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A New Look into the Partial-Wave Decomposition of Three-Nucleon Forces

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Abstract. We demonstrate that the partial-wave decomposition of three-nucleon forces used up to now in momentum space has to be necessarily unstable for high partial waves. This does not affect the applications performed up to now, which were restricted to low partial waves. We present a new way to perform the partial-wave decomposition free of that defect. This is exemplified for the most common two-pion-exchange Tucson-Melbourne three-nucleon force. For the lower partial waves the results of the old method are reproduced.

1 Introduction

Three-nucleon forces (3NF) act for more than two nucleons. The interesting questions are after their strengths and their signatures.

A first observable where 3NF clearly show up is the binding energy of the triton. Here it is known that the most recent realistic nucleon-nucleon (*NN*) forces cannot produce the binding energy and 3NF are needed in order to get the experimental number [1, 2].

The next logical step is to look into the $3N$ continuum. Our results based on numerically precise solutions of the three-nucleon ($3N$) Faddeev equations and realistic *NN* forces agree overall very well with experimental data [3]. In elastic nucleon-deuteron (*Nd*) scattering there is only one discrepancy that sticks out clearly, namely the low-energy vector analyzing power, which depends sensitively on the ^3P_j *NN* force components. There is either an ambiguity in their determination from *NN* data or one really sees a 3NF effect. The inclusion of the 3NF, which have been worked out up to now, does not diminish that discrepancy [3, 4]. Right now it remains a puzzle [5]. At very low energies, near the *Nd* threshold, one has to expect 3NF effects, connected with the accompanying shift of the triton binding energy. But we have found also scattering observables that do not scale with the triton binding energy [6, 3]. The threshold region is an interesting energy domain to be studied further experimentally. At higher energies, up to about 60 MeV, the 3NF effects we find for cross sections are mostly small (of the and

$$G_{\alpha_J\alpha'_J}(qq'x) = \sum_k P_k(x) \sum_{l_1+l_2=l} \sum_{l'_1+l'_2=l'} q^{l_2+l'_2} q'^{l_1+l'_1} g^{kl_1l_2l'_1l'_2}_{\alpha_J\alpha'_J}. \tag{A.3}$$

The purely geometrical quantity $g^{kl_1l_2l'_1l'_2}_{\alpha_J\alpha'_J}$ has now to be taken without isospin:

$$\begin{aligned} g^{kl_1l_2l'_1l'_2}_{\alpha_J\alpha'_J} = &- \sqrt{\hat{l}\hat{s}\hat{j}\hat{\lambda}\hat{I}\hat{l}'\hat{s}'\hat{j}'\hat{\lambda}'\hat{I}'} \\ &\times \sum_{LS} \hat{L}\hat{S} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s \\ \frac{1}{2} & S & s' \end{Bmatrix} \begin{Bmatrix} l & s & j \\ \lambda & \frac{1}{2} & I \\ L & S & J \end{Bmatrix} \begin{Bmatrix} l' & s' & j' \\ \lambda' & \frac{1}{2} & I' \\ L & S & J \end{Bmatrix} \\ &\times \hat{k}\, (\tfrac{1}{2})^{l_2+l'_1} \sqrt{\frac{(2l+1)!}{(2l_1)!(2l_2)!}} \sqrt{\frac{(2l'+1)!}{(2l'_1)!(2l'_2)!}} \\ &\times \sum_{ff'} \begin{Bmatrix} l_1 & l_2 & l \\ \lambda & L & f \end{Bmatrix} \begin{Bmatrix} l'_2 & l'_1 & l' \\ \lambda' & L & f' \end{Bmatrix} C(l_2 0\ \lambda 0, f0) C(l'_1 0\ \lambda' 0, f'0) \\ &\times \begin{Bmatrix} f & l_1 & L \\ f' & l'_2 & k \end{Bmatrix} C(k0\ l_1 0, f'0) C(k0\ l'_2 0, f0). \end{aligned} \tag{A.4}$$

The very left recoupling coefficient has to be taken in the form where both δ-functions act to the right,

$$_1\langle pq\alpha|P_{12}P_{23}|p'q'\alpha'\rangle_1 = \tfrac{1}{2}(-)^{l'+s'+t'+1} \int_{-1}^{+1} dx \frac{\delta(p'-\tilde{\pi})}{p'^{l'+2}} \frac{\delta(q'-\tilde{\chi})}{q'^{\lambda'+2}} \tilde{G}_{\alpha\alpha'}(pqx) \tag{A.5}$$

with

$$\begin{aligned} \tilde{\pi} &= \sqrt{\tfrac{1}{4}p^2 + \tfrac{9}{16}q^2 + \tfrac{3}{4}pqx}, \\ \tilde{\chi} &= \sqrt{p^2 + \tfrac{1}{4}q^2 - pqx} \end{aligned} \tag{A.6}$$

and $\tilde{G}_{\alpha\alpha'}(pqx)$ can be taken, for instance, from ref. [3].

Finally, the recoupling coefficient from the states of type 1 to 3 require a form where both δ-functions act to the left,

$$\langle pq\alpha|P_{12}P_{23}|p'q'\alpha'\rangle = \tfrac{1}{2}(-)^{l'+s'+t'+1} \int_{-1}^{+1} dx \frac{\delta(p-\tilde{\tilde{\pi}})}{p^{l+2}} \frac{\delta(q-\tilde{\tilde{\chi}})}{q^{\lambda+2}} \tilde{G}_{\alpha'\alpha}(p'q'x) \tag{A.7}$$

with

$$\begin{aligned} \tilde{\tilde{\pi}} &= \sqrt{\tfrac{1}{4}p'^2 + \tfrac{9}{16}q'^2 + \tfrac{3}{4}p'q'x}, \\ \tilde{\tilde{\chi}} &= \sqrt{p'^2 + \tfrac{1}{4}q'^2 + p'q'x}. \end{aligned} \tag{A.8}$$

In Eq. (A.7) we need the same quantity $\tilde{G}$ as in Eq. (A.5) but with interchanged arguments.

Appendix B. Cubic Hermitean Splines

In Appendix A we encountered two-fold interpolations. They have to be performed for very many channels and should be as good as possible. We found that our usual basis splines [14] are not efficient enough to perform these two-fold interpolations within a reasonable time. Therefore we sought a more efficient interpolation algorithm.

Such an algorithm can be constituted by using cubic Hermitean splines. Although cubic Hermitean splines are well-known in the literature (see, for example, ref. [21]), we shall give here a short introduction in order to explain our way to use them.

Consider a function $f(x)$ given at certain grid points x_i, $i = 1, \ldots, n$. Let x be positioned in the interval $[x_i, x_{i+1}]$. For the sake of simpler notation we call the end points $x_i \equiv x_1$ and $x_{i+1} \equiv x_2$. Then one defines a unique cubic polynomial $f_i(x)$ by the following constraints:

$$\begin{aligned} f_i(x_1) &= f(x_1), \\ f_i(x_2) &= f(x_2), \\ f_i{}'(x_1) &= f'(x_1), \\ f_i{}'(x_2) &= f'(x_2). \end{aligned} \tag{B.1}$$

Therefore these interpolating functions $f_i(x)$ and their derivatives $f_i{}'(x)$ are continuous at the grid points x_i. They are given by

$$f_i(x) = f(x_1)\phi_1(x) + f(x_2)\phi_2(x) + f'(x_1)\phi_3(x) + f'(x_2)\phi_4(x) \tag{B.2}$$

in terms of the spline functions

$$\begin{aligned} \phi_1(x) &= \left(\frac{(x_2 - x)^2}{(x_2 - x_1)^3}((x_2 - x_1) + 2(x - x_1))\right), \\ \phi_2(x) &= \left(\frac{(x_1 - x)^2}{(x_2 - x_1)^3}((x_2 - x_1) + 2(x_2 - x))\right), \\ \phi_3(x) &= \frac{(x - x_1)(x_2 - x)^2}{(x_2 - x_1)^2}, \\ \phi_4(x) &= \frac{(x - x_1)^2(x - x_2)}{(x_2 - x_1)^2}. \end{aligned} \tag{B.3}$$

We approximate the derivatives $f'(x_1)$ and $f'(x_2)$ with the help of a quadratic polynomial, which is uniquely defined by the function values at a grid point and its two neighbours. Calling $x_{i-1} = x_0$ and $x_{i+1} = x_3$ we get

$$\begin{aligned} f'(x_1) \approx{}& f(x_2)\frac{x_1 - x_0}{x_2 - x_1}\frac{1}{x_2 - x_0} - f(x_0)\frac{x_2 - x_1}{x_1 - x_0}\frac{1}{x_2 - x_0} \\ &+ f(x_1)\left(\frac{x_2 - x_1}{x_1 - x_0} - \frac{x_1 - x_0}{x_2 - x_1}\right)\frac{1}{x_2 - x_0}, \\ f'(x_2) \approx{}& f(x_3)\frac{x_2 - x_1}{x_3 - x_2}\frac{1}{x_3 - x_1} - f(x_1)\frac{x_3 - x_2}{x_2 - x_1}\frac{1}{x_3 - x_1} \\ &+ f(x_2)\left(\frac{x_3 - x_2}{x_2 - x_1} - \frac{x_2 - x_1}{x_3 - x_2}\right)\frac{1}{x_3 - x_1}. \end{aligned} \tag{B.4}$$

At the end points x_1 and x_n we define the quadratic polynomial by $f(x_1)$, $f(x_2)$, and $f(x_3)$ and by $f(x_{n-2})$, $f(x_{n-1})$, and $f(x_n)$, respectively. This is achieved by putting $x_0 = x_3$ in the first case and $x_3 = x_{n-2}$ in the second case.

Insertion of Eq. (B.4) into Eq. (B.2) yields

$$f_i(x) = \sum_{j=0}^{3} S_j(x) f(x_j) \tag{B.5}$$

for the interpolating function in the i-th interval of the grid points. Thereby we are led to the modified spline functions

$$\begin{aligned} S_0(x) &= -\phi_3(x)\frac{x_2 - x_1}{x_1 - x_0}\frac{1}{x_2 - x_0}, \\ S_1(x) &= \phi_1(x) + \phi_3(x)\left(\frac{x_2 - x_1}{x_1 - x_0} - \frac{x_1 - x_0}{x_2 - x_1}\right)\frac{1}{x_2 - x_0} - \phi_4(x)\frac{x_3 - x_2}{x_2 - x_1}\frac{1}{x_3 - x_1}, \end{aligned}$$

$$S_2(x) = \phi_2(x) + \phi_3(x)\frac{x_1 - x_0}{x_2 - x_1}\frac{1}{x_2 - x_0} + \phi_4(x)\left(\frac{x_3 - x_2}{x_2 - x_1} - \frac{x_2 - x_1}{x_3 - x_2}\right)\frac{1}{x_3 - x_1},$$

$$S_3(x) = \phi_4(x)\frac{x_2 - x_1}{x_3 - x_2}\frac{1}{x_3 - x_1}. \tag{B.6}$$

Eq. (B.5) is very well suited for the numerical usage. The modified spline functions $S_j(x)$ are independent of the function values and depend only on the grid points and the actual position x. Therefore they can be prepared beforehand. This is very important if one has to interpolate very many functions given at the same grid points as we have to do in our 3NF code.

The form of Eq. (B.5) is the same as the one found in ref. [14] for basis splines. The difference is that the sum for the basis splines runs over the whole grid, whereas the sum for the Hermitean splines in Eq. (B.5) has only four terms related to the four grid points nearest to the interpolation point x. (Basis splines are global splines, whereas Hermitean splines are local.) Assuming a grid of typically 20 points the one-dimensional interpolation using Hermitean splines needs only $\frac{1}{5}$ operations as compared to basis splines. For a two-dimensional interpolation the number of operations is reduced by a factor of $\frac{1}{25}$.

For the two-dimensional interpolation one has to make a bi-cubic ansatz for the interpolating functions $f_{ij}(x,y)$. To define a bi-cubic function uniquely we need 16 constraints, which we choose as

$$\begin{aligned} f_{ij}(x_1,y_1) &= f(x_1,y_1), \\ \frac{\partial f_{ij}(x,y_1)}{\partial x}\Big|_{x=x_1} &= \frac{\partial f(x,y_1)}{\partial x}\Big|_{x=x_1}, \\ \frac{\partial f_{ij}(x_1,y)}{\partial y}\Big|_{y=y_1} &= \frac{\partial f(x_1,y)}{\partial y}\Big|_{y=y_1}, \\ \frac{\partial^2 f_{ij}(x,y)}{\partial x\,\partial y}\Big|_{x=x_1,y=y_1} &= \frac{\partial^2 f(x,y)}{\partial x\,\partial y}\Big|_{x=x_1,y=y_1} \end{aligned} \tag{B.7}$$

and identical expressions for the other three points (x_1,y_2), (x_2,y_1), and (x_2,y_2), respectively. Hereby the four grid points (x_1,y_1), (x_1,y_2), (x_2,y_1), and (x_2,y_2) are the nearest neighbours for the interpolation point (x,y) in the xy-plane.

The partial derivatives are approximated as in the one-dimensional case. The second derivative is estimated by a bi-quadratic polynomial, which is uniquely given by the function value at the specific grid point and the function values of the eight surrounding grid points.

Following these steps one obtains

$$f_{ij}(x,y) = \sum_{k=0}^{3}\sum_{l=0}^{3} S_{kl}^{(2)}(x,y)\,f(x_k,y_l) \tag{B.8}$$

for the interpolating function. It is a fairly easy exercise to show that the two-dimensional spline functions $S_{kl}^{(2)}(x,y)$ are simply given by

$$S_{kl}^{(2)}(x,y) = S_k(x)S_l(y). \tag{B.9}$$

Analogous equations hold for interpolations in more than two dimensions.

According to our experience one- and two-dimensional interpolations using Hermitean splines are at least of the same accuracy as interpolations based on basis splines.

References

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