Computational challenges in the relativistic few-nucleon problem

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Abstract

I discuss computational challenges in the relativistic few-nucleon problem and the resolution of some of these challenges. I also discuss the outlook for the future.

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1 Introduction

Studying nuclear physics at distance scales that are potentially sensitive to sub-nucleon physics requires a relativistic treatment of the dynamics. This scale is interesting because QCD is non-perturbative at this scale; of particular concern is that it is not yet known how to compute mathematical error bounds, even for non-perturbative methods, making the accuracy of calculations based directly on QCD difficult to assess. This is also the scale where transition from meson-nucleon to sub-nucleon degrees of freedom is poorly understood.

Relativistic quantum mechanics provides a means for studying few-body problems at this scale. It provides a quantum mechanical description of the dynamics of the relevant degrees of freedom consistent with the exact Poincaré symmetry of underlying theory. Because few-body models can be solved exactly, comparison of these computations to experiment provides the direct feedback needed to construct realistic models based on a given set of degrees of freedom.

Normally the relevant degrees of freedom are the experimental degrees of freedom which are the particle spins and momenta that are observed in reactions at this scale. A suitable model Hilbert space is the direct sum of tensor products of the single-nucleon spaces,

$$H = \bigoplus (\otimes H_{m,j})$$

which are irreducible representation spaces for the Poincaré group.

Any relativistic model formulated on this space is necessarily characterized by a unitary representation of the Poincaré group [1]

$$U(\Lambda, a) : H \rightarrow H.$$ (2)

The dynamical unitary representation $U(\Lambda, a)$ of the Poincaré group necessarily differs from the natural free-particle representation, $U_{0}(\Lambda, a)$, given by the direct sum of tensor products free-particle irreducible representations on $H$.

The ability to perform local tests of special relativity requires that the unitary representations of the Poincaré group corresponding to different subsystems be related to $U(\Lambda, a)$ by cluster properties

$$\lim_{|r_{ij} - r_{kj}| \rightarrow \infty} \| (U(\Lambda, a) - U_{ij}(\Lambda, a) \otimes U_{kj}(\Lambda, a)) |\psi\rangle \| = 0.$$ (3)

The problem of relativistic few-body physics is to construct mathematical models $U(\Lambda, a)$ with the above properties that provide a realistic quantitative and consistent
description of few-GeV scale structure and reactions for few-hadron systems. This problem is a natural extension of the corresponding non-relativistic problem; but the relativistic treatment leads to a number of computational issues that do not arise in the non-relativistic formulation of the same problem.

In the non-relativistic case it is useful to work in a frame where the total momentum $P$ is zero. In that frame the Hamiltonian is replaced by the center of mass Hamiltonian, $h = H - P^2/2M$, where $M$ is the Galilean mass of the system. In the relativistic case the corresponding operator is the invariant mass operator, which is the rest energy of the system. We denote the mass operator by $M$.

The first complication in formulation of a relativistic few-body dynamics arises because the Hamiltonian appears on the right-hand side of three different commutators. As a consequence, the Poincaré commutation relations require that at least three of the Poincaré generators have an interaction dependence. The commutation relations impose a set of non-linear constraints on these interactions. One way to satisfy these constraints is to notice that all ten generators can be expressed in terms of the two Casimir operators (mass and spin), four commuting functions of the generators, and four functions of the generators that are conjugate to the four commuting functions of the generators. If interactions are added to the non-interacting mass operator, keeping these other nine operators free of interactions, and the ten generators are expressed and functions of these nine operators and the interacting invariant mass, the resulting generators will satisfy the Poincaré commutation relations provided the interaction terms commute with these nine-non-interacting operators. This is the assumption that defines the Bakamjian Thomas [2] method. These nine commutators with the relativistic interaction are the relativistic equivalent of the nine constraints on the non-relativistic interactions that result from the requirements that the interactions be translationally invariant, rotationally invariant, and independent of the total momentum.

Solving for the mass eigenvalue problem in a suitable irreducible free-particle basis leads to an explicit dynamical unitary representation of the Poincaré group, $\tilde{U}_{ij}(\Lambda, a)$ on the two particle Hilbert space.

If this method is applied to the three-nucleon system the resulting three-nucleon mass operator [3] has the form

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

$$\tilde{M}_{i,j,k} = M_0 + \tilde{V}_{ij}$$

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

where the relativistic Jacobi momenta

$$q_i := \Lambda(P/M_0)^{-1}p_i \quad k_{ij} := \Lambda(q_i + q_j)^{-1}m_{ij}$$

are obtained by Lorentz transforming single-particle momenta to the two and three-body rest frames with non-interacting Lorentz transformations. We call these relativistic Jacobi momenta because the usual Jacobi momenta can be constructed in the same manner by replacing the Lorentz boost by a Galilean boost.

Because all three of the interactions commute with the same nine functions of the three-nucleon Poincaré generators, the interactions can be combined algebraically in the three-nucleon mass operator and the result will commute with these same nine operators. Poincaré generators can then be expressed in terms of the interacting mass operator and the nine-other three-body kinematic operators. Again, diagonalizing $\tilde{M}$
in a suitable irreducible free-particle basis gives a dynamical unitary representation of the Poincaré group, $\tilde{U}(\Lambda, a)$, for a system of three interacting particles.

The commutator of the interaction with the free spin operator, $\hat{J}_0^2$

$$[\hat{V}_{ij}, \hat{J}_0^2] = 0,$$  

is incompatible with cluster properties of the three-body Poincaré generators. The problem is that the relative orbital angular momentum, which contributes to the total spin, gets modified as a consequence of the interactions. Here the failure means that

$$\tilde{U}(\Lambda, a) \to \tilde{U}_{ij,k}(\Lambda, a) \neq \tilde{U}_{ij} \otimes U_k(\Lambda, a).$$  \hspace{1cm} (9)

where $\tilde{U}_{ij,k}(\Lambda, a)$ is obtained from $\tilde{U}(\Lambda, a)$ by turning off the interactions involving particle $k$. The way that cluster properties fail at the operator level is that interactions that should survive in the cluster limit actually vanish.

While cluster properties of $\tilde{U}(\Lambda, a)$ in the sense the equation (3) do not hold, it turns our that the $S$ matrices associated with the $2 + 1$ representations of $\tilde{U}_{ij,k}(\Lambda, a)$ and $\tilde{U}_{ij} \otimes U_k(\Lambda, a)$ are identical.

The equivalence of the $2+1$ $S$ matrices to the corresponding $S$ matrices for the tensor product dynamics

$$\tilde{S}_{ij,k} = S_{ij} \otimes I_k$$  \hspace{1cm} (10)

implies the existence [4] of an $S$-matrix preserving unitary transformation, $A_{ij,k}$, satisfying

$$A_{ij,k} \tilde{U}_{ij,k}(\Lambda, a) A_{ij,k}^\dagger = \tilde{U}_{ij} \otimes U_k(\Lambda, a)$$  \hspace{1cm} (11)

$$A_{ij,k} \tilde{M}_{ij,k} A_{ij,k}^\dagger = M_{ij} \otimes I_k$$  \hspace{1cm} (12)

$$A_{ij,k} \hat{J}_0^2 A_{ij,k}^\dagger = \hat{J}_0^2 \neq I_k.$$  \hspace{1cm} (13)

Using these unitary operators for each pair of interacting particles we construct their Cayley transforms, add the Cayley transforms, and inverse Cayley transform the sum of the individual Cayley transforms to get a new unitary operator $A$[5]:

$$C_{ij,k} := i(A_{ij,k} - I)(A_{ij,k} + I)^{-1}$$  \hspace{1cm} (14)

$$C := C_{12,3} + C_{23,1} + C_{31,2}$$  \hspace{1cm} (15)

$$A := (I - iC)(I + iC)^{-1} \quad A \to A_{ij,k} \to I.$$  \hspace{1cm} (16)

The resulting transformation $A$ is an $S$-matrix preserving unitary transformation. Using it to transform $\tilde{U}(\Lambda, a)$ gives a new unitary representation[6] of the Poincaré group

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

satisfying cluster properties (3) of the unitary representation of the Poincaré group

$$U(\Lambda, a) \to \tilde{U}_{ij}(\Lambda, a) \otimes U_k(\Lambda, a).$$  \hspace{1cm} (17)

The Poincaré generators for this representation include sums of the different pairwise interactions. The operators $A$ and $A_{ij,k}$ also generate additional three-nucleon forces that are needed to satisfy the commutation relations. These three-nucleon forces are different from standard three-nucleon forces because they are frame-dependent and are explicit functions of the underlying two-nucleon forces.

The resulting invariant mass operator has the form

$$M = A(\sum A_{ij,k}^\dagger M_{ij} \otimes k A_{ij,k} - 2M_0)A^\dagger = A \tilde{M} A^\dagger.$$  \hspace{1cm} (18)

The important property is that because $A$ is $S$-matrix preserving it means the $\tilde{M}$ leads to the same $S$ matrix as $M$, so even though the representation $\tilde{U}(\Lambda, a)$ fails to
It has the same \( S \) matrix as the model satisfying cluster properties. This means that for scattering and bound state calculations, \textit{it is sufficient to solve the Faddeev equations for \( M \).}

This avoids that complications of computing the additional three-nucleon interaction that appears in \( M \) in the three-body case, however it is important to remark that this equivalence does not extend to the four-nucleon case unless the corresponding generated three-body interactions appear in the four-body mass operator. We also remark the two-body interactions \( \tilde{V}_\gamma \) are really three-body operators due to the role of the spectator momentum - one can think of them as frame-dependent two-body interactions.

The next set of complications are more technical. In order to formulate relativistic Faddeev equations for the dynamics given by the mass operator \( \tilde{M} \) we define the operators

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

(19)

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

(20)

Using time-dependent methods \cite{12} it is possible to show that the \( S \) matrix can be expressed in terms of the following relativistic transition operator

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

(21)

The input to (23) equation is the \( 2 + 1 \) transition operators

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

(24)

As in the non-relativistic case the Faddeev equation can be solved with mathematically controlled errors because the iterated kernel is compact and can be uniformly approximated by a finite dimensional matrix:

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

(25)

\[
\tilde{T} (z) = (I - \tilde{K} (z)^2)^{-1} (\tilde{D} (z) + \tilde{K} (z) \tilde{T} (z)).
\]

(26)

The first technical problem is to construct realistic two-nucleon interactions. Repeating what was done for the non-relativistic problem, by carefully fitting models to two-nucleon phase shifts, can also be done in the relativistic case, but because both the relativistic and non-relativistic interactions are fit to the same data, refitting is not necessary. The trick was first given by Coester, Pieper and Serduke\cite{7}.

The mass operator in the Bakamjian-Thomas representation has the form

\[
\tilde{M} := M_0 + \tilde{V}_{12} + \tilde{V}_{23} + \tilde{V}_{31}
\]

(27)

where

\[
\tilde{V}_{ij} := \sqrt{q_i^2 + (\sqrt{k_i^2 + m_i^2} + 2\mu_{ij} v_{nr_{ij}} + \sqrt{k_{ij}^2 + m_j^2 + \mu_{ij} v_{nr_{ij}}}^2 -}
\]

\[
\sqrt{q_i^2 + (\sqrt{k_i^2 + m_i^2} + \sqrt{k_{ij}^2 + m_j^2}^2)^2}
\]
and \( \mu_{ij} \) is the two-nucleon reduced mass. The important property of this interaction is the corresponding \( 2 + 1 \) mass operator is a function of the non-relativistic nucleon-nucleon rest Hamiltonian, \( h_{ij} = H_{ij} - \frac{(p_i + p_j)^2}{2(m_i + m_j)} \). This means that the \( S \) matrix in both the relativistic and non-relativistic models have the same internal wave functions and phase shifts as a function of the center of mass momentum \( k \):

\[
\langle p, q, k_r| S_{ij,k_r} | p', q', k'_r \rangle = \delta(p - p')\delta(q - q')\langle k_r | s_{ij} | k'_r \rangle \quad (29)
\]

\[
\langle p, q_{nr}, k_{nr}| S_{ij,k_{nr}} | p', q'_{nr}, k'_{nr} \rangle = \delta(p - p')\delta(q_{nr} - q'_{nr})\langle k_{nr} | s_{ij} | k'_{nr} \rangle. \quad (30)
\]

In order to take advantage of this relationship we recall that the two-body input to the relativistic Faddeev equation can be expressed in the following ways

\[
\langle p, q_r, k_r| \tilde{T}_\alpha | p', q'_r, k'_r \rangle = \langle p, q_r, k_r | \tilde{V}_\alpha | p', q'_r, k'_r \rangle = \langle p, q_r, k_r | \tilde{M}_\alpha - M_0 | p', q'_r, k'_r \rangle. \quad (31)
\]

Since for the above choice of interaction the internal relativistic and non-relativistic wave functions are identical we get the identifications

\[
\langle k| k'_{nr}^- \rangle = \langle k| k'_r \rangle. \quad (32)
\]

Using this it follows that the Faddeev kernel can be written as

\[
\langle q_\alpha, k_\alpha | T_\alpha(z)(z - \tilde{M}_0)^{-1} | q'_\alpha, k'_\alpha \rangle = \delta(q_\alpha - q'_\alpha) \frac{m_{\alpha\alpha}(k) + m_{\alpha\alpha}(k')}{(\sqrt{q_\alpha^2 + m_{\alpha\alpha}^2(k)}) + (\sqrt{q_\alpha^2 + m_{\alpha\alpha}^2(k')})} \times \frac{1}{M_0(q_\alpha, k_\alpha) - M_0(q_\alpha, k'_\alpha) + i0^+} \quad (33)
\]

where

\[
m_{\alpha\alpha}(k) := \sqrt{k_i^2 + m_i^2} + \sqrt{k_j^2 + m_j^2} \quad (34)
\]

and

\[
z = M_0(q_\alpha, k_\alpha) + i0^+, \quad \langle k_\alpha | t_r(z) | k'_\alpha \rangle = \frac{2\mu}{\sqrt{k_i^2 + m_i^2} + \sqrt{k_j^2 + m_j^2}} + \frac{2\mu}{\sqrt{k_i^2 + m_i^2} + \sqrt{k_j^2 + m_j^2}} \times \langle k_\alpha | t_{nr}(k_j^2/2\mu + i0^+) | k'_\alpha \rangle. \quad (35)
\]

These relations express the Faddeev kernel in terms of the non-relativistic transition matrix elements. The identity of the wave functions, which was used to derive the result, is limited to the case that the transition matrix elements are half-on shell. This relations does not extend to the off-shell transition matrix elements which appear in the Faddeev kernel.

The fully off-shell two-body \( \tilde{T}_\alpha(z) \) embedded in the three-nucleon Hilbert space can be computed by solving the first resolvent equation[8]:

\[
\tilde{T}_\alpha(z) = \tilde{T}_\alpha(z') + \tilde{T}_\alpha(z)' \frac{z' - z}{(z - M_0)(z' - M_0)} \tilde{T}_\alpha(z'). \quad (36)
\]

Finally we note that while it is natural to use variables to label two-nucleon interactions to be associated with the two-nucleon rest frames, with these variables the permutation operators involve Wigner rotations. The Wigner rotations can be
removed from the permutation operators by expressing everything in terms of variables associated with the three-nucleon rest frame. In this representation the Wigner rotations appear in the elementary nucleon-nucleon interactions:

$$\langle \mathbf{q}_i, \mu_i, \mathbf{q}_j, \mu_j \mid t_\nu(z) \mid \mathbf{q}_i', \mu_i', \mathbf{q}_j', \mu_j' \rangle =$$

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

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

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

$$D_{\nu_i',\mu_i'}^{\nu_j',\mu_j'}[R_{wc}(B_c^{-1}(q_{ij}), q_i)] D_{\mu_j',\nu_j'}^{\mu_i',\nu_i'}[R_{wc}(B_c^{-1}(q_{ij}), q_j)] \times$$

$$\left( \frac{\omega_i(\mathbf{q}_i) + \omega_j(\mathbf{q}_j)}{\omega_i(\mathbf{k}_{ij}) + \omega_j(\mathbf{k}_{ji})} \right)^{1/2}.$$  (37)

The final technical challenge is that at the few-hundred MeV scale partial-wave projections begin to lose their underlying advantage. This is in part because the transition operator is a relatively smooth operator, so there are necessarily a lot of cancellations involved in the partial wave expansions, especially at large angles. As a practical matter double precision three-nucleon calculations based on partial wave methods are limited to about 300 MeV. Direct integration calculations are stable over a wider range of energies [8], extending to the few-GeV scale.

The final computational challenge is that the natural input to direct-interaction three-nucleon calculations is a momentum-space interaction in operator form. One of the few realistic interactions in operator form is the Argonne V18 interaction which is given in a configuration-space representation.

It has been Fourier transformed [9] in an operator form. The resulting interaction can be expanded in terms of 24 spin-isospin operators.

It is possible to reduce the number of required operators using symmetry properties. The most general nucleon-nucleon interactions can be expanded in terms of the following spin operators:

$$\langle \mathbf{k} | v_{mn} | \mathbf{k}' \rangle = \sum V_n W_n$$  (38)

$$W_1 := I$$  (39)

$$W_2 := j_1 \cdot j_2$$  (40)

$$W_3 := (j_1 \cdot \mathbf{K}) \otimes (j_2 \cdot \mathbf{K})$$  (41)

$$W_4 := (j_1 \cdot \mathbf{Q}) \otimes (j_2 \cdot \mathbf{Q})$$  (42)

$$W_5 := (j_1 \cdot \mathbf{N}) \otimes I_2 + I_1 \otimes (j_2 \cdot \mathbf{N})$$  (43)

$$W_6 := (j_1 \cdot \mathbf{K}) \otimes (j_2 \cdot \mathbf{Q}) + (j_1 \cdot \mathbf{Q}) \otimes (j_2 \cdot \mathbf{K})$$  (44)

where

$$\mathbf{K} := k' - k \quad \mathbf{Q} := k' + k \quad \mathbf{N} := k' \times k.$$  (45)

The coefficients of these operator expansions are simply related to the Wolfenstein parameters [11], which facilitates the computation of spin observables. The remaining
computational difficulty is related to the observation that there are five independent operators on shell, and one more off shell.

Numerical instabilities can arise when the independent on-shell and off-shell operators are not simply related[10]. For the choice above five of the off-shell operators become the five on-shell operators in the on-shell limit.

The last dynamical consideration is the computation of current matrix elements, which are needed to study few-nucleon systems with few-GeV scale hadronic probes. The important observation is that any change of representation of the Poincaré generators requires a corresponding change of representation of the current operator in order leave the physical observables unchanged. In principle one expects both the strong dynamics and electromagnetic current to satisfy cluster properties. This suggest that using currents that have well-behaved cluster expansions should not be used in Bakamjian-Thomas representation of the dynamics. In general one expects that one must first transform either the current operator or the dynamics with an operator like (16):

\[
\langle \Psi_f | J^\mu(0) | \Psi_i \rangle = \langle \bar{\Psi}_f | A^\dagger J^\mu(0) A | \bar{\Psi}_i \rangle \approx \langle \bar{\Psi}_f | J^\mu(0) | \bar{\Psi}_i \rangle. \tag{46}
\]

When \( A \) is close to the identity, which appears to be the case for nuclear physics scales ([12]), this operator can be ignored, resulting in a significant increase in computational efficiency.

As a result of these various simplifications and tricks it has been possible to perform three-nucleon calculations with realistic interactions [13]. Figure 1 show the differential cross section for \( p - d \) elastic scattering for relativistic and non-relativistic three-nucleon models with realistic two- (CD Bonn) and three-nucleon (TM99) interactions. The calculations show that for elastic scattering the relativistic effects are small, except at back angles, where there is some enhancement due to relativity for the 250 MeV curves. Comparison of these calculations with measurements from [14] shows that there is missing physics that is not explained by the combination of the TM99 three-nucleon force and relativity. Elastic spin observables at these also show a weak dependence on relativistic effects. This is in part the comparison that we show is only sensitive to the difference in how the two-nucleon subsystem is embedded in the three nucleon system. Breakup calculations, on the other hand, exhibit strong relativistic effects in certain observables. The calculations in figure 2 [15] provide a beautiful illustration of some of these effects. These calculations were at a much higher energy than the calculations of figure 1 however they only use spin-independent Malfliet-Tjon interaction. The figure show the fivefold differential cross section where the scattered protons emerge symmetric at different angles relative to the beam line. These are plotted against the energy of one of the scattered protons. This figure shows a dramatic crossing of the non-relativistic and relativistic results as the angle is changed. The data is from [16].

In this manuscript we have discussed many of the complications involved in making realistic relativistic three-nucleon calculations. We have discussed tricks that make realistic calculations possible at relativistic energies. The calculations suggest that the relativistic effects are small for nucleon-meson degrees of freedom, except in certain areas of breakup phase space, however realistic relativistic calculations have not been performed at the few-GeV scale. The discrepancy of the calculated large-angle elastic scattering cross section with data suggests some missing short distance physics in the three-nucleon forces.

We anticipate that relativistic few-body methods will be an important tool for understanding physics at scales between the Chiral perturbation theory and perturbative QCD scales. Modern computers have made realistic few-GeV scale few-body calculations feasible. The approach that we advocate, using models with the dominant degrees of freedom and symmetries is similar to the approach used in condensed matter physics. It is far easier than attempting to get mathematical convergent approximations of QCD at the Few GeV scale.
Figure 1: Relativistic effects in elastic p-d scattering

Figure 2: Relativistic effects in n-d breakup reactions
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References