T_{rel} and the NCSD Importance-Truncation Code

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1 Introduction

The purpose of this composition is to record the exact modifications I made to the No-Core Shell Model importance truncation code (`it-code-111815.f`) and the motivation behind them.

2 Two definitions of T_{rel}

For an A-particle system with an effective mass A_{eff}, relative kinetic energy, T_{rel}, may be defined in two different ways [3].

The first way to define relative kinetic energy is by subtracting the center of mass kinetic energy from the total kinetic energy. The sums are over the number of particles, A, but an effective particle number, A_{eff}, is used in the center of mass term.

Definition 2.1. *Let the relative kinetic energy with respect to an effective mass A_{eff} be defined by the total kinetic energy minus the kinetic energy of the center of mass, where the effective term is used in the center of mass kinetic energy.*

$$T_{\text{rel},1} = T^A - T_{\text{CM}}^{A_{\text{eff}}}$$

Expanding this in terms of particle momenta gives

$$T_{\text{rel},1} = \left(\sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} \right) - \frac{\boldsymbol{p}_{\text{tot}}^2}{2mA_{\text{eff}}},$$

where

$$\boldsymbol{p}_{\text{tot}} = \sum_{i=1}^{A} \boldsymbol{p}_i.$$

This can be rewritten into the form

$$T_{\text{rel},1} = \left(1 - \frac{1}{A_{\text{eff}}}\right) \sum_{i=1}^{A} \tau_i - \frac{1}{2A_{\text{eff}}} \sum_{i \neq j=1}^{A} \tau_{ij}, \tag{1}$$

where

$$\tau_i = \frac{\boldsymbol{p}_i^2}{2m}, \quad \tau_{ij} = \frac{\boldsymbol{p}_i \cdot \boldsymbol{p}_j}{m}. \tag{2}$$

The second way to define relative kinetic energy is by adding the relative momentum differences of all of the particles. The sum, again, is over the true particle number, A, while A_{eff} is used as the effective particle number for defining the mass.

Definition 2.2. *Let the relative kinetic energy with respect to an effective mass A_{eff} be defined by the sum of differences of momenta of individual particles according to*

$$T_{\text{rel},2} = \sum_{i<j=1}^{A} \frac{\left(\boldsymbol{p}_i - \boldsymbol{p}_j\right)^2}{2mA_{\text{eff}}}$$

This can be rewritten into the form

$$T_{\text{rel},2} = \frac{A-1}{A_{\text{eff}}} \sum_{i=1}^{A} \tau_i \; - \frac{1}{2A_{\text{eff}}} \sum_{i \neq j=1}^{A} \tau_{ij}, \tag{3}$$

where τ_i and τ_{ij} are defined as in Equation (2).

The two definitions are clearly equal when $A_{\text{eff}} = A$; however, they are different in general.

3 Mixed 1,2-body operators based on T_{rel} definitions

We can translate the coordinate forms of the the two kinetic energy definitions into their occupation number representation according to the following equations [4].

One body operator in occupation number representation:

$$\begin{aligned} T &= \sum_{i=1}^{A} t_i(\boldsymbol{x}_i) = \sum_{ab} t_{ab} \; a_a^\dagger a_b, \\ t_{ab} &= \langle a|T|b\rangle \end{aligned} \tag{4}$$

Two body operator in occupation number representation:

$$\begin{aligned} V &= \frac{1}{2} \sum_{i \neq j} v\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \frac{1}{4} \sum_{abcd} v_{abcd} \; a_a^\dagger a_b^\dagger a_d a_c, \\ v_{abcd} &= \langle ab|V|cd\rangle - \langle ab|V|dc\rangle \end{aligned} \tag{5}$$

3.1 Mixed 1,2-body operator for Definition 2.1

The following is the mixed 1,2-body operator based on Definition 2.1. The operator is obtained by translating Equation (1) to occupation number representation using Equations (4) and (5).

$$\hat{T}_{\mathrm{rel},1}^{(1,2)} = \left(1 - \frac{1}{A_{\mathrm{eff}}}\right) \sum_{abJT} \tau_{ab}^{JT}\ a_a^\dagger a_b - \frac{1}{4A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau_{abcd}^{JT}\ a_a^\dagger a_b^\dagger a_d a_c, \tag{6}$$

where

$$\tau_{ab}^{JT} = \left\langle a \middle| \frac{\boldsymbol{p}^2}{2m} \middle| b \right\rangle_{JT}, \quad \tau_{abcd}^{JT} = \left\langle ab \middle| \frac{\boldsymbol{p}_1 \cdot \boldsymbol{p}_2}{m} \middle| cd \right\rangle_{JT}, \tag{7}$$

and

$$\left\langle a \middle| \frac{\boldsymbol{p}^2}{2m} \middle| b \right\rangle_{JT} = \begin{cases} \frac{1}{2}(2n_a + l_a + 3/2), & n_a = n_b, l_a = l_b, j_a = j_b \\ \frac{1}{2}\sqrt{n_a(n_a + l_a + 1/2)}, & n_a = n_b + 1, l_a = l_b, j_a = j_b \\ 0, & \text{else} \end{cases}.$$

3.2 Mixed 1,2-body operator for Definition 2.2

The following is the mixed 1,2-body operator based on Definition 2.2. The operator is obtained by translating Equation (3) to occupation number representation using Equations (4) and (5).

$$\hat{T}_{\mathrm{rel},2}^{(1,2)} = \frac{A-1}{A_{\mathrm{eff}}} \sum_{abJT} \tau_{ab}^{JT}\ a_a^\dagger a_b - \frac{1}{4A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau_{abcd}^{JT}\ a_a^\dagger a_b^\dagger a_d a_c \tag{8}$$

where τ_{ab}^{JT} and τ_{abcd}^{JT} are as defined in Equation (7).

4 Fully 2-body operators from mixed 1,2-body operators

We now look to translate the 1,2-body $\hat{T}_{\mathrm{rel}}$ operators into fully 2-body operators. A general 1,2-body operator $\mathcal{O}$ may be translated into a fully 2-body operator according to the equation

$$\mathcal{O} = \sum_{ab} o_{ab}\ a_a^\dagger a_b = \frac{1}{4} \sum_{abcd} \tilde{o}_{abcd}\ a_a^\dagger a_b^\dagger a_d a_c,$$

where $\tilde{o}_{abcd}$ is the antisymmetrized two-body matrix element defined by

$$\tilde{o}_{abcd} = \mathcal{N}\left(o_{ac}\delta_{bd} + o_{bd}\delta_{ac} - (o_{ad}\delta_{bc} + o_{bc}\delta_{ad})\right)$$

for some normalization $\mathcal{N}$ [2]. In the case where this is coupled to some J and T (as here), the transformation for an operator $\mathcal{T}^{JT}$ is

$$\mathcal{T}^{JT} = \sum_{abJT} \tau_{ab}^{JT}\ a_a^\dagger a_b = \frac{1}{4} \cdot \frac{1}{A-1} \sum_{\substack{abcd\\JT}} \tilde{\tau}_{abcd}^{JT}\ a_a^\dagger a_b^\dagger a_d a_c, \tag{9}$$

where

$$\tilde{\tau}_{abcd}^{JT} = \mathcal{N}_{abcd}\left(\rho_{abcd}^{JT} - (-1)^{\phi_{ab}^{JT}} \rho_{abdc}^{JT}\right) \triangle\left(j_a, j_b, J\right) \triangle\left(t_a, t_b, T\right), \tag{10}$$

and I have defined

$$
\begin{aligned}
\mathcal{N}_{abcd} &= \sqrt[-1]{(1-\delta_{ab})(1-\delta_{cd})} \\
\rho^{JT}_{abcd} &= \tau^{JT}_{ac}\delta_{bd} + \tau^{JT}_{bd}\delta_{ac} \\
\phi^{JT}_{ab} &= j_a + j_b - J + t_a + t_b - T \\
\triangle(x,y,z) &= \begin{cases} 1, & |x-y| \le z \le x+y \\ 0, & \text{else} \end{cases}
\end{aligned}
$$

4.1 Fully 2-body operator for Definition 2.1

The following is the fully 2-body operator based on Definition 2.1. The operator is obtained by translating the mixed 1,2-body operator in Equation (6) using Equation (9).

$$
\begin{aligned}
\hat{T}^{(2)}_{\mathrm{rel},1} &= \left(1 - \frac{1}{A_{\mathrm{eff}}}\right) \sum_{\substack{abcd\\JT}} \frac{1}{4(A-1)} \tilde{\tau}^{JT}_{abcd}\ a^\dagger_a a^\dagger_b a_d a_c - \frac{1}{4A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau^{JT}_{abcd}\ a^\dagger_a a^\dagger_b a_d a_c \\
&= \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \frac{1}{8} \left(\frac{A_{\mathrm{eff}}-1}{A-1}\, \tilde{\tau}^{JT}_{abcd} - \tau^{JT}_{abcd} \right) a^\dagger_a a^\dagger_b a_d a_c,
\end{aligned}
\tag{11}
$$

where τ^{JT}_{abcd} is as defined in Equation (7) and $\tilde{\tau}^{JT}_{abcd}$ is as defined in Equation (10).

4.2 Fully 2-body operator for Definition 2.2

The following is the fully 2-body operator based on Definition 2.2. The operator is obtained by translating the mixed 1,2-body operator in Equation (8) using Equation (9).

$$
\begin{aligned}
\hat{T}^{(2)}_{\mathrm{rel},2} &= \left(\frac{A-1}{A_{\mathrm{eff}}}\right) \sum_{\substack{abcd\\JT}} \frac{1}{4(A-1)} \tilde{\tau}^{JT}_{abcd}\ a^\dagger_a a^\dagger_b a_d a_c - \frac{1}{4A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau^{JT}_{abcd}\ a^\dagger_a a^\dagger_b a_d a_c \\
&= \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \frac{1}{8} \left(\tilde{\tau}^{JT}_{abcd} - \tau^{JT}_{abcd} \right) a^\dagger_a a^\dagger_b a_d a_c.
\end{aligned}
\tag{12}
$$

5 Importance truncation code

The kinetic energy term in the `it-code-111815.f` file is based on Defintion 2.2. This is also multiplied by $2/A_{\mathrm{eff}}$ in the code, so we define

$$
(\tau_{\mathrm{file}})^{JT}_{abcd} = \frac{1}{8}\left(\tilde{\tau}^{JT}_{abcd} - \tau^{JT}_{abcd}\right), \tag{13}
$$

so that Equation (12) can be simplified to

$$
\hat{T}^{(2)}_{\mathrm{rel},2} = \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} (\tau_{\mathrm{file}})^{JT}_{abcd}\ a^\dagger_a a^\dagger_b a_d a_c. \tag{14}
$$

We also define

$$
(\tau_{\mathrm{add}})^{JT}_{abcd} = \frac{1}{8} \cdot \frac{A_{\mathrm{eff}} - A}{A-1}\, \tilde{\tau}^{JT}_{abcd}, \tag{15}
$$

so that Equation (11), the two-body operator based on Definition 2.2, can be simplified to

$$
\hat{T}^{(2)}_{\mathrm{rel},1} = \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \left[(\tau_{\mathrm{file}})^{JT}_{abcd} + (\tau_{\mathrm{add}})^{JT}_{abcd} \right] a^\dagger_a a^\dagger_b a_d a_c. \tag{16}
$$

Now since Definition 2.1 for relative kinetic energy is the definition that we take to be truely fundamental, $(\tau_{\text{add}})^{JT}_{abcd}$ defines the modification to the code in order to produce the correct kinetic energy when $A_{\text{eff}} \neq A$. This is the modification I *will soon* implement in `it-code-111815.f` [1].

References

[1] D. Fullerton, *Original and modified no-core slater determinant importance truncation codes*, GitHub, Available at `https://github.com/dilynfullerton/tr-c-ncsm/tree/master/nuclear_codes`.

[2] S. R. Stroberg and J. D. Holt, *Promoting a one-body operator to a two-body operator*, TRIUMF IMSRG Wiki, Available at `http://wiki.triumf.ca/wiki/IMSRG/index.php/Promoting_a_one-body_operator`.

[3] ———, *Relative kinetic energy*, TRIUMF IMSRG Wiki, Available at `http://wiki.triumf.ca/wiki/IMSRG/index.php/Relative_kinetic_energy`.

[4] J. Suhonen, *From nucleons to nuclei*, ch. 4, pp. 69–71, Springer-Verlag Berlin Heidelberg, 2007.