2N and 3N systems in three dimensional formalism

Kacper Topolnicki

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INTERNATIONAL PHD PROJECTS IN APPLIED NUCLEAR PHYSICS AND INNOVATIVE TECHNOLOGIES
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DECENT QM

- Calculations within the confines of a well defined set of DOF. The proton and the neutron are two states of the spin $\frac{1}{2}$ isospin $\frac{1}{2}$ nucleon. We use three dimensional states:

$$|\,\mathbf{k}_1\mathbf{k}_2\rangle\otimes\,|\uparrow\downarrow\rangle^{\mathrm{isospin}}\otimes\,|\uparrow\uparrow\rangle^{\mathrm{spin}},|\,\mathbf{Kp}\rangle\otimes\,|\uparrow\downarrow\rangle^{\mathrm{isospin}}\otimes\,|\uparrow\downarrow\rangle^{\mathrm{spin}}$$

$$|\,\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\rangle\otimes\,|\uparrow\downarrow\downarrow\rangle^{\mathrm{isospin}}\otimes\,|\uparrow\downarrow\downarrow\rangle^{\mathrm{spin}},|\,\mathbf{Kpq}\rangle\otimes\,|\uparrow\downarrow\downarrow\rangle^{\mathrm{isospin}}\otimes\,|\downarrow\uparrow\downarrow\rangle^{\mathrm{spin}}.$$

DECENT QM

- Classical QM - always start with the Schrödinger (or Faddeev) equation:

$$i\hbar\partial_t \mid \psi(t)\rangle = \check{H} \mid \psi(t)\rangle$$

$$\mid \psi(t)\rangle = \exp(-i\check{H}(t - t_0)) \mid \psi(t_0)\rangle.$$

or LSE:

$$t = t + \check{V}\check{G}_0 t$$

COMPLEXITY

- Classical non-relativistic QM, but calculations get quite complicated.
- A lot of pieces of the puzzle must fit together.
  - Gargantuan mathematical expressions make analytical calculations practically impossible. This is especially true for 3N systems.
  - Code for the numerical solution (that uses the complicated expressions) must not contain errors. Depending on the problem - possibly thousands of lines of FORTRAN code to be generated (implements eg. momentum dependent matrix elements). 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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WHY 3D CALCULATIONS?

- Basic idea - given a linear operator $\check{O}$ (any implementation will do, no explicit matrix representation necessary) and a starting vector $\mathbf{v}$ calculate the KRYLOV subspace:

$$K(\check{O}, \mathbf{v}) = span(\mathbf{v}, \check{O}\mathbf{v}, \check{O}\check{O}\mathbf{v}, \ldots)$$

- More sophisticated numerically stable algorithms are available eg. Arnoldi iteration - they produce the same space.
- Work with $\check{O}$ projected onto this subspace.

WHY 3D CALCULATIONS?

- The choice of partial wave channels is to *some* degree arbitrary.
  - More precise predictions $\rightarrow$ take a larger number of channels (matrix elements of operators not necessarily organized by their magnitude).
  - Using Krylov subspace methods and 3D representation automatically organizes matrix elements according to their size. This gives hope for better precision.
  - 3D calculations utilize all partial waves.
- Why not! Rare opportunity to gain direct insight into the nuclear processes.

OUR SCHEME

- Chose a potential (2N, 3N) and a problem (2N bound state, transition operator (NN t matrix), 3N bound state).
- Calculate the hard part (analytical expressions and FORTRAN code) using Mathemaica.
- 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.

DEUTERON

- ϕ_1, ϕ_2 describe the 2N bound state.
- Linear operator (acing in the space of scalar functions ϕ).
- Expressed in terms of integrals but an explicit matrix representation is also available.

$$\left(\check{K}^d(E_d)\phi\right)_q(|\mathbf{p}|) =$$

$$\frac{1}{E_d - \frac{\mathbf{p}^2}{m}} \int d^3\mathbf{p}' \sum_{j=1}^{6} v_j^{00}(\mathbf{p}, \mathbf{p}') \sum_{k''=1}^{2}$$

$$\left(\sum_k \left(A^d(\mathbf{p})\right)^{-1}_{qk} B^d_{kjk''}(\mathbf{p}, \mathbf{p}') \right) \phi_{k''}(|\mathbf{p}'|)$$

$\check{K} \leftrightarrow$ operator

$\phi \leftrightarrow \phi_1, \phi_2$

$\left(\check{K}\phi\right)_q(|\mathbf{p}|), \phi_q(|\mathbf{p}|) \leftrightarrow$ take value at ...

Time independent Schrödinger equation
$\rightarrow \left(\check{K}^d(E)\phi\right)_q(|\mathbf{p}|) = \lambda\phi_q(|\mathbf{p}|)$ - find E such that $\lambda \approx 1$ ($E \approx E_d$).

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DEUTERON

- $\phi_q(|\mathbf{p}|)$ - $2 \cdot 40 = 80$ dimensional vector.
- $\check{K}^d(E_d)$ - 80×80 matrix.
- $\left(\sum_k \left(A^d(\mathbf{p})\right)^{-1}_{qk} B^d_{kjk''}(\mathbf{p}, \mathbf{p}') \right)$ - calculated in Mathematica.
- $v_j^{00}(\mathbf{p}, \mathbf{p}')$ - 2N potential (decomposed).
- Small problem, a chance to test our Krylov subspace method approach.

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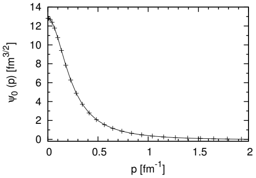
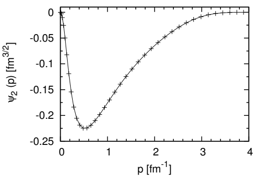
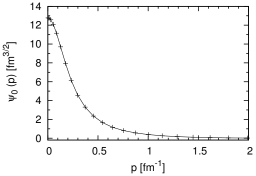
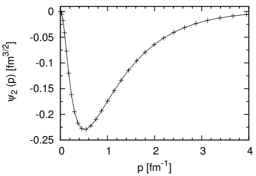
DEUTERON





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
Phys. Rev. C 81 3 (2010)
Golak, J. and Glöckle, W. and Skibiński R. and Witała H. and Rozpędzik 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.

$$(\check{\mathcal{B}}t)_k^{\{\gamma\}}\left(\{E\}, |\mathbf{p}'|, \{|\mathbf{p}|\}, x'\right) = \int_0^{+\infty} \mathrm{d}|\mathbf{p}''| \int_{-1}^{1} \mathrm{d}x'' \int_0^{2\pi} \mathrm{d}\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6} \frac{|\mathbf{p}''|^2}{\{E\} - \frac{|\mathbf{p}''|^2}{m} + i\epsilon}$$
$$v_j^{\{\gamma\}}\left(|\mathbf{p}'|, |\mathbf{p}''|, \sqrt{1-x'^2}\sqrt{1-x''^2}\cos\phi'' + x'x''\right)$$
$$\mathcal{B}_{kjj'}\left(|\mathbf{p}'|, \{|\mathbf{p}|\}, x', |\mathbf{p}''|, x'', \phi''\right)$$
$$t_{j'}^{\{\gamma\}}\left(\{E\}, |\mathbf{p}''|, \{|\mathbf{p}|\}, x''\right)$$

$$(\check{f}(|\mathbf{p}''|)t)_k^{\{\gamma\}}\left(\{E\}, |\mathbf{p}'|, \{|\mathbf{p}|\}, x'\right) = m \int_{-1}^{1} \mathrm{d}x'' \int_0^{2\pi} \mathrm{d}\phi'' \sum_{j=1}^{6} \sum_{j'=1}^{6}$$
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LSE $\rightarrow t = v + \check{\mathcal{B}}t$

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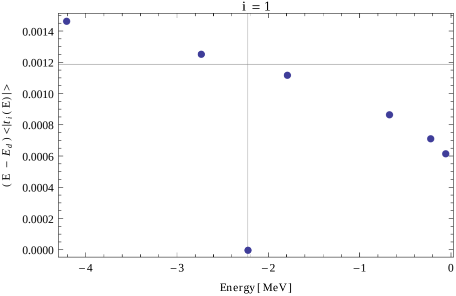
$$\boxed{\text{LSE} \rightarrow t = v + \check{\mathcal{B}}t}$$

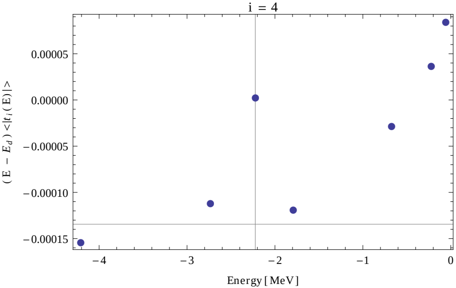
TRANSITION OPERATOR

- $t_k^{\{\gamma\}}\left(_{\{E\}}, |\mathbf{p}'|, _{\{|\mathbf{p}|\}}, x'\right)$ - for each $\gamma, E, |\mathbf{p}|$ - $6 \cdot 40 \cdot 40 = 9600$ dimensional vector.
- $\left(\check{\mathcal{B}} t\right)_k^{\{\gamma\}}\left(_{\{E\}}, |\mathbf{p}'|, _{\{|\mathbf{p}|\}}, x'\right)$ - $4 \cdot 40 \cdot <$ number of energies $>$ 9600×9600 dimensional independent problems 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 $\check{V} \mid \phi_d\rangle \frac{1}{E-E_b} \langle\phi_d \mid \check{V}$. All expressions simple to calculate with our tools.
  - $E > 0$ - problem with singularity in $\check{\mathcal{B}}$ (we introduce $\check{f}$).

TRANSITION OPERATOR $E < 0$

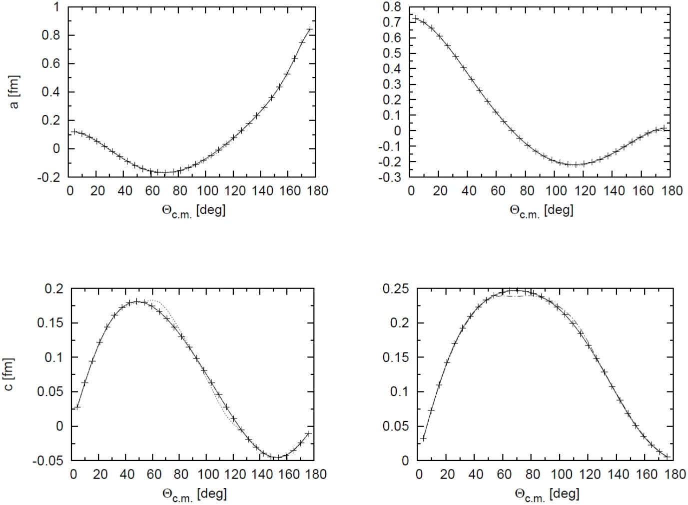
A slice through $t_i^{\{\gamma\}}\left(_{\{E\}}, |\mathbf{p}'|, _{\{|\mathbf{p}|\}}, x'\right)$ (the cross represents deuteron substitution):

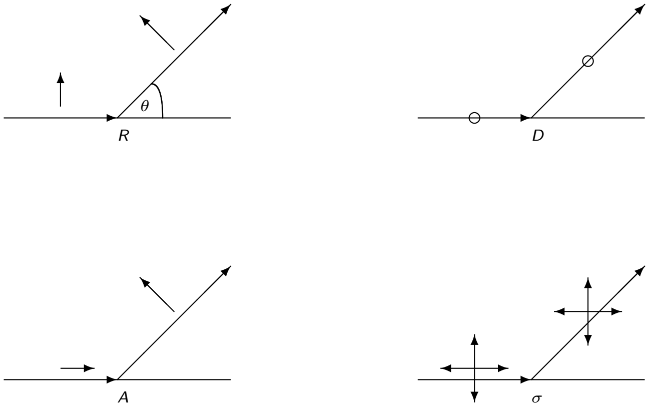




T OPERATOR ON SHELL - $E = 300\,\text{MeV}$

Different Methods for the Two-Nucleon T-Matrix in the Operator Form
Few-Body Systems 2012 (53 237-252)
Golak, J. and Skibiński, R. and Witała, H. and Topolnicki, K. and Glöckle, W. and Nogga, A. and Kamada, H.





The Quantum Mechanical Few-Body Problem. Walter Glöckle (Springer-Verlag)

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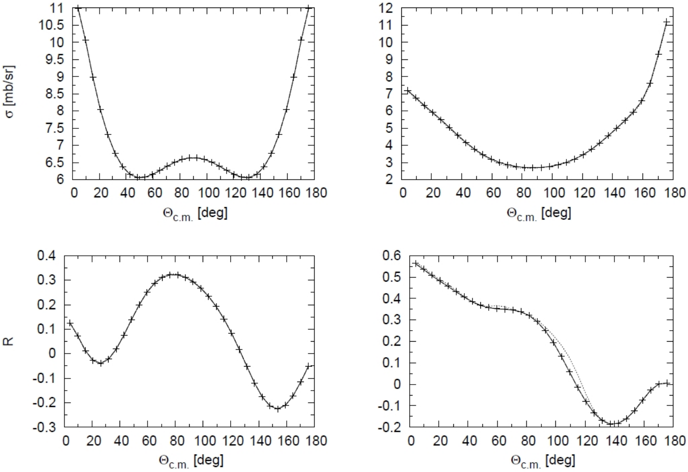

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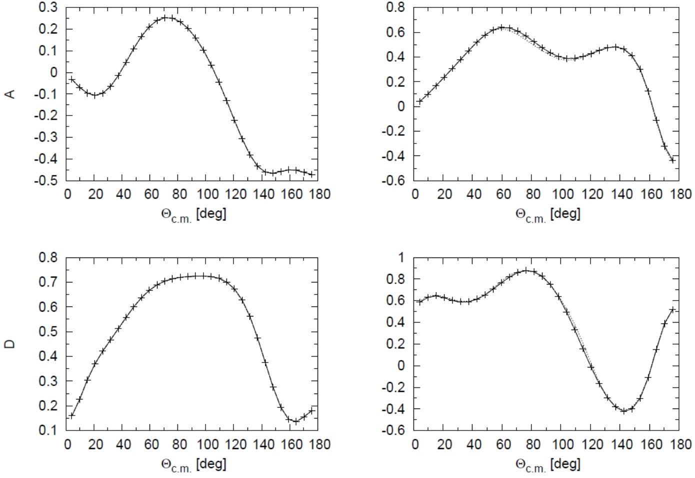

Different Methods for the Two-Nucleon T-Matrix in the Operator Form Few-Body Systems 2012 Golak, J. and Skibiński, R. and Witała, H. and Topolnicki, K. and Glöckle, W. and Nogga, A. and Kamada, H.

3N BOUND STATE

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

$$\left(\check{P}^{\rm scalar}_{1223}\beta\right)^{(k)}_{t'T'}(|\mathbf{p}'|,|\mathbf{q}'|,\hat{\mathbf{p}}'\cdot\hat{\mathbf{q}}') = \sum_{tT}\sum_{i=1}^{8}\beta^{(i)}_{tT}(|\mathbf{P}^{2312}(\mathbf{p}',\mathbf{q}')|,|\mathbf{Q}^{2312}(\mathbf{p}',\mathbf{q}')|, \hat{\mathbf{P}}^{2312}(\mathbf{p}',\mathbf{q}')\cdot\hat{\mathbf{Q}}^{2312}(\mathbf{p}',\mathbf{q}')) \, C^{1223}_{t'T'k;tTi}(\mathbf{p}',\mathbf{q}')$$

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Schrödinger (Faddeev) equation
$\rightarrow \left(\check{G}_0(E)\left(\check{V}^{\rm scalar}+\check{V}^{(1){\rm scalar}}\right)\left(\check{1}+\check{P}^{\rm scalar}_{1223}+\check{P}^{\rm scalar}_{1323}\right)\right)\beta = \lambda\beta$ solve and find E such that $\lambda \approx 1$.

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$$\left(\check{V}^{\mathrm{scalar}}\beta\right)^{(k)}_{t'T'}(|\mathbf{p}'|,|\mathbf{q}'|,\hat{\mathbf{p}}'\cdot\hat{\mathbf{q}}') =$$

$$\int \mathrm{d}^3\mathbf{p}' \sum_{i=1}^{8}\sum_{T}\sum_{j=1}^{6} \beta^{(i)}_{tT'}(|\mathbf{p}'|,|\mathbf{q}|,\hat{\mathbf{p}}'\cdot\hat{\mathbf{q}}) v_j^{tTtT'}(|\mathbf{p}|,|\mathbf{p}'|,\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')$$

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

$$(\check{V}^{(1)\mathrm{scalar}}\beta)^{(i)}_{tT}(|\mathbf{p}|,|\mathbf{q}|,\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}) =$$

$$\sum_{i=1}^{8}\int \mathrm{d}^3\mathbf{p}\int \mathrm{d}^3\mathbf{q}\sum_{t'} \beta^{(i)}_{tT}(|\mathbf{p}|,|\mathbf{q}|,\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})$$

$$\sum_{r=1}^{8} C^{-1}_{kr}(\mathbf{p},\mathbf{q}) E^{ttT}_{ri}(\mathbf{pq};\mathbf{pqpq};\mathbf{pq}) \equiv$$

$$\sum_{i=1}^{8}\int \mathrm{d}^3\mathbf{p}\int \mathrm{d}^3\mathbf{q}\sum_{t'} \beta^{(i)}_{tT}(|\mathbf{p}|,|\mathbf{q}|,\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})(C^{-1}E)^{ttT}_{ri}(\mathbf{pq};\mathbf{pqpq};\mathbf{pq})$$

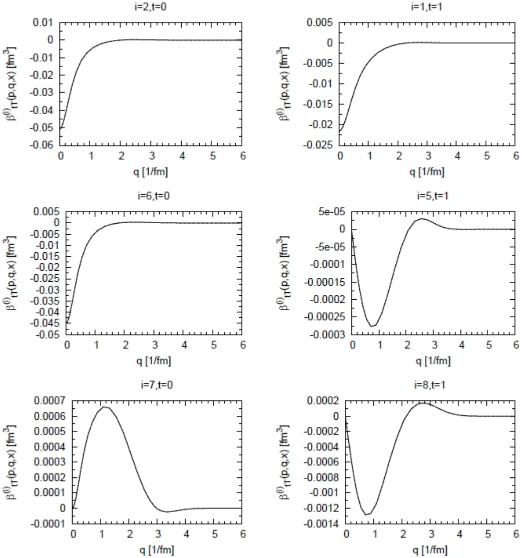
Schrödinger equation
$\rightarrow \left(\check{G}_0(E)\left(\check{V}^{\mathrm{scalar}} + \check{V}^{(1)\mathrm{scalar}}\right)\left(\check{1} + \check{P}^{\mathrm{scalar}}_{1223} + \check{P}^{\mathrm{scalar}}_{1323}\right)\right)\beta = \lambda\beta$ solve and find E such that $\lambda \approx 1$.

3N BOUND STATE

- $\beta^{(k)}_{t'T'}(|\mathbf{p}'|, |\mathbf{q}'|, \hat{\mathbf{p}}' \cdot \hat{\mathbf{q}}')$ - $3 \cdot 8 \cdot 40 \cdot 40 \cdot 40 = 1536000$ dimensional vectors.
- $\check{V}^{\mathrm{scalar}}, \check{V}^{(1)\mathrm{scalar}}, \check{P}^{\mathrm{scalar}}_{1223}, \check{P}^{\mathrm{scalar}}_{1323}$ - 1536000×1536000 dimensional operators.
- Large computational resources necessary - JUQUEEN in FZJ JUELICH.

A Three-Dimensional Treatment of the Three-Nucleon Bound State
Few-Body Systems 2012
Golak, J. and Topolnicki, K. and Skibiński, R. and Glöckle, W. and Kamada, H. and Nogga, A.

	PWD	3D
λ	1.0	0.99976
$< E_{\rm kin} >$	33.448	33.412
$< E_{\rm pot}^{\rm 2N} >$	-41.329	-41.273
$< E_{\rm pot}^{\rm 3N} >$	-0.765	- 0.770
total energy	-8.646	-8.631



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:
  - *Phys. Rev. C 81 3 (2010)*
  - *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 emploing our three dimensional tools to study the decay of the muonic atom in $\mu^- + d \to \nu_\mu + n + n$ and other electro-weak processes.