Numerical Implementation of Three-Body Forces in Bound State Faddeev Calculations in Three Dimensions

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Abstract

The Faddeev equations for the three-body bound state are solved directly as three-dimensional integral equations without employing partial wave decomposition. Two-body forces of the Malfliet-Tjon type and simple spin independent genuine three-body forces are considered for the calculation of the three-body binding energy.

Key words: Faddeev equations, three-body forces
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1. Introduction

Three nucleon (3N) bound state calculations are traditionally carried out by solving Faddeev equations on a partial wave basis. After truncation this leads to a set of a finite number of coupled equations in two variables for the amplitude. The calculations are performed either in momentum space \cite{1–3}, in configuration space \cite{4,5}, or in a hybrid fashion using both spaces \cite{6}. Though a few partial waves often provide qualitative insight, modern three nucleon bound state calculations need 34 or more different isospin, spin and orbital angular momentum combinations \cite{3}. It appears therefore natural to avoid a partial wave representation completely and work directly with vector variables \cite{7}. This is especially the case, if one wants to consider genuine three-nucleon force (3NF) effects. The true advantage stems from the fact that a 3N calculation is carried out in Jacobi variables, whereas a typical 3NF has the form of two consecutive meson-exchange propagators between e.g. particles 1 and 2, then particles 2 and 3. Using vector variables, the necessary coordinate transformations are numerically realized by interpolations, whereas in a partial wave based calculation a large amount of coupling coefficients has to be evaluated and stored \cite{8}, requiring large storage and memory capabilities of a computer architecture.

2. Bound State Equation with a Three-Body Force

The Faddeev component describing the bound state of three identical particles interacting via pairwise forces as well as genuine three-body forces...
can be written as
\[ \psi_i = G_0 t_i \psi_i + (1 + G_0 t_i) G_0 W^{(i)}(1 + P) \psi_i, \quad (1) \]
where \( i = 1, 2, 3 \). In the following, we choose \( i = 1 \) without loss of generality. The operator \( t_i \) stands for the two-body \( t \)-matrix in the subsystem (\( jk \)) summing up the pair interaction in this system. The quantity \( W^{(i)} \), shown diagrammatically in Fig. 1, is defined via
\[ V_{123} = W^{(1)} + W^{(2)} + W^{(3)}, \quad (2) \]
where \( W^{(i)} \) is that part of the full 3N force \( V_{123} \) which is symmetric for the exchange of nucleons \( j \) and \( k \) (\( j \neq i \neq k \)). The decomposition of Eq. (2) is natural, e.g. for the \( \pi \pi \) exchange 3N force which is present in all currently available 3N forces. The free 3N propagator is given by
\[ G^{-1}_0 = E - \frac{p^2}{m} - \frac{3}{4m} q^2, \quad (3) \]
where \( p \) and \( q \) are the standard Jacobi momenta
\[ p_i = \frac{1}{2}(k_j - k_k) \]
\[ q_i = \frac{2}{3}(k_j - \frac{1}{2}(k_j + k_k)), \quad (4) \]
where \( ijk = 123 \) and cyclic permutations thereof.

The permutation operator \( P \) is given as \( P = P_{12}P_{23} + P_{13}P_{21} \), and the full 3N wave function is related to the Faddeev component by
\[ |\Psi\rangle = (1 + P)|\psi\rangle. \quad (5) \]
The solution of Eq. (1) with \( W^{(1)} = 0 \) is described in detail in Ref. [7] and shall not be discussed here. For our model calculations we also use Yukawa interactions of the Malfliet-Tjon type here, however, we modify the interaction with a cutoff function of a dipole type [9].

In order to develop the algorithm, we concentrate on a model 3N force of scalar meson exchange character, which can be written as
\[ |\Psi\rangle = (1 + P)|\psi\rangle. \quad (5) \]

The function \( F(Q^2) = \left[ (\Lambda_s^2 - m_s^2)/(\Lambda_s^2 + Q^2) \right]^2 \) represents a cutoff function for large momenta \( Q^2 \). The parameters of the 3NF used in the presented calculation are given in Table 1. For evaluating Eq. (1) we need to calculate matrix elements like
\[ (pq|G_0 W^{(1)}|\Psi). \quad (8) \]

Considering the momentum dependence in the meson propagators of \( W^{(1)} \), one can easily imagine that the efficiency of any algorithm will crucially depend on the choice of coordinate system(s) when carrying out the integrations over the intermediate momenta. Our numerical evaluation of Eq. (8) is based on the realization that \( W^{(1)} \) can be interpreted as two independent interactions, first in the subsystem (12), then in (31). Explicitly, we write
\[ (pq|W^{(1)}|\Psi) = \int d^3 p' \int d^3 p'' \ z(p' ' | p'' | q'| q'') \langle p' ' q'| p'' | q'' | \Psi \rangle \]
\[ \int d^3 p'' \frac{F((p' - p'')^2)}{(p' - p'')^2 + m_s^2} \]
\[ \int d^3 p''' \int d^3 q''' \ z(p'' | p''' | q''') \langle p'' | p''' | q''' | \Psi \rangle. \quad (9) \]

Here the subscripts 1, 2, 3 of the bra and ket vectors define the meaning of the related vectors \( p \) and \( q \), namely the particle number \( i \) singled out by \( q_i \) as indicated in Eq. (4). We would like to point out that in each integration over a piece of the 3NF we only integrate over three variables,

\[
\begin{array}{llll}
g_s^2/4\pi m_s (\text{MeV}) & \Lambda_s (\text{MeV}) & a_s & \\
5.0 & 305.8593 & 1000.0 & -1.73
\end{array}
\]
\[
\frac{g_\alpha^2}{4\pi} m_\alpha (\text{MeV}) \Lambda_\alpha (\text{MeV}) \frac{g_\alpha^2}{4\pi} m_\alpha (\text{MeV}) \Lambda_\alpha (\text{MeV})
\]

| \(g_\alpha^2/4\pi\) | \(m_\alpha (\text{MeV})\) | \(\Lambda_\alpha (\text{MeV})\) |
|-----------------|-----------------|-----------------|
| -3.5775         | 330.2104        | 1500            |
| 9.4086          | 612.4801        | 1500            |

Table 2
The parameters of the two nucleon pair force.

namely the magnitude of a momentum and two angle variables. It turns out that it is most favorable to choose momenta \(q', q''\) parallel to the \(z\)-axis, so that no interpolation on the unknown function \(\Psi(p, q', \hat{p} \cdot \hat{q}')\) needs to be performed. The calculation of the transformation from one subsystem to another, e.g. \(2\langle p'' q' | p''' q''' \rangle_3\), requires three-dimensional interpolations. We employ cubic Hermite splines [8], which prove to be both accurate and fast.

3. Computational Approach

The discretized Faddeev equation for a bound state (neglecting spin degrees of freedom) is an integral equation in three variables on a typical grid size of \(65 \times 65 \times 42\) (momentum magnitudes, \(p, q\), and angle between the momentum vectors). A priori the multidimensionality of the integral equation to be solved requires more memory. However, on an MPP system the number of variables and thus the memory do not pose a computational problem, since a variable defining a specific dimension of the grid can be distributed over a number of processors, leaving a lower dimensional grid on each processor. As such, our three-dimensional approach is ideally suited as MPP application, and we can achieve an almost perfect load balance in our runs.

The eigenvalue equation for the bound state is solved iteratively by using Lanczo’s type techniques, here the method of iterated orthogonal eigenvectors [2]. For a typical run ten orthogonal eigenvectors are calculated per energy. We need about 5 to 7 energy iterations to find the ground state energy.

The calculation of the kernel of the integral equation means evaluating the matrix elements given on the right-hand side of Eq. (1) on a fixed grid \(p, q, \text{ and angle } x = \cos(\hat{p} \cdot \hat{q})\). The two-body t-matrix (with the two-nucleon pair interaction as the driving term) is obtained by solving a system of linear equations of the form \(A \cdot x = b\), where \(A\) is typically a \(2500 \times 2500\) matrix. This system is solved for about 60 different vectors \(b\), distributed over correspondingly many processors. The integrations over the 3NF terms are also distributed over the same number of processors, which depends on the size of the \(q\)-grid. Details about the different grid sizes and the dependence of the numerical accuracy on them can be found in Ref. [7].

4. Results and Discussion

For our model calculation we use Yukawa interactions of the Malfliet-Tjon [10] type

\[
V(p', p) = \sum_{\alpha=a,r} \frac{g_\alpha^2}{(p' - p)^2 + m_\alpha^2} \left( \frac{\Lambda_\alpha^2 - m_\alpha^2}{\Lambda_\alpha^2 + (p' - p)^2} \right)^2
\]

with a short-ranged repulsive and a long-ranged attractive piece. The parameters used in our calculation are given in Table 2. A calculation of the three-body binding energy with this pair force gives \(E_t = 7.699\) MeV. The parameters of the 3NF are then adjusted such that its inclusion in the calculation gives a binding energy \(E_t = 8.590\) MeV, a value close to the measured one. The full 3N wave function is calculated from the solution of Eq. (1) using Eq. (5) and shown in Fig. 2 as a function of \(x\).
of the momenta $p$ and $q$ at the fixed angle $x = 1$. A comparison of the 3N wave functions calculated with the 2N pair forces alone and with the inclusion of the 3NF is shown in Figs. 3 and 4. Both figures depict slices through the wave functions at specific values.

The 3NF in our model calculation is attractive, as expressed by the larger binding energy. One would expect that the system becomes slightly smaller and acquires more high momentum components. Since the wave functions are both normalized to one, an increase of high momentum components will be seen as a decrease in low momentum components, as seen in Fig. 3. Once the wave function decreases by some orders of magnitude, the differences disappear.

In summary, an alternative approach to state-of-the-art three-nucleon bound state calculations, which are based on solving the Faddeev equations on a partial wave basis, is to work directly with momentum vectors. We formulate the Faddeev equations for identical particles as a function of vector Jacobi momenta, specifically the magnitudes of the momenta and the angle between them, for the case when not only pair forces act between the particles but also genuine three-body forces. As model forces we concentrate on scalar forces, a superposition of an attractive and repulsive Yukawa interaction for the pair force and an attractive Yukawa interaction for the three-body force. We demonstrate the numerical feasibility and accuracy of the solution. We want to point out that the incorporation of the 3N forces is less cumbersome in a three-dimensional approach, and the algorithm can be made quite efficient on parallel architectures.

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