Space Ordering the Numerical Problem

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1 Background

Note that in this document I didn't consider either the cumulent average or replica trick.

We would like to calculate

$$\tilde{S}^{(n)}_{1...n} = v^n \sum_{j_n=1}^{N} .... \sum_{j_1=1}^{N} \sum_{k_n=1}^{N_m} ... \sum_{k_n=1}^{N_m} \left\langle \left\langle \sigma_1^{\alpha_1} \exp\left(i\vec{k}_1 \cdot \vec{r}_{j_1,k_1}\right) ... \sigma_n^{\alpha_n} \exp\left(i\vec{k}_n \cdot \vec{r}_{j_n,k_n}\right) \right\rangle \right\rangle$$

where the averages are defined as

$$\langle X(\alpha_i) \rangle_\sigma = \frac{\sum_{j=1}^{N} \sum_{\alpha_j = A,B} f_{\alpha_1} p(\alpha_2|\alpha_1) p(\alpha_3|\alpha_2) ... p(\alpha_N|\alpha_{N-1}) X(\alpha_i)}{\sum_{j=1}^{N} \sum_{\alpha_j = A,B} f_{\alpha_1} p(\alpha_2|\alpha_1) p(\alpha_3|\alpha_2) ... p(\alpha_N|\alpha_{N-1})}$$

$$\langle X(\vec{r}_{i,j}) \rangle_0 = \int \prod_{jk} \prod_{\xi=1}^{m} d\vec{r}^{\,\xi}_{jk} \exp\left(- \sum_{\xi=1}^{m} \beta e_0^\xi \left(\left\{ \vec{r}^{\,\xi}_{j,k} \right\} \right) \right) X(\vec{r}_{i,j})$$

Separating out the average over chemical identity σ

$$\tilde{S}^{(n)}_{1...n} = v^n \sum_{j_n=1}^{N} .... \sum_{j_1=1}^{N} \sum_{k_n=1}^{N_m} ... \sum_{k_n=1}^{N_m} \langle \sigma_{j_1}^{\alpha_1} \sigma_{j_2}^{\alpha_2} ... \sigma_{j_n}^{\alpha_n} \rangle \left\langle \exp\left(i\vec{k}_1 \cdot \vec{r}_{j_1,k_1}\right) ... \exp\left(i\vec{k}_n \cdot \vec{r}_{j_n,k_n}\right) \right\rangle_0$$

1.1 Configuration propagator

Consider the expression

$$\left\langle \exp\left(i\vec{k}_1 \cdot \vec{r}_{j_1,k_1} + i\vec{k}_2 \cdot \vec{r}_{j_2,k_2} + i\vec{k}_3 \cdot \vec{r}_{j_3,k_3} + i\vec{k}_4 \cdot \vec{r}_{j_4,k_4} \right) \right\rangle_0 \tag{1}$$

We can rearrange the exponent into pairs of $\Delta\vec{r}$'s

$$\left\langle \exp\left(i\left(\vec{k}_1 + \vec{k}_2 + \vec{k}_3 + \vec{k}_4\right) \cdot \vec{r}_{j_1 k_1} + i\left(\vec{k}_2 + \vec{k}_3 + \vec{k}_4\right) \cdot \left(\vec{r}_{j_2 k_2} - \vec{r}_{j_1,k_1}\right) + i\left(\vec{k}_3 + \vec{k}_4\right) \cdot \left(\vec{r}_{j_3,k_3} - \vec{r}_{j_2,k_2}\right) + i\vec{k}_4 \left(\vec{r}_{j_4,k_4} - \vec{r}_{j_3,k_3}\right) \right) \right\rangle_0 \tag{2}$$

we have the translational invariance condition $0 = \vec{k}_4 + \vec{k}_3 + \vec{k}_2 + \vec{k}_1$ so

$$\left\langle \exp\left(-i\vec{k}_1 \cdot \left(\vec{r}_{j_2 k_2} - \vec{r}_{j_1,k_1}\right) - i\left(\vec{k}_1 + \vec{k}_2\right) \cdot \left(\vec{r}_{j_3,k_3} - \vec{r}_{j_2,k_2}\right) + i\vec{k}_4 \left(\vec{r}_{j_4,k_4} - \vec{r}_{j_3,k_3}\right) \right) \right\rangle_0 \tag{3}$$

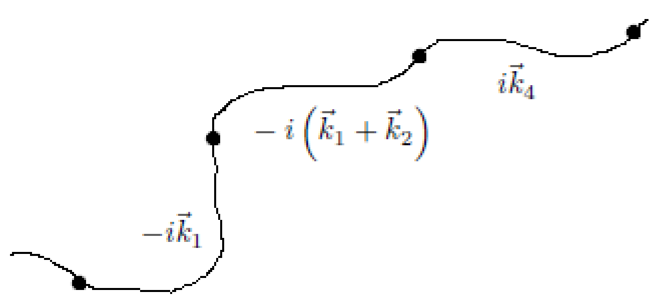


Figure 1: $-\vec{k}_1$, the forier transform of $\vec{r}_1$, connects $\vec{r}_{j_2 k_2}$ and $\vec{r}_{j_1,k_1}$.

we want to break this up into 3 propagators but in order to do so we need $j_4 > j_3 > j_2 > j_1$. Suppose instead we had $j_4 > j_3 > j_1 > j_2$. We could make an expression similar to expression 3.

$$\left\langle \exp\left(i\left(\vec{k}_1+\vec{k}_2+\vec{k}_3+\vec{k}_4\right)\cdot\vec{r}_{j_2k_2}+i\left(\vec{k}_1+\vec{k}_3+\vec{k}_4\right)\cdot\left(\vec{r}_{j_1k_1}-\vec{r}_{j_2,k_2}\right)+i\left(\vec{k}_3+\vec{k}_4\right)\cdot\left(\vec{r}_{j_3,k_3}-\vec{r}_{j_1,k_1}\right)+i\vec{k}_4\left(\vec{r}_{j_4,k_4}-\vec{r}_{j_3,k_3}\right)\right)\right\rangle_0$$

which you can easily verify is mathematically the same thing as expression 1. Once again use $0=\vec{k}_4+\vec{k}_3+\vec{k}_2+\vec{k}_1$ and see that

$$\left\langle \exp\left(-i\vec{k}_2\cdot\left(\vec{r}_{j_1k_1}-\vec{r}_{j_2,k_2}\right)-i\left(\vec{k}_2+\vec{k}_1\right)\cdot\left(\vec{r}_{j_3,k_3}-\vec{r}_{j_1,k_1}\right)+i\vec{k}_4\left(\vec{r}_{j_4,k_4}-\vec{r}_{j_3,k_3}\right)\right)\right\rangle_0$$

Instead of working this out for each different order of $\vec{r}$ locations visited by the polymer we simply note that we need only two swap k_1 and k_2. In order to get every combination of j orderings we need each of the $n!$ arrangement of the k values.

$$\tilde{S}^{(n)}_{1\ldots n}=v^n\sum_{\text{orders}}^{n!}\underbrace{\sum_{j_n=1}^{N}....\sum_{j_1=1}^{N}\sum_{k_n=1}^{N_m}...\sum_{k_1=1}^{N_m}}_{\text{ordered}}\left\langle\sigma^{\alpha_1}_{j_1}\sigma^{\alpha_2}_{j_2}...\sigma^{\alpha_n}_{j_n}\right\rangle G\left(1\to2\to3\to4\right) \tag{4}$$

where $\sum_{\text{orders}}^{n!}$ means a sum over the different arrangements of the k vectors. There are $n!$ such orders. Each order changes has the respective order of $\vec{k}$ vectors plugged into $G\left(1\to2\to3\to4\right)$ and also changes the expression $\langle\sigma...\rangle$ as will be discussed below. The ordered sum requires either the j values be increasing or respective s values are ordered. I.e

$$j_{n+1}>j_n\ \vee\ \left(j_{n+1}=j_n\ \wedge\ k_{n+1}\geq k_n\right)\ \forall\ n$$

I have defined

$$\begin{aligned}
G\left(1\to2\to3\to4\right)\equiv&\left\langle\exp\left(-i\left(\vec{k}_1\right)\cdot\left(\vec{r}_{j_2k_2}-\vec{r}_{j_1,k_1}\right)-i\left(\vec{k}_1+\vec{k}_2\right)\cdot\left(\vec{r}_{j_3,k_3}-\vec{r}_{j_2,k_2}\right)+i\vec{k}_4\left(\vec{r}_{j_4,k_4}-\vec{r}_{j_3,k_3}\right)\right)\right\rangle_0\\
=&G\left(-\vec{k}_1,\left|N_m\left(j_2-j_1\right)+\left(s_2-s_1\right)\right|\right)G\left(-\vec{k}_1-\vec{k}_2,\left|N_m\left(j_3-j_2\right)+\left(s_3-s_2\right)\right|\right)G\left(\vec{k}_4,\left|N_m\left(j_4-j_3\right)+\left(s_4-s_3\right)\right|\right)\\
=&e^{-\frac{k_1^2b^2}{2}\left|N_m(j_2-j_1)+(s_2-s_1)\right|}e^{-\frac{k_{12}^2b^2}{2}\left|N_m(j_3-j_2)+(s_3-s_2)\right|}e^{-\frac{k_4^2b^2}{2}\left|N_m(j_4-j_3)+(s_4-s_3)\right|}\\
=&z_1^{\left|N_m(j_2-j_1)+(s_2-s_1)\right|}z_{12}^{\left|N_m(j_3-j_2)+(s_3-s_2)\right|}z_4^{\left|N_m(j_4-j_3)+(s_4-s_3)\right|}
\end{aligned}$$

Note that I have make the transformation

$$\sum_{k_n=1}^{N_m}...\sum_{k_1=1}^{N_m}\to\int_0^{N_m}ds_n...\int_0^{N_m}ds_1$$

Notice that I have not discussed the effects of ordering on the $\left\langle\sigma^{\alpha_1}_{j_1}\sigma^{\alpha_2}_{j_2}...\sigma^{\alpha_n}_{j_n}\right\rangle$ portion of the equation 4; we turn to this next.

1.1.1 WLC propagator

In the case of worm like chain

$$G\left(1\to2\to3\to4\right)=\int d\vec{u}_1\int d\vec{u}_2\int d\vec{u}_3G\left(\vec{u}_1,\vec{u}_0,-\vec{k}_1,L_{12}\right)G\left(\vec{u}_2,\vec{u}_1-\vec{k}_1-\vec{k}_2,L_{23}\right)G\left(\vec{u}_3,\vec{u}_2,\vec{k}_4,L_{34}\right)$$

where $L_{12}=\left|N_m\left(j_2-j_1\right)+\left(s_2-s_1\right)\right|$, $L_{23}=\left|N_m\left(j_3-j_2\right)+\left(s_3-s_2\right)\right|$, and $L_{34}=\left|N_m\left(j_4-j_3\right)+\left(s_4-s_3\right)\right|$.
This propagator is discussed in more detial elsewhere.

1.2 Chemical propagator

Because the σ average is done with propagators that follow the chain as well it will use same propagator path lengths $|j_n-j_{n-1}|$ as the confrontational average.
The chemical transition probability [e.g. $\left\langle\sigma^{\alpha_1}_{j_1}\sigma^{\alpha_2}_{j_2}\right\rangle$]is calculated via

transition	probability
$A\to A$	$f_A+f_B\lambda^{\lvert j_2-j_1\rvert}$
$A\to B$	$f_B-f_B\lambda^{\lvert j_2-j_1\rvert}$
$B\to A$	$f_A-f_A\lambda^{\lvert j_2-j_1\rvert}$
$B\to B$	$f_B+f_A\lambda^{\lvert j_2-j_1\rvert}$

$$\left\langle \sigma_{j_1}^{\alpha_1}\sigma_{j_2}^{\alpha_2}\right\rangle = \begin{cases} f_A^2 + f_A f_B \lambda^{|j_2-j_1|} & \alpha_1=\alpha_2=A \\ f_A f_B - f_A f_B \lambda^{|j_2-j_1|} & \alpha_1\neq\alpha_2 \\ f_B^2 + f_A f_B \lambda^{|j_2-j_1|} & \alpha_1=\alpha_2=B \end{cases}$$

which we will write as

$$\left\langle \sigma_{j_1}^{\alpha_1}\sigma_{j_2}^{\alpha_2}\right\rangle = \gamma_1 + \gamma_2 \lambda^{|j_2-j_1|}$$

where γ_i is implicitly a function $\gamma_i\left(\alpha_1,\alpha_2,n\right)$.
In the three point case

$$\left\langle \sigma_{j_1}^{\alpha_1}\sigma_{j_2}^{\alpha_2}\sigma_{j_3}^{\alpha_3}\right\rangle = \begin{cases} f_A\left(f_A + f_B\lambda^{|j_2-j_1|}\right)\left(f_A + f_B\lambda^{|j_3-j_2|}\right) & AAA \\ f_A\left(f_A + f_B\lambda^{|j_2-j_1|}\right)\left(f_B - f_B\lambda^{|j_3-j_2|}\right) & AAB \\ f_A\left(f_B - f_B\lambda^{|j_2-j_1|}\right)\left(f_A - f_A\lambda^{|j_3-j_2|}\right) & ABA \\ f_A\left(f_B - f_B\lambda^{|j_2-j_1|}\right)\left(f_B + f_A\lambda^{|j_3-j_2|}\right) & ABB \\ f_B\left(f_A - f_A\lambda^{|j_2-j_1|}\right)\left(f_A + f_B\lambda^{|j_3-j_2|}\right) & BAA \\ f_B\left(f_A - f_A\lambda^{|j_2-j_1|}\right)\left(f_B - f_B\lambda^{|j_3-j_2|}\right) & BAB \\ f_B\left(f_B + f_A\lambda^{|j_2-j_1|}\right)\left(f_A - f_A\lambda^{|j_3-j_2|}\right) & BBA \\ f_B\left(f_B + f_A\lambda^{|j_2-j_1|}\right)\left(f_B + f_A\lambda^{|j_3-j_2|}\right) & BBB \end{cases}$$

which can also be expanded

$$\left\langle \sigma_{j_1}^{\alpha_1}\sigma_{j_2}^{\alpha_2}\sigma_{j_3}^{\alpha_3}\right\rangle = \gamma_1 + \gamma_2\lambda^{|j_2-j_1|} + \gamma_3\lambda^{|j_3-j_2|} + \gamma_4\lambda^{|j_2-j_1|}\lambda^{|j_3-j_2|}$$

and likewise with the fourth

$$\left\langle \sigma_{j_1}^{\alpha_1}\sigma_{j_2}^{\alpha_2}\sigma_{j_3}^{\alpha_3}\sigma_{j_4}^{\alpha_4}\right\rangle = \gamma_1 + \gamma_2\lambda^{|j_2-j_1|} + \gamma_3\lambda^{|j_3-j_2|} + \gamma_4\lambda^{|j_4-j_3|} + \gamma_5\lambda^{|j_2-j_1|}\lambda^{|j_3-j_2|} + ...$$

A convenient way to make sure we get all the 2^{n-1} terms is to write the sum

$$\sum_{\{I\}=1}^{2^{n-1}} \gamma_{\{I\}}\lambda^{func(\{I\})}$$

in the case of $n=4$ there are a set of 3 binary I values which choose which side of each binomial to take.

$$\gamma_{\{I\}}\lambda^{func(\{I\})} = f_{\alpha_1}\left(\underbrace{f_{\alpha_2}}_{I_1=0} + \Delta_{\alpha_1,\alpha_2}\underbrace{\left(1-f_{\alpha_1}\right)\lambda^{|j_2-j_1|}}_{I_1=1}\right)\left(\underbrace{f_{\alpha_3}}_{I_2=0} + \Delta_{\alpha_2,\alpha_3}\underbrace{\left(1-f_{\alpha_2}\right)\lambda^{|j_3-j_2|}}_{I_2=1}\right)\left(\underbrace{f_{\alpha_4}}_{I_3=0} + \Delta_{\alpha_3,\alpha_4}\underbrace{\left(1-f_{\alpha_3}\right)\lambda^{|j_4-j_3|}}_{I_3=1}\right)$$

where

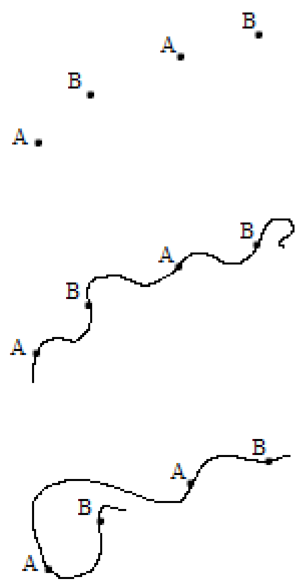
$$\Delta_{\alpha_1,\alpha_2} \equiv \begin{cases} 1 & \text{if } \alpha_1=\alpha_2 \\ -1 & \text{if } \alpha_1\neq\alpha_2 \end{cases}$$

or to be more mathematical

$$\gamma_{\{I\}} = f_{\alpha_1}\left(f_{\alpha_2}\delta_{I_1,0} + \Delta_{\alpha_1,\alpha_2}\left(1-f_{\alpha_1}\right)\delta_{I_1,1}\right)\left(f_{\alpha_3}\delta_{I_2,0} + \Delta_{\alpha_1,\alpha_2}\left(1-f_{\alpha_2}\right)\delta_{I_2,1}\right)\left(f_{\alpha_4}\delta_{I_2,0} + \Delta_{\alpha_1,\alpha_2}\left(1-f_{\alpha_3}\right)\delta_{I_3,1}\right) \tag{5}$$

$$func\left(\{I\}\right) = I_1\left|j_2-j_1\right| + I_2\left|j_3-j_2\right| + I_3\left|j_4-j_3\right| \tag{6}$$

$$\sum_{\{I\}=1}^{2^{n-1}} \equiv \sum_{I_1=0}^{1}\sum_{I_2=0}^{1}...\sum_{I_n=0}^{1}$$



$$S\left(\overbrace{A,B,A,B}^{\alpha_{spacial}}\right)$$

$$\alpha_{path}=\begin{bmatrix}A\\B\\A\\B\end{bmatrix}\qquad -i\vec{k}_1\vec{r}_{12}-i\left(\vec{k}_1+\vec{k}_2\right)\vec{r}_{23}+i\vec{k}_4\vec{r}_{34}$$

$$\alpha_{path}=\begin{bmatrix}B\\A\\A\\B\end{bmatrix}\qquad -i\vec{k}_2\vec{r}_{21}-i\left(\vec{k}_2+\vec{k}_1\right)\vec{r}_{13}+i\vec{k}_4\vec{r}_{34}$$

Figure 2: Suppose we are calculating $S\left(A,B,A,B\right)$. Space ordering has two effects, one is to order the α values along the path, the other is to reorder the $\vec{k}$ values. S is a function of $\alpha_{spacial}$ while γ is a function of α_{path} so a different mapping must occure for each term in $\sum_{\text{orders}}^{n!}$.

1.3 Put the two together

Each of the different terms in $\sum_{\text{orders}}^{n!}$ differs from the others in two ways: a different order of the $\vec{k}$ vectors as well as a different order of the α values.

$$\tilde{S}^{(n)}_{1\ldots n}\left(\alpha_{space}\right)=v^n\sum_{\text{orders}}^{n!}\underbrace{\sum_{\{j\}}\int\{ds\}}_{\text{ordered}}\sum_{\{I\}=1}^{2^{n-1}}\gamma\left(\{I\},\alpha_{path}\right)\lambda^{func(\{I\})}z_1^{|N_m(j_2-j_1)+(s_2-s_1)|}z_{12}^{|N_m(j_3-j_2)+(s_3-s_2)|}z_4^{|N_m(j_4-j_3)+(s_4-s_3)|}$$

here α_{path} is a function of α_{space} and term in we may $\sum_{\text{orders}}^{n!}$ it is in. We may separate the sum and integral[1]

$$\tilde{S}^{(n)}_{1\ldots n}=v^n\sum_{\text{orders}}^{n!}\sum_{\{I\}=1}^{2^{n-1}}\gamma\left(\{I\},\alpha_{path}\right)\overbrace{\underbrace{\sum_{\{j\}}}_{\text{ordered}}\lambda^{func(\{I\})}z_1^{|N_m(j_2-j_1)|}z_{12}^{|N_m(j_3-j_2)|}z_4^{|N_m(j_4-j_3)|}}^{\text{valne}}\overbrace{\underbrace{\int\{ds\}}_{\text{ordered}}z_1^{|s_2-s_1|}z_{12}^{|s_3-s_2|}z_4^{|s_4-s_3|}}^{\text{valeq}}$$

recalling the definition 6 we may write

$$\tilde{S}^{(n)}_{1\ldots n}=v^n\sum_{\text{orders}}^{n!}\sum_{\{I\}=1}^{2^{n-1}}\gamma\left(\{I\},\alpha_{path}\right)\underbrace{\sum_{\{j\}}}_{\text{ordered}}\left(z_1^{N_m}\lambda^{I_1}\right)^{|j_2-j_1|}\left(z_{12}^{N_m}\lambda^{I_{12}}\right)^{|j_3-j_2|}\left(z_4^{N_m}\lambda^{I_{12}}\right)^{|j_4-j_3|}\underbrace{\int_0^{N_m}ds_{1-4}}_{\text{ordered}}z_1^{|s_2-s_1|}z_{12}^{|s_3-s_2|}z_4^{|s_4-s_3|}$$

Also separate the ordered sums by case

[1] The separation of the sum and the intigral would be complicated by the absolute value signs if it had occured prior to space ordering. After ordering the sum and intigral the separation is simple.

$$\underbrace{\sum_{\{j\}}}_{\text{ordered}} = \begin{cases} N & case = 1: \; j_1 = j_2 = j_3 = j_4 \\ \sum_{j_2=2}^{N} \sum_{j_1=1}^{j_2-1} & case = 2: \; j_1 \neq j_2 = j_3 = j_4 \\ \sum_{j_3=2}^{N} \sum_{j_1=1}^{j_3-1} & case = 3: \; j_1 = j_2 \neq j_3 = j_4 \\ \sum_{j_4=2}^{N} \sum_{j_1=1}^{j_4-1} & case = 4: \; j_1 = j_2 = j_3 \neq j_4 \\ \sum_{j_3=3}^{N} \sum_{j_2=2}^{j_3-1} \sum_{j_1=1}^{j_2-1} & case = 5: \; j_1 \neq j_2 \neq j_3 = j_4 \\ \sum_{j_4=3}^{N} \sum_{j_3=2}^{j_4-1} \sum_{j_1=1}^{j_3-1} & case = 6: \; j_1 = j_2 \neq j_3 \neq j_4 \\ \sum_{j_4=3}^{N} \sum_{j_2=2}^{j_4-1} \sum_{j_1=1}^{j_2-1} & case = 7: \; j_1 \neq j_2 = j_3 \neq j_4 \\ \sum_{j_4=4}^{N} \sum_{j_3=3}^{j_4-1} \sum_{j_2=2}^{j_3-1} \sum_{j_1=1}^{j_2-1} & case = 8: \; j_1 \neq j_2 \neq j_3 \neq j_4 \end{cases}$$

$$\underbrace{\int_0^{N_m} ds_{1-4}}_{\text{ordered}} = \begin{cases} \int_0^{N_m} \int_0^{s_4} \int_0^{s_3} \int_0^{s_2} ds_1 ds_2 ds_3 ds_4 & case = 1: \; j_1 = j_2 = j_3 = j_4 \\ \int_0^{N_m} \int_0^{s_4} \int_0^{s_3} \int_0^{N_m} ds_1 ds_2 ds_3 ds_4 & case = 2: \; j_1 \neq j_2 = j_3 = j_4 \\ \int_0^{N_m} \int_0^{s_4} \int_0^{N_m} \int_0^{s_2} ds_1 ds_2 ds_3 ds_4 & case = 3: \; j_1 = j_2 \neq j_3 = j_4 \\ \int_0^{N_m} \int_0^{N_m} \int_0^{s_3} \int_0^{s_2} ds_1 ds_2 ds_3 ds_4 & case = 4: \; j_1 = j_2 = j_3 \neq j_4 \\ \int_0^{N_m} \int_0^{s_4} \int_0^{N_m} \int_0^{N_m} ds_1 ds_2 ds_3 ds_4 & case = 5: \; j_1 \neq j_2 \neq j_3 = j_4 \\ \int_0^{N_m} \int_0^{N_m} \int_0^{N_m} \int_0^{s_2} ds_1 ds_2 ds_3 ds_4 & case = 6: \; j_1 = j_2 \neq j_3 \neq j_4 \\ \int_0^{N_m} \int_0^{N_m} \int_0^{s_3} \int_0^{N_m} ds_1 ds_2 ds_3 ds_4 & case = 7: \; j_1 \neq j_2 = j_3 \neq j_4 \\ \int_0^{N_m} \int_0^{N_m} \int_0^{N_m} \int_0^{N_m} ds_1 ds_2 ds_3 ds_4 & case = 8: \; j_1 \neq j_2 \neq j_3 \neq j_4 \end{cases}$$

Notice that the way I have chosen to express things there is some redundancy. If $j_1 = j_2$ than the sum doesn't depend on I_1 so we may add together the two terms $f_{\alpha_2}\delta_{I_1,0} + \Delta_{\alpha_1,\alpha_2}(1 - f_{\alpha_1})\delta_{I_1,1}$ from equation 5. In the even that $\alpha_1 = \alpha_2$ this will simply be 1 and when $\alpha_1 \neq \alpha_2$ it will be zero.

2 Numerical Problem

Fortunately the above $\underbrace{\sum_{\{j\}}}_{\text{ordered}}$ sums and $\underbrace{\int_0^{N_m} ds_{1-4}}_{\text{ordered}}$ integrals have simple closed form values. Unfortunately there is a numerical problem that appears in both the integrals and the sums.

2.1 In the sum

Consider 4 point, case 8. We would like to perform a sum of the form:

$$valne = \sum_{j_4=4}^{N} \sum_{j_3=3}^{j_4-1} \sum_{j_2=2}^{j_3-1} \sum_{j_1=1}^{j_2-1} a^{|j_2-j_1|} b^{|j_3-j_2|} c^{|j_4-j_3|} \tag{7}$$

In particular $a = e^{-\frac{k_1^2 b^2}{2} N_m} \lambda^{I_1}$. By using truncated geometric series [or your favorite algebra system] one may verify that

$$valne = \frac{-abc}{(1-a)(1-b)(1-c)} \left(\frac{(a-1)(c-1)\left(b^3 - b^N\right)}{(a-b)(b-c)(b-1)} + \frac{(b-1)(c-1)\left(a^3 - a^N\right)}{(a-b)(c-a)(a-1)} + \frac{(a-1)(b-1)\left(c^3 - c^N\right)}{(c-a)(b-c)(c-1)} - N + 3 \right) \tag{8}$$

One will notice that if a, b, and/or c is close to 1 or they are close to each other the terms in parenthesis will become large. By taking limits one may verify that even though individual terms go to infinity their sum does not due to cancellation. This spells disaster for numerical evaluation. This problem can be remedied by replacing the values in the vicinity of these singularities by the value at the singularity with some cutoff limit. In order to improve accuracy I replace regions near singularities by limiting functions rather than limiting values. For example when a, b, and c are all near 1 I use:

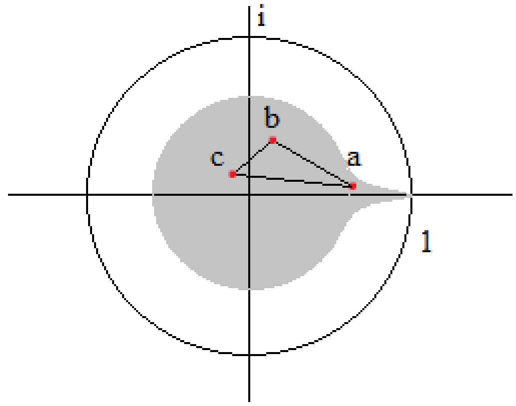


Figure 3: The values $e^{\epsilon N_m}$ must fall in the shadded area.

$$
\begin{aligned}
valne &= \sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left(1-\delta_{1a}\right)^{|j_2-j_1|}\left(1-\delta_{1b}\right)^{|j_3-j_2|}\left(1-\delta_{1c}\right)^{|j_4-j_3|}\\
&\approx \sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left(1-\left(j_2-j_1\right)\delta_{1a}\right)\left(1-\left(j_3-j_2\right)\delta_{1b}\right)\left(1-\left(j_4-j_3\right)\delta_{1c}\right)\\
&= -\frac{N\left(N-1\right)\left(N-2\right)\left(N-3\right)\left(\left(N+1\right)\left(\delta_{1a}+\delta_{1b}+\delta_{1c}\right)-5\right)}{120}\\
&= -\frac{N\left(N-1\right)\left(N-2\right)\left(N-3\right)\left(\left(N+1\right)\left(3-a-b-c\right)-5\right)}{120}
\end{aligned}
$$

A similar such approximation can be made in other limits as will be tabulated below.

2.1.1 Ordering a, b, and c

Here I address the equestion of how to list the possible limits to be tabulated later. When evaluting the sum 7 we need make an exception when any of the set $\{a, b, c, 1\}$ gets close to any other member of that set so that a zero in the denominator of 8. Making an exception for each combination would result in a large number of exceptions. This is simplifed by fact that *valne* is invariant with respect to swapping a, b, and c. If a,b, and c are all real we can simply order such that $1 > a > b > c > 0$. This is possible because $\mathrm{Re}\left(-\epsilon N_m\right) < 0$. After this ordering we only need to check the size of $\delta_{1a} = 1 - a$, $\delta_{ab} = a - b$, $\delta_{b-c} = b - c$ for a total of $2^3 = 8$ different expressions.

When a, b, and/or c is complex things gets more complicated. Fortionatly we still have $\mathrm{Re}\left(-\epsilon N_m\right) < 0$ and when ϵ is close to zero it happens to be purly real [citation needed]. Hence a,b, and c fall in the shadded region in the complex plain.

The procedure we use for ordering a,b, and c. Choose a as the value with the largest real part. Next choose b to be the value closer to a in absolute value distance. For the purposes of deciding which expression to use the absolute value of the δ values are used.

2.2 In the integral

Once again consider 4 point, case 8.

$$valeq = \int_0^{N_m}\int_0^{N_m}\int_0^{N_m}\int_0^{N_m} e^{\epsilon_1(s_2-s_1)}e^{\epsilon_{12}(s_3-s_2)}e^{\epsilon_3(s_4-s_3)}ds_1ds_2ds_3ds_4$$

This is a doable integral

$$valeq = \frac{1}{\left(\epsilon_1-\epsilon_2\right)\epsilon_3}\left(\left(\frac{N_m\epsilon_3 - z_3 + 1}{\epsilon_3}\right)\left(\frac{1}{\epsilon_1}-\frac{1}{\epsilon_2}\right)+\frac{\epsilon_2\left(e^{N_m\epsilon_3}-1\right)-\epsilon_3\left(e^{N_m\epsilon_2}-1\right)}{\epsilon_2^2\left(\epsilon_2-\epsilon_3\right)}+\frac{\epsilon_3\left(e^{N_m\epsilon_1}-1\right)-\epsilon_1\left(e^{N_m\epsilon_3}-1\right)}{\epsilon_1^2\left(\epsilon_1-\epsilon_3\right)}\right)$$

once again this has numerical issues if the ϵ's are close to each other or 0. Once again these bad spots will need to be replace by a limiting value or function.

2.3 A partial solution

Performing cancellation can serve as a partial solution to this problem. I don't know how to cancel everything that needs to be canceled so I still need to use limiting cases. However, performing at least some cancellation improves accuracy. Consider the the two point integral for $j_1 = j_2$

$$\int_0^{N_m}\int_0^{s_2} e^{\epsilon_1(s_2-s_1)}ds_1 ds_2 = \frac{e^{N_m\epsilon_1} - N_m\epsilon_1 - 1}{\epsilon_1^2}$$

if we evaluate the right hand side of this equation with small values of $N_m\epsilon_1$ we will have numerical issues. These issues can be resolved by expanding the exponent as a power series and then canceling the first two terms.

$$\int_0^{N_m}\int_0^{s_2} e^{\epsilon_1(s_2-s_1)}ds_1 ds_2 = \frac{1}{\epsilon_1^2}\sum_{j=2}^{\infty}\frac{(N_m\epsilon_1)^j}{j!}$$

because we will use it a lot I define

$$\mathrm{expl}\,(m,x) = \sum_{j=m}^{\infty}\frac{x^j}{j!}$$

so

$$\int_0^{N_m}\int_0^{s_2} e^{\epsilon_1(s_2-s_1)}ds_1 ds_2 = \frac{\mathrm{expl}\,(2, N_m\epsilon_1)}{\epsilon_1^2}$$

In this particular case [except when $\epsilon_1 = 0$ exactly] this cancellation has solved the numerical issue. Unfortunately in the higher point calculations this will not be so easy because the number of therms one would have to write in order to do such cancellation is impractically large.

In a similar fashion we may perform cancellation on the sum. For example take case 2 $j_1 \neq j_2$

$$\begin{aligned}\sum_{j_2=2}^{N}\sum_{j_1=1}^{j_2-1} a^{j_2-j_1} &= -a\frac{-a^N + 1 - N + aN}{(1-a)^2}\\ &= -a\frac{-e^{\ln(a)N} + 1 - N + e^{\ln(a)}N}{(1-a)^2}\\ &= -a\frac{-\mathrm{expl}\,(2, N\ln(a)) + N\mathrm{expl}\,(2,\ln(\mathrm{a}))}{(1-a)^2}\end{aligned}$$

this isn't complete cancellation but it is numerically accurate closer to $a = 1$.

2.4 How to choose cutoffs

Looking at the expression for the sum in case 8, 8, we see that it becomes numerically troublesome when a, b, and c are close to each other or 1. We fixed the problem by switching to approximations for the various regions. The approximations are only accurate in the vicinity of their respective singularity while equation 8 is only numerically stable far from the singularities. Choosing between the approximations is not trivial because the optimal crossover point is a complicated function of a,b,c, N, and the accuracy of double precision variables. A useful way to particularize parameter space [no pun intended] is to order $a > b > c$ and then define

$$\delta_{1a} = 1 - a$$

$$\delta_{ab} = a - b$$

$$\delta_{b-c} = b - c$$

as well as N. In this 4 dimensional parameter space the singularities occur along the surfaces $\delta_{1a} = 0$, $\delta_{ab} = 0$, and $\delta_{bc} = 0$ and the edges that make the intersections between these surfaces. Each surface and edge is approximated with a different approximation. Once could, in principle, determine a regions in this space where various methods are more accurate. Rather than work this out the current version of the code calculates each method as well as a rough upper estimate for the relative error of each method may have due to either numerics or some approximation. The code then chooses the result with the smallest estimated error. For example:

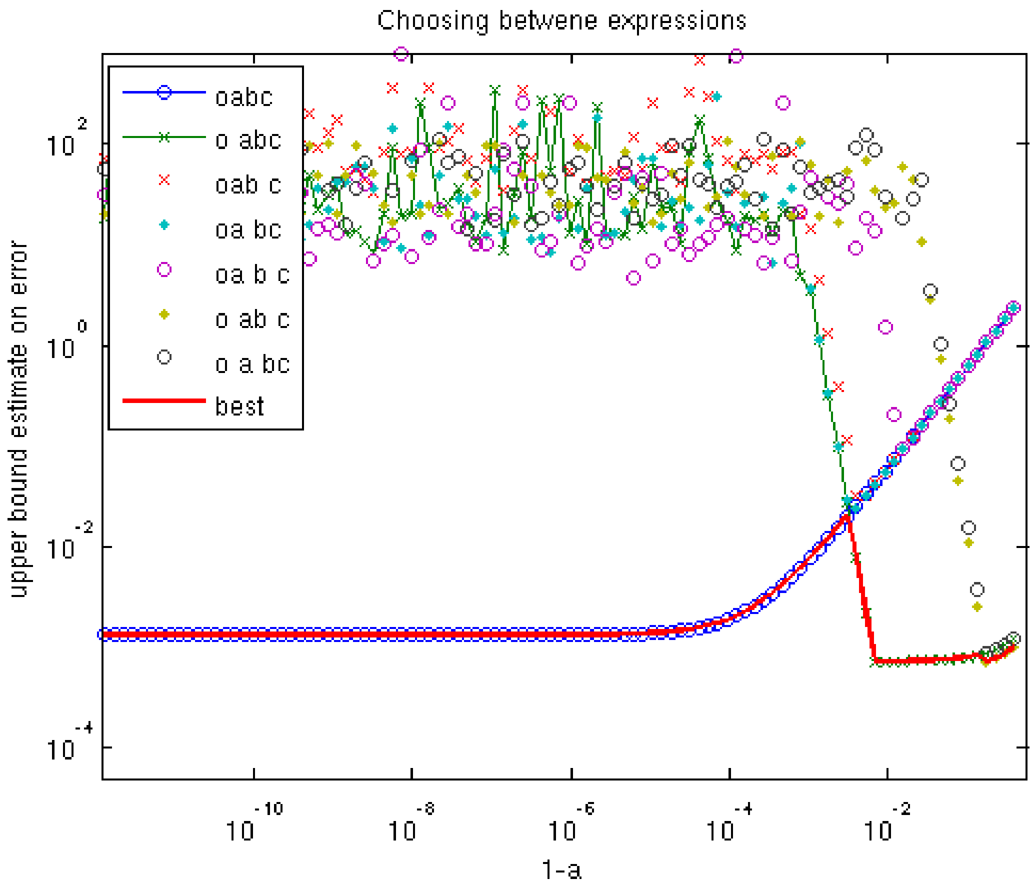


Figure 4: An estimate for the upper bound on the relative error for the various methods of calculating the sum in case 8. A curve though parameter space is shown: $1 - a = variable$, $a - b = 0.0001$, and $b - c = 0.00012$. The thick red line shows the chosen method for calculating the result.

This rather cumbersome method for choosing which approximation to use was used for calculating *valne* in cases five though eight. Simple expressions for switching points where used for *valne* in cases 1-4 and for *valeq* in all cases.

3 Tabulated Integrals

The attached Mathcad document as selected sums and integral approximation expressions. Not every one is listed, for those that are missing see the MatLab code.

Valeq

Two point,

$j_1 = j_2$

$$\int_0^{N_m}\int_0^{s_2} e^{\varepsilon_1 (s_2-s_1)}\, ds_1\, ds_2 \qquad \frac{\mathrm{expl}(2, \varepsilon_1 N_m)}{\varepsilon_1^2}$$

$j_1 \neq j_2$

$$\int_0^{N_m}\int_0^{N_m} e^{\varepsilon_1 (s_2-s_1)}\, ds_2\, ds_1 \qquad \frac{\mathrm{expl}(2, \varepsilon_1 N_m) + \mathrm{expl}(2, -\varepsilon_1 N_m)}{\varepsilon_1^2}$$

Three point

$j_1 = j_2 = j_3$ $\quad \int_0^{N_m}\int_0^{s_3}\int_0^{s_2} e^{\varepsilon_2 (s_3-s_2)}\, e^{\varepsilon_1 (s_2-s_1)}\, ds_1\, ds_2\, ds_3$

$\varepsilon_1 \neq \varepsilon_2$ $\quad \dfrac{\varepsilon_2^{-2}\,\mathrm{expl}(2, N_m \varepsilon_2) - \varepsilon_1^{-2}\,\mathrm{expl}(2, N_m \varepsilon_1)}{\varepsilon_2 - \varepsilon_1}$

$\varepsilon_1 = \varepsilon_2$ $\quad \dfrac{-2\,\mathrm{expl}(3, N_m \varepsilon_1) + N_m \varepsilon_1\,\mathrm{expl}(2, N_m \varepsilon_1)}{\varepsilon_1^3}$

$j_1 = j_2 < j_3$ $$\int_0^{N_m}\int_0^{N_m}\int_0^{s_2} e^{\varepsilon_2 (s_3 - s_2)} e^{\varepsilon_1 (s_2 - s_1)}\, ds_1\, ds_2\, ds_3$$

$\varepsilon_1 \neq \varepsilon_2$ $$\frac{-\frac{1}{\varepsilon_2}\left(\mathrm{expl}(2, N_m\,\varepsilon_2) + \mathrm{expl}(2, -N_m\,\varepsilon_2)\right) - \frac{1}{\varepsilon_1}\,\mathrm{expl}(1, -N_m\,\varepsilon_2)\,\mathrm{expl}(1, N_m\,\varepsilon_1)}{\varepsilon_2\left(\varepsilon_1 - \varepsilon_2\right)}$$

$\varepsilon_1 = \varepsilon_2$ $$\frac{-\mathrm{expl}(4, N_m\,\varepsilon_1) - \mathrm{expl}(4, -N_m\,\varepsilon_1) + \mathrm{expl}(2, N_m\,\varepsilon_1)\, N_m\,\varepsilon_1}{\varepsilon_1^{\,3}}$$

$j_1 < j_2 < j_3$ $$\int_0^{N_m}\int_0^{N_m}\int_0^{N_m} e^{\varepsilon_1 (s_3 - s_2)} e^{\varepsilon_1 (s_2 - s_1)}\, ds_1\, ds_2\, ds_3$$

$\varepsilon_1 \neq \varepsilon_2$ $$\frac{\mathrm{expl}(1, -\varepsilon_1\, N_m)\left(\mathrm{expl}(2, \varepsilon_2\, N_m) + \mathrm{expl}(2, -\varepsilon_2\, N_m)\right) - \mathrm{expl}(1, -\varepsilon_2\, N_m)\left(\mathrm{expl}(2, \varepsilon_1\, N_m) + \mathrm{expl}(2, -\varepsilon_1\, N_m)\right)}{\left(\varepsilon_1\,\varepsilon_2^{\,2} - \varepsilon_1^{\,2}\,\varepsilon_2\right)}$$

$\varepsilon_1 = \varepsilon_2$ $$\frac{N_m\left(\mathrm{expl}(2, \varepsilon_1\, N_m) + \mathrm{expl}(2, -\varepsilon_1\, N_m)\right)}{\varepsilon_1^{\,2}}$$

Four point

Case 1

$j_1 = j_2 = j_3 = j_4$ $$\int_0^{N_m}\int_0^{s_4}\int_0^{s_3}\int_0^{s_2} e^{\varepsilon_3 (s_4-s_3)} e^{\varepsilon_2 (s_3-s_2)} e^{\varepsilon_1 (s_2-s_1)} ds_1\, ds_2\, ds_3\, ds_4$$

$\varepsilon_1 \neq \varepsilon_2 \neq \varepsilon_3$ $$\frac{\left(\frac{\varepsilon_2-\varepsilon_3}{\varepsilon_1^{\,2}}\right)\mathrm{expl}(2, N_m\,\varepsilon_1) + \left(\frac{\varepsilon_3-\varepsilon_1}{\varepsilon_2^{\,2}}\right)\mathrm{expl}(2, N_m\,\varepsilon_2) + \left(\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_3^{\,2}}\right)\mathrm{expl}(2, N_m\,\varepsilon_3)}{(\varepsilon_1-\varepsilon_2)(\varepsilon_1-\varepsilon_3)(\varepsilon_2-\varepsilon_3)}$$

$\varepsilon_1 \neq \varepsilon_2 = \varepsilon_3$

$$\frac{-N_m\,\varepsilon_2\,\mathrm{expl}(3, N_m\,\varepsilon_2)\,\varepsilon_1^{\,3} + 2\,\mathrm{expl}(4, N_m\,\varepsilon_2)\,\varepsilon_1^{\,3} + \mathrm{expl}(4, N_m\,\varepsilon_1)\,\varepsilon_2^{\,3} - 3\,\mathrm{expl}(4, N_m\,\varepsilon_2)\,\varepsilon_1^{\,2}\,\varepsilon_2 + N_m\,\varepsilon_2\,\mathrm{expl}(3, N_m\,\varepsilon_2)\,\varepsilon_1^{\,2}\,\varepsilon_2}{\varepsilon_1^{\,4}\,\varepsilon_2^{\,3} - 2\,\varepsilon_1^{\,3}\,\varepsilon_2^{\,4} + \varepsilon_1^{\,2}\,\varepsilon_2^{\,5}}$$

$\varepsilon_1 = \varepsilon_2 \neq \varepsilon_3$ similar to above

$\varepsilon_1 = \varepsilon_3 \neq \varepsilon_2$ similar to above

$\varepsilon_1 = \varepsilon_2 = \varepsilon_3$ $$\frac{-6\,\mathrm{expl}(4, N_m\,\varepsilon_1) - N_m^{\,2}\,\varepsilon_1^{\,2}\,\mathrm{expl}(2, N_m\,\varepsilon_1) + 4\,N_m\,\varepsilon_1\,\mathrm{expl}(3, N_m\,\varepsilon_1)}{2\,\varepsilon_1^{\,4}}$$

$0 = \varepsilon_1 = \varepsilon_2 = \varepsilon_3$ $$\frac{N_m^{\,4}\,(N_m\,\varepsilon_1 + N_m\,\varepsilon_2 + N_m\,\varepsilon_3 + 5)}{120}$$

$0 = \varepsilon_1 = \varepsilon_2$ see code

$0 = \varepsilon_3 = \varepsilon_2$ same as above except swap 1 and 3

$0 = \varepsilon_1 = \varepsilon_3$

$$\frac{\left(-3\,\varepsilon_1\,\mathrm{expl}(3,N_m\,\varepsilon_1) + N_m\,\varepsilon_1^{\,2}\,\mathrm{expl}(2,N_m\,\varepsilon_1)\right)\varepsilon_2^{\,2} + \left(2\,\mathrm{expl}(3,N_m\,\varepsilon_1) - N_m\,\varepsilon_1\,\mathrm{expl}(2,N_m\,\varepsilon_1)\right)\varepsilon_2^{\,3} + \varepsilon_1^{\,3}\,\mathrm{expl}(3,N_m\,\varepsilon_2)}{\varepsilon_1^{\,3}\,\varepsilon_2^{\,2}\,(\varepsilon_1-\varepsilon_2)^2}$$

$0 = \varepsilon_1 \neq \varepsilon_2 = \varepsilon_3$

$$\frac{-6\,\mathrm{expl}(3,N_m\,\varepsilon_2) + 2\,N_m\,\varepsilon_2\,\mathrm{expl}(2,N_m\,\varepsilon_2)}{2\,\varepsilon_2^{\,4}}$$ This is a limit only, not an expression

$0 = \varepsilon_2 \neq \varepsilon_1 = \varepsilon_3$ or $0 = \varepsilon_3 \neq \varepsilon_1 = \varepsilon_2$ same as above except re-ordered

$0 = \varepsilon_1$

$$\frac{\dfrac{\mathrm{expl}(4,N_m\,\varepsilon_2)}{\varepsilon_2^{\,3}} - \dfrac{\mathrm{expl}(4,N_m\,\varepsilon_3)}{\varepsilon_3^{\,3}}}{(\varepsilon_2-\varepsilon_3)}$$

$0 = \varepsilon_2$ or $0 = \varepsilon_3$ same as above except re-ordered

Case 2

$j_1 < j_2 = j_3 = j_4$ $$\int_0^{N_m}\int_0^{s_4}\int_0^{s_3}\int_0^{N_m} e^{\varepsilon_3\,(s_4-s_3)}\,e^{\varepsilon_2\,(s_3-s_2)}\,e^{\varepsilon_1\,(s_2-s_1)}\,ds_1\,ds_2\,ds_3\,ds_4$$

same as case 4 with E1 and E3 switched

Case 3

$j_1 = j_2 < j_3 = j_4$ $$\int_0^{N_m}\int_0^{s_4}\int_0^{N_m}\int_0^{s_2} e^{\varepsilon_3 (s_4 - s_3)} e^{\varepsilon_2 (s_3 - s_2)} e^{\varepsilon_1 (s_2 - s_1)}\, ds_1\, ds_2\, ds_3\, ds_4$$

$0 = \varepsilon_1 = \varepsilon_2 = \varepsilon_3$ $$\frac{N_m^{\ 4}\left(N_m \varepsilon_1 - N_m \varepsilon_2 + N_m \varepsilon_3 + 3\right)}{12}$$

$0 = \varepsilon_3 = \varepsilon_2$ $$\frac{-N_m^{\ 2}}{12\,\varepsilon_1^{\ 3}}\left[\left[N_m^{\ 2}\left(2\varepsilon_3 - \varepsilon_2\right) + 6N_m\right]\varepsilon_1^{\ 2} + 2N_m\varepsilon_1\left[\left(1 + 2e^{N_m \varepsilon_1}\right)\varepsilon_2 + \left(1 - e^{N_m \varepsilon_1}\right)\varepsilon_3\right] + 6\left(1 - e^{N_m \varepsilon_1}\right)\left(\varepsilon_1 + \varepsilon_2\right)\right]$$

$0 = \varepsilon_1 = \varepsilon_2$

same as above just switch 1 and 3

$0 = \varepsilon_1 = \varepsilon_3$

$$\frac{\left[2N_m^{\ 2} + N_m^{\ 3}\left(\varepsilon_1 + \varepsilon_3\right)\right]e^{-N_m \varepsilon_2}\,\varepsilon_2^{\ 3} + 2N_m^{\ 2}\left(\varepsilon_1 + \varepsilon_3\right)\varepsilon_2^{\ 2} + \left(e^{-N_m \varepsilon_2} - 1\right)\left[\left[3N_m^{\ 2}\left(\varepsilon_1 + \varepsilon_3\right) + 4N_m\right]\varepsilon_2^{\ 2} + 4N_m\left(\varepsilon_1 + \varepsilon_3\right)\varepsilon_2 - 2\left(\varepsilon_1 + \varepsilon_2 + \varepsilon_3\right)\left(e^{N_m \varepsilon_2} - \right.\right.}{2\,\varepsilon_2^{\ 5}}$$

$\varepsilon_1 = 0$ $\qquad \varepsilon_2 = \varepsilon_3$

$$-\frac{2\,\mathrm{coshl}\left(4, N_m \varepsilon_3\right) - 2N_m \varepsilon_3\,\mathrm{sinhl}\left(3, N_m \varepsilon_3\right)}{\varepsilon_3^{\ 4}}$$

$\varepsilon_3 = 0$ $\qquad \varepsilon_1 = \varepsilon_2$ $\qquad$ notice same as above with 1,3 swap

$$-\frac{2\,\mathrm{coshl}\left(4, N_m \varepsilon_1\right) - 2N_m \varepsilon_1\,\mathrm{sinhl}\left(3, N_m \varepsilon_1\right)}{\varepsilon_1^{\ 4}}$$

$\varepsilon_2 = 0$ $\qquad \varepsilon_1 = \varepsilon_3$

$$\frac{\mathrm{expl}\left(3, 2N_m \varepsilon_1\right) - 2\,\mathrm{expl}\left(3, N_m \varepsilon_1\right) - 2N_m \varepsilon_1\,\mathrm{expl}\left(2, N_m \varepsilon_1\right)}{\varepsilon_1^{\ 4}}$$

$\varepsilon_1 = 0$

$$\frac{\varepsilon_3\ \mathrm{expl}(4, N_m\, \varepsilon_2) + \varepsilon_3\ \mathrm{expl}(4, -N_m\, \varepsilon_2) + \varepsilon_2\ \mathrm{expl}(2, -N_m\, \varepsilon_2)\ \mathrm{expl}(1, N_m\, \varepsilon_3) + N_m\, \varepsilon_2\, \varepsilon_3\ \mathrm{expl}(2, -N_m\, \varepsilon_2) + N_m\, \varepsilon_2^{\,2}\ \mathrm{expl}(1, -N_m\, \varepsilon_2)\ \mathrm{expl}(1, N_m\, \varepsilon_3)}{\varepsilon_2^{\,3}\, \varepsilon_3\, (\varepsilon_2 - \varepsilon_3)} = 1.132$$

$\varepsilon_3 = 0$ notice case as above with 1,3 swap

$$\frac{\varepsilon_1\ \mathrm{expl}(4, N_m\, \varepsilon_2) + \varepsilon_1\ \mathrm{expl}(4, -N_m\, \varepsilon_2) + \varepsilon_2\ \mathrm{expl}(2, -N_m\, \varepsilon_2)\ \mathrm{expl}(1, N_m\, \varepsilon_1) + N_m\, \varepsilon_2\, \varepsilon_1\ \mathrm{expl}(2, -N_m\, \varepsilon_2) + N_m\, \varepsilon_2^{\,2}\ \mathrm{expl}(1, -N_m\, \varepsilon_2)\ \mathrm{expl}(1, N_m\, \varepsilon_1)}{\varepsilon_2^{\,3}\, \varepsilon_1\, (\varepsilon_2 - \varepsilon_1)} = 0.988$$

$\varepsilon_2 = 0$

$$\frac{\mathrm{expl}(2, N_m\, \varepsilon_1)\ \mathrm{expl}(2, N_m\, \varepsilon_3)}{\varepsilon_1^{\,2}\, \varepsilon_3^{\,2}} = 4.377$$

Case 4

$j_1 = j_2 = j_3 < j_4$ $$\int_0^{N_m}\int_0^{N_m}\int_0^{s_3}\int_0^{s_2} e^{\varepsilon_3 (s_4 - s_3)}\, e^{\varepsilon_2 (s_3 - s_2)}\, e^{\varepsilon_1 (s_2 - s_1)}\, ds_1\, ds_2\, ds_3\, ds_4 = 1.856$$

$\varepsilon_1 \neq \varepsilon_2 \neq \varepsilon_3$ $$\frac{\mathrm{expl}(1, N_m\, \varepsilon_1)\,\left(\mathrm{expl}(1, -N_m\, \varepsilon_1) - \mathrm{expl}(1, -N_m\, \varepsilon_2)\right)\left(\mathrm{expl}(2, N_m\, \varepsilon_3)\, \varepsilon_2 - \mathrm{expl}(2, N_m\, \varepsilon_2)\, \varepsilon_3\right)}{\varepsilon_1\, \varepsilon_2\, \varepsilon_3\, (\varepsilon_2 - \varepsilon_3)\, (\varepsilon_1 - \varepsilon_2)}$$

$\varepsilon_1 = \varepsilon_2 = \varepsilon_3$ $$\frac{N_m^{\,4}\,(N_m\, \varepsilon_1 - N_m\, \varepsilon_3 + N_m\, \varepsilon_{12} + 4)}{24}$$

$\varepsilon_3 = 0 \quad \varepsilon_1 = \varepsilon_{12}$

$$\frac{N_m\left(N_m \varepsilon_{12} - 2 e^{N_m \varepsilon_{12}} + N_m \varepsilon_{12} e^{N_m \varepsilon_{12}} + 2\right)}{\varepsilon_{12}^{3}}$$

$\varepsilon_1 = 0 \quad \varepsilon_{12} = \varepsilon_3$

$$\frac{2\left(N_m \varepsilon_3 \operatorname{sinhl}(3, N_m \varepsilon_3) - 2 \operatorname{coshl}(4, N_m \varepsilon_3)\right)}{\varepsilon_3^{4}}$$

$\varepsilon_{12} = 0 \quad \varepsilon_1 = \varepsilon_3$

$$\frac{2\left(N_m \varepsilon_1 \operatorname{sinhl}(3, N_m \varepsilon_1) - 2 \operatorname{coshl}(4, N_m \varepsilon_1)\right)}{\varepsilon_1^{4}}$$

$\varepsilon_1 = 0$

$$\frac{\left(\operatorname{expl}(3, N_m \varepsilon_3) + \operatorname{expl}(3, -N_m \varepsilon_3) + N_m \varepsilon_3 \operatorname{expl}(2, -N_m \varepsilon_3)\right) \varepsilon_{12}^{2} + \left(\operatorname{expl}(1, -N_m \varepsilon_3) \operatorname{expl}(2, N_m \varepsilon_{12})\right) \varepsilon_3^{2}}{\varepsilon_3^{3} \varepsilon_{12}^{2} \left(\varepsilon_3 - \varepsilon_{12}\right)}$$

$\varepsilon_2 = 0$

same as above with 1 and 2 flipped

$\varepsilon_3 = 0$

$$\frac{N_m\left(\varepsilon_1^{2} \operatorname{expl}(3, N_m \varepsilon_{12}) - \varepsilon_{12}^{2} \operatorname{expl}(3, N_m \varepsilon_1)\right)}{-\varepsilon_1^{2} \varepsilon_{12}^{2} \left(\varepsilon_1 - \varepsilon_{12}\right)}$$

Case 5

$j_1 < j_2 < j_3 = j_4$

The 5 intigral is the same as the case 6 with 1 and 3 flipped

Case 6

$j_1 = j_2 < j_3 < j_4$

$$\int_0^{N_m}\int_0^{N_m}\int_0^{N_m}\int_0^{s_2} e^{\varepsilon_3 (s_4 - s_3)} e^{\varepsilon_2 (s_3 - s_2)} e^{\varepsilon_1 (s_2 - s_1)} \, ds_1 \, ds_2 \, ds_3 \, ds_4$$

$$0 = \varepsilon_1 = \varepsilon_2 = \varepsilon_3 \quad \frac{N_m^{\,4}\left(2\,N_m\,\varepsilon_1 - N_m\,\varepsilon_2 + 6\right)}{12}$$

$$0 = \varepsilon_1 = \varepsilon_2 \quad \frac{N_m^{\,2}\,e^{N_m\,\varepsilon_3}\left(e^{-N_m\,\varepsilon_3} - 1\right)\left[3\left(\varepsilon_2 + \varepsilon_3\right)\left(e^{-N_m\,\varepsilon_3} + N_m\,\varepsilon_3 - 1\right) - 3\,N_m\,\varepsilon_3^{\,2} + N_m\left(\varepsilon_1 + \varepsilon_2\right)\varepsilon_3\left(e^{-N_m\,\varepsilon_3} - 1\right)\right]}{6\,\varepsilon_3^{\,3}}$$

$$\varepsilon_3 = \varepsilon_2 = 0 \quad \frac{N_m^{\,2}\left[\left(\varepsilon_1 + \varepsilon_2\right)\left(e^{N_m\,\varepsilon_1} - N_m\,\varepsilon_1 - 1\right) - \dfrac{N_m\,\varepsilon_1\,\varepsilon_2\left(e^{N_m\,\varepsilon_1} - 1\right)}{2}\right]}{\varepsilon_1^{\,3}}$$

$$0 = \varepsilon_1 = \varepsilon_3$$

$$\frac{N_m}{\left(2\,\varepsilon_2^{\,4}\right)}\left[2\left(\varepsilon_1 + \varepsilon_2 + \varepsilon_3\right)\left(\mathrm{expl}\left(3, N_m\,\varepsilon_2\right) + \mathrm{expl}\left(3, -N_m\,\varepsilon_2\right) + N_m\,\varepsilon_2\,\mathrm{expl}\left(2, -N_m\,\varepsilon_2\right)\right) + N_m^{\,2}\left(\varepsilon_1 + \varepsilon_3\right)\varepsilon_2^{\,2}\,\mathrm{expl}\left(1, -N_m\,\varepsilon_2\right) + N_m\,\varepsilon_2\,\varepsilon_3\left(\mathrm{expl}\left(2, -N_m\,\varepsilon_2\right) - \mathrm{expl}(2, N\right.\right.$$

Case 7

$j_1 < j_2 = j_3 < j_4$ $$\int_0^{N_m}\int_0^{N_m}\int_0^{s_3}\int_0^{N_m} e^{\varepsilon_3 (s_4-s_3)}\, e^{\varepsilon_2 (s_3-s_2)}\, e^{\varepsilon_1 (s_2-s_1)}\, ds_1\, ds_2\, ds_3\, ds_4$$

$0 = \varepsilon_1 = \varepsilon_2 = \varepsilon_3$

$$\frac{N_m^{\ 4}\left[-N_m\left(\varepsilon_1 - 2\,\varepsilon_2 + \varepsilon_3\right) + 6\right]}{12}$$

$0 = \varepsilon_2 = \varepsilon_3$

$$\frac{N_m\left[2\left(\varepsilon_1 + \varepsilon_2 + \varepsilon_3\right)\left(e^{N_m\,\varepsilon_1} + e^{-N_m\,\varepsilon_1} - 2\right) + N_m\,\varepsilon_1\left[2\,\varepsilon_1 + N_m\,\varepsilon_1\,\varepsilon_2 + 2\,\varepsilon_2 + \varepsilon_3\left(e^{N_m\,\varepsilon_1} + 1\right)\right]\left(e^{-N_m\,\varepsilon_1} - 1\right)\right]}{2\,\varepsilon_1^{\ 4}}$$

$0 = \varepsilon_1 = \varepsilon_2$

same as above except exchange ε1 and ε3

$0 = \varepsilon_1 = \varepsilon_3$

$$-\frac{N_m^{\ 2}\left[2\left(\varepsilon_1 + \varepsilon_2 + \varepsilon_3\right)\left(1 + N_m\,\varepsilon_2 - e^{N_m\,\varepsilon_2}\right) + N_m\left(\varepsilon_1 + \varepsilon_3\right)\varepsilon_2\left(e^{N_m\,\varepsilon_2} - 1\right)\right]}{2\,\varepsilon_2^{\ 3}}$$

$0 = \varepsilon_1$

$$\frac{N_m\left[-\varepsilon_3\,\operatorname{expl}\left(1, N_m\,\varepsilon_2\right)\,\operatorname{expl}\left(1, -N_m\,\varepsilon_3\right) - \varepsilon_2\left(\operatorname{expl}\left(2, N_m\,\varepsilon_3\right) + \operatorname{expl}\left(2, -N_m\,\varepsilon_3\right)\right)\right]}{\varepsilon_2\,\varepsilon_3^{\ 2}\left(\varepsilon_2 - \varepsilon_3\right)}$$ may not use

not all three orders are the same

$0 = \varepsilon_1$ $\quad \varepsilon_2 = \varepsilon_3$

$$\frac{N_m^{\ 2}\,\varepsilon_2\,\operatorname{expl}\left(1, N_m\,\varepsilon_2\right) - N_m\left(\operatorname{expl}\left(2, N_m\,\varepsilon_2\right) + \operatorname{expl}\left(2, -N_m\,\varepsilon_2\right)\right)}{\varepsilon_2^{\ 3}}$$

may not use
not all three orders are the same

Case 8

$$j_1 < j_2 < j_3 < j_4 \qquad \int_0^{N_m}\int_0^{N_m}\int_0^{N_m}\int_0^{N_m} e^{\varepsilon_3 (s_4-s_3)}\, e^{\varepsilon_2 (s_3-s_2)}\, e^{\varepsilon_1 (s_2-s_1)}\, ds_1\, ds_2\, ds_3\, ds_4$$

$$0 = \varepsilon_1 = \varepsilon_2 = \varepsilon_3 \qquad {N_m}^4$$

$$0 = \varepsilon_1 = \varepsilon_2 \qquad \frac{{N_m}^2}{2\,{\varepsilon_3}^3}\left[2\left(\varepsilon_2 + \varepsilon_3\right)\left(\mathrm{expl}\left(2, N_m\,\varepsilon_3\right) + \mathrm{expl}\left(2, -N_m\,\varepsilon_3\right)\right) - 2\,N_m\,\varepsilon_2\,\varepsilon_3\,\sinh\left(N_m\,\varepsilon_3\right)\right]$$

$0 = \varepsilon_2 = \varepsilon_3$ same as above except swap 1 and 3

$$0 = \varepsilon_1 = \varepsilon_3 \qquad \frac{{N_m}^2}{{\varepsilon_2}^3}\left[4\left(\varepsilon_1 + \varepsilon_2 + \varepsilon_3\right)\sinh\left(\frac{N_m\,\varepsilon_2}{2}\right)^2 - N_m\left(\varepsilon_1 + \varepsilon_3\right)\varepsilon_2\,\sinh\left(N_m\,\varepsilon_2\right)\right]$$

Valne

Four point

Case 8

$$\sum_{j_4=4}^{N}\ \sum_{j_3=3}^{j_4-1}\ \sum_{j_2=2}^{j_3-1}\ \sum_{j_1=1}^{j_2-1}\left(c^{j_4-j_3}\, b^{j_3-j_2}\, a^{j_2-j_1}\right)$$

When 1~ a~b~c

$$-\frac{N (N-1) (N-2) (N-3) [(N+1) (3-a-b-c)-5]}{120}$$

When 1~ a~b, c~0

$$\frac{c (N-3) (N-2) (N-1)}{24} [N (a+b-2)+4]$$

When 1~ a, b~c~0

$$b\, c\left[\frac{(N+1) \left(10 N+18 a+N^2 a-N^2-7 N a-36\right)}{6}-4 a+10\right]$$

When 1 !~ a~b~c

$$\frac{\begin{pmatrix} a^{N+4} & a^{N+3} & a^{N+2} & a^{N+1} & a^{N} & a^{5} & a^{4} & a^{3} & a^{2} \end{pmatrix}\left[\begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & 6 & -11 & 6 \\ 3 & -12 & 3 & 18 \\ -3 & 6 & 9 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -6 & -6 \\ 0 & 0 & 6 & -18 \end{pmatrix}\left(\delta_{bc}+2\,\delta_{ab}\right)+\begin{pmatrix} 0 & 3 & -15 & 18 \\ 0 & -9 & 33 & -18 \\ 0 & 9 & -21 & 0 \\ 0 & -3 & 3 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -6 & 0 \\ 0 & 0 & 12 & -18 \\ 0 & 0 & -6 & 18 \\ 0 & 0 & 0 & 0 \end{pmatrix}\right]\begin{pmatrix} N^3 \\ N^2 \\ N \\ 1 \end{pmatrix}}{6 (a-1)^5}$$

Now 1~a~b !~ c

$$\sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left(c^{j_4-j_3}\,b^{j_3-j_2}\,a^{j_2-j_1}\right) = 1.411\times 10^{3}$$

$$\frac{\left(\delta_{ab}+2\,\delta_{1a}\right)\begin{pmatrix} c^5 & c^4 & c^3 & c^2 & c & 1\end{pmatrix}\begin{pmatrix} 1 & -2 & -1 & 2 & 0 \\ -4 & 12 & 4 & -12 & 0 \\ 6 & -24 & 6 & 36 & 0 \\ -4 & 20 & -20 & -20 & 24 \\ 1 & -6 & 11 & -6 & 0 \\ 0 & 0 & 0 & 0 & -24\,c^{N+2}\end{pmatrix}\begin{pmatrix} N^4 \\ N^3 \\ N^2 \\ N \\ 1\end{pmatrix} - 2\left[\begin{pmatrix} c^5 & c^4 & c^3 & c^2 & c & 1\end{pmatrix}\begin{pmatrix} 0 & 2 & -6 & 4 & 0 \\ 0 & -8 & 30 & -22 & 0 \\ 0 & 12 & -54 & 54 & 0 \\ 0 & -8 & 42 & -58 & 12 \\ 0 & 2 & -12 & 22 & -12 \\ 0 & 0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix} N^4 \\ N^3 \\ N^2 \\ N \\ 1\end{pmatrix} + \left(12\,c^{N+1} - 12\,c^{N+2}\right)\right]}{24\,(c-1)^5}$$

Now 1~a !~ b~c

$$\sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left[\left[b^{j_4} - \left(j_4-j_3\right)\delta_{bc}\,b^{\left(j_4-1\right)} - b^{j_4}\left(j_2-j_1\right)\delta_{1a}\right]b^{-j_2}\right]$$

$$\frac{\begin{pmatrix} b^{N+3} & b^{N+2} & b^{N+1} & b^{N} & b^{5} & b^{4} & b^{3} & b^{2} & b^{1}\end{pmatrix}\left[\begin{pmatrix} 0 & 0 & -6 & 18 \\ 0 & 0 & 6 & 6 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 3 & -6 & -9 & 0 \\ -3 & 12 & -3 & -18 \\ 1 & -6 & 11 & -6 \\ 0 & 0 & 0 & 0\end{pmatrix}\delta_{1a} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -3 & 15 & -18 \\ 0 & 6 & -12 & -18 \\ 0 & -3 & -3 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 3 & 3 & 0 \\ 0 & -6 & 12 & 18 \\ 0 & 3 & -15 & 18\end{pmatrix}\delta_{bc} + \begin{pmatrix} 0 & 0 & 6 & -18 \\ 0 & 0 & -12 & 18 \\ 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 3 & -3 & 0 \\ 0 & -9 & 21 & 0 \\ 0 & 9 & -33 & 18 \\ 0 & -3 & 15 & -18 \\ 0 & 0 & 0 & 0\end{pmatrix}\right]\begin{pmatrix} N^3 \\ N^2 \\ N \\ 1\end{pmatrix}}{6\,(b-1)^5}$$

Now 1~a !~ b !~ c

$$\sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left[c^{j_4-j_3}\,b^{j_3-j_2}\left[1-\delta_{1a}\left(j_2-j_1\right)\right]\right]$$

$$\alpha_1 := \begin{pmatrix} c^5 & c^4 & c^3 & c^2 \end{pmatrix} \ldots$$

$$\ldots\left[\begin{pmatrix} 1 & 0 & -1 & -6 \\ -3 & 3 & 6 & 18 \\ 3 & -6 & -3 & -12 \\ -1 & 3 & -2 & 6 \end{pmatrix}\delta_{1a}\,b^3+\begin{pmatrix} 0 & -3 & 3 & 6 \\ 0 & 9 & -15 & -18 \\ 0 & -9 & 21 & 12 \\ 0 & 3 & -9 & 0 \end{pmatrix}b^3+\begin{pmatrix} -2 & 3 & 5 & -6 \\ 6 & -15 & -15 & 24 \\ -6 & 21 & 3 & -36 \\ 2 & -9 & 7 & 6 \end{pmatrix}\delta_{1a}\,b^2+\begin{pmatrix} 0 & 6 & -12 & 0 \\ 0 & -18 & 48 & -6 \\ 0 & 18 & -60 & 24 \\ 0 & -6 & 24 & -18 \end{pmatrix}b^2+\begin{pmatrix} 1 & -3 & 2 & 0 \\ -3 & 12 & -9 & 0 \\ 3 & -15 & 18 & 0 \\ -1 & 6 & -11 & 6 \end{pmatrix}\delta_{1a}\,b+\begin{pmatrix} 0 & -3 & 9 & -6 \\ 0 & 9 & -33 & 24 \\ 0 & -9 & 39 & -36 \\ 0 & 3 & -15 & 18 \end{pmatrix}b\right]\begin{pmatrix} N^3 \\ N^2 \\ N \\ 1 \end{pmatrix}$$

$$\alpha_2 := b^3\left[\left(18\,c-6-18\,c^2\right)c^N\,\delta_{1a}+\left(12\,c^2+6-18\,c\right)c^N\right]+b^2\left[\left(18\,c^2-6\,c\right)c^N\delta_{1a}+\left(24\,c-6-18\,c^2\right)c^N\right]+b\left[-6\,c^{N+2}\,\delta_{1a}+(6\,c-6)\,c^{N+1}\right]$$

$$-\frac{1}{(b-1)^3}\left[\frac{\alpha_1+\alpha_2}{6\,c\,(c-1)^4}-\frac{b\left(b\,\delta_{1a}-b+1\right)\left(b^2\,c^3-b^3\,c^2-b^2\,c^N+b^N\,c^2+b^3\,c^N-b^N\,c^3\right)}{c\,(b-c)\,(b-1)\,(c-1)}\right]$$

Now 1 !~ a~b !~ c

$$\sum_{j_4=4}^{N}\sum_{j_3=3}^{j_4-1}\sum_{j_2=2}^{j_3-1}\sum_{j_1=1}^{j_2-1}\left[c^{j_4-j_3}\,b^{j_3-j_2}\left[b^{\left(j_2-j_1\right)}-\left(j_2-j_1\right)\delta_{ba}\,b^{\left(j_2-j_1-1\right)}\right]\right]$$

$$T_1 := \frac{c}{(b-1)^2}\left[\begin{pmatrix} b^{N+4} & b^{N+3} & b^{N+2} & b^{N+1} & b^{N} & b^{5} & b^{4} & b^{3}\end{pmatrix}\begin{pmatrix} 0 & 0 & N^2-5N+6 \\ 0 & 8N-2N^2-6 & 6N-2N^2 \\ N^2-3N+2 & 4N^2-8N-8 & N^2-N-2 \\ 2N-2N^2+4 & 6-2N^2 & 0 \\ N^2+N-2 & 0 & 0 \\ -2 & -4 & -4 \\ 8 & 12 & 0 \\ -10 & 0 & 0 \end{pmatrix}\begin{pmatrix} c^2 \\ c \\ 1 \end{pmatrix}\right]$$

$$T_2 := -\frac{2b^2\left(c^3-c^N\right)(b-2c+bc)}{c-1}$$

$$T_3 := -\frac{c^2(1-c)\left(b^4-b\,b^N\right)}{1-b}+\frac{b^2(1-b)\left(c^4-c\,c^N\right)}{1-c}+b^2c^2(b-c)(N-3)$$

$$T_4 := \frac{bc}{(b-c)^2(b-1)^3(c-1)^2}\begin{pmatrix} b^{N+2} & b^{N+1} & b^{N} & b^{4} & b^{3} & b^{2} & b\end{pmatrix}\begin{pmatrix} 0 & 0 & 3-N & 2N-6 & 3-N \\ 0 & N-2 & 3-N & -N & N-1 \\ 0 & -N & 2N & -N & 0 \\ -1 & 0 & 0 & N & 1-N \\ 3 & 0 & -2N & N & N-3 \\ -3 & N & N-3 & 6-2N & 0 \\ 1 & 2-N & N-3 & 0 & 0 \end{pmatrix}\begin{pmatrix} c^N \\ c^3 \\ c^2 \\ c \\ 1 \end{pmatrix}$$

$$-\delta_{ba}\left[\frac{T_1 - T_2}{2\,(b-1)^2\,(b-c)^3} + \frac{T_3}{b\,c\,(b-c)\,(b-1)^3\,(c-1)}\right] - T_4$$

1 !~ a !~ b !~ c

$$\frac{-a\,b\,c}{(1-a)\,(1-b)\,(1-c)}\left[\left[-\frac{b^2\,(1-a)}{(b-a)\,(c-b)} + \frac{a^2\,(1-b)}{(b-a)\,(c-a)} + \frac{1}{(c-1)}\right]\left(\frac{c^3 - c^N}{-c^2}\right) + \left(\frac{a}{b-a} + \frac{1}{1-b}\right)\frac{c-1}{c-b}\left(\frac{b^3 - b^N}{b}\right) + \frac{1-b}{b-a}\,\frac{1-c}{c-a}\,\frac{a^3 - a^N}{1-a} - (N-3)\right]$$