

T_{rel} and the 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.

2.1 Definition 1

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.

$$\begin{aligned} T_{\text{rel},1} &= T - T_{\text{CM}} \\ &= \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m} - \frac{\mathbf{p}_{\text{tot}}^2}{2mA_{\text{eff}}}, \end{aligned}$$

where

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

This can be written in 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

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

2.2 Definition 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.

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

The can be written in 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 (2).

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

3 Operators based on Definition 1

We find the operators that stem from defining T_{rel} according to (1).

3.1 Mixed 1,2-body operator

Equation (1) translates easily into a 1,2-body operator.

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

where

$$\begin{aligned} \tau_{ab}^{JT} &= \left\langle a \left| \frac{\mathbf{p}^2}{2m} \right| b \right\rangle_{JT}, \quad \tau_{abcd}^{JT} = \left\langle ab \left| \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{m} \right| cd \right\rangle_{JT} \\ \left\langle a \left| \frac{\mathbf{p}^2}{2m} \right| b \right\rangle_{JT} &= \begin{cases} \frac{1}{2}(2n_a + l_a + 3/2), & n_a = n_b, l_a = l_b, j_a = j_b \\ \frac{1}{2}\sqrt{n_a(n_a + l_a + 1/2)}, & n_a = n_b + 1, l_a = l_b, j_a = j_b \\ 0, & \text{else} \end{cases} \end{aligned} \quad (5)$$

3.2 Fully 2-body operator

The 1,2-body operator defined above (4) can be refactored into a fully 2-body operator.

$$\begin{aligned} \hat{T}_{\text{rel},1}^{(2)} &= \left(1 - \frac{1}{A_{\text{eff}}}\right) \sum_{\substack{abcd \\ JT}} \frac{\alpha}{4(A-1)} \tilde{\tau}_{abcd}^{JT} a_a^\dagger a_b^\dagger a_c a_d - \frac{1}{2A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \tau_{abcd}^{JT} a_a^\dagger a_b^\dagger a_c a_d \\ &= \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \left(\frac{\alpha}{8} \cdot \frac{A_{\text{eff}} - 1}{A - 1} \tilde{\tau}_{abcd}^{JT} - \frac{1}{4} \tau_{abcd}^{JT} \right) a_a^\dagger a_b^\dagger a_c a_d, \end{aligned} \quad (6)$$

where

$$\tilde{\tau}_{abcd}^{JT} = N_{abcd} (\rho_{abcd}^{JT} - (-1)^{\phi_{ab}} \rho_{abdc}^{JT}) \triangle (j_a, j_b, J) \triangle (t_a, t_b, T) \quad (7)$$

$$\begin{aligned} \alpha &= 2 \\ N_{abcd} &= \sqrt[4]{(1 - \delta_{ab})(1 - \delta_{cd})} \\ \rho_{abcd}^{JT} &= \tau_{ac}^{JT} \delta_{bd} + \tau_{bd}^{JT} \delta_{ac} \\ \phi_{ab} &= j_a + j_b - J + t_a + t_b - T \\ \triangle(a, b, c) &= \begin{cases} 1, & 0 \leq c \leq a + b \\ 0, & \text{else} \end{cases} \end{aligned}$$

4 Operators based on Definition 2

We find the operators that stem from defining T_{rel} according to (3).

4.1 Mixed 1,2-body operator

Equation (3) translates easily into a 1,2-body operator.

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

4.2 Fully 2-body operator

The 1,2-body operator defined above (8) can be refactored into a fully 2-body operator.

$$\begin{aligned} \hat{T}_{\text{rel},2}^{(2)} &= \left(\frac{A-1}{A_{\text{eff}}} \right) \sum_{\substack{abcd \\ JT}} \frac{\alpha}{4(A-1)} \tilde{\tau}_{abcd}^{JT} a_a^\dagger a_b^\dagger a_c a_d - \frac{1}{2A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \tau_{abcd}^{JT} a_a^\dagger a_b^\dagger a_c a_d \\ &= \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} \left(\frac{\alpha}{8} \tilde{\tau}_{abcd}^{JT} - \frac{1}{4} \tau_{abcd}^{JT} \right) a_a^\dagger a_b^\dagger a_c a_d. \end{aligned} \quad (9)$$

5 Importance truncation code

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

$$(\tau_{\text{file}})_{abcd}^{JT} = \frac{1}{4} \left(\frac{\alpha}{2} \tilde{\tau}_{abcd}^{JT} - \tau_{abcd}^{JT} \right), \quad (10)$$

so that (9) can be simplified to

$$\hat{T}_{\text{rel},2}^{(2)} = \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} (\tau_{\text{file}})_{abcd}^{JT} a_a^\dagger a_b^\dagger a_c a_d. \quad (11)$$

We also define

$$(\tau_{\text{add}})_{abcd}^{JT} = \frac{\alpha}{8} \cdot \frac{A_{\text{eff}} - A}{A - 1} \tilde{\tau}_{abcd}^{JT}, \quad (12)$$

so that (6), the two-body operator based on Definition 1, can be simplified to

$$\hat{T}_{\text{rel},1}^{(2)} = \frac{2}{A_{\text{eff}}} \sum_{\substack{abcd \\ JT}} [(\tau_{\text{file}})_{abcd}^{JT} + (\tau_{\text{add}})_{abcd}^{JT}] a_a^\dagger a_b^\dagger a_c a_d. \quad (13)$$

Now since Definition 1 for relative kinetic energy is the definition that is 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 have implemented in `it-code-111815.f`.

6 References

Original and modified NCSM codes:

<https://github.com/dilynfullerton/tr-c-ncsm/>

More general discussion of definitions of T_{rel} :

http://wiki.triumf.ca/wiki/IMSRG/index.php/Relative_kinetic_energy

Promoting a one-body to a two-body operator:

http://wiki.triumf.ca/wiki/IMSRG/index.php/Promoting_a_one-body_operator

Occupation number representation of 1- and 2-body operators:
Suhonen. *From Nucleons to Nucleus*. Chapter 4.2.