A numerical code to generate the nucleon-nucleon and three-nucleon matrix elements, NuHamil

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We introduce the numerical code NuHamil that generates the nucleon-nucleon (NN) and three-nucleon (3N) matrix elements. The code is written in the modern Fortran, and OpenMP+MPI hybrid parallelization is available for the 3N matrix element generation. The generated files can be served as inputs of the many-body solvers. The code is distributed on GitHub (XXXX) under the GPL 3.0 license.

I. INTRODUCTION

The atomic nucleus is a system dominated by the strong interaction, quantum chromodynamics. It is well established that the nucleon can be an effective degree of freedom, starting point of nuclear ab initio calculations. To perform an ab initio computation, the matrix elements of the nuclear Hamiltonian (and relevant operators) are essential. However, the development of a numerical code for matrix element generation can be an obstacle for practitioners. The goal of the NuHamil code is to provide an easy way to generate the NN and 3N matrix elements expressed in the spherical harmonic oscillator (HO) basis. The generated files can be used as inputs of the many-body calculations, such as the no-core shell model with the Bigstick code [1], the in-medium similarity renormalization group with imsrg++ code [2], and many-body perturbation theory with HartreeFock code [3]. In this document, a quick introduction of the NuHamil code is given.

II. NN AND 3N MATRIX ELEMENTS

Here, we briefly show the way to compute the NN and 3N matrix elements in the product of single-particle HO basis. In the second quantization form, the Hamiltonian H is

$$H = \sum_{\tilde{p}'\tilde{p}} T_{\tilde{p}'\tilde{p}} c^\dagger_{\tilde{p}'} c_{\tilde{p}} + \left(\frac{1}{2!}\right)^2 \sum_{\tilde{p}'\tilde{q}'\tilde{p}\tilde{q}} V^{\rm NN}_{\tilde{p}'\tilde{q}'\tilde{p}\tilde{q}} c^\dagger_{\tilde{p}'} c^\dagger_{\tilde{q}'} c_{\tilde{q}} c_{\tilde{p}} + \left(\frac{1}{3!}\right)^2 \sum_{\tilde{p}'\tilde{q}'\tilde{r}'\tilde{p}\tilde{q}\tilde{r}} V^{\rm 3N}_{\tilde{p}'\tilde{q}'\tilde{r}'\tilde{p}\tilde{q}\tilde{r}} c^\dagger_{\tilde{p}'} c^\dagger_{\tilde{q}'} c^\dagger_{\tilde{r}'} c_{\tilde{r}} c_{\tilde{q}} c_{\tilde{p}} + \cdots , \tag{1}$$

with the creation (annihilation) operator $c^\dagger$ (c). The subscripts $\tilde{p}$, $\tilde{q}$, ... indicate the single-particle states, and we usually use the harmonic oscillator quantum numbers, i.e. $\tilde{p} = \{n_p, l_p, j_p, m_p, t_{z,p}\}$. Here, n_p, l_p, j_p, m_p, and $t_{z,p}$ are the nodal quantum number, orbital angular momentum, total angular momentum, z-component of j_p, and the label distinguishing proton or neutron, respectively. The objects $T_{\tilde{p}'\tilde{p}}$, $V^{\rm NN}_{\tilde{p}'\tilde{q}'\tilde{p}\tilde{q}}$, and $V^{\rm 3N}_{\tilde{p}'\tilde{q}'\tilde{r}'\tilde{p}\tilde{q}\tilde{r}}$ are the kinetic, NN, and 3N matrix elements, respectively. Owing to the rotational invariance of the Hamiltonian, the numbers of matrix elements we need to compute are greatly reduced, and we need to compute the J-coupled matrix element because of the following relation:

$$T_{\tilde{p}'\tilde{p}} = T_{p'p}\delta_{m_{p'}m_p}, \tag{2}$$

$$V^{\rm NN}_{\tilde{p}'\tilde{q}'\tilde{p}\tilde{q}} = \sum_J \mathcal{C}^{j_{p'}j_{q'}J}_{m_{p'}m_{q'}M} \mathcal{C}^{j_p j_q J}_{m_p m_q M} V^{{\rm NN},J}_{p'q'pq}, \tag{3}$$

$$V^{\rm 3N}_{\tilde{p}'\tilde{q}'\tilde{r}'\tilde{p}\tilde{q}\tilde{r}} = \sum_{JJ_{p'q'}J_{pq}} \mathcal{C}^{j_{p'}j_{q'}J_{p'q'}}_{m_{p'}m_{q'}M_{p'q'}} \mathcal{C}^{j_p j_q J_{pq}}_{m_p m_q M_{pq}} \mathcal{C}^{J_{p'q'}j_{r'}J}_{M_{p'q'}m_{r'}M} \mathcal{C}^{J_{pq}j_r J}_{M_{pq}m_r M} V^{{\rm 3N},J_{p'q'}J_{pq}J}_{p'q'r'pqr}, \tag{4}$$

with the J-coupled matrix elements $T_{p'p}$, $V^{{\rm NN},J}_{p'q'pq}$, and $V^{{\rm 3N},J}_{p'q'r'pqr}$. Here the subscript p is the quantum number set without m_p, i.e. $p = \{n_p, l_p, j_p, t_{z,p}\}$. Note that the one-body kinetic matrix element $T_{\tilde{p}'\tilde{p}}$ is trivial to compute and

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not discussed here. The NN and 3N matrix elements can be obtained through the Talmi-Moshinsky transformation:

$$V^{\mathrm{NN},J}_{p'q'pq} = \sum_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} J^{\mathrm{NN}}_{\mathrm{rel}} S} \sum_{n'l'nl} T^{p'q'J}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} n'l'SJ^{\mathrm{NN}}_{\mathrm{rel}}} \; V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{n'l'nl} \; T^{pqJ}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nlSJ^{\mathrm{NN}}_{\mathrm{rel}}}, \tag{5}$$

$$V^{\mathrm{3N},J_{p'q'}J_{pq}J}_{p'q'r'pqr} = \sum_{N^{\mathrm{3N}}_{\mathrm{cm}} L^{\mathrm{3N}}_{\mathrm{cm}} J^{\mathrm{3N}}_{\mathrm{rel}}} \sum_{n'_{12} n'_3 \alpha' n_{12} n_3 \alpha} T^{p'q'r'J_{p'q'}J}_{N^{\mathrm{3N}}_{\mathrm{cm}} L^{\mathrm{3N}}_{\mathrm{cm}} n'_{12} n'_3 \alpha' J^{\mathrm{3N}}_{\mathrm{rel}}} \; V^{J^{\mathrm{3N}}_{\mathrm{rel}}}_{n'_{12} n'_3 \alpha' n_{12} n_3 \alpha} \; T^{pqrJ_{pq}J}_{N^{\mathrm{3N}}_{\mathrm{cm}} L^{\mathrm{3N}}_{\mathrm{cm}} n_{12} n_3 \alpha J^{\mathrm{3N}}_{\mathrm{rel}}}. \tag{6}$$

The quantum numbers introduced for the NN transformation $N^{\mathrm{NN}}_{\mathrm{cm}}$, $L^{\mathrm{NN}}_{\mathrm{cm}}$, n, l, S, and $J^{\mathrm{NN}}_{\mathrm{rel}}$ are the cm radial quantum number, cm orbital angular momentum, relative radial quantum number, relative orbital angular momentum, total spin, and total angular momentum of the relative motion, respectively. Likewise, $N^{\mathrm{3N}}_{\mathrm{cm}}$, $L^{\mathrm{3N}}_{\mathrm{cm}}$, $J^{\mathrm{3N}}_{\mathrm{rel}}$, n_{12}, n_3, and α are the cm radial quantum number, cm orbital angular momentum, total angular momentum of the relative motion, radial quantum number of relative motion of particles 1 and 2, radial quantum number of particle 3 relative to the cm of the particles 1 and 2, and the set of quantum numbers $\alpha = \{l_{12}, s_{12}, j_{12}, l_3, j_3\}$ respectively. As assigned in the radial quantum numbers, the quantum numbers with the index 12 are the numbers for the relative motion of particles 1 and 2, and the quantum numbers with the index 3 are the numbers for the particles 3 with respect to the cm of particles 1 and 2. The transformation coefficients are

$$\begin{aligned} T^{pqJ}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nlSJ^{\mathrm{NN}}_{\mathrm{rel}}} &= \sum_{\Lambda} [\Lambda] \sqrt{[j_p][j_q][S][J^{\mathrm{NN}}_{\mathrm{rel}}]} (-1)^{L^{\mathrm{NN}}_{\mathrm{cm}} + l + S + J} \begin{Bmatrix} l_p & 1/2 & j_p \\ l_q & 1/2 & j_q \\ \Lambda & S & J \end{Bmatrix} \\ &\quad \times \begin{Bmatrix} L^{\mathrm{NN}}_{\mathrm{cm}} & l & \Lambda \\ S & J & J^{\mathrm{NN}}_{\mathrm{rel}} \end{Bmatrix} \langle N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nl : \Lambda | n_p l_p n_q l_q : \Lambda \rangle_1, \end{aligned} \tag{7}$$

$$\begin{aligned} T^{pqrJ_{pq}J}_{N^{\mathrm{3N}}_{\mathrm{cm}} L^{\mathrm{3N}}_{\mathrm{cm}} n_{12} n_3 \alpha J^{\mathrm{3N}}_{\mathrm{rel}}} &= (-1)^{L^{\mathrm{3N}}_{\mathrm{cm}} + j_3 + 3/2} \sqrt{[J_{pq}][j_r][J^{\mathrm{3N}}_{\mathrm{rel}}][j_3]} \sum_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}}} T^{pqJ_{pq}}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} n_{12} l_{12} s_{12} j_{12}} \\ &\quad \times \sum_{\Lambda} (-1)^{\Lambda} [\Lambda] \langle N^{\mathrm{3N}}_{\mathrm{cm}} L^{\mathrm{3N}}_{\mathrm{cm}} n_3 l_3 : \Lambda | N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} n_r l_r : \Lambda \rangle_2 \begin{Bmatrix} j_{12} & L^{\mathrm{NN}}_{\mathrm{cm}} & \Lambda & L^{\mathrm{3N}}_{\mathrm{cm}} \\ J_{pq} & l_r & l_3 & J^{\mathrm{3N}}_{\mathrm{rel}} \\ J & j_r & 1/2 & j_3 \end{Bmatrix}. \end{aligned} \tag{8}$$

In the above equation, $6j$-, $9j$-, and $12j$-symbols are used with the standard notation [4]. The symbol $\langle NLnl : \Lambda | n_1 l_1 n_2 l_2 : \Lambda \rangle_d$ is the HO bracket defined with the notation in Ref. [5]. The inner summations in Eqs. (5) and (6) can be performed with the efficient matrix multiplication. Note that the antisymmetrization is not taken into account in Eqs. (5) and (6). For the NN system the antisymmetrization is trivial, while it is accomplished with the diagonalization coefficient of the antisymmetrizer for the 3N system [6–9]. The output NN matrix elements are in the proton-neutron formalism, while the 3N matrix elements are in isospin coupled formalism. The projection to the proton-neutron basis of 3N matrix elements should be done in a many-body solver.

The NN matrix element in the relative HO basis $V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{n'l'nl}$ can be obtained through the transformation:

$$V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{n'l'nl} = \int d\pi'_1 d\pi_1 \; \pi'^2_1 \pi^2_1 R_{n'l'}(\pi'_1) R_{nl}(\pi_1) V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{l'l}(\pi'_1, \pi_1), \tag{9}$$

with the radial HO wave function:

$$R_{nl}(\pi_1) = (-1)^n \sqrt{\frac{2b\Gamma(n+1)}{\Gamma(n+l+3/2)}} b(\pi_1 b)^l e^{-\pi^2_1 b^2/2} L^{(l+1/2)}_n(\pi^2_1 b^2). \tag{10}$$

Here the oscillator length b is defined as $b^2 = \hbar/m\omega$ with the nucleon mass m and oscillator frequency ω. The momentum π_1 is defined as $\pi_1 = |(\boldsymbol{p}_1 - \boldsymbol{p}_2)|/\sqrt{2}$, different from the usual relative momentum definition $p = |\boldsymbol{p}_1 - \boldsymbol{p}_2|/2$. The momentum-space matrix element is stored with the p notation, and $V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{l'l}(p', p)$ of some selected interactions are in the `input_nn_files` directory. The available chiral EFT NN interactions are listed in the following.

- LO interaction with 500 MeV regulator cutoff [10].
- NLO interaction with 500 MeV regulator cutoff [10].
- N^{2}LO interaction with 500 MeV regulator cutoff [10].
- N^{3}LO interaction with 500 MeV regulator cutoff [10].

- N^{4}LO interaction with 500 MeV regulator cutoff [10].
- N^{3}LO interaction with 500 MeV regulator cutoff [11].
- N^{2}LO$_{\rm opt}$ interaction [12].
- N^{2}LO$_{\rm sat}$ interaction [13].
- Δ-full N^{2}LO$_{\rm GO}$ interaction with 394 MeV regulator cutoff [14].
- Δ-full NLO$_{\rm GO}$ interaction with 450 MeV regulator cutoff [14].
- Δ-full N^{2}LO$_{\rm GO}$ interaction with 450 MeV regulator cutoff [14].

The 3N matrix element in the Jacobi HO basis $V^{J^{\rm 3N}_{\rm rel}}_{n'_{12}n'_3\alpha' n_{12}n_3\alpha}$ can be obtained through the transformation:

$$V^{J^{\rm 3N}_{\rm rel}}_{n'_{12}n'_3\alpha' n_{12}n_3\alpha} = \int d\pi'_1 d\pi'_2 d\pi_1 d\pi_2 \ \pi'^2_1\pi'^2_2\pi^2_1\pi^2_2 R_{n'_{12}l'_{12}}(\pi'_1)R_{n_{12}l_{12}}(\pi_1)R_{n'_3l'_3}(\pi'_2)R_{n_3l_3}(\pi_2)V^{J^{\rm 3N}_{\rm rel}}_{\alpha'\alpha}(\pi'_1,\pi'_2,\pi_1,\pi_2). \quad (11)$$

Here, the momentum π_2 is defined as $\pi_2 = \sqrt{2/3}|(\boldsymbol{p}_1+\boldsymbol{p}_2)/2-\boldsymbol{p}_3|$. The code has the capability to read the momentum-space matrix element $V^{J^{\rm 3N}_{\rm rel}}_{\alpha'\alpha}(\pi'_1,\pi'_2,\pi_1,\pi_2)$ from the HDF files created by Hebeler et al. [15, 16]. However, the code does not generate the matrix element $V^{J^{\rm 3N}_{\rm rel}}_{\alpha'\alpha}(\pi'_1,\pi'_2,\pi_1,\pi_2)$, and the HDF files are required if one needs fully non-locally regulated 3N interaction. On the other hand, the code supports the local 3N interaction. Owing to the diagonality in the coordinate-space matrix element, the transformation to the HO basis is relatively simple and given as

$$V^{J^{\rm 3N}_{\rm rel}}_{n'_{12}n'_3\alpha' n_{12}n_3\alpha} = \int d\xi_1 d\xi_2 \ \xi^2_1\xi^2_2 \tilde{R}_{n'_{12}l'_{12}}(\xi_1)\tilde{R}_{n_{12}l_{12}}(\xi_1)\tilde{R}_{n'_3l'_3}(\xi_2)\tilde{R}_{n_3l_3}(\xi_2)V^{J^{\rm 3N}_{\rm rel}}_{\alpha'\alpha}(\xi_1,\xi_2), \quad (12)$$

with the Jacobi coordinates $\xi_1 = |\boldsymbol{r}_1-\boldsymbol{r}_2|/\sqrt{2}$ and $\xi_2 = \sqrt{2/3}|(\boldsymbol{r}_1+\boldsymbol{r}_2)/2-\boldsymbol{r}_3|$. Also, the coordinate space radial function is

$$\tilde{R}_{nl}(\xi) = \sqrt{\frac{2\Gamma(n+1)}{b\Gamma(n+l+3/2)}}\frac{1}{b}\left(\frac{\xi}{b}\right)^l e^{-\xi^2_1/2b^2}L^{(l+1/2)}_n(\xi^2/b^2). \quad (13)$$

The coordinate-space matrix element $V^{J^{\rm 3N}_{\rm rel}}_{\alpha'\alpha}(\xi_1,\xi_2)$ is computed in the way shown in Ref. [17].

III. INSTALLATION

The `NuHamil` code is written in the fortran. It requires some standard libraries, `BLAS`, `LAPACK`, GNU scientific library (`gsl`), `zlib`, and `hdf5`. Once the requirements are satisfied, one can install the code in the following way.

Download the code with the `git` command:

```
$ cd ~
$ git clone XXXXXX
```

Note that downloading the code in the home directory is not mandatory, but it is recommended. Change the directory and download the submodules:

```
$ cd NuHamil
$ git submodule init
$ git submodule update
```

With the `make` command, the execution file will be build up, and the symbolic link will be created by the `make install` command.

```
$ make -j
$ make install
$ echo 'export PATH=$PATH:$HOME/bin' >> $HOME/.bashrc
$ source $HOME/.bashrc
```

IV. HOW TO RUN

Jobs can be controlled by a `python` script. Some example scripts are prepared in the `exe` directory. See below for simple explanations of the sample scripts.

- `exe/NuHamil_2BME.py` : generate the two-body interaction matrix element file of chiral EFT N^{3}LO (EM500) [11] softened by SRG up to $\lambda = 2$ fm^{-1}, in the gzipped **me2j** format at $e_{\max} = 14$ and $\hbar\omega = 16$ MeV.
- `exe/NuHamil_3BME.py` : generate the three-body interaction matrix element file of chiral EFT N^{3}LO NN (EM500) +3N N^{2}LO 3N (local-non-locally regulated) [18] softened by SRG up to $\lambda = 2$ fm^{-1}, in the gzipped **me3j** format at $e_{\max} = 14$, $E_{3\max} = 16$ and $\hbar\omega = 16$ MeV. The frequency conversion technique [8] is used with the parent frequency of 30 MeV.
- `exe/phase-shift-analysis/calc_phase_shift.py` : the phase-shift analysis using the chiral EFT NN at N^{3}LO (EM500) interaction [11].
- `exe/few-body/deuteron.py` : Calculate the deuteron properties with the diagonalization using the chiral EFT NN at N^{3}LO (EM500) interaction [11].
- `exe/few-body/triton_helium3.py` : calculate the ^{3}H or ^{3}He properties with the Jacobi-NCSM [19, 20] using the chiral EFT N^{3}LO (EM500) NN + N^{2}LO 3N (local-non-locally regulated) interaction [11, 18].
- `exe/few-body/helium4.py` : calculate the ^{4}He properties with the Jacobi-NCSM using the chiral EFT N^{3}LO NN (EM500)+ N^{2}LO 3N (local-non-locally regulated) interaction [11, 18].

V. MAJOR INPUT PARAMETERS

Here is the list of parameters that one might want to change.

- `rank`: particle number of the system
- `hw`: frequency of the HO basis in the unit of MeV. The typical range is $10 \lesssim$ `hw` $\lesssim 40$.
- `hw_target`: target frequency for the frequency conversion technique. The parameter is valid if `rank` > 2. To turn off the frequency conversion, remove the argument in a job submission script or set `hw_target` $= -1$.
- `emax`: $e_{\max}$ truncation for the output lab-frame HO matrix element file. One can take `emax` $\lesssim 18$.
- `e2max`: $e_{2\max}$ truncation for the output lab-frame HO matrix element file. It is recommended to use `e2max` $= 2 \times$ `emax`
- `e3max`: $E_{3\max}$ truncation for the output 3N lab-frame HO matrix element file. A typical limit is `e3max` $= 16$, and it will not work for the larger `e3max` because of the memory requirements. If only the matrix elements relevant for the NO2B approximation are needed [9], `e3max` $= 24$ would be a typical choice without the MPI parallelization.
- `file_name_nn`: file name of the output lab-frame NN HO matrix elements.
- `file_name_3n`: file name of the output lab-frame 3N HO matrix elements.
- `renorm`: renormalization method; one can take `bare`, `srg`, or `Vlowk`.
- `input_nn_file`: file name of the NN interaction represented in the relative momentum space. The files are in the input_nn_files directory.
- `NNInt`: name of the NN interaction.
- `N2max`: $N_{\max}$ truncation for the NN system.
- `only_no2b_element`: If it is set `True`, only the matrix elements relevant for the NO2B approximation will be computed [9].

- `ramp`: Jacobi 3N angular momentum dependent $N_{\max}$ truncation for the 3N SRG space. See Ref. [8] for the details. For example, one can use `ramp` = "ramp40-7-38-9-36". This means $N_{\max} = 40$ for $1/2 \leq J \leq 7/2$ channels, $N_{\max} = 38$ for $J = 9/2$ channels, and $N_{\max} = 36$ for the higher J channels. Also, it is supported the J-independent 3N $N_{\max}$ with, for instance, `ramp` = "flat40" (equivalent to `ramp` = "ramp40").
- `jmax3`: maximum value of the 3N Jacobi angular momentum taken into account. This has to be an integer and twice of the actual angular momentum.
- `genuine_3bf`: set `True` if the bare 3N interaction needs to be included. If it is set `False` and `renorm=srg`, the SRG induced 3N interaction will be computed.
- `Regulator` and `RegulatorPower`: regulator functional. One can choose "Local", "NonLocal", or "LNL" [18] for `Regulator`. `RegulatorPower` is the power of the regulator function.
- `LECs`: 5 dimensional array providing the low-energy constants appear in N^{2}LO 3N interaction in the chiral EFT, $\{c_1, c_3, c_4, c_D, c_E\}$. Note that c_1, c_3, and c_4 are in the unit of GeV^{-1}, while c_D and c_E are dimensionless.
- `lambda_3nf_local`: cutoff of the 3N local regulator in the unit of MeV.
- `lambda_3nf_nonlocal`: cutoff of the 3N non-local regulator in the unit of MeV.

ACKNOWLEDGMENTS

The `NuHamil` code is greatly inspired by the `manyeff` code by P. Navrátil and `VRenormalize` in Computational Environment for Nuclear Structure (CENS) project. The code uses VODE library (https://www.radford.edu/ thompson/vodef90web/). The author thanks P. Navrátil, N. Shimizu, and N. Tsunoda for the discussions, optimizations, and parallelizations. The author also thanks P. Arthuis, A. Belly, M. Heinz, B. S. Hu, S. R. Stroberg, and A. Tichai for testing the code and useful feedback. This work was in part supported by JSPS KAKENHI Grant No. JP16J05707, the Program for Leading Graduate Schools, MEXT, Japan, and the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 279384907 – SFB 1245. The author was affiliated with TRIUMF, receiving funding via a contribution through the National Research Council of Canada. The code was in part developed and tested with an allocation of computing resources on Cedar at WestGrid and Compute Canada, at the Jülich Supercomputing Center, and the Oak Cluster at TRIUMF managed by the University of British Columbia department of Advanced Research Research Computing (ARC).

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