T_{rel} and the Importance-Truncation Code

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2016-06-01

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.

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

where

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

This can be written in the form

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

where

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

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.

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

The can be written in the form

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

where τ_i and τ_{ij} are defined as in (2).
The two definitions are clearly equal when $A_{\mathrm{eff}} = A$; 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.

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

where

$$\tau^{JT}_{ab} = \left\langle a \middle| \frac{\mathbf{p}^2}{2m} \middle| b \right\rangle_{JT}, \quad \tau^{JT}_{abcd} = \left\langle ab \middle| \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{m} \middle| cd \right\rangle_{JT} \tag{5}$$

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

3.2 Fully 2-body operator

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

$$\begin{aligned} \hat{T}^{(2)}_{\mathrm{rel},1} &= \left(1 - \frac{1}{A_{\mathrm{eff}}}\right) \sum_{\substack{abcd\\JT}} \frac{\alpha}{4(A-1)} \tilde{\tau}^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d - \frac{1}{2A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d \\ &= \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \left(\frac{\alpha}{8} \cdot \frac{A_{\mathrm{eff}} - 1}{A-1} \tilde{\tau}^{JT}_{abcd} - \frac{1}{4} \tau^{JT}_{abcd} \right) a^\dagger_a a^\dagger_b a_c a_d, \end{aligned} \tag{6}$$

where

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

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

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.

$$\hat{T}^{(1,2)}_{\mathrm{rel},2} = \frac{A-1}{A_{\mathrm{eff}}} \sum_{abJT} \tau^{JT}_{ab} a^\dagger_a a_b - \frac{1}{2A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d. \tag{8}$$

4.2 Fully 2-body operator

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

$$\begin{aligned}\hat{T}^{(2)}_{\mathrm{rel},2} &= \left(\frac{A-1}{A_{\mathrm{eff}}}\right) \sum_{\substack{abcd\\JT}} \frac{\alpha}{4(A-1)} \tilde{\tau}^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d - \frac{1}{2A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \tau^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d \\ &= \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \left(\frac{\alpha}{8}\tilde{\tau}^{JT}_{abcd} - \frac{1}{4}\tau^{JT}_{abcd}\right) a^\dagger_a a^\dagger_b a_c a_d.\end{aligned} \tag{9}$$

5 Importance truncation code

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

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

so that (9) can be simplified to

$$\hat{T}^{(2)}_{\mathrm{rel},2} = \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} (\tau_{\mathrm{file}})^{JT}_{abcd} a^\dagger_a a^\dagger_b a_c a_d. \tag{11}$$

We also define

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

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

$$\hat{T}^{(2)}_{\mathrm{rel},1} = \frac{2}{A_{\mathrm{eff}}} \sum_{\substack{abcd\\JT}} \left[(\tau_{\mathrm{file}})^{JT}_{abcd} + (\tau_{\mathrm{add}})^{JT}_{abcd}\right] a^\dagger_a a^\dagger_b a_c a_d. \tag{13}$$

Now since Definition 1 for relative kinetic energy is the definition that is truely fundamental, $(\tau_{\mathrm{add}})^{JT}_{abcd}$ defines the modification to the code in order to produce the correct kinetic energy when $A_{\mathrm{eff}} \neq A$. 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.