing protons

\[ \frac{d\sigma}{d\Omega_1 d\Omega_2 dE_1} \text{ [mb/(MeV sr)]} \]

\[ E_1 \text{ [MeV]} \]

\[ \theta_1 = 38.1^\circ, \theta_2 = 38.0^\circ, \phi_{12} = 180^\circ \]

\[ \theta_1 = 41.5^\circ, \theta_2 = 41.4^\circ, \phi_{12} = 180^\circ \]

\[ \theta_1 = 44.1^\circ, \theta_2 = 44.0^\circ, \phi_{12} = 180^\circ \]

\[ \theta_1 = 47.1^\circ, \theta_2 = 47.0^\circ, \phi_{12} = 180^\circ \]
Selected polarization observables comparing relativistic and non-relativistic pd scattering with and without 3NFs.


Data from:

- **red** - non-relativistic - CD Bonn
- **blue dots** - non-relativistic - CD Bonn + TM 3Nf
- **blue dashes** - relativistic - CD Bonn - no Wigner rotations
- **brown dash-dot** - relativistic - CD Bonn + TM 3Nf - no Wigner rotations
As a large scale computational problem.

- Few-nucleon physics has traditionally been associated with large-scale computing.

- A relativistic treatment presents additional challenges.

- This talk will discuss the resolution of some of the additional computational challenges that arise in the relativistic three-nucleon problem.
Model structure

Relativistic quantum theory (Wigner)

\[ \mathcal{H} = \bigoplus (\bigotimes \mathcal{H}_{m,j_i}) \]

\[ U(\Lambda, a) : \mathcal{H} \rightarrow \mathcal{H} \]

Cluster properties

\[ \lim_{|r_{ij} - r_k| \to \infty} [U(\Lambda, a) - U_{ij}(\Lambda, a) \otimes U_k(\Lambda, a)] = 0 \]

Challenges
New computational issues

• The Poincaré commutation relations put non-linear dynamical constraints on the interactions.

• Cluster properties require the addition of three (many)-body interactions to the cluster expansions of generators to preserve Poincaré CRs.

• Partial-wave expansions have numerical issues above about 250 MeV.

• Numerous interaction-related complications.

• Permutation operators involve momentum-dependent spin rotations.

• Large singular matrix equations.
Structure of dynamical 3N models (Coester)

\[ \tilde{M} := \tilde{M}_{12,3} + \tilde{M}_{23,1} + \tilde{M}_{31,2} - 2M_0 \]

\[ \tilde{M}_{ij,k} = M_0 + \tilde{V}_{ij} \]

\[ M_0 = \sqrt{q_k^2 + (\sqrt{k_{ij}^2 + m_i^2} + \sqrt{k_{ij}^2 + m_j^2})^2 + \sqrt{q_k^2 + m_k^2}} \]

\[ q_i := \Lambda(P/M_0)^{-1}p_i \quad k_{ij} := \Lambda\left(\frac{q_i + q_j}{m_{0ij}}\right)^{-1}q_i \]

\[ [\tilde{V}_{ij},j_0^2] = 0 \]
• One Casimir operator, $\tilde{M}$, has interactions.

• Diagonalize $\tilde{M}$ in invariant subspaces of $j_0^2$. (Bakamjian-Thomas)

\[
\tilde{U}(\Lambda, a) = \sum_j \oplus U_{j_0, m}(\Lambda, a)
\]

• Problem - $\tilde{U}(\Lambda, a)$ violates cluster properties.

• No loss of generality - $\exists$ $S$-matrix-preserving unitary transformations $A$: $Aj^2A^\dagger = j_0^2$. 
\( \bar{U}(\Lambda, a) \rightarrow \bar{U}_{ij,k}(\Lambda, a) \neq \bar{U}_{ij} \otimes U_k(\Lambda, a) \)

however

\[ \bar{S}_{ij,k} = \bar{S}_{ij} \otimes I_k \]

\[ \downarrow \]

\[ \exists A_{ij,k} \quad (\text{Ekstein}) \]

\[ A_{ij,k} \bar{U}_{ij,k}(\Lambda, a) A_{ij,k}^\dagger = \bar{U}_{ij} \otimes U_k(\Lambda, a) \]

\[ A_{ij,k} \bar{M}_{ij,k} A_{ij,k}^\dagger = M_{ij} \otimes k \]

\[ A_{ij,k} j_0^2 A_{ij,k}^\dagger = j_{ij \otimes k}^2 \neq j_0^2 \]
\[ C_{ij,k} := i(A_{ij,k} - I)(A_{ij,k} + I)^{-1} \]

\[ C := C_{12,3} + C_{23,1} + C_{31,2} \]

\[ A := (I - iC)(I + iC)^{-1} \quad A \rightarrow A_{ij,k} \rightarrow I \]

\[ U(\Lambda, a) := A^\dagger \bar{U}(\Lambda, a)A \]

\[ U(\Lambda, a) \rightarrow \bar{U}_{ij}(\Lambda, a) \otimes U_k(\Lambda, a) \]

\[ M = A(\sum_{ij,k} A_{ij,k}^\dagger M_{ij} \otimes k A_{ij,k} - 2M_0)A^\dagger = A\bar{M}A^\dagger \]

(Sokolov)
Simplifications:

- $A$, $A_{ij,k}^\dagger$ generate many-body forces that restore Poincaré CR to cluster expansions of generators.

$$A(p = 0) = I \quad S(p) = S(p = 0) = \bar{S}(p = 0) = \bar{S}(p)$$

- To calculate 3N $S$ no need to calculate 3NFs generated by $A$, $A_{ij,k}^\dagger$!

\[\Downarrow\]

To calculate on-shell $S$ set $A \rightarrow I$, diagonalize $\bar{M}$
Three-Particle Scattering (Operator Equations)

\[ \tilde{M} = M_0 + \tilde{V} \quad \tilde{V} = \sum_\alpha \tilde{V}_\alpha \quad \alpha \in \{(12, 3), (23, 1), (31, 2)\} \]

\[ \tilde{V}_\alpha = \tilde{M}_\alpha - M_0 \quad \tilde{V}^\alpha = \tilde{M} - \tilde{M}_\alpha \]

\[ \tilde{T}^{\alpha\beta}(m) := \tilde{V}^\beta + \tilde{V}^\alpha (m - \tilde{M} + i0^+)^{-1} \tilde{V}^\beta \]

\[ \langle a_0|S^{\alpha\beta}|b_0\rangle = \langle a_0|b_0\rangle - 2\pi i \delta(m_a - m_b) \langle a_0|\tilde{T}^{\alpha\beta}(m_a + i0^+)|b_0\rangle \]
Faddeev Equations

\[ \bar{T}^{\alpha\beta}(z) = \bar{V}^\beta + \sum_{\gamma \neq \alpha} \bar{T}_\gamma(z - M_0)^{-1} \bar{T}^{\gamma\beta}(z) \]

\[ \bar{T}_\gamma(z) = \bar{V}_\gamma + \bar{V}_\gamma(z - M_0)^{-1} \bar{T}_\gamma(z) \]

Iterated kernel of coupled equations compact

\[ \bar{T}(z) = \bar{D}(z) + \bar{K}(z) \bar{T}(z) \quad \bar{K}(z)^2 \text{ compact} \]

\[ \bar{T}(z) = (I - \bar{K}(z)^2)^{-1}(\bar{D}(z) + \bar{K}(z) \bar{T}(z)) \]
\[ \bar{M} := M_0 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31} \]

\[ \bar{V}_{ij} := \sqrt{q_k^2 + (\sqrt{k_{ij}^2 + m_i^2 + 2\mu_{ij}v_{nr\ ij}} + \sqrt{k_{ij}^2 + m_j^2 + 2\mu_{ij}v_{nr\ ij}})^2} - \sqrt{q_k^2 + (\sqrt{k_{ij}^2 + m_i^2} + \sqrt{k_{ij}^2 + m_j^2})^2} \]

\[ \bar{M}_{ij,k} = M_{ij,k}(h_{nr\ ij}) \]

\[ \langle \mathbf{p}, \mathbf{q}_r, \mathbf{k}_r | S_{ij,k_r} | \mathbf{p}', \mathbf{q}'_r, \mathbf{k}'_r \rangle = \delta(p - p')\delta(q_r - q'_r) \langle \mathbf{k}_r | s_{ij} | \mathbf{k}'_r \rangle \]

\[ \langle \mathbf{p}, \mathbf{q}_{nr}, \mathbf{k}_{nr} | S_{ij,k_{nr}} | \mathbf{p}', \mathbf{q}'_{nr}, \mathbf{k}'_{nr} \rangle = \delta(p - p')\delta(q_{nr} - q'_{nr}) \langle \mathbf{k}_{nr} | s_{ij} | \mathbf{k}'_{nr} \rangle \]
• $\tilde{V}_{\alpha}$ is a complicated operator involving square roots of the non-relativistic interaction.

$$\langle \Phi_0 | \bar{T}_\alpha | \psi \rangle = \langle \Phi_0 | \bar{V}_\alpha | \psi^- \rangle = \langle \Phi_0 | (\bar{M}_\alpha - M_0) | \psi^- \rangle$$

• Using the identity of the NN wave functions, the half-shell relativistic Faddeev kernel can be expressed exactly in terms of the non-relativistic half-shell two-body transition matrix elements!

$$\langle k | \psi^-_{nr} \rangle = \langle k | \psi^-_r \rangle$$

• The two-nucleon subsystem is not at rest in the three-nucleon rest frame.
\[ \langle q_\alpha, k_\alpha | T_\alpha(z)(z - \bar{M}_0)^{-1} | q'_\alpha, k'_\alpha \rangle = \]

\[ \delta(q_\alpha - q'_\alpha) \frac{m_{0\alpha}(k) + m_{0\alpha}(k')}{(\sqrt{q^2_\alpha + m^2_{0\alpha}(k)} + \sqrt{q^2_\alpha + m^2_{0\alpha}(k')})} \times \]

\[ \langle k_\alpha | t_r(z) | k'_\alpha \rangle \frac{1}{M_0(q_\alpha, k_\alpha) - M_0(q_\alpha, k'_\alpha) + i0^+} \]

where

\[ m_{0\alpha}(k_\alpha) := \sqrt{k^2_\alpha + m_i^2} + \sqrt{k^2_\alpha + m_j^2} \]

and

\[ z = M_0(q_\alpha k_\alpha) + i0^+ \]
\begin{align*}
\langle k_\alpha | t_r(z) | k'_\alpha \rangle &= \left( \frac{2\mu}{\sqrt{k_\alpha^2 + m_i^2} + \sqrt{k'_\alpha^2 + m_j^2}} + \frac{2\mu}{\sqrt{k_\alpha^2 + m_i^2} + \sqrt{k'_\alpha^2 + m_j^2}} \right) \times \\
&\quad \langle k_\alpha | t_{nr}(k_\alpha^2/2\mu + i0^+) | k'_\alpha \rangle
\end{align*}
Permutation operators - different NN rest frames

$$\langle q_i, \mu_i, q_j, \mu_j | t_r(z) | q'_i, \mu'_i, q'_j, \mu'_j \rangle =$$

$$\delta(q_k - q'_k) \left( \frac{\omega_i(q_i) + \omega_j(q_j)}{\omega_i(k_{ij}) + \omega_j(k_{ji})} \right)^{1/2} \times$$

$$\sum D_{\mu_i \nu_i}^{ji} [R_{wc}(B_c(q_{ij}), k_{ij})] D_{\mu_j \nu_j}^{ij} [R_{wc}(B_c(q_{ij}), k_{ji})] \times$$

$$\langle k_{ij}, \nu_i, \nu_j | t_r(z) | k'_{ij}, \nu'_i, \nu'_j \rangle \times$$

$$D_{\nu'_j \mu'_j}^{ji} [R_{wc}(B^{-1}_c(q_{ij}), q_i)] D_{\nu'_i \mu'_i}^{ij} [R_{wc}(B^{-1}_c(q_{ij}), q_j)] \times$$

$$\left( \frac{\omega_i(q'_i) + \omega_j(q'_j)}{\omega_i(k'_{ij}) + \omega_j(k'_{ji})} \right)^{1/2} \times$$

$$\left( \frac{\omega_i(k'_{ij}) \omega_j(k'_{ji})}{\omega_i(q'_i) \omega_j(q'_j)} \right)^{1/2}$$
• The relation to the half-shell non-relativistic transition operator avoids the problem of explicitly computing square roots of non-commuting operators.

• The fully off-shell transition operator is needed in the Faddeev kernel. It can be obtained by solving the first resolvent equation in the form

\[
\bar{T}_\alpha(z) = \bar{T}_\alpha(z') + \bar{T}_\alpha(z)\frac{z' - z}{(z - M_0)(z' - M_0)} \bar{T}_\alpha(z')
\]
Interactions III

- Partial-wave expansion numerically difficult above 250 MeV.

- Use direct three-dimensional integration.
  - Adds continuous variables (larger matrices).
  - One channel (Malfliet-Tjon) model convergent at 2 GeV.
  - Requires realistic momentum-space interaction in operator form.
  - Fourier transform of Argonne V18
\[ \langle k|v_{nr}|k' \rangle = \sum V_n W_n \]

\[ W_1 := I \]

\[ W_2 := \sigma_1 \cdot \sigma_2 \]

\[ W_3 := (\sigma_1 \cdot \hat{K}) \otimes (\sigma_2 \cdot \hat{K}) \]

\[ W_4 := (\sigma_1 \cdot \hat{Q}) \otimes (\sigma_2 \cdot \hat{Q}) \]

\[ W_5 := i(\sigma_1 \cdot \hat{N}) \otimes l_2 + l_1 \otimes (\sigma_2 \cdot \hat{N}) \]

\[ W_6 := (\sigma_1 \cdot \hat{K}) \otimes (\sigma_2 \cdot \hat{Q}) + (\sigma_1 \cdot \hat{Q}) \otimes (\sigma_2 \cdot \hat{K}) \]

\[ K = k' - k \quad Q = k' + k \quad N = k' \times k \]
• Spins and continuous variables must be chosen to Wigner rotate together.

• Six independent spin operators off shell, five on shell - can lead to numerical instabilities.

• Choose the 5 off-shell operators to match smoothly with the 5 on-shell operators.

• Generate three-nucleon spin operators by iteration.

• Faddeev equation has $24^3$ traces - developed dedicated symbolic package (using GiNaC) to perform traces.

• $NN$ scattering tested against PW calculations and GW database.
V18 results pp 350 MeV

Wolfenstein Amplitudes pp

\[ E_{\text{lab}} = 350 \text{ MeV} \]
• Established computational methods can still be applied.

• Use powers of kernel on driving term plus Gram-Schmidt orthogonalization to generate a small basis (Krylov method).

• Use rotational covariance simplify the computation of the kernel (Balian - Brezin method).
Summary

- Poincaré invariance - choose to add interactions to only one Casimir operator.
- Cluster properties in the rest frame is sufficient to get cluster properties for $S$.
- Realistic NN interactions parameterize 2-body data - can be used to construct equivalent relativistic interactions.
- Identity of $nr$ and $r$ wave functions gives half-shell relativistic Faddeev kernel in terms of $nr$ half-shell transition matrix.
- First resolvent equation must be solved to get relativistic off-shell kernel.
Permutation operators involve Jacobians and Wigner rotations. Permutations can be made trivial by including these factors in the relativistic two-nucleon transition matrices.

Partial-wave expansions unstable - need a realistic interaction. Fourier transform AV18.

Expand in terms of Wolfensteinn parameters to easily extract cross sections, extra operator needed. Must be chosen carefully for stability.

Many traces needed. Can be automated.

Standard computational methods can still be applied.

Non-relativistic Faddeev equation arises by setting relativistic corrections to 1.
To do

- GeV-scale 3N calculations with V18 in progress (Mohammadreza).

- Many-body forces (cluster corrections) are needed for 4N systems or electroweak probes of 3N system.

- Production channels need to be included in a manner consistent with cluster properties.
Thanks!
Andrey, Bruce, Pieter
and the Organizing Committee.