Computational aspects of the relativistic three-nucleon problem

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Happy Birthday James!

Your leadership in initiating collaborations to solve difficult problems in nuclear physics using leadership class computational facilities has been transformational to the field and is appreciated by the nuclear physics community. It is only matched by your tireless efforts to develop and mentor the careers of students and young physicists.

Thanks!

Collaborators

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

Outline

- **Motivation.**
- **Relativistic effects - examples.**
- **The structure of relativistic models.**
- **Computational issues in the relativistic 3N problem.**

Motivation

- **Understand few-GeV-scale hadronic physics using few-body methods.**
- **At this scale:**
  - **Sub-nucleon degrees of freedom should be relevant.**
  - **QCD is non-perturbative.**
  - **Relativistic effects are important.**
- **Assumption: dynamics dominated by a small number of degrees of freedom.**

Examples of relativistic effects in scattering reactions below the few-GeV scale.

Models are constrained so (1) two-body

$$S_{2b\,r}(\mathbf{p}=0) = S_{2b\,nr}(\mathbf{p}=0)$$

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

$$S_{3b} \to S_{2b\,ij} \otimes I_k$$

Example 1

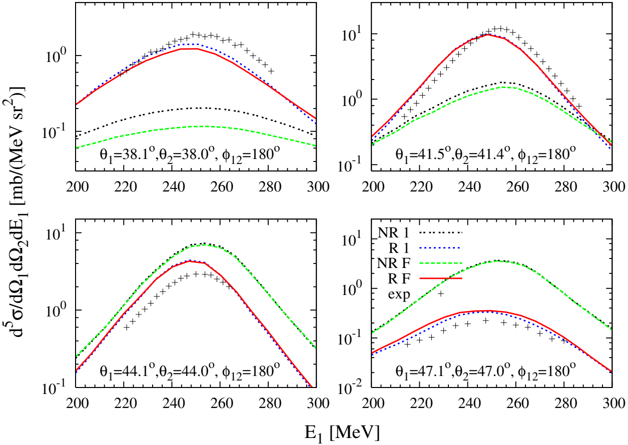
pd **breakup reactions at** $508 MeV$**.**

Calculations from T. Lin, et. al.
Phys. Lett. B660,345,2008.

Data from V. Punjabi et al.,
Phys. Rev. C 38, 2728 (1988).

- **solid red lines: relativistic calculation.**
- **dashed green lines: non-relativistic calculation**

symmetric outgoing protons



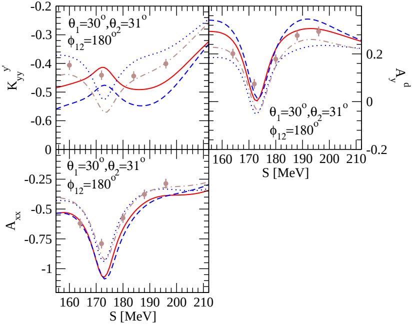
Example 2

Selected spin-dependent pd breakup observables at 270 MeV with and without 3N forces.

Calculations: H. Witała, et al, Phys. Rev. C.83.044001(2011).

Data from: K. Sekiguchi et al., Phys. Rev. C79, 054008(2009).

- **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



θ1=30o,θ2=31o
φ12=180o
K_yy^y'
A_y^d
A_xx
S [MeV]
S [MeV]

Model structure

Relativistic quantum theory (Wigner)

$$\mathcal{H} = \oplus(\otimes\mathcal{H}_{m_i\,j_i})$$

$$U(\Lambda, a) : \mathcal{H} \to \mathcal{H}$$

Cluster properties

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

Computational issues

- **Few-nucleon physics has traditionally been associated with large-scale computing.**
- **A relativistic treatment presents additional challenges.**

New computational issues (relativistic n=3)

- **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.**

Structure of dynamical 3N models (Coester)

$$\bar{M} := \bar{M}_{12,3} + \bar{M}_{23,1} + \bar{M}_{31,2} - 2M_0$$

$$\bar{M}_{ij,k} = M_0 + \bar{V}_{ij}$$

$$M_0 = \sqrt{\mathbf{q}_k^2 + (\sqrt{\mathbf{k}_{ij}^2 + m_i^2} + \sqrt{\mathbf{k}_{ij}^2 + m_j^2})^2} + \sqrt{\mathbf{q}_k^2 + m_k^2}$$

$$\mathbf{q}_i := \mathbf{\Lambda}(P/M_0)^{-1} p_i \qquad \mathbf{k}_{ij} := \mathbf{\Lambda}(\frac{q_i + q_j}{m_{0ij}})^{-1} q_i$$

$$[\bar{V}_{ij}, \mathbf{j}_0^2] = 0$$

$$\downarrow$$

- **One Casimir operator, $\bar{M}$, has interactions.**

- **Diagonalize $\bar{M}$ in invariant subspaces of $\mathbf{j}_0^2$. (Bakamjian-Thomas)**

$$\bar{U}(\Lambda, a) = \sum\!\!\!\!\!\!\int \oplus U_{\mathbf{j}_0,m}(\Lambda, a)$$

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

- **No loss of generality - $\exists\, S$-matrix-preserving unitary transformations A: $A\mathbf{j}^2 A^\dagger = \mathbf{j}_0^2$.**

$$\bar{U}(\Lambda, a) \to \bar{U}_{ij,k}(\Lambda, a) \neq \bar{U}_{ij} \otimes U_k(\Lambda, a)$$

however

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

$$\Downarrow$$

$$\exists\, A_{ij,k} \qquad (\textbf{Ekstein})$$

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

$$A_{ij,k} \bar{M}_{ij,k} A^{\dagger}_{ij,k} = M_{ij \otimes k}$$

$$A_{ij,k} \mathbf{j}_0^2 A^{\dagger}_{ij,k} = \mathbf{j}^2_{ij \otimes k} \neq \mathbf{j}_0^2$$

$$C_{ij,k} := i(A_{ij,k} - I)(A_{ij,k} + I)^{-1}$$

$$C := C_{12,3} + C_{23,1} + C_{31,2}$$

$$A := (I - iC)(I + iC)^{-1} \qquad A \to A_{ij,k} \to I$$

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

$$U(\Lambda, a) \to \bar{U}_{ij}(\Lambda, a) \otimes U_k(\Lambda, a)$$

$$M = A(\sum A^{\dagger}_{ij,k} M_{ij\otimes k} A_{ij,k} - 2M_0)A^{\dagger} = A\bar{M}A^{\dagger}$$

(Sokolov)

Simplifications:

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

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

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

$$\Downarrow$$

To calculate on-shell S **set** $A \to I$, **diagonalize** $\bar{M}$

Three-Particle Scattering (Operator Equations)

$$\bar{M} = M_0 + \bar{V} \qquad \bar{V} = \sum_{\alpha} \bar{V}_{\alpha} \qquad \alpha \in \{(12,3),(23,1),(31,2)\}$$

$$\bar{V}_{\alpha} = \bar{M}_{\alpha} - M_0 \qquad \bar{V}^{\alpha} = \bar{M} - \bar{M}_{\alpha}$$

$$\bar{T}^{\alpha\beta}(m) := \bar{V}^{\beta} + \bar{V}^{\alpha}(m - \bar{M} + i0^{+})^{-1}\bar{V}^{\beta}$$

$$\langle a_0|S^{\alpha\beta}|b_0\rangle = \langle a_0|b_0\rangle - 2\pi i\delta(m_a - m_b)\langle a_0|\bar{T}^{\alpha\beta}(m_a + i0^{+})|b_0\rangle$$

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

$$\bar{T}(z) = \bar{D}(z) + \bar{K}(z)\,\bar{T}(z) \qquad \bar{K}(z)^2 \quad \textbf{compact}$$

$$\bar{T}(z) = (I - \bar{K}(z)^2)^{-1}(\bar{D}(z) + \bar{K}(z)\,\bar{T}(z))$$

Interactions I
(Coester, Pieper & Serduke)

$$\bar{M} := M_0 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31}$$

$$\bar{V}_{ij} :=$$

$$\sqrt{\mathbf{q}_k^2 + (\sqrt{\mathbf{k}_{ij}^2 + m_i^2 + 2\mu_{ij} v_{nr\,ij}} + \sqrt{\mathbf{k}_{ij}^2 + m_j^2 + 2\mu_{ij} v_{nr\,ij}})^2} -$$

$$\sqrt{\mathbf{q}_k^2 + (\sqrt{\mathbf{k}_{ij}^2 + m_i^2} + \sqrt{\mathbf{k}_{ij}^2 + m_j^2})^2}$$

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

$$\langle \mathbf{p}, \mathbf{q}_r, \mathbf{k}_r | S_{ij,k\,r} | \mathbf{p}', \mathbf{q}'_r, \mathbf{k}'_r \rangle = \delta(\mathbf{p} - \mathbf{p}')\delta(\mathbf{q}_r - \mathbf{q}'_r)\langle \mathbf{k}_r | s_{ij} | \mathbf{k}'_r \rangle$$

$$\langle \mathbf{p}, \mathbf{q}_{nr}, \mathbf{k}_{nr} | S_{ij,k\,nr} | \mathbf{p}', \mathbf{q}'_{nr}, \mathbf{k}'_{nr} \rangle = \delta(\mathbf{p} - \mathbf{p}')\delta(\mathbf{q}_{nr} - \mathbf{q}'_{nr})\langle \mathbf{k}_{nr} | s_{ij} | \mathbf{k}'_{nr} \rangle$$

Interactions II

- $\bar{V}_\alpha$ **is a complicated operator involving square roots of the non-relativistic interaction.**

$$\langle \Phi_0 | \bar{T}_\alpha | \Psi_0 \rangle = \langle \Phi_0 | \bar{V}_\alpha | \Psi^- \rangle = \langle \Phi_0 | (\bar{M}_\alpha - M_0) | \Psi^- \rangle$$

- **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!**

$$\langle \mathbf{k} | \Psi_{nr}^- \rangle = \langle \mathbf{k} | \Psi_r^- \rangle$$

- **The two-nucleon subsystem is not at rest in the three-nucleon rest frame.**

$$\langle \mathbf{q}_\alpha, \mathbf{k}_\alpha | T_\alpha(z)(z - \bar{M}_0)^{-1} | \mathbf{q}'_\alpha, \mathbf{k}'_\alpha \rangle =$$

$$\delta(\mathbf{q}_\alpha - \mathbf{q}'_\alpha) \frac{m_{0\alpha}(\mathbf{k}) + m_{0\alpha}(\mathbf{k}')}{(\sqrt{\mathbf{q}_\alpha^2 + m_{0\alpha}^2(\mathbf{k}_\alpha)} + \sqrt{\mathbf{q}_\alpha^2 + m_{0\alpha}^2(\mathbf{k}'_\alpha)})} \times$$

$$\langle \mathbf{k}_\alpha | t_r(z) | \mathbf{k}'_\alpha \rangle \frac{1}{M_0(\mathbf{q}_\alpha, \mathbf{k}_\alpha) - M_0(\mathbf{q}_\alpha, \mathbf{k}'_\alpha) + i0^+}$$

where

$$m_{0\alpha}(\mathbf{k}_\alpha) := \sqrt{\mathbf{k}_\alpha^2 + m_i^2} + \sqrt{\mathbf{k}_\alpha^2 + m_j^2}$$

and

$$z = M_0(\mathbf{q}_\alpha \mathbf{k}_\alpha) + i0^+$$

$$\langle \mathbf{k}_\alpha | t_r(z) | \mathbf{k}'_\alpha \rangle =$$

$$\left(\frac{2\mu}{\sqrt{\mathbf{k}_\alpha^2 + m_i^2} + \sqrt{\mathbf{k}_\alpha'^2 + m_j^2}} + \frac{2\mu}{\sqrt{\mathbf{k}_\alpha^2 + m_i^2} + \sqrt{\mathbf{k}_\alpha'^2 + m_j^2}}\right) \times$$

$$\langle \mathbf{k}_\alpha | t_{nr}(\mathbf{k}_\alpha^2 / 2\mu + i0^+) | \mathbf{k}'_\alpha \rangle$$

Permutation operators - different NN rest frames

$$\langle \mathbf{q}_i, \mu_i, \mathbf{q}_j, \mu_j | t_r(z) | \mathbf{q}'_i, \mu'_i, \mathbf{q}'_j, \mu'_j \rangle =$$

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

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

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

$$D^{j_i}_{\nu'_i \mu'_i}[R_{wc}(B_c^{-1}(q_{ij}), q_i)] D^{j_j}_{\nu'_j \mu'_j}[R_{wc}(B_c^{-1}(q_{ij}), q_j)] \times$$

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

- **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

$$\langle \mathbf{k} | v_{nr} | \mathbf{k}' \rangle = \sum V_n W_n$$

$$W_1 := I$$

$$W_2 := \mathbf{j}_1 \cdot \mathbf{j}_2$$

$$W_3 := (\mathbf{j}_1 \cdot \hat{\mathbf{K}}) \otimes (\mathbf{j}_2 \cdot \hat{\mathbf{K}})$$

$$W_4 := (\mathbf{j}_1 \cdot \hat{\mathbf{Q}}) \otimes (\mathbf{j}_2 \cdot \hat{\mathbf{Q}})$$

$$W_5 := (\mathbf{j}_1 \cdot \hat{\mathbf{N}}) \otimes I_2 + I_1 \otimes (\mathbf{j}_2 \cdot \hat{\mathbf{N}})$$

$$W_6 := (\mathbf{j}_1 \cdot \hat{\mathbf{K}}) \otimes (\mathbf{j}_2 \cdot \hat{\mathbf{Q}}) + (\mathbf{j}_1 \cdot \hat{\mathbf{Q}}) \otimes (\mathbf{j}_2 \cdot \hat{\mathbf{K}})$$

$$\mathbf{K} = \mathbf{k}' - \mathbf{k} \qquad \mathbf{Q} = \mathbf{k}' + \mathbf{k} \qquad \mathbf{N} = \mathbf{k}' \times \mathbf{k}$$

- **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.**

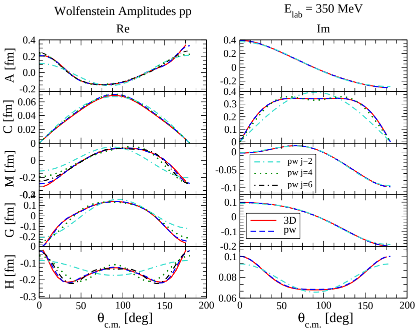
- **Choose the 6 off-shell operators to match smoothly with the 5 on-shell operators.**

- **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



- **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 Wolfenstein 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.**

Future

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

- Cluster expansions for generators and consistent covariant conserved currents.

- Inclusion of production channels in a manner consistent with cluster properties.

Thanks!
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