

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

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

where

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

This can be rewritten into the form

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

where

$$\tau_i = \frac{\mathbf{p}_i^2}{2m}, \quad \tau_{ij} = \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{m}. \quad (2)$$

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*

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

This can be rewritten into the form

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

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 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:

$$T = \sum_{i=1}^A t_i(\mathbf{x}_i) = \sum_{ab} t_{ab} a_a^\dagger a_b, \quad (4)$$

$$t_{ab} = \langle a|T|b \rangle$$

Two body operator in occupation number representation:

$$V = \frac{1}{2} \sum_{i \neq j} v(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{2} \sum_{abcd} v_{abcd} a_a^\dagger a_b^\dagger a_d a_c, \quad (5)$$

$$v_{abcd} = \langle ab|V|cd \rangle$$

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).

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

where

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

and

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

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).

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

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}_{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

$$\mathcal{O} = \sum_{ij} o_{ij} a_i^\dagger a_j = \frac{1}{4} \sum_{ijkl} \tilde{o}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

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

$$\tilde{o}_{ijkl} = \mathcal{N} (o_{ik}\delta_{jl} + o_{jl}\delta_{ik} - (o_{il}\delta_{jk} + o_{jk}\delta_{il}))$$

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

$$\mathcal{T}^{JT} = \sum_{ij} \tau_{ij}^{JT} a_i^\dagger a_j = \frac{1}{4} \cdot \frac{1}{A-1} \sum_{ijkl} \tilde{\tau}_{ijkl}^{JT} a_i^\dagger a_j^\dagger a_l a_k, \quad (9)$$

where

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

and I have defined

$$\begin{aligned}
\mathcal{N}_{abcd} &= \sqrt[3]{(1 - \delta_{ab})(1 - \delta_{cd})} \\
\rho_{abcd}^{JT} &= \tau_{ac}^{JT} \delta_{bd} + \tau_{bd}^{JT} \delta_{ac} \\
\phi_{ab}^{JT} &= j_a + j_b - J + t_a + t_b - T \\
\Delta(a, b, c) &= \begin{cases} 1, & |a - b| \leq c \leq a + b \\ 0, & \text{else} \end{cases}
\end{aligned}$$

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).

$$\begin{aligned}
\hat{T}_{\text{rel},1}^{(2)} &= \left(1 - \frac{1}{A_{\text{eff}}}\right) \sum_{\substack{abcd \\ JT}} \frac{1}{4(A-1)} \tilde{\tau}_{abcd}^{JT} a_a^\dagger a_b^\dagger a_d a_c - \frac{1}{2A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \tau_{abcd}^{JT} a_a^\dagger a_b^\dagger a_d a_c \\
&= \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \left(\frac{1}{8} \cdot \frac{A_{\text{eff}} - 1}{A - 1} \tilde{\tau}_{abcd}^{JT} - \frac{1}{4} \tau_{abcd}^{JT} \right) a_a^\dagger a_b^\dagger a_d a_c,
\end{aligned} \tag{11}$$

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

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

5 Importance truncation code

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

$$(\tau_{\text{file}})_{abcd}^{JT} = \frac{1}{4} \left(\frac{1}{2} \tilde{\tau}_{abcd}^{JT} - \tau_{abcd}^{JT} \right), \tag{13}$$

so that Equation (12) can be simplified to

$$\hat{T}_{\text{rel},2}^{(2)} = \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} (\tau_{\text{file}})_{abcd}^{JT} a_a^\dagger a_b^\dagger a_d a_c. \tag{14}$$

We also define

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

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

$$\hat{T}_{\text{rel},1}^{(2)} = \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \left[(\tau_{\text{file}})_{abcd}^{JT} + (\tau_{\text{add}})_{abcd}^{JT} \right] a_a^\dagger a_b^\dagger a_d a_c. \quad (16)$$

Now since Definition 2.1 for relative kinetic energy is the definition that we take to be truly fundamental, $(\tau_{\text{add}})_{abcd}^{JT}$ 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

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