2N and 3N systems in three dimensional formalism - a compilation.

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Classical QM - always start with the Schrödinger equation:

\[ i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \]

or

\[ |\psi(t)\rangle = \exp(-i\hat{H}(t - t_0)) |\psi(t_0)\rangle. \]

Hands on approach - the proton and the neutron are two states of the spin $\frac{1}{2}$ isospin $\frac{1}{2}$ nucleon. We use three dimensional states:

\[ |k_1 k_2\rangle \otimes |\uparrow \downarrow\rangle_{\text{isospin}} \otimes |\uparrow \uparrow\rangle_{\text{spin}}, |Kp\rangle \otimes |\uparrow \downarrow\rangle_{\text{isospin}} \otimes |\uparrow \rangle_{\text{spin}} \]

or

\[ |k_1 k_2 k_3\rangle \otimes |\uparrow \downarrow \downarrow\rangle_{\text{isospin}} \otimes |\uparrow \downarrow \downarrow\rangle_{\text{spin}}, |Kpq\rangle \otimes |\uparrow \downarrow \downarrow\rangle_{\text{isospin}} \otimes |\downarrow \uparrow \downarrow\rangle_{\text{spin}}. \]
COMPLEXITY

- Classical non-relativistic QM, but calculations get quite complicated.
- A lot of pieces of the puzzle must fit together.
  - Analytical calculations are practically impossible. This is especially true for 3N systems.
  - Numerical code implementing analytical results must not contain errors. Typically thousands of lines of FORTRAN code. Each +, − must be in the proper place. This process must be automated.
  - Our solution - extensive use of symbolic programming within the Mathematica system.
- Exponential increase in efficiency. What used to take months now takes 15 min and a click of a button.
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OUR SCHEME

- Chose a potential (2N, 3N) and a problem (2N bound state, 3N bound state, transition operator calculation).

- Calculate the hard part (analytical expressions and FORTRAN code) using Mathematica.

- Construct a FORTRAN implementation of linear operators (resulting directly from the Schrödinger equation with some additional constraints on the states of the system under consideration) from automatically generated code.

- Use Krylov subspace methods to reduce the size of the operators (this is especially needed for large 3N systems and requires the use of powerful computing clusters - JUQUEEN in FZJ).

- Solve the reduced (say 40 × 40 dimensional) linear (eigen) equation using classical methods. We use LAPACK or Mathematica linear solvers.

- Compare results with classical PWD calculations.
The choice of partial wave channels is to some degree arbitrary. If we want more precise predictions, we take a larger number of channels but it is not always true that PWD states are organized in such a way that taking a large number of channels produces matrix elements of operators organized by their magnitude. 3D calculations utilize all partial waves.

Using Krylov subspace methods and 3D representation automatically organizes matrix elements according to their size. This gives hope for better precision.

Why not! Rare opportunity to gain direct insight into the nuclear processes.
DEUTERON

- $\phi_1, \phi_2$ describe the 2N bound state.
- Linear operator (acting in the space of scalar functions $\phi$).
- Expressed in terms of integrals but an explicit matrix representation is also available.

$$\left( \tilde{K}^d(E_d)\phi \right)_q(|p|) = \frac{1}{E_d - \frac{p^2}{m}} \int d^3p' \sum_{j=1}^6 \nu_j^{00}(p, p') \sum_{k''=1}^2 \left( \sum_k \left( A^d(p) \right)_{qk}^{-1} B^d_{kjk''}(p, p') \right) \phi_{k''}(|p'|)$$

Time independent Schrödinger equation

$$\rightarrow (\tilde{K}^d(E)\phi)_q(|p|) = \lambda \phi_q(|p|)$$ - find $E$ such that $\lambda \approx 1$ ($E \approx E_d$).
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\[
\left( \mathcal{K}^d(E_d)\phi \right)_q(|p|) = \frac{1}{E_d - \frac{p^2}{m}} \int d^3p' \sum_{j=1}^{6} v_{j00}(p, p') \sum_{k''=1}^{2} \left( \sum_{k} (A^d(p))_{qk}^{-1} B_{kk''}^d(p, p') \right) \phi_{k''}(|p'|)
\]

Time independent Schrödinger equation

\[\rightarrow \left( \mathcal{K}^d(E)\phi \right)_q(|p|) = \lambda \phi_q(|p|) - \text{find } E \text{ such that } \lambda \approx 1 \ (E \approx E_d).\]
• $\phi_q(|p|) - 2 \cdot 40 = 80$ dimensional vector.
• $\tilde{K}^d(E_d) - 80 \times 80$ matrix.
• $\left( \sum_k (A^d(p))^{-1}_{qk} B^d_{kk''}(p, p') \right)$ - calculated in Mathematica.
• $v_{j}^{00}(p, p')$ - $2N$ potential (decomposed).
• Small problem, a chance to test our Krylov subspace method approach.
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- $\tilde{K}^d(E_d)$ - $80 \times 80$ matrix.
- $\left( \sum_k (A^d(p))^{-1}_{qk} B^d_{kj} (p, p') \right)$ - calculated in Mathematica.
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The $s$-wave (left) and $d$-wave (right) component of the deuteron wave function - chiral NNLO potential.

The same but for the Bonn B potential.

Two-nucleon systems in three dimensions
Golak, J. and Glöckle, W. and Skibiński R. and Witała H. and Rozpedzik D. and Topolnicki, K. and Fachruddin, I. and Elster, Ch. and Nogga, A.
TRANSITION OPERATOR (T MATRIX)

Linear operators in the space of scalar functions $t$.

The transition operator is fully determined by the set of 6 $t$ functions.

An explicit matrix representation is available.

$$
(\tilde{\mathcal{B}} t)_{k}^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x') = \\
\int_{0}^{+\infty} d|p''| \int_{-1}^{1} dx'' \int_{0}^{2\pi} d\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6} \frac{|p''|^2}{|E| - |p''|^2/m + i\epsilon}$$

$$
\tilde{v}^{\{\gamma\}}_{j} (|p'|, |p''|, \sqrt{1 - x'^2} \sqrt{1 - x''^2} \cos \phi'' + x' x'')$$

$$
\mathcal{B}_{kjj'}(|p'|, \{|p|\}, x', |p''|, x'', \phi'')$$

$$
(\tilde{t}(|p''|) t)_{k}^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x') = \\
m \int_{-1}^{1} dx'' \int_{0}^{2\pi} d\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6}$$

$$
\tilde{v}^{\{\gamma\}}_{j} (|p'|, |p''|, \sqrt{1 - x'^2} \sqrt{1 - x''^2} \cos \phi'' + x' x'')$$

$$
\mathcal{B}_{kjj'}(|p'|, \{|p|\}, x', |p''|, x'', \phi'')$$

$$
\tilde{t}^{\{\gamma\}}_{j'} (\{E\}, |p''|, \{|p|\}, x'')$$

$LSE \rightarrow t = \nu + \tilde{\mathcal{B}} t$
Linear operators in the space of scalar functions \( t \).

The transition operator is fully determined by the set of 6 \( t \) functions.

An explicit matrix representation is available.

\[
\begin{align*}
(\mathcal{B}t)_{k}^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x') &= \\
&= \int_{0}^{+\infty} d|p''| \int_{-1}^{1} dx'' \int_{0}^{2\pi} d\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6} \frac{|p''|^2}{|E| - \frac{|p''|^2}{m} + i\epsilon} \gamma_j \{E\}, |p'|, \{|p|\}, x'') \\
&= t_j^{\{\gamma\}} (\{E\}, |p''|, \{|p|\}, x'')
\end{align*}
\]

\[
\begin{align*}
(\tilde{\mathcal{B}}t)_{k}^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x') &= \\
&= \int_{0}^{1} dx'' \int_{0}^{2\pi} d\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6} \frac{m}{|E|} \gamma_j \{E\}, |p'|, \{|p|\}, x''') \\
&= t_j^{\{\gamma\}} (\{E\}, |p''|, \{|p|\}, x''')
\end{align*}
\]

\[\text{LSE} \rightarrow t = \nu + \mathcal{B}t\]
TRANSITION OPERATOR

- $t_k^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x')$ - for each $\gamma$, $E$, $|p|$ - $6 \cdot 40 \cdot 40 = 9600$ dimensional vector.

- $(\mathcal{B} t)_k^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x')$ - $4 \cdot 40 \cdot \langle \text{number of energies} \rangle$ $9600 \times 9600$ dimensional independent problems.

- Cases with $E > 0$ and $E < 0$ need to be considered separately.
  
  - $E < 0$ - singularity around the deuteron binding energy, we need to substitute $\mathcal{V} |\phi_d\rangle \frac{1}{E - E_b} \langle \phi_d | \mathcal{V}$. All expressions simple to calculate with our tools.
  
  - $E > 0$ - problem with singularity in $\mathcal{B}$ (we introduce $\tilde{f}$).
TRANSITION OPERATOR $E < 0$

A slice through $t_i^{\{\gamma\}} (\{E\}, |p'|, \{|p|\}, x')$ (the cross represents deuteron substitution):

(i) $E < 0$

- $i = 1$

- $i = 4$

Energy [MeV]
Different Methods for the Two-Nucleon T-Matrix in the Operator Form
Few-Body Systems 2012 (53 237-252)
The Quantum Mechanical Few-Body Problem. Walter Glöckle (Springer-Verlag)
Different Methods for the Two-Nucleon T-Matrix in the Operator Form
Few-Body Systems 2012
T OPERATOR ON SHELL - $E = 300\text{MeV}$

Different Methods for the Two-Nucleon T-Matrix in the Operator Form
Few-Body Systems 2012
3N BOUND STATE

- Linear operator in the space of $\beta$ scalar functions.
- The 3N bound state is determined by the 8 $\beta$ functions.
- Currently no explicit matrix representation is available - it is constructed from integrals.

\[
\begin{align*}
\left( \hat{P}_{1223}^{\text{scalar}} \beta \right)^{(k)}_{t'T'} (|p', q'|) &= \sum_{i=1}^{8} \sum_{tT} \beta^{(i)}_{tT} (|P_{1231}^{2312}(p', q')|, |Q_{2312}^{2312}(p', q')|), \\
\hat{P}_{1223}^{2312}(p', q') \cdot \hat{Q}_{2312}^{2312}(p', q') \\
C_{t'T'k; tTi}^{1223}(p', q')
\end{align*}
\]

\[
\begin{align*}
\left( \hat{P}_{1323}^{\text{scalar}} \beta \right)^{(k)}_{t'T'} (|p', q'|) &= \sum_{i=1}^{8} \sum_{tT} \beta^{(i)}_{tT} (|P_{1231}^{2313}(p', q')|, |Q_{2313}^{2313}(p', q')|), \\
\hat{P}_{1323}^{2313}(p', q') \cdot \hat{Q}_{2313}^{2313}(p', q') \\
C_{t'T'k; tTi}^{1323}(p', q')
\end{align*}
\]

Schrödinger equation

\[
\rightarrow \left( \hat{G}_0(E) \left( \hat{V}^{\text{scalar}} + \hat{V}^{(1)\text{scalar}} \right) (\hat{1} + \hat{P}_{1223}^{\text{scalar}} + \hat{P}_{1323}^{\text{scalar}}) \right) \beta = \lambda \beta \text{ solve and find } E \text{ such that } \lambda \approx 1.
\]
3N BOUND STATE

- Linear operator in the space of $\beta$ scalar functions.
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\[
\left( \mathcal{V}^{\text{scalar}}_{\beta} \right)_{i, j}^{(k)} (|p', q', \hat{p}' \cdot \hat{q}'\rangle = \int d^3 p' \sum_{i=1}^{8} \sum_{T} \sum_{j=1}^{6} \beta_{i T}^{(j)} (|p', q|, \hat{p}' \cdot \hat{q}) \mathcal{V}_{j}^{T t} (|p|, |p'|, \hat{p} \cdot \hat{p}')
\]

\[
(C^{-1} L)_{kji} (p, q; p', p'; p', q)
\]

\[
(\mathcal{V}^{(1)\text{scalar}}_{\beta})_{i T} (|p|, |q|, \hat{p} \cdot \hat{q}) = \sum_{i=1}^{8} \int d^3 p \int d^3 q \sum_{T'} \beta_{i T}^{(j)} (|p|, |q|, \hat{p} \cdot \hat{q}) \mathcal{V}_{j}^{T t} (|p|, |q|, \hat{p} \cdot \hat{q})
\]

\[
\sum_{r=1}^{8} C_{kr}^{-1} (p, q) E_{ri}^{tt} (pq; pqpq; pq) \equiv \sum_{i=1}^{8} \int d^3 p \int d^3 q \sum_{T'} \beta_{i T}^{(j)} (|p|, |q|, \hat{p} \cdot \hat{q}) (C^{-1} E)_{ri}^{tt} (pq; pqpq; pq)
\]

Schrödinger equation
\[
\rightarrow \left( \mathcal{G}_0 (E) \left( \mathcal{V}^{\text{scalar}} + \mathcal{V}^{(1)\text{scalar}} \right) \left( \mathcal{I} + \mathcal{P}^{\text{scalar}}_{1223} + \mathcal{P}^{\text{scalar}}_{1323} \right) \right) \beta = \lambda \beta \text{ solve and find } E \text{ such that } \lambda \approx 1.
\]
3N BOUND STATE

- $\beta_{T'}^{(k)}(\left|p'\right|, \left|q'\right|, \hat{p}' \cdot \hat{q}') - 3 \cdot 8 \cdot 40 \cdot 40 \cdot 40 = 1536000$ dimensional vectors.
- $\tilde{\mathcal{V}}_{\text{scalar}}, \tilde{\mathcal{V}}_{(1)\text{scalar}}, \tilde{\mathcal{P}}_{1223}, \tilde{\mathcal{P}}_{1323} - 1536000 \times 1536000$ dimensional operators.
- Large computational resources necessary - JUQUEEN in FZJ JUELICH.
A Three-Dimensional Treatment of the Three-Nucleon Bound State
Few-Body Systems 2012

\[
\begin{array}{|c|c|c|}
\hline
& \text{PWD} & \text{3D} \\
\hline
\lambda & 1.0 & 0.99976 \\
\langle E_{\text{kin}} \rangle & 33.448 & 33.412 \\
\langle E_{\text{pot}}^{2N} \rangle & -41.329 & -41.273 \\
\langle E_{\text{pot}}^{3N} \rangle & -0.765 & -0.770 \\
\text{total energy} & -8.646 & -8.631 \\
\hline
\end{array}
\]
SUMMARY AND OUTLOOK

- We developed a new framework for dealing with 2N and 3N systems.
- The results for the deuteron, t-matrix and 3N bound state have been verified and published in:
  - Few-Body Systems 2012 (53 237-252)
  - Few-Body Systems 2012 (1-20)
- Current work is focused on compiling a collection of FORTRAN codes, Mathematica notebooks and packages that can, together with a comprehensive description (aka phd thesis), be used by anyone to reconstruct 2N and 3N calculations.
- Our tools can also be deployed in processes involving EM probes:
  - Deuteron Disintegration in Three Dimensions, Few-Body Systems 2012
- We start employing our three dimensional tools to study the decay of the muonic atom in $\mu^- + d \rightarrow \nu_\mu + n + n$ and other electro-weak processes.