DBG Notes

Mark Boyer, Feb. 8 2024

These are a collection of notes for an upcoming paper on the use of distributed Gaussian bases in an AIMD context. Most code and figures have been hidden.

Generic algorithms and expressions for integrals involving a product of a multidimensional Gaussian with arbitrary rotation (covariance matrix) and complex phases are provided, as well as specific symmetrizations that allow for entirely real integrals.

Miscellaneous other proofs and algorithms are provided, like tensor derivatives for inverse-distance weighted interpolants, some code for handling arbitrary tensor product derivatives, and a convenient way to defined reduced dimensional coordinate spaces

Everything is *caveat emptor*, these are personal notes, although well-tested implementations of most derivations are provided here [https://github.com/McCoyGroup/Psience]

DGB Definition

Our basis functions are given by

$$\phi(x, \xi, \alpha) = N(\alpha)\, e^{-\alpha(x-\xi)^2}$$

where

$$N(\alpha) = \left(\frac{2\,\alpha}{\pi}\right)^{1/4}$$

The real saving grace of a DGB approach is that the product of two DGB functions is again a DGB function, just centered around the weighted average of the original DGB points

$$\phi(x, \xi_i, \alpha_i)\,\phi\left(x, \xi_j, \alpha_j\right) = W\left(\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j}, \xi_i-\xi_j\right)\phi\left(x, \frac{\alpha_i\xi_i+\alpha_j\xi_j}{\alpha_i+\alpha_j}, \alpha_i+\alpha_j\right)$$

where

$$W(A, \Delta x) = N(A)\, e^{-\mathrm{A}\Delta x^2}$$

which it should be noted is equivalent to $\phi\left(\xi_i, \xi_j, {}^{\alpha_i\,\alpha_j}\!/_{\alpha_i+\alpha_j}\right)$

Functional Form

Overlaps

As we have

$$\phi(x,\,\xi_i,\,\alpha_i)\,\phi\big(x,\,\xi_j,\,\alpha_j\big) \;=\; W\!\left(\frac{\alpha_i\,\alpha_j}{\alpha_i{+}\alpha_j},\,\xi_i{-}\xi_j\right)\phi\!\left(x,\,\frac{\alpha_i\xi_i{+}\alpha_j\xi_j}{\alpha_i{+}\alpha_j},\,\alpha_i{+}\alpha_j\right)$$

it is straightforward to note that

$$\begin{aligned}
\big\langle\varphi_i\big|\varphi_j\big\rangle &= \int P_{nm}^{(i,j)}(x)\,\phi^{(i)}(x)\,\phi^{(j)}(x)\\
&= W^{(i,j)}\int\phi\!\left(x,\,\frac{\alpha_i\xi_i{+}\alpha_j\xi_j}{\alpha_i{+}\alpha_j},\,\alpha_i{+}\alpha_j\right)\\
&= W^{(i,j)}\left(\frac{2\,\pi}{\alpha_i{+}\alpha_j}\right)^{1/4}\\
&= \left(\frac{2\,\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j}}{\pi}\right)^{1/4}\left(\frac{2\,\pi}{\alpha_i{+}\alpha_j}\right)^{1/4}\exp\!\left(-\frac{\alpha_i\,\alpha_j}{\alpha_i{+}\alpha_j}\,\big(\xi_i{-}\xi_j\big)^2\right)\\
&= \left(\frac{4\,\alpha_i\,\alpha_j}{\big(\alpha_i{+}\alpha_j\big)^2}\right)^{1/4}\exp\!\left(-\frac{\alpha_i\,\alpha_j}{\alpha_i{+}\alpha_j}\,\big(\xi_i{-}\xi_j\big)^2\right)
\end{aligned}$$

Using Mass-Weighted Coordinates

Integration of the Potential (Non-Rotated)

We start with our multivariate Gaussian basis function centered around a point $\xi^{(i)}$

$$\varphi_i(\boldsymbol{x}){=}\prod_{j=1}^{3N}\phi\big(x_j,\,\xi_j^{(i)},\,\alpha_i\big)$$

the integral we then want to evaluate is

$$\int_{\mathbb{R}^N}\varphi_i(\boldsymbol{x})\;V(\boldsymbol{x})\,\varphi_j(\boldsymbol{x})\,d\boldsymbol{x}$$

where then

$$\varphi_i(\boldsymbol{x})\,\varphi_j(\boldsymbol{x}){=}\prod_{k=1}^{3N}\phi\big(x_k,\,\xi_k^{(i)},\,\alpha_i\big)\,\phi\big(x_k,\,\xi_k^{(j)},\,\alpha_j\big)$$

$$= \prod_{k=1}^{3N} W\left(\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j},\, \xi_k^{(i)}-\xi_k^{(j)}\right) \prod_{k=1}^{3N} \phi\left(x_{k,}\, \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j},\, \alpha_i+\alpha_j\right)$$

and so

$$\int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x})\; V(\boldsymbol{x})\, \varphi_j(\boldsymbol{x})\, d\boldsymbol{x} = \prod_{k=1}^{3N} W\left(\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j},\, \xi_k^{(i)}-\xi_k^{(j)}\right) \int_{\mathbb{R}^N} V(\boldsymbol{x}) \prod_{k=1}^{3N} \phi\left(x_{k,}\, \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j},\, \alpha_i+\alpha_j\right) d\boldsymbol{x}$$

When evaluating this final integral, we then have a few approaches

Quadrature

- Straightforward
- The relevant Gauss-Hermite quadrature weights are built into **`scipy`**
- Scales poorly with dimension

Expansions

Taylor Series

ALTERNATE EXPRESSION

Final Expression

Local Expansions

The local expansion context is largely the same as the Taylor series context, except instead of picking one point to expand about, we expand locally around every integration point, i.e. we choose

$$\zeta_k = \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j}$$

which means our final integrals end up as

$$\int_{\mathbb{R}^N} \prod_{k=1}^{3N} \phi\left(x_{k,}\, \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j},\, \alpha_i+\alpha_j\right) (x_k-\zeta_k)^{p_k}\, d\boldsymbol{x} = \prod_{k=1}^{3N} \int \phi\left(x_{k,}\, 0,\, \alpha_i+\alpha_j\right) {x_k}^{p_k}\, dx_k$$

which is easy to integrate

In[1695]:=

```
baseInt = Assuming[
  n ∈ Integers && n ≥ 0 && α > 0,
  Integrate[DGB[0, α][x] x^n, {x, -∞, ∞}]
 ]
```

Out[1695]=

$$\frac{\left(1+(-1)^{n}\right)\alpha^{-\frac{1}{4}-\frac{n}{2}}\,\mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4}\,\pi^{1/4}}$$

And notably, this says the *odd-degree* contribution vanishes, giving us

$$\int \phi(x_k, 0, \alpha)\, x_k{}^{p_k} = \begin{cases} \left(\frac{2\,\alpha^{-(2\,p_k+1)}}{\pi}\right)^{1/4} \Gamma\!\left(\frac{p_k+1}{2}\right) & p_k \text{ even} \\ 0 & \text{else} \end{cases}$$

and then for even order terms we have

$$\Gamma\!\left(\frac{p_k+1}{2}\right) = \frac{\sqrt{\pi}}{2^{p_k/2}} \prod_{m=1}^{p_k/2} (2m-1)$$

giving us, for even p_k,

$$\begin{aligned}\int \phi(x_k, 0, \alpha)\, x_k{}^{p_k} &= \left(\frac{2\,\alpha^{-(2\,p_k+1)}}{\pi}\right)^{1/4} \frac{\sqrt{\pi}}{2^{p_k/2}} \prod_{m=1}^{p_k/2} (2m-1) \\ &= \frac{1}{\sqrt{2^{p_k/2}\,\alpha^{p_k/2}}} \left(\frac{2\,\pi}{\alpha}\right)^{1/4} \prod_{m=1}^{p_k/2} (2m-1)\end{aligned}$$

which we can also make proportional to contribution from the overlap, $S_{ij}^{(k)} = (2\,\pi/\alpha)^{1/4}$

$$\int \phi(x_k, 0, \alpha)\, x_k{}^{p_k} = \frac{S_{ij}^{(k)}}{\sqrt{2^{p_k}\,\alpha^{p_k}}} \prod_{m=1}^{p_k/2} (2m-1)$$

Then expanding back out we get (for entirely even p_k w/ $\sum_k p_k = m$)

$$\begin{aligned}\int_{\mathbb{R}^N} \prod_{k=1}^{3N} \phi(x_k, 0, \alpha_i+\alpha_j)\, x_k{}^{p_k} &= \prod_{k=1}^{3N} \frac{S_{ij}^{(k)}}{\sqrt{2^{p_k}\,(\alpha_i+\alpha_j)_k{}^{p_k}}} \prod_{l=1}^{p_k/2} (2l-1) \\ &= \frac{S_{ij}}{\sqrt{2^m}} \prod_{k=1}^{3N} \frac{1}{(\alpha_i+\alpha_j)_k{}^{p_k/2}} \prod_{l=1}^{p_k/2} (2l-1)\end{aligned}$$

so finally

$$\int_{\mathbb{R}^N} V(\boldsymbol{x}) \prod_{k=1}^{3N} \phi\!\left(x_k, \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j}, \alpha_i+\alpha_j\right) d\boldsymbol{x} =$$

$$S_{ij}\sum_{m=0}^{M}\sum_{p\in P_E(m)}\frac{1}{W_p\,\sqrt{2^m}}\,\frac{\partial V(\zeta)}{\partial x_1^{p_1}\dots\partial x_{3N}^{p_{3N}}}\prod_{k=1}^{3N}\frac{1}{{(\alpha_i+\alpha_j)_k}^{p_k/2}}\prod_{l=1}^{p_k/2}(2l-1)$$

where we pick $P_E(m)$ to be the *entirely even* partitions of m

For a quadratic expansion this becomes

$$\begin{aligned}\xi^{(ij)} &= \frac{\alpha^{(i)}\,\xi_k^{(i)}+\alpha^{(j)}\,\xi_k^{(j)}}{\alpha^{(i)}+\alpha^{(j)}}\\ \alpha^{(ij)} &= \alpha^{(i)}+\alpha^{(j)}\\ V_{ij} &= S_{ij}\left(V\left(\boldsymbol{\xi}^{(ij)}\right)+\frac{1}{4}\sum_{k=1}^{3N}\frac{1}{\alpha_k^{(ij)}}\,\frac{\partial^2}{\partial x_k^2}\,V(\boldsymbol{\zeta})\right)\end{aligned}$$

Equivalence to Taylor Series

Integration of the Kinetic Energy (Non-Rotated)

We start with our multivariate Gaussian basis function centered around a point $\xi^{(i)}$

$$\varphi_i(\boldsymbol{x})=\prod_{j=1}^{3N}\phi\left(x_j,\,\xi_j^{(i)},\,\alpha_i\right)$$

the integral we then want to evaluate is

$$\begin{aligned}T_{ij} &= -\int_{\mathbb{R}^N}\varphi_i(\boldsymbol{x})\,\frac{\nabla^2}{2\boldsymbol{m}}\,\varphi_j(\boldsymbol{x})\,d\boldsymbol{x}\\ &= -\sum_k\frac{1}{2m_k}\int_{\mathbb{R}^N}\varphi_i(\boldsymbol{x})\,\frac{\partial}{\partial x_k}\,\varphi_j(\boldsymbol{x})\,d\boldsymbol{x}\end{aligned}$$

where we note that

$$\frac{\partial}{\partial x_k}\varphi_j(\boldsymbol{x}) = 2\,\alpha_k^{(j)}\left(2\,\alpha_k^{(j)}\left(x_k-\xi_k^{(j)}\right)^2-1\right)\,\varphi_j(\boldsymbol{x})$$

so we have

$$\begin{aligned}\xi^{(ij)} &= \frac{\alpha^{(i)}\,\xi_k^{(i)}+\alpha^{(j)}\,\xi_k^{(j)}}{\alpha^{(i)}+\alpha^{(j)}}\\ \alpha^{(ij)} &= \alpha^{(i)}+\alpha^{(j)}\end{aligned}$$

$$\begin{aligned}T_{ij} &= -\int_{\mathbb{R}^N}\varphi_i(\boldsymbol{x})\,\frac{\nabla^2}{2\boldsymbol{m}}\,\varphi_j(\boldsymbol{x})\,d\boldsymbol{x}\\ &= -\sum_k\frac{1}{2m_k}\int_{\mathbb{R}^N}2\,\alpha_k^{(j)}\left(2\,\alpha_k^{(j)}\left(x_k-\xi_k^{(j)}\right)^2-1\right)\phi_i(\boldsymbol{x})\,\phi_j(\boldsymbol{x})\,d\boldsymbol{x}\end{aligned}$$

$$=\sum_k \frac{1}{2m_k}\; W^{(ij)} \int_{\mathbb{R}^N} 2\,\alpha_k^{(j)}\left(1-2\,\alpha_k^{(j)}\left(x_k-\xi_k^{(j)}\right)^2\right)\phi^{(ij)}(\boldsymbol{x})\,d\boldsymbol{x}$$

Shifted Approach

We will now introduce the shift $\chi^{(ij)} = x - \xi^{(ij)}$, giving us

$$\alpha_k^{(j)}\left(1-2\,\alpha_k^{(j)}\left(x_k-\xi_k^{(j)}\right)^2\right) = \alpha_k^{(j)}\left(1-2\,\alpha_k^{(j)}\left(\chi^{(ij)} + \left(\xi_k^{(ij)} - \xi_k^{(j)}\right)\right)^2\right)$$

where

$$\begin{aligned}\xi^{(ij)} - \xi^{(j)} &= \frac{\alpha^{(i)}}{\alpha^{(i)} + \alpha^{(j)}}\left(\xi^{(i)} - \xi^{(j)}\right)\\ &=\frac{\alpha^{(i)}}{\alpha^{(ij)}}\;\Delta\xi^{(ij)}\end{aligned}$$

and so

$$\alpha^{(j)}\left(1-2\,\alpha^{(j)}\left(x-\xi^{(j)}\right)^2\right) = \alpha^{(j)} - 2\,\alpha^{(j)^2}\chi^{(ij)2} + 4\,\frac{\alpha^{(j)^2}\,\alpha^{(i)}}{\alpha^{(ij)}}\,\chi^{(ij)}\,\Delta\xi^{(ij)} - 2\left(\frac{\alpha^{(j)}\alpha^{(i)}}{\alpha^{(ij)}}\right)^2\Delta\xi^{(ij)^2}$$

Next we'll note that the linear term in $\chi^{(ij)}$ will vanish when integrating its product with $\phi^{(ij)}$, and so we are left with

$$\begin{aligned}T_{ij} &= \sum_k \frac{1}{m_k}\; W^{(ij)}\int_{\mathbb{R}^N}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\Delta\xi_k^{(ij)^2}\right)\phi^{(ij)}(\boldsymbol{x}) \;- 2\,\alpha^{(j)^2}\chi_k^{(ij)2}\,d\boldsymbol{x}\\ &= \sum_k \frac{1}{m_k} S_{ij}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\Delta\xi_k^{(ij)^2}\right) - 2\,\alpha_k^{(j)^2}\int_{\mathbb{R}^N}\chi_k^{(ij)2}\,\phi^{(ij)}(\boldsymbol{x})\,d\boldsymbol{x}\end{aligned}$$

where, as $\phi^{(ij)}(\boldsymbol{x})$ is really centered around $\chi_k^{(ij)}$ we get (from the portion on local expansions)

$$\int_{\mathbb{R}^N}\chi_k^{(ij)2}\,\phi^{(ij)}(\boldsymbol{x})\,d\boldsymbol{x} = \frac{S_{ij}}{2\,\alpha_k^{(ij)}}$$

giving us

$$\begin{aligned}T_{ij} &= S_{ij}\sum_k \frac{1}{m_k}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\Delta\xi_k^{(ij)^2}\right) - \frac{\alpha_k^{(j)^2}}{\alpha_k^{(ij)}}\\ &= S_{ij}\sum_k \frac{1}{m_k}\left(\frac{\alpha_k^{(j)}\,\alpha_k^{(ij)} - \alpha_k^{(j)^2}}{\alpha_k^{(ij)}} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\Delta\xi_k^{(ij)^2}\right)\\ &= S_{ij}\sum_k \frac{1}{m_k}\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(ij)}} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\Delta\xi_k^{(ij)^2}\right)\end{aligned}$$

$$= S_{ij} \sum_k \frac{1}{m_k} \frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(ij)}} \left(1 - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2}\right)$$

Direct Strategy

Rotated Basis

By supplying a full covariance matrix we can use everything developed by the statistics community in arbitrary dimensions. Given a covariance matrix Σ, which will be by default the diagonal matrix with $1/2\alpha_i$ as its values, we have

$$\phi(x,\, \xi,\, \Sigma) = N(\Sigma)\, e^{-\frac{1}{2}\left(\Sigma^{-1}\odot(x-\xi)^2\right)}$$

where

$$N(\Sigma) = \left(\pi^{-d}\det\left(\Sigma^{-1}\right)\right)^{1/4}$$

we'll note that we are off from the standard Gaussian normalization by a factor of $2^{-d/2}\, N(\Sigma)$

Then we have (from the Matrix Cookbook)

$$\phi(x,\, \xi_i,\, \Sigma_i)\, \phi\left(x,\, \xi_j,\, \Sigma_j\right) = W\left(\Sigma_i{+}\Sigma_j,\, \xi_i{-}\xi_j\right)\phi(x,\, \xi_c,\, \Sigma_c)$$

where

$$\begin{aligned} \Sigma_c^{-1} &= \Sigma_i^{-1}{+}\Sigma_j^{-1} \\ \xi_c &= \Sigma_c\left(\Sigma_i^{-1}\xi_i + \Sigma_j^{-1}\xi_j\right) \end{aligned}$$

plus we'll add in the helpful identity that

$$\begin{aligned} \left(\Sigma_i{+}\Sigma_j\right)^{-1} &= \left(\left(\Sigma_i^{-1}\right)^{-1}{+}\left(\Sigma_j^{-1}\right)^{-1}\right)^{-1} \\ &= \Sigma_i^{-1}\left(\Sigma_i^{-1}{+}\Sigma_j^{-1}\right)^{-1}\Sigma_j^{-1} \\ &= \Sigma_i^{-1}\,\Sigma_c\,\Sigma_j^{-1} \end{aligned}$$

and to figure out exactly what W must be, we first note that for standard Gaussians we would have

$$W_N = \frac{1}{\sqrt{2^d\,\pi^d\left|\Sigma_i{+}\Sigma_j\right|}}\; e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

but letting $\varphi^{(i)}$ be a properly normalized Gaussian,

$$\phi^{(i)} = \frac{1}{2^{-d/2}\, N\left(\Sigma^{(i)}\right)}\,\varphi^{(i)}$$

so we have

$$
\begin{aligned}
\phi(x,\,\xi_i,\,\Sigma_i)\,\phi\big(x,\,\xi_j,\,\Sigma_j\big) &= \frac{1}{2^{-d/2}\,N\big(\Sigma^{(i)}\big)}\,\frac{1}{2^{-d/2}\,N\big(\Sigma^{(j)}\big)}\,\varphi^{(i)}\,\varphi^{(j)} \\
&= \frac{1}{2^{-d}\,N\big(\Sigma^{(i)}\big)\,N\big(\Sigma^{(j)}\big)}\,W_N\,\varphi^{(c)} \\
&= \frac{2^{-d/2}\,N\big(\Sigma^{(c)}\big)}{2^{-d}\,N\big(\Sigma^{(i)}\big)\,N\big(\Sigma^{(j)}\big)}\,W_N\,\phi^{(c)} \\
&= \frac{2^{-d/2}\left(\pi^{-d}\det\big(\Sigma^{(c)-1}\big)\right)^{1/4}}{2^{-d}\left(\pi^{-d}\det\big(\Sigma^{(i)-1}\big)\right)^{1/4}\left(\pi^{-d}\det\big(\Sigma^{(j)-1}\big)\right)^{1/4}}\,W_N\,\phi^{(c)} \\
&= \frac{1}{2^{-d/2}\left(\pi^{-d}\det\big(\Sigma^{(i)-1}\,\Sigma^{(c)}\,\Sigma^{(j)-1}\big)\right)^{1/4}}\,W_N\,\phi^{(c)} \\
&= \frac{2^{d/2}\left(\pi^{d}\,\big|\Sigma_i+\Sigma_j\big|\right)^{1/4}}{\sqrt{2^d\,\pi^d\,\big|\Sigma_i+\Sigma_j\big|}}\,e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}\,\phi^{(c)} \\
&= N\big(\Sigma_i+\Sigma_j\big)\,e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}\,\phi^{(c)}
\end{aligned}
$$

giving us

$$
W\big(\Sigma_i+\Sigma_j,\,\xi_i-\xi_j\big) = N\big(\Sigma^{(i)}+\Sigma^{(j)}\big)\,e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}
$$

and as a final note, this can be made more useful by considering that

$$
\begin{aligned}
\det\Big(\big(\Sigma_i+\Sigma_j\big)^{-1}\Big) &= \det\big(\Sigma_i^{-1}\big)\det(\Sigma_c)\det\big(\Sigma_j^{-1}\big) \\
\Rightarrow \det(\Sigma_c) &= \frac{\det\Big(\big(\Sigma_i+\Sigma_j\big)^{-1}\Big)}{\det\big(\Sigma_i^{-1}\big)\det\big(\Sigma_j^{-1}\big)}
\end{aligned}
$$

And to confirm we're on the right track, we can note that in the case that Σ_i is diagonal with diagonal entries $1/2\alpha_k^{(i)}$ and similarly with Σ_j we get

$$
\begin{aligned}
W\big(\Sigma_i+\Sigma_j,\,\xi_i-\xi_j\big) &= \left(\frac{1}{\pi^d}\prod_k 2\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\right)\right)^{1/4}\prod_k \exp\!\left(-\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right) \\
&= \left(\frac{2}{\pi}\right)^{d/4}\prod_k\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\right)^{1/4}\exp\!\left(-\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right)
\end{aligned}
$$

which is of course our original expression.

Finally, by diagonalizing Σ_c^{-1} we can get a new set of normal effective modes and alphas, returning to a decoupled form, with $\alpha^{(c)} = \left(\Lambda^{(c)}\right)^{-1}\big/2$ for $\Lambda^{(c)}$ the vector of eigenvalues

Functional Form

Overlaps

Just for the heck of it,

$$N(\Sigma) = \left(\pi^{-d} \det\left(\Sigma^{-1}\right)\right)^{1/4}$$

$$\begin{aligned}
&\int_{\mathbb{R}^d} \phi(x,\, \xi_i,\, \Sigma_i)\, \phi\left(x,\, \xi_j,\, \Sigma_j\right) dx \\
&\quad = W\left(\Sigma_i+\Sigma_j,\, \xi_i-\xi_j\right) \int_{\mathbb{R}^d} \phi(x,\, \xi_c,\, \Sigma_c)\, dx \\
&\quad = \frac{N\left(\Sigma^{(i)}+\Sigma^{(i)}\right)}{2^{-d/2}\, N\left(\Sigma^{(c)}\right)}\; e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \odot\left(\xi_i-\xi_j\right)^2\right)} \\
&\quad = 2^{d/2} \left(\frac{\left|\Sigma^{(c)}\right|}{\left|\Sigma^{(i)}+\Sigma^{(j)}\right|}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \odot\left(\xi_i-\xi_j\right)^2\right)} \\
&\quad = 2^{d/2} \left(\frac{\left|\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\right|^2}{\left|\Sigma^{(i)}\right| \left|\Sigma^{(j)}\right|}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \odot\left(\xi_i-\xi_j\right)^2\right)} \\
&\quad = 2^{d/2} \left(\frac{\left|\Sigma^{(i)-1}\right| \left|\Sigma^{(j)-1}\right|}{\left|\Sigma^{(c)-1}\right|^2}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \odot\left(\xi_i-\xi_j\right)^2\right)}
\end{aligned}$$

and then just to confirm that this makes sense, in the case that Σ_i and Σ_j are diagonal with $1/2\, \alpha_k^{(i)}$ we get

$$2^{d/2} \left(\frac{\left|\Sigma^{(i)-1}\right| \left|\Sigma^{(j)-1}\right|}{\left|\Sigma^{(c)-1}\right|^2}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1} \odot\left(\xi_i-\xi_j\right)^2\right)} =$$

$$2^{d/2} \prod_k \left(\frac{\alpha_k^{(i)}\, \alpha_k^{(j)}}{\left(\alpha_k^{(i)}+\alpha_k^{(j)}\right)^2}\right)^{1/4} \exp\left(-\frac{\alpha_k^{(i)}\, \alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}} \left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right)$$

which ends up being the correct result

Tests

Kinetic Energy

Shifted Approach

As in the direct approach we note that

$$T_{ij}=-\frac{1}{2}\ W\left(\Sigma_i+\Sigma_j,\ \xi_i-\xi_j\right)\int_{\mathbb{R}^d}\phi(x,\ \xi_c,\ \Sigma_c)\ \mathrm{Tr}\left(M^{-1}\,\mathcal{T}_j\right)dx$$

where

$$\mathcal{T}_j = \left(\nabla_x\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\right)^2 - \nabla_{x^2}\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)$$

then we'll note that

$$\Sigma_j^{-1} = \Sigma_c^{-1} - \Sigma_i^{-1}$$

and as before we'll write

$$x = x - \xi_c + \xi_c$$

which admittedly seems unhelpful, but we'll plow on, noting

$$\begin{aligned}
\xi_c &= \Sigma_c\left(\Sigma_i{}^{-1}\xi_i + \Sigma_j{}^{-1}\xi_j\right)\\
\xi_j &= \Sigma_c\left(\Sigma_c{}^{-1}\ \xi_j\right)\\
&= \Sigma_c\left(\Sigma_i{}^{-1}\xi_j + \Sigma_j{}^{-1}\xi_j\right)\\
\Rightarrow \xi_c-\xi_j &= \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)
\end{aligned}$$

So then when we have

$$\begin{aligned}
\nabla_x\left(\frac{1}{2}\ \Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right) &= \Sigma_j^{-1}\left(x-\xi_j\right)\\
\nabla_{x^2}\left(\frac{1}{2}\ \Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right) &= \Sigma_j^{-1}\\
\nabla_x\left(\frac{1}{2}\ \Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)^2 &= \left(\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\right)
\end{aligned}$$

we can replace $x-\xi_j$ with $x-\xi_c$

$$\Sigma_j^{-1}\left(x-\xi_c+\xi_c-\xi_j\right) = \Sigma_j^{-1}(x-\xi_c) + \Sigma_j^{-1}\ \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)$$

and so

$$\begin{aligned}
\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right] &= \left[\Sigma_j^{-1}(x-\xi_c)\right]\otimes\left[\Sigma_j^{-1}(x-\xi_c)\right]\\
&\quad+\ \left[\Sigma_j^{-1}\ \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\ \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\\
&\quad+\text{ linear terms}
\end{aligned}$$

Therefore we have

$$\begin{aligned}
\mathcal{T}_j &= \left(\nabla_x\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\right)^2 - \nabla_{x^2}\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\\
&= \left[\Sigma_j^{-1}(x-\xi_c)\right]\otimes\left[\Sigma_j^{-1}(x-\xi_c)\right]\\
&\quad+\left[\Sigma_j^{-1}\ \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\ \Sigma_c\ \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right] - \Sigma_j^{-1}\\
&\quad+\text{ linear terms}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_n \left[\Sigma_j^{-1}(x-\xi_c)\right]_n^2 \\
&\quad + \left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right]\otimes\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right] - \Sigma_j^{-1} \\
&\quad + \text{linear terms}
\end{aligned}
$$

Next so we can actually integrate, we'll make the substitution

$$q = L(x-\xi_c)$$

where L diagonalizes Σ_c, i.e.

$$L\,\Sigma_c^{-1}\,L^T = A_c$$

and so

$$L\,\Sigma_i^{-1}\,L^T + L\,\Sigma_j^{-1}\,L^T = A_c$$

Putting this together,

$$\Sigma_j^{-1}(x-\xi_c) = \Sigma_j^{-1}\,L^T q$$

Giving us

$$
\begin{aligned}
\mathcal{T}_j &= \sum_n \left[\Sigma_j^{-1}\,L^T q\right]_n^2 \\
&\quad + \left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right]\otimes\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right] - \Sigma_j^{-1} \\
&\quad + \text{linear terms}
\end{aligned}
$$

and when we evaluate the proper Laplacian we have

$$\mathrm{Tr}\big(M^{-1}\,\mathcal{T}_j\big) = \sum_n \frac{1}{m_n}\Big[\ \left[\Sigma_j^{-1}\,L^T q\right]_n^2 + \left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right]_n^2 - \Sigma_j^{-1}{}_{nn}\ \Big]$$

This is again, not manifestly symmetric, but we'll consider the integration here where since the linear terms vanish we get

$$\int\left[\Sigma_j^{-1}\,L^T q\right]_n^2 \phi_c(q) = S^{(c)} \sum_k \frac{\big(\Sigma_j^{-1}\,L^T\big)_{nk}^2}{\alpha_k^{(c)}}$$

so in total we have

$$\int_{\mathbb{R}^d}\phi(x,\,\xi_c,\,\Sigma_c)\,\mathrm{Tr}\big(M^{-1}\,\mathcal{T}_j\big)\,dx = \sum_n \frac{1}{m_n}\Big[\ \sum_k \frac{\big(\Sigma_j^{-1}\,L^T\big)_{nk}^2}{\alpha_k^{(c)}} + \left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\big(\xi_i-\xi_j\big)\right]_n^2 - \Sigma_j^{-1}{}_{nn}\Big]$$

and now I have to do some gymnastics to figure out how everything cancels, in particular I guess I have something like

$$\sum_k \frac{\big(\Sigma_j^{-1}\,L^T\big)_{nk}^2}{\alpha_k^{(c)}} = \big(\Sigma_j^{-1}\big)_{n:}\,\big(L^T\,A_c^{-1}\,L\big)\,\big(\Sigma_j^{-1}\big)_{:n}$$

$$= \left(\Sigma_j^{-1}\right)_{n:} \Sigma_c \left(\Sigma_j^{-1}\right)_{:n}$$
$$= \left(\Sigma_j^{-1}\right)_{n:} \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} \left(\Sigma_j^{-1}\right)_{:n}$$

Next we'll use the Woodbury identity to write

$$\begin{aligned}\left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} &= \left(L^{(i)} A_i L^{(i)T}+\Sigma_j^{-1}\right)^{-1} \\ &= \Sigma_j - \Sigma_j L^{(i)}\left(A_i^{-1} + L^{(i)T} \Sigma_j L^{(i)}\right)^{-1} L^{(i)T} \Sigma_j\end{aligned}$$

which seems nasty, but we'll note that

$$\begin{aligned}A_i^{-1} + L^{(i)} \Sigma_j L^{(i)T} &= L^{(i)T} \Sigma_i L^{(i)} + L^{(i)T} \Sigma_j L^{(i)} \\ &= L^{(i)T}\left(\Sigma_i+\Sigma_j\right) L^{(i)} \\ \left(L^{(i)T}\left(\Sigma_i+\Sigma_j\right) L^{(i)}\right)^{-1} &= L^{(i)T}\left(\Sigma_i+\Sigma_j\right)^{-1} L^{(i)}\end{aligned}$$

and so

$$\Sigma_c = \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} = \Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1} \Sigma_j$$

Then,

$$\begin{aligned}\left(\Sigma_j^{-1}\right)_{n:} \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} \left(\Sigma_j^{-1}\right)_{:n} &= \left(\Sigma_j^{-1}\right)_{n:} \left(\Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1} \Sigma_j\right) \left(\Sigma_j^{-1}\right)_{:n} \\ &= \left(\Sigma_j^{-1}\right)_{n:} \delta_{:n} - \delta_{n:}\left(\Sigma_i+\Sigma_j\right)^{-1} \delta_{:n} \\ &= \left(\Sigma_j^{-1}\right)_{nn} - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\end{aligned}$$

so in total

$$T_{ij} = S_{ij} \sum_n \frac{1}{m_n}\left[\left[\Sigma_j^{-1} \Sigma_c \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]_n^2 - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\right]$$

Finally, we'll consider

$$\begin{aligned}\Sigma_j^{-1} \Sigma_c \Sigma_i{}^{-1} &= \Sigma_j^{-1}\left(\Sigma_i{}^{-1}+\Sigma_j{}^{-1}\right)^{-1} \Sigma_i{}^{-1} \\ &= \left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\end{aligned}$$

which is clearly symmetric

Therefore, we know that once and for all, T is symmetric with

$$T_{ij} = -\frac{1}{2} S_{ij} \sum_n \frac{1}{m_n}\left[\left[\Sigma_j^{-1} \Sigma_c \Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]_n^2 - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\right]$$

and to confirm for the diagonal case, we have

$$T_{ij} = S_{ij} \sum_k \frac{1}{m_k} \frac{\alpha_k^{(i)} \alpha_k^{(j)}}{\alpha_k^{(ij)}} \left(1 - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2}\right)$$

$$= -\frac{1}{2}\, S_{ij} \sum_k \frac{1}{m_k}\, 2\, \frac{\alpha_k^{(i)}\, \alpha_k^{(j)}}{\alpha_k^{(ij)}} \left(2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2} - 1\right)$$

where

$$\begin{aligned}
\left(\Sigma_i{+}\Sigma_j\right)^{-1} &= 2\left(\frac{1}{\alpha^{(i)}}+\frac{1}{\alpha^{(j)}}\right)^{-1} \\
&= 2\,\frac{\alpha^{(i)}\,\alpha^{(j)}}{\alpha^{(i)}{+}\alpha^{(j)}} \\
&= \Sigma_j^{-1}\,\Sigma_c\,\Sigma_i^{-1}
\end{aligned}$$

Tests

Misc Old Shit

Direct Approach

Alternate Formulation

Potential Energy

We're able to use everything from before, not even needing to rotate the derivatives. To confirm this, we'll consider our integral

$$V_{ij} = W\!\left(\Sigma_i{+}\Sigma_j,\, \xi_i{-}\xi_j\right) \int_{\mathbb{R}^N} V(\boldsymbol{x})\; \phi(x,\, \xi_c,\, \Sigma_c)\, d\boldsymbol{x}$$

where we'll expand $V(\boldsymbol{x})$ as

$$V(\boldsymbol{x}) = \sum_{m=0}^{M} \frac{1}{W}\; \nabla_{X^m} V(\boldsymbol{\zeta}) \odot (x{-}\zeta)^m$$

so giving us

$$\int_{\mathbb{R}^N} V(\boldsymbol{x})\; \phi(x,\, \xi_c,\, \Sigma_c)\, d\boldsymbol{x} = \sum_{m=0}^{M} \int_{\mathbb{R}^N} \frac{1}{W}\; \nabla_{X^m} V(\boldsymbol{\zeta}) \odot (x{-}\zeta)^m\; \phi(x,\, \xi_c,\, \Sigma_c)\, d\boldsymbol{x}$$

where for simplicity we'll first shift by ζ to give

$$\int_{\mathbb{R}^N} V(\boldsymbol{x})\; \phi(x,\, \xi_c,\, \Sigma_c)\, d\boldsymbol{x} = \sum_{m=0}^{M} \int_{\mathbb{R}^N} \frac{1}{W}\; \nabla_{X^m} V(\boldsymbol{\zeta}) \odot (x)^m\; \phi(x,\, \xi_c{-}\zeta,\, \Sigma_c)\, d\boldsymbol{x}$$

then by applying L_c as our change of basis, we get up with

$$\int_{\mathbb{R}^N} \frac{1}{W}\; \nabla_{X^m} V(\zeta) \odot (x)^m\; \phi(x,\, \xi_c{-}\zeta,\, \Sigma_c)\, d\boldsymbol{x} =$$

$$= \int_{\mathbb{R}^N} \frac{1}{W} \nabla_{Q^m} V(\boldsymbol{\zeta}) \odot (q)^m \; \phi(q, \; L_c(\xi_c - \zeta), \; \Lambda_c) \, d\boldsymbol{q}$$

which can be evaluated using what we did previously after recognizing that we have a linear transformation between $\boldsymbol{q}$ and $\boldsymbol{x}$ and so

$$\nabla_{Q^m} V(\boldsymbol{\zeta}) = L_c \langle 2, \; m\rangle (L_c \langle 2, \; m\rangle (\ldots (L_c \langle 2, \; m\rangle \nabla_{X^m} V(\boldsymbol{\zeta}))))$$

which is equivalent to just rotating the derivatives as claimed previously

---

Internal Coordinates

We likely will want to work in internals at some point, for which we have

$$H = pGp + V(r) + V'(r)$$

The integrals induced by G and V' now require some thought

Considering just one matrix element, we get

$$\langle \phi_i | \; T \; | \phi_j \rangle = \sum_{a,b} \langle \phi_i | \; p_a G_{ab} p_b \; | \phi_j \rangle$$

$$\langle \phi_i | \; p_a G_{ab} p_b \; | \phi_j \rangle = \int G_{ab}(r) \, \phi_i(r) \, p_a p_b \; \phi_j(r)$$

where we have assumed the internal coordinates live on the $[-\infty, \infty]$ range, ignoring the considerations given in Section IV of Frederick and Woywood

Such integrals are very difficult to handle generically, but we can approximate them by again doing local expansions of the G and V' terms

Rotations

It is straightforward to use the ideas developed previously for a rotated basis in this context, as these are all just polynomial and polynomial-product integrals.

Watson Coordinates

An alternative to proper internal coordinates is to use a rotated Cartesian-displacement normal mode coordinates. To start, we'll note that these coordinates can be expressed as

$$q_i = \sum_n L_{in} \Delta x_n$$

and their overlaps may be computed just like any Gaussian product basis

The difficulty arises in integrating the kinetic energy, where we have

$$T = P^2 + \frac{1}{2}\sum_{\alpha} I_{\alpha}^{-1}\, {p_{\alpha}}^2$$

for

$$p_{\alpha} = \sum_{r,s} \zeta_{rs}^{\alpha}(Q_r P_s - Q_s P_r)$$

where

$$\zeta_{rs}^{\alpha} = (-1)^{\beta} \sum_{k} L_{r\ (k,\beta)}\, L_{s\ (k,\gamma)} - L_{r\ (k,\gamma)}\, L_{s\ (k,\beta)}$$

for the cyclic permutations $\beta = \alpha{+}1 \bmod 3$, $\gamma = \alpha{+}2 \bmod 3$

This is clearly coming from the a cross-product like term (this is classically expressed with the Levi Cevita symbol), which is basically just a generator of rotation

Notably,

$$\begin{aligned} \zeta_{sr}^{\alpha} &= -\zeta_{rs}^{\alpha} \\ \zeta_{rr}^{\alpha} &= 0 \end{aligned}$$

This gives us

$$T = P^2 + \frac{1}{2}\sum_{i,j,k,l}\sum_{\alpha} I_{\alpha}^{-1}\, \zeta_{ij}^{\alpha}\, \zeta_{kl}^{\alpha}\, Q_i P_j\, Q_k P_l$$

We will note that under our approximation, L is *definitional*, which is to say our choice of L will not change no matter what value of Q we choose. Therefore

$$\left\langle \phi_n \right| I_{\alpha}^{-1}\, \zeta_{ij}^{\alpha}\, \zeta_{kl}^{\alpha}\, Q_i P_j\, Q_k P_l \left| \phi_m \right\rangle = \zeta_{ij}^{\alpha}\, \zeta_{kl}^{\alpha} \left\langle \phi_n \right| I_{\alpha}^{-1}\, Q_i P_j\, Q_k P_l \left| \phi_m \right\rangle$$

and then for simplicity, we will also assume I_{α}^{-1} is independent of Q, although this is simply an approximation (I think)

This gives us a 4D tensor described by

$$Q\,P\,Q\,P \left| \phi_j \right\rangle = K_j(q) \left| \phi_j \right\rangle$$

which we then element-wise multiply into

$$Z = \sum_{\alpha} I_{\alpha}^{-1} (\zeta^{\alpha} \otimes \zeta^{\alpha})$$

and then we can integrate the tensor expansion induced by $Z \circ K_j$

Tests

Symmetry Proof

But maybe we want to see that we truly get a symmetric form out of K_j after we integrate?

Computer Assisted Expressions

Hand Simplification: Case 0

In[4409]:=

```
niceExpr // pruneLinear[#, Q[ξ[c]]] & // watFmt /@ #[0] & // Column
```

Out[4409]=

$$-\left(\xi^{(c)} \otimes \mathrm{TQ}\left[\left(\xi^{(c)} \otimes \Sigma^{(j)^{-1}}\right),\ 2 \to 1\right]\right)$$
$$\xi^{(c)} \otimes \mathrm{I} \otimes \Sigma^{(d)} \Delta$$
$$\xi^{(c)} \otimes \Sigma^{(d)} \Delta \otimes \xi^{(c)} \otimes \Sigma^{(d)} \Delta$$

Annoyingly, all of these terms survive, although we *can* write

$$\Sigma^{(j)^{-1}} = \sum_s 2\, \alpha_s^{(j)}\, L_s^{(j)} \otimes L_s^{(j)}$$

to get the first term to become

$$\sum_s 2\, \alpha_s^{(j)}\, \xi^{(c)} \otimes L_s^{(j)} \otimes \xi^{(c)} \otimes L_s^{(j)}$$

we can do the same trick with the second one if we want, too giving us

$$\sum_s \xi^{(c)} \otimes e_s \otimes e_s \otimes \left(\Sigma^{(d)}\, \Delta^{(i,j)}\right)$$

Term Expressions

Old Pretranspose Note ;____;

Old Tests

Hand Simplification: Case 2

Base Expressions

Integration

We can integrate any term of the form

$$L^{(1)}\, Q^{(c)} \otimes A \otimes L^{(2)}\, Q^{(c)} \otimes B$$

by doing the classic rotation (see old integration attempt)

$$R = L Q^{(c)}$$

giving us

$$L^{(1)}\, L^T R \otimes A \otimes L^{(2)} L^T R \otimes B$$

and since only the even order terms contribute we can consider that end up with integrals of the form

$$\int \left(L^{(1)}\, L^T R\right)_i \left(L^{(2)} L^T R\right)_k A_j\, B_l = \int A_j\, B_l \left(\left(L^{(1)}\, L^T\right)_i \otimes \left(L^{(2)}\, L^T\right)_k\right) \odot R^2$$
$$= S^{(c)}\, A_j\, B_l \sum_s \frac{\left(\left(L^{(1)}\, L^T\right)_i \otimes \left(L^{(2)}\, L^T\right)_k\right)_{ss}}{2\, \alpha_s^{(c)}}$$

and generically we can write this as

$$\begin{aligned}
\sum_s \frac{\left(\left(L^{(1)}\, L^T\right)_i \otimes \left(L^{(2)}\, L^T\right)_j\right)_{ss}}{2\, \alpha_s^{(c)}} &= \sum_s \left(L^{(1)}\, L^T\right)_{is} \left(A^{(c)}\right)_{ss} \left(L^{(2)}\, L^T\right)_{js} \\
&= \sum_s \left(L^{(1)}\, L^T\right)_{is} \left(A^{(c)}\right)_{ss} \left(L^{(2)}\, L^T\right)^T{}_{sj} \\
&= \sum_{u,v} \sum_s \left(L^{(1)}\right)_{iu} L^T{}_{us} \left(A^{(c)}\right)_{ss} (L)_{sv} \left(L^{(2)}\right)_{vj} \\
&= \left(L^{(1)}\, \Sigma^{(c)}\, L^{(2)}\right)_{ij}
\end{aligned}$$

$$\left\langle \phi_n \right| I_\alpha^{-1} (\zeta^\alpha \otimes \zeta^\alpha) \left(L^{(1)}\, Q^{(c)} \otimes A \otimes L^{(2)} Q^{(c)} \otimes B\right) \left| \phi_m \right\rangle =$$
$$S^{(c)} \sum_{ijkl} I_\alpha^{-1} (\zeta^\alpha \otimes \zeta^\alpha)_{ijkl}\, A_j\, B_l \left(L^{(1)}\, \Sigma^{(c)}\, L^{(2)}\right)_{ik}$$

and obviously there was nothing special about the way we ordered the A and B so this works generically, giving us a quadratic contributions that looks like

Term 1:

$$\begin{aligned}
-\sum_s 2\, \alpha_s^{(j)}\, Q^{(c)} \otimes L_s^{(j)} \otimes Q^{(c)} \otimes L_s^{(j)} &= -\sum_{numv} \zeta_{nu}^\alpha\, \zeta_{mv}^\alpha \sum_s 2\, \alpha_s^{(j)} \left(L_s^{(j)}{}_u\, L_s^{(j)}{}_v\right) \left(\Sigma^{(c)}\right)_{nm} \\
&= -\sum_{numv} \zeta_{nu}^\alpha\, \zeta_{mv}^\alpha \left(\Sigma^{(c)}\right)_{nm} \sum_s 2\, \alpha_s^{(j)} \left(L_s^{(j)}{}_u\, L_s^{(j)}{}_v\right) \\
&= -\sum_{numv} \zeta_{nu}^\alpha\, \zeta_{mv}^\alpha \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}$$

Term 2:

$$\begin{aligned}
-\sum_s Q^{(c)} \otimes e_s \otimes e_s \otimes \left(\Sigma^{(j)^{-1}}\, Q^{(c)}\right) &= -\sum_{numv} \zeta_{nu}^\alpha\, \zeta_{mv}^\alpha \sum_s (e_s)_u\, (e_s)_m \left(\Sigma^{(c)}\, \Sigma^{(j)^{-1}}\right)_{nv} \\
&= -\sum_{nmv} \zeta_{nm}^\alpha\, \zeta_{mv}^\alpha\, \delta_{um} \left(\Sigma^{(c)}\, \Sigma^{(j)^{-1}}\right)_{nv}
\end{aligned}$$

Term 3:

$$Q^{(c)} \otimes \Sigma^{(d)}\, \Delta^{(i,j)} \otimes Q^{(c)} \otimes \Sigma^{(d)}\, \Delta^{(i,j)} = \sum_{numv} \zeta_{nu}^\alpha\, \zeta_{mv}^\alpha \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(d)}\, \Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\, \Delta^{(i,j)}\right)_v$$

Term(s) 4:

$$-2\left((Q-\xi^{(c)})\otimes\Sigma^{(d)}\Delta\otimes\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}(Q-\xi^{(c)})\right)$$

$$Q^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)}\otimes\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}\,Q^{(c)} = -2\sum_{numv}\zeta^{\alpha}_{nu}\,\zeta^{\alpha}_{mv}\left(\Sigma^{(c)}\,{\Sigma^{(j)}}^{-1}\right)_{nv}\left(\xi^{(c)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m}$$

$$Q^{(c)}\otimes{\Sigma^{(j)}}^{-1}\,Q^{(c)}\otimes\xi^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)} = -2\sum_{numv}\zeta^{\alpha}_{nv}\,\zeta^{\alpha}_{mu}\left(\Sigma^{(c)}\,{\Sigma^{(j)}}^{-1}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m}$$

Term 5:

$$\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}(Q-\xi^{(c)})\otimes\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}(Q-\xi^{(c)})$$

$$\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}\,Q^{(c)}\otimes\xi^{(c)}\otimes{\Sigma^{(j)}}^{-1}\,Q^{(c)} = \sum_{numv}\zeta^{\alpha}_{nu}\,\zeta^{\alpha}_{mv}\left({\Sigma^{(j)}}^{-1}\Sigma^{(c)}\,{\Sigma^{(j)}}^{-1}\right)_{uv}(\xi^{c})_{n}\,(\xi^{c})_{m}$$
$$= \sum_{numv}\zeta^{\alpha}_{nu}\,\zeta^{\alpha}_{mv}\left({\Sigma^{(j)}}^{-1}\Sigma^{(c)}\,{\Sigma^{(j)}}^{-1}\right)_{nm}(\xi^{c})_{u}\,(\xi^{c})_{v}$$

Integral Test

Sad Tests

Old Pretranspose Note ;_____;

Old Tests

Hand Simplification: Case 4

In[4269]:=

```
niceExpr // pruneLinear[#, Q[ξ[c]]] & // watFmt /@ #[4] & // Column
```

Out[4269]=

$$(\mathrm{Q}-\xi^{(\mathrm{c})})\otimes{\Sigma^{(\mathrm{j})}}^{-1}(\mathrm{Q}-\xi^{(\mathrm{c})})\otimes(\mathrm{Q}-\xi^{(\mathrm{c})})\otimes{\Sigma^{(\mathrm{j})}}^{-1}(\mathrm{Q}-\xi^{(\mathrm{c})})$$

Integration

In[3475]:=

$$\left(\frac{\left(1+(-1)^{n}\right)\alpha^{-\frac{1}{4}-\frac{n}{2}}\,\mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4}\,\pi^{1/4}}\;/.\;n\to 4\right)\Big/\left(\frac{\left(1+(-1)^{n}\right)\alpha^{-\frac{1}{4}-\frac{n}{2}}\,\mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4}\,\pi^{1/4}}\;/.\;n\to 0\right)$$

Out[3475]=

$$\frac{3}{4\,\alpha^{2}}$$

This will be somewhat tedious, but we have

$$L^{(1)}\,L^{T}R\;\otimes L^{(2)}\,L^{T}R\otimes L^{(3)}L^{T}R\otimes L^{(4)}L^{T}R$$

and since only the even order terms contribute we can consider that writing

$$\int\left(L^{(1)}\,L^{T}R\right)_{i}\left(L^{(2)}L^{T}R\right)_{j}\left(L^{(3)}\,L^{T}R\right)_{k}\left(L^{(4)}L^{T}R\right)_{l}$$

$$= \int\Big(\big(L^{(1)}\,L^T\big)_i \otimes \big(L^{(2)}\,L^T\big)_j \otimes \big(L^{(3)}\,L^T\big)_k \otimes \big(L^{(4)}\,L^T\big)_l\Big) \odot R^4$$

$$= S^{(c)}\,3\sum_s \frac{\Big(\big(L^{(1)}\,L^T\big)_i \otimes \big(L^{(2)}\,L^T\big)_j \otimes \big(L^{(3)}\,L^T\big)_k \otimes \big(L^{(4)}\,L^T\big)_l\Big)_{ssss}}{4\,\alpha_s^{(c)}} + \text{quadratics}$$

and now

$$\begin{aligned}
\sum_s \frac{([\text{see above}])_{ss}}{4\,\alpha_s^{(c)}} &= \sum_s \big(L^{(1)}\,L^T\big)_{is}\big(A^{(c)}\big)_{ss}\big(L^{(2)}\,L^T\big)_{js}\big(L^{(3)}\,L^T\big)_{ks}\big(A^{(c)}\big)_{ss}\big(L^{(4)}\,L^T\big)_{ls}\\
&= \sum_s \big(L^{(1)}\,L^T\big)_{is}\big(A^{(c)}\big)_{ss}\big(L^{(2)}\,L^T\big)^T{}_{sj}\big(L^{(3)}\,L^T\big)_{ks}\big(A^{(c)}\big)_{ss}\big(L^{(4)}\,L^T\big)^T{}_{sl}\\
&= \big(L^{(1)}\,\Sigma^{(c)}\,L^{(2)}\big)_{ij}\big(L^{(3)}\,\Sigma^{(c)}\,L^{(4)}\big)_{kl}
\end{aligned}$$

and accounting for the quadratic products we have have to take all the different possible permutations of $(s,\ s,\ t,\ t)$ to get terms like

$$\big(L^{(1)}\,L^T R\big)_{is}\big(L^{(2)}L^T R\big)_{js}\big(L^{(3)}\,L^T R\big)_{kt}\big(L^{(4)}L^T R\big)_{lt}$$

which means we will get

$$\begin{aligned}
\sum_s \sum_{t\neq s} &\frac{\big(L^{(1)}\,L^T R\big)_{is}\big(L^{(2)}L^T R\big)_{js}\big(L^{(3)}\,L^T R\big)_{kt}\big(L^{(4)}L^T R\big)_{lt}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}}\\
&+\frac{\big(L^{(1)}\,L^T R\big)_{is}\big(L^{(2)}L^T R\big)_{jt}\big(L^{(3)}\,L^T R\big)_{ks}\big(L^{(4)}L^T R\big)_{lt}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}}\\
&+\frac{\big(L^{(1)}\,L^T R\big)_{is}\big(L^{(2)}L^T R\big)_{jt}\big(L^{(3)}\,L^T R\big)_{kt}\big(L^{(4)}L^T R\big)_{ls}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}}
\end{aligned}$$

which is unfortunate because we need the $t{=}s$ term to simplify, but then we can realize that we can actually add it in since *from above* the quartic term just pops in a 3!

and each of these will reduce to give us a form like and so in total we have

$$\begin{aligned}
\int\big(L^{(1)}\,L^T R\big)_i\big(L^{(2)}L^T R\big)_j\big(L^{(3)}\,L^T R\big)_k\big(L^{(4)}L^T R\big)_l &= \big(L^{(1)}\Sigma^{(c)}\,L^{(2)}\big)_{ij}\big(L^{(3)}\,\Sigma^{(c)}\,L^{(4)}\big)_{kl}\\
&+ \big(L^{(1)}\Sigma^{(c)}\,L^{(3)}\big)_{ik}\big(L^{(2)}\,\Sigma^{(c)}\,L^{(4)}\big)_{jl}\\
&+ \big(L^{(1)}\Sigma^{(c)}\,L^{(4)}\big)_{il}\big(L^{(2)}\,\Sigma^{(c)}\,L^{(3)}\big)_{jk}
\end{aligned}$$

Test

Term

giving us

$$Q^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} \otimes Q^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} \to= \sum_{numv} \zeta^{\alpha}_{nu} \zeta^{\alpha}_{mv} ($$

$$\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nu} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mv}$$
$$+ \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{uv}$$
$$+ \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)}\right)_{um}$$
$$)$$

which we can contract further by noting that (by symmetry)

$$\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)}\right)_{um} = \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mu}$$

giving us

$$Q^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} \otimes Q^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} \to= \sum_{numv} \zeta^{\alpha}_{nu} \zeta^{\alpha}_{mv} ($$

$$\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nu} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mv}$$
$$+ \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mu}$$
$$+ \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{uv}$$
$$)$$

Sad Tests

Old Pretranspose Note ;____;

Adding all terms

Setup

Our total term list is

$$.=-\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\right)_{uv}$$
$$.= \delta_{um}\left(\xi^{(c)}\right)_n \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_v$$
$$.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_u \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_v$$
$$.= -\left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\right)_{uv}$$
$$.= -\delta_{um}\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv}$$
$$.= \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_u \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_v$$
$$.= \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nm} (\xi^{c})_u (\xi^{c})_v$$
$$.= -2\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\xi^{(c)}\right)_u \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_m$$
$$.= -2\left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nu} \left(\xi^{(c)}\right)_v \left(\Sigma^{(d)} \Delta^{(i,j)}\right)_m$$
$$.= \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nu} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mv} + \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{mu} + \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{uv}$$

Test

Simplification

Now we'll collect everything with two ξ terms,

$$\begin{aligned}
&.= -\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\right)_{uv} \\
&.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v \\
&.= \left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nm} \left(\xi^{c}\right)_u \left(\xi^{c}\right)_v
\end{aligned}$$

and we'll swap $u\to m$ and $n\to v$ (two flips $\Rightarrow$ no sign change) to get

$$\begin{aligned}
&.= -\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\right)_{uv} \\
&.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v \\
&.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}$$

Now we note that by the Woodbury identity

$$\Sigma_c = \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} = \Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1}\Sigma_j$$

so

$$\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma_j - \left(\Sigma_i+\Sigma_j\right)^{-1}$$

and so we get

$$\left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(j)^{-1}}\right)_{uv} = -\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

and in total we have

$$\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

which is clearly symmetric with respect to index interchange

We get to do the same simplification with the terms

$$\begin{aligned}
&.= -\left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\right)_{uv} \\
&.= \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v \\
&.= \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}$$

giving us

$$\left(\Sigma^{(c)}\right)_{nm} \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

and so this whole block becomes

$$\left(\Sigma^{(c)} + \xi^{(c)}\otimes\xi^{(c)}\right)_{nm} \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv} \tag{1}$$

Through experimentation we also find the following are symmetric when added up

$$
\begin{aligned}
.&= -\delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} \\
.&= \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} \\
.&= \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu}
\end{aligned}
$$

It is initially strange that this works, but perhaps we try an initial condensation

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu} - \delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} = \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - I\right)_{mu}$$

and we'll recall that we can write

$$\Sigma^{(c)-1} = \Sigma^{(i)-1} + \Sigma^{(j)^{-1}}$$

$$\alpha^{(c)} = \alpha^{(i)} + \alpha^{(j)}$$

$$\Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma^{(c)}\left(\Sigma^{(c)-1} - \Sigma^{(i)-1}\right)$$

so we get

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - I\right)_{mu} = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mu}$$

which is clearly symmetric once we add up every term

And similarly

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} = \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(I - \Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}$$

which isn't an issue for the very, very subtle reason that $m = v \Rightarrow \zeta^{(\alpha)}_{mv} = 0$ and so the asymmetric term disappears, which *also* means that we get away with just writing

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}$$

And these two can be condensed into

$$-\left(\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mu} + \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}\right) \tag{2}$$

Finally, we have

$$
\begin{aligned}
.&= \delta_{um}\left(\xi^{(c)}\right)_{n}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{v} \\
.&= -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\xi^{(c)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m} \\
.&= -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m}
\end{aligned}
$$

which will cancel for a very similar reason to what we had above, first off we have

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m} = -\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m}$$

by the exact same argument as before, *and then* we note that $\Delta^{(i,j)} = -\Delta^{(j,i)}$ and so

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m} = -2\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(j,i)}\right)_{m}$$

which gives us the symmetry we need

We'll handle the other term by first swapping $n \rightarrow u$ and $m \rightarrow v$ which doesn't change the sign, this means we have

$$\left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(\delta_{nv} - 2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\right) = \left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(I - 2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)\right)_{nv}$$

which isn't exactly the pattern we had before, but here's a mind-blowing fact

$$2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right) = \Sigma^{(c)}\,\Sigma^{(j)^{-1}} + \Sigma^{(c)}\,\Sigma^{(j)^{-1}}$$

and so we can use the first copy to perform the previous trick

$$I - \Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma^{(c)}\,\Sigma^{(i)^{-1}}$$

and so we get to do the same double negative as before, giving us

$$\begin{aligned}\left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(i)^{-1}} - \Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} &= -\left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv} \\ &= \left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(j,i)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv}\end{aligned}$$

And we can combine some of this to make for less typing, first using the same mind blowing $2\,x = x + x$ trick to write

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu} \left(\xi^{(c)}\right)_v \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu} \left(\xi^{(c)}\right)_v \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m$$

and so we get

$$\begin{aligned}&\left(\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv} \left(\xi^{(c)}\right)_u - \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu} \left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \\ &= \left(\Sigma^{(c)}\right)_n \left(\left(\Sigma^{(j)^{-1}} - \Sigma^{(i)-1}\right)_v \left(\xi^{(c)}\right)_u - \left(\Sigma^{(j)^{-1}} - \Sigma^{(i)-1}\right)_u \left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \\ &= \left(\Sigma^{(c)}\right)_n \left(\Delta\Sigma_v \left(\xi^{(c)}\right)_u - \Delta\Sigma_u \left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m\end{aligned} \tag{3}$$

Full Expression

From above we get three classes of terms (I dropped a negative on part of the third expression initially and a 1/2 on the second...)

$$\left(\Sigma^{(c)} + \xi^{(c)} \otimes \xi^{(c)}\right)_{nm} \left(\Delta\xi \otimes \Delta\xi - \Sigma^{+}\right)_{uv} \tag{4}$$

$$-\frac{1}{2}\left(\Gamma^{(j)}_{nv}\Gamma^{(i)}_{mu} + \Gamma^{(j)}_{nu}\Gamma^{(i)}_{mv}\right) \tag{5}$$

$$-\Sigma^{(c)}_n \left(\Delta\Sigma_v\,\xi^{(c)}_u + \Delta\Sigma_u\,\xi^{(c)}_v\right) \Delta\xi_m \tag{6}$$

where

$$\begin{aligned}\Sigma^{+} &= \left(\Sigma^{(i)} + \Sigma^{(j)}\right)^{-1} \\ \Delta\xi &= \Sigma^{+}\left(\xi^{(i)} - \xi^{(j)}\right) \\ \Gamma^{(i)} &= \Sigma^{(c)}\,\Sigma^{(i)^{-1}} \\ \Delta\Sigma &= \Sigma^{(i)^{-1}} - \Sigma^{(j)^{-1}}\end{aligned}$$

Test 2

Full Integration (old)

Bad Symmetry, Good Math

Value Test

Momentum Inclusion

To account for the momentum we change our Gaussian definition to include a momentum dependent phase as

$$\varphi^{(i)} = \mathcal{N}\left(\Sigma^{(i)}\right) \exp\left(-\frac{1}{2}\left(q-\xi^{(i)}\right)\Sigma^{(i)-1}\left(q-\xi^{(i)}\right) + \mathbb{i}\, J^{(i)}\, q\right)$$

where $J = Q_{\Sigma}\, p_0$ are chosen to be the momenta along the rotated Gaussian axes

The normalization will not need to change

Rephasing

Function

Generic Shifted Integral

In[1023]:=

```
baseShiftedIntegral =
 Assuming[a > 0 && p > 0 && k > 0 && k ∈ Integers && c ∈ Reals,
  Integrate[q^k Exp[-a q^2 + I p (q - c)], {q, -∞, ∞}]
 ]
```

Out[1023]=

$$\frac{1}{2} a^{-1-\frac{k}{2}} e^{-\mathbb{i}\, c\, p} \left(-\mathbb{i} \left(-1+(-1)^k\right) p\, \text{Gamma}\left[1+\frac{k}{2}\right] \text{Hypergeometric1F1}\left[1+\frac{k}{2}, \frac{3}{2}, -\frac{p^2}{4 a}\right] + \left(1+(-1)^k\right) \sqrt{a}\, \text{Gamma}\left[\frac{1+k}{2}\right] \text{Hypergeometric1F1}\left[\frac{1+k}{2}, \frac{1}{2}, -\frac{p^2}{4 a}\right]\right)$$

Solving for Hypergeometric Expressions

We start out by noting that the even term is just built off a Hermite polynomial, so we’ll ignore it. The second term

$$\text{Gamma}\left[1+\frac{k}{2}\right] \text{Hypergeometric1F1}\left[\frac{2+k}{2}, \frac{3}{2}, -x\right]$$

is rather more annoying, so we return to the definition of the HGF

$$ {}_1F_1(a;\ b;\ x) = \sum_{m=0}^{\infty} \frac{(a)_m}{(b)_m}\ \frac{x^m}{m!} $$

where $(a)_m$ is the rising factorial starting at a and going to $a{+}m{-}1$

Noting that

$$ (a)_m = \frac{\Gamma(a+m)}{\Gamma(a)} $$

and that in our case, $a = b + k$, we have

$$ \frac{(a)_m}{(b)_m} = \frac{\Gamma(b+k+m)}{\Gamma(b+k)}\ \frac{\Gamma(b)}{\Gamma(b+m)} = \frac{(b+m)_k}{(b)_k} $$

and the $(b)_k$ can be factored and $(b{+}m)_k$ can be expressed as a polynomial with

$$ (b+m)_k = \sum_{j=1}^{k} |S_1(k,\ j)|\ (b+m)^j $$

and then we can express this in terms of m alone by writing

$$ (b+m)_k = \sum_{j=1}^{k} \sum_{l=0}^{j} |S_1(k,\ j)| \binom{j}{j-l}\ b^{(j-l)}\ m^l $$

and then we flip the sum to get

$$ (b+m)_k = \sum_{l=0}^{k} \sum_{j=l}^{k}\ |S_1(k,\ j)| \binom{j}{j-l}\ b^{(j-l)}\ m^l $$

where we've explicitly taken advantage of the fact that $S_1(k,\ 0) = 0$, so now we have

$$ {}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k} \sum_{l=0}^{k} \sum_{j=l}^{k} |S_1(k,\ j)| \binom{j}{j-l}\ b^{(j-l)}\ \sum_{m=0}^{\infty} m^l\ \frac{x^m}{m!} $$

and then that final sum actually has a simple form as

$$ \sum_{m=0}^{\infty} m^l\ \frac{x^m}{m!} = e^x \sum_{n=1}^{l} S_2(l,\ n)\ x^n $$

which means in total we get

$$ {}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k}\ e^x \sum_{l=0}^{k} \sum_{j=l}^{k} \sum_{n=1}^{l} |S_1(k,\ j)| \binom{j}{j-l}\ b^{(j-l)}\ S_2(l,\ n)\ x^n $$

and then flipping the sum once more we have

$$ {}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k}\ e^x \sum_{n=1}^{k} \sum_{l=n}^{k} \sum_{j=l}^{k}\ |S_1(k,\ j)| \binom{j}{j-l}\ b^{(j-l)}\ S_2(l,\ n)\ x^n $$

finally, flipping that rising factorial back around we have (I dropped a power but otherwise everything is fine)

$$\begin{aligned}{}_1F_1(b{+}k;\ b;\ x) &= \frac{(b{-}1)!}{(k{+}b{-}1)!}\ e^x \sum_{n=0}^{k}\sum_{l=n}^{k}\sum_{j=l}^{k}\ |S_1(k,\ j)| \binom{j}{l} b^{(j-l)}\ S_2(l,\ n)\ x^n \\ &= \frac{(b{-}1)!}{(k{+}b{-}1)!}\ e^x \sum_{n=0}^{k}\sum_{l=n}^{k}\sum_{j=l}^{k}\ S_1(k,\ j) \binom{j}{l} b^{(j-l)}\ S_2(l,\ n)\ (-x)^n\end{aligned}$$

and we can view this as a type of matrix transform in the basis of rising/falling factorials, which leads us to

$$\begin{aligned}{}_1F_1(b{+}k;\ b;\ x) &= \frac{1}{(b)_k}\ e^x \sum_{n=0}^{k} \binom{k{+}b{-}1}{n} [k]_{k-n}\ x^n \\ &= e^x \sum_{n=0}^{k} \binom{k{+}b{-}1}{n} \frac{[k]_{(k-n)}}{(b)_k}\ x^n\end{aligned}$$

Finally, we have the prefactor, so

$$\begin{aligned}\Gamma(b{+}k)\,{}_1F_1(b{+}k;\ b;\ x) &= \Gamma(b{+}k)\ \frac{\Gamma(b)}{\Gamma(b{+}k)}\ e^x \sum_{n=0}^{k} \binom{k{+}b{-}1}{k{-}n} [k]_{(k-n)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k{+}b)}{\Gamma(k{-}n{+}1)\,\Gamma(n{+}b)}\ [k]_{(k-n)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k{+}b)}{\Gamma(n{+}b)}\ \frac{\Gamma(k{+}1)}{\Gamma(k{-}n{+}1)\,\Gamma(n{+}1)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k{+}b)}{\Gamma(n{+}b)} \binom{k}{n} x^n\end{aligned}$$

And then to clean up the $\Gamma(b)$ terms we get

$$\begin{aligned}\Gamma(b{+}k)\,{}_1F_1(b{+}k;\ b;\ x) &= \Gamma(b{+}k)\ \frac{\Gamma(b)}{\Gamma(b{+}k)}\ e^x \sum_{n=0}^{k} \binom{k{+}b{-}1}{k{-}n} [k]_{(k-n)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k{+}b)}{\Gamma(k{-}n{+}1)\,\Gamma(n{+}b)}\ [k]_{(k-n)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k{+}b)}{\Gamma(n{+}b)}\ \frac{\Gamma(k{+}1)}{\Gamma(k{-}n{+}1)\,\Gamma(n{+}1)}\ x^n \\ &= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(b{+}k)}{\Gamma(n{+}b)} \binom{k}{n} x^n\end{aligned}$$

which actually just shows that

$$ {}_1F_1(b+k;\ b;\ x) = e^x \sum_{n=0}^{k} \frac{1}{(b)_{(n)}} \binom{k}{n} x^n $$

then adding on that pre-factor we get

$$ \Gamma(b+k)\,{}_1F_1(b+k;\ b;\ x) = e^x \sum_{n=0}^{k} \frac{\Gamma(b+k)}{(b)_{(n)}} \binom{k}{n} x^n $$

where letting $b = c + 1/2$

$$ \frac{\Gamma(b+k)}{(b)_{(n)}} = \frac{\sqrt{\pi}}{2^{c+k-n}} \frac{(2\,(c+k)-1)!!\,(2c-1)!!}{(2(n+c)-1)!!} $$

Derivation Work

Generic Integral Form

We get in total

$$ \int_{-\infty}^{\infty} (q-c)^k \exp\!\left(-\alpha(q-c)^2 + ipq\right) = e^{-icp} \begin{cases} \alpha^{-(1+k/2)}\ ip\ \Gamma\!\left(\frac{2+k}{2}\right) F_1\!\left(\frac{2+k}{2};\ \frac{3}{2};\ -\frac{p^2}{4\alpha}\right) & k \text{ odd} \\ \alpha^{-(1/2+k/2)}\ \Gamma\!\left(\frac{1+k}{2}\right) F_1\!\left(\frac{1+k}{2};\ \frac{1}{2};\ -\frac{p^2}{4\alpha}\right) & k \text{ even} \end{cases} $$

where both of these branches use the symbolic form from above, as

$$ \begin{aligned} \frac{2+k}{2} - \frac{3}{2} &= \frac{3}{2} + \frac{(k-1)}{2} \\ \frac{1+k}{2} - \frac{1}{2} &= \frac{1}{2} + \frac{k}{2} \end{aligned} $$

and therefore, letting $m = \lfloor k/2 \rfloor$ we have both integrals having the form of powers in p

$$ \Gamma(b+m)\ F_1\!\left(b+m;\ b+m;\ -\frac{p^2}{4\alpha}\right) = \exp\!\left(-\frac{p^2}{4\alpha}\right) \sum_{n=0}^{m} (-1)^n \frac{\Gamma(b+m)}{(b)_{(n)}} \binom{m}{n} \left(\frac{p}{2\sqrt{\alpha}}\right)^{2\,n} $$

and in the case that $p = 0$, letting $0^0 = 1$ we recover the original form

$$ \Gamma(b+m)\ F_1\!\left(b+m;\ b+m;\ -\frac{p^2}{4\ a}\right) = \Gamma(b+m) $$

for convenience, we will write

$$ G_b^k(\alpha,\ p) = \Gamma(b+\lfloor k/2 \rfloor)\ F_1\!\left(b+\lfloor k/2 \rfloor;\ b+\lfloor k/2 \rfloor;\ -\frac{p^2}{4\alpha}\right) $$

and so our total integral is

$$\int_{-\infty}^{\infty}(q-c)^k \exp\left(-\alpha(q-c)^2+ \mathbb{i}pq\right) = e^{-\mathbb{i}cp}\begin{cases} \alpha^{-(1+k/2)}\ \mathbb{i}p\ G_{3/2}^k(\alpha,\ p) & k \text{ odd} \\ \alpha^{-(1/2+k/2)}\ G_{1/2}^k(\alpha,\ p) & k \text{ even}\end{cases}$$

Rephasing

Generic form for M

To make the derivations simpler, we will introduce the notation

$$M_b^k(\alpha,\ p) = \frac{2^{\lceil k/2\rceil}}{\sqrt{\pi}} \sum_{n=0}^{\lfloor k/2\rfloor}\left(-\frac{1}{2}\right)^n \frac{\Gamma(b+\lfloor k/2\rfloor)}{(b)_{(n)}}\binom{\lfloor k/2\rfloor}{n}\left(\frac{p^2}{2\,\alpha}\right)^n$$

and more specifically,

$$M_k^{(i,j)} = \begin{cases} M_{3/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ odd} \\ M_{1/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ even}\end{cases}$$

we'll also take this chance to figure out what the two relevant values of M_k evaluate to

First we have

$$\begin{aligned}\frac{\Gamma(3/2+k)}{(3/2)_{(n)}} &= \frac{\sqrt{\pi}}{2^{k+1-n}}\frac{2k!!}{2n!!} \\ \frac{\Gamma(1/2+k)}{(1/2)_{(n)}} &= \frac{\sqrt{\pi}}{2^{k-n}}\frac{(2\,k-1)!!}{(2n-1)!!}\end{aligned}$$

then we get

$$\begin{aligned}M_{1/2}^k(\alpha,\ p) &= \frac{2^{k/2}}{\sqrt{\pi}}\sum_{n=0}^{k/2}\left(-\frac{1}{2}\right)^n \frac{\sqrt{\pi}}{2^{k/2-n}}\frac{(k-1)!!}{(2n-1)!!}\binom{k/2}{n}\left(\frac{p^2}{2\,\alpha}\right)^n \\ &= \sum_{n=0}^{k/2}(-1)^n \frac{(k-1)!!}{(2n-1)!!}\binom{k/2}{n}\left(\frac{p^2}{2\,\alpha}\right) \\ &= \sum_{n=0}^{k/2}(-1)^n\left(\prod_{j=n+1}^{k/2}2j-1\right)\binom{k/2}{n}\left(\frac{p^2}{2\,\alpha}\right) \\ M_{3/2}^k(\alpha,\ p) &= \sum_{n=0}^{(k-1)/2}(-1)^n\frac{(k-1)!!}{2n!!}\binom{(k-1)/2}{n}\left(\frac{p^2}{2\,\alpha}\right)^n \\ &= \sum_{n=0}^{(k-1)/2}(-1)^n\left(\prod_{j=n}^{(k-1)/2}2j+1\right)\binom{(k-1)/2}{n}\left(\frac{p^2}{2\,\alpha}\right)^n\end{aligned}$$

this then provides a recurrence relation in k on the coefficients as we have the generic form

$$\mu_n^k = (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j + (-1)^{k+1} \right) \binom{\lfloor k/2 \rfloor}{n}$$

and

$$\binom{\lfloor k/2 \rfloor}{n} = \binom{\lfloor (k-2)/2 \rfloor}{n} + \binom{\lfloor (k-2)/2 \rfloor}{n-1}$$

$$\left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j + (-1)^{k+1} \right) = \left(2 \lfloor k/2 \rfloor - (-1)^k\right) \left(\prod_{j=n+1}^{\lfloor (k-2)/2 \rfloor} 2j + (-1)^{k+1} \right)$$

therefore

$$\begin{aligned}
\mu_n^k &= (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j + (-1)^{k+1} \right) \binom{\lfloor k/2 \rfloor}{n} \\
&= (-1)^n \left(2 \lfloor k/2 \rfloor + (-1)^{k+1}\right) \left(\prod_{j=n+1}^{\lfloor (k-2)/2 \rfloor} 2j - (-1)^k \right) \left(\binom{\lfloor (k-2)/2 \rfloor}{n} + \binom{\lfloor (k-2)/2 \rfloor}{n-1} \right) \\
&= \left(2 \lfloor k/2 \rfloor + (-1)^{k+1}\right) \left(\mu_n^{k-2} - \left(\prod_{j=n+1}^{\lfloor (k-2)/2 \rfloor} 2j - (-1)^k \right) \binom{\lfloor (k-2)/2 \rfloor}{n-1} \right) \\
&= \left(2 \lfloor k/2 \rfloor + (-1)^{k+1}\right) \left(\mu_n^{k-2} - \frac{1}{2n - (-1)^k} \mu_{n-1}^{k-2} \right)
\end{aligned}$$

and finally

$$\begin{aligned}
\left(2 \lfloor k/2 \rfloor + (-1)^{k+1}\right) &= 2\left(k - \left(1 - (-1)^k\right)/2\right)/2 - (-1)^k \\
&= k - \left(1 - (-1)^k\right)/2 - (-1)^k \\
&= \lceil k/2 \rceil
\end{aligned}$$

so we get

$$\mu_n^k = \lceil k/2 \rceil \left(\mu_n^{k-2} - \frac{1}{2n - (-1)^k} \mu_{n-1}^{k-2} \right)$$

where it should be noted that $\lceil k/2 \rceil$ is always odd and so the first term will always just be the product of odd integers

Tests

Notation

Old

Final Integrals

$$\int_{-\infty}^{\infty}\left(q_s - \xi_s^{(i,j)}\right)^k \varphi^{(i)}\,\varphi^{*(j)} = \frac{X_0^{(i,j)}}{\left(2\,\alpha_s^{(i,j)}\right)^{\lceil k/2\rceil}}\begin{cases} \mathbb{i}\,p^{(i,j)} M_{3/2}^{k}\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ odd} \\ M_{1/2}^{k}\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ even}\end{cases}$$

where

$$\begin{aligned} X_0^{(i,j)} &= S_0^{(i,j)} \exp\left(-\frac{1}{2}\,J^{(i,j)}\,\Sigma^{(i,j)}\,J^{(i,j)\mathrm{T}}\right)\exp\left(-\mathbb{i}\xi^{(i,j)}\cdot J^{(i,j)}\right) \\ p^{(i,j)} &= \left(J^{(i)} - J^{(j)}\right) L^{(i,j)\mathrm{T}} = J^{(i,j)}\,L^{(i,j)\mathrm{T}} \end{aligned}$$

for convenience we will enumerate the relevant values of M

$$\begin{aligned} M_1^{(i,j)} &= 1 \\ M_2^{(i,j)} &= 1 - \frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}} \\ M_3^{(i,j)} &= 3 - \frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}} \\ M_4^{(i,j)} &= 3 - \frac{6\,p_s^{(i,j)2}}{2\,\alpha_s^{(i,j)}} + \frac{p_s^{(i,j)4}}{4\alpha_s^{(i,j)}} \end{aligned}$$

where generically

$$M_k = \sum_{n=0}^{\lfloor k/2\rfloor} \mu_n^{(k)} \left(\frac{p_m^2}{2\,\alpha_m}\right)^n$$

with

$$\begin{aligned} \mu_n^{(k)} &= \lceil k/2\rceil\left(\mu_n^{(k-2)} - \frac{1}{2n - (-1)^k}\,\mu_{n-1}^{(k-2)}\right) \\ &= (-1)^n\left(\prod_{j=n+1}^{\lfloor k/2\rfloor} 2j - (-1)^k\right)\binom{\lfloor k/2\rfloor}{n} \end{aligned}$$

which is just a binomial coefficient times the appropriate falling factorial in odd numbers

This means the generic integral form is

$$\int_{-\infty}^{\infty}\left(q_s - \xi_s^{(i,j)}\right)^k \varphi^{(i)}\,\varphi^{*(j)} = \frac{X_0^{(i,j)}}{\left(2\,\alpha_s^{(i,j)}\right)^{\lceil k/2\rceil}}\left(\sum_{n=0}^{\lfloor k/2\rfloor} \mu_n^{(k)}\left(\frac{p_s^{(i,j)^2}}{2\,\alpha_s^{(i,j)}}\right)^n\right)\begin{cases} \mathbb{i}\,p^{(i,j)} & k \text{ odd} \\ 1 & k \text{ even}\end{cases}$$

Tests

Rotated Integrations

We can integrate along the rotated coordinates, but it is perhaps more useful to have expressions in terms of the covariance matrices

The basic form of the integrals will be, e.g.,

$$\int A\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{*(j)}$$

and the $\phi^{(i)}\,\phi^{(j)}$ component will provide the Gaussian axes and all the usual data such that

$$\left(Q-\xi^{(i,j)}\right) = L^T R$$

at the phase factors will combine to give

$$\exp\left(\mathbb{i}\left(J^{(i)}-J^{(j)}\right)Q\right)$$

To that end, we'll consider the different forms of expressions we have. In the k=0 case, we'll have terms like

Constants

$$\int_{-\infty}^{\infty} V^{(0)}\,\varphi^{(i)}\,\varphi^{*(j)} = V^{(0)}\,X_0^{(i,j)}$$

Linear Terms

We'll have things like

$$\begin{aligned}
\int_{-\infty}^{\infty} V_n^{(1)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{*(j)} &= \mathbb{i}\,X_0^{(i,j)}\sum_s \frac{\left(V^{(1)}L^{\mathrm{T}}\right)_{ns}}{2\,\alpha_s^{(i,j)}}\;p_s^{(i,j)} \\
&= \mathbb{i}\,X_0^{(i,j)}\sum_s \left(V^{(1)}L^{\mathrm{T}}\right)_{ns}\Lambda_{ss}^{(i,j)}\left(J^{(i,j)}\,L^{\mathrm{T}}\right)_s \\
&= \mathbb{i}\,X_0^{(i,j)}\sum_s V_n^{(1)}(L^{\mathrm{T}})_{:s}\,\Lambda_{ss}^{(i,j)}(L)_{s:}\,J^{(i,j)\mathrm{T}} \\
&= \mathbb{i}\,X_0^{(i,j)}\;V_n^{(1)}\,\Sigma^{(i,j)}\;J^{(i,j)\mathrm{T}}
\end{aligned}$$

and we'll shorthand momentum correlation vector as

$$\rho^{(i,j)} = \Sigma^{(i,j)}\;J^{(i,j)\mathrm{T}}$$

so we get

$$\int_{-\infty}^{\infty} V^{(1)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{*(j)} = \mathbb{i}\,X_0^{(i,j)}\;V_n^{(1)}\,\rho^{(i,j)}$$

Quadratic Terms

We have

$$\frac{\int V_n^{(1)}\left(Q-\xi^{(i,j)}\right)\,V_m^{(2)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{(j)}}{X_0^{(i,j)}} = \sum_s\sum_t \frac{\left(V^{(1)}L^{(i,j)\mathrm{T}}\right)_{ns}\left(V^{(2)}L^{(i,j)\mathrm{T}}\right)_s}{2\,\alpha_s^{(i,j)}}\begin{cases} M_2^{(i,j)} & s=t \\ -\dfrac{p_s^{(i,j)}\,p_t^{(i,j)}}{2\,\alpha_t^{(i,j)}}\,M_1^{(i,j)} & s\neq t\end{cases}$$

but then we note that

$$M_2^{(i,j)} = 1-\frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}}$$

and the momentum contributions add, giving us

$$\begin{aligned}\frac{\int \cdots}{X_0^{(i,j)}} &= \sum_s \frac{V_n^{(1)}L_s^{(i,j)\mathrm{T}}\otimes V_m^{(2)}L_t^{(i,j)\mathrm{T}}}{2\,\alpha_s^{(i,j)}} - \sum_s \frac{V_n^{(1)}L_s^{(i,j)\mathrm{T}}\,p_s^{(i,j)}}{2\,\alpha_s^{(i,j)}}\sum_t \frac{V_m^{(2)}L_t^{(i,j)\mathrm{T}}\,p_t^{(i,j)}}{2\,\alpha_t^{(i,j)}} \\ &= \left(V^{(1)}\Sigma^{(i,j)}V^{(2)}\right)_{nm} - \left(V^{(1)}\rho^{(i,j)}\right)_n\left(V^{(2)}\rho^{(i,j)}\right)_m\end{aligned}$$

General Term

$$\frac{\int_{-\infty}^{\infty}\left[\prod_{n=1}^{d} V_{b_n}^{(a_n)}\left(Q-\xi^{(i,j)}\right)\right]\varphi^{(i)}\,\varphi^{(j)}}{X_0^{(i,j)}} =$$

$$\sum_{k\in\mathcal{P}(d)}\left(\sum_{s=\mathcal{D}(k)}\left(\prod_{n=1}^{d}V_{b_n}^{(a_n)}L_{s_n}^{(i,j)\mathrm{T}}\right)\right)\prod_{m=1}^{d}\frac{X_0^{(i,j)}}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k/2\rceil}}\begin{cases}\mathbb{i}\,p_m^{(i,j)}M_m^{k_m} & k_m \text{ odd}\\ M_m^{k_m} & k_m\text{ even}\end{cases}$$

which is just the classic way of saying we sum over $\mathcal{P}(d)$, the set of partitions of permutations of the total order of the polynomial, to figure out what order polynomial we have in each dimension. Then for each order we sum over the ways to distribute these across the $V^{(a_n)}$ boxes. Finally, each order partition permutation gets the appropriate prefactor.

We'll probably want to show how to construct this whole deal via induction, but first we should look at the function

$$\begin{aligned}Z(k) &= \prod_{m=1}^{d}\frac{X_0^{(i,j)}}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k/2\rceil}}\begin{cases}\mathbb{i}\,p_m^{(i,j)}M_m^{k_m} & k_m\text{ odd}\\ M_m^{k_m} & k_m\text{ even}\end{cases}\\ &= \mathbb{i}^d(-1)^{z(k)-1}\,X_0^{(i,j)}\prod_{m=1}^{d}\frac{1}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k_m/2\rceil}}\sum_{n=0}^{\lfloor k_m/2\rfloor}\mu_n^{k_m}\left(\frac{p_m^2}{2\,\alpha_m}\right)^n\end{aligned}$$

where $z(k)$ is the number of odd partitions in k and μ_n^k is given by

$$\mu_n^{(k)} = \lceil k/2\rceil\left(\mu_n^{(k-2)} - \frac{1}{2n-(-1)^k}\,\mu_{n-1}^{(k-2)}\right)$$

$$= (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j - (-1)^k \right) \binom{\lfloor k/2 \rfloor}{n}$$

therefore we get a product of expansions in $p_m^2/2\,\alpha_m$ for each dimension

Next we'll note that for any $s \in \mathcal{D}(k)$, we can isolate the product of the form

$$\prod_{n=1}^{k_m} V_{b_n}^{(a_n)} L_m^{(i,j)\mathrm{T}}$$

where we WLOG chose n to start at 1

And so we have $\lfloor k_m/2 \rfloor$ terms like

$$\frac{\left(V_{b_{n_1}}^{(a_{n_1})} L_m^{(i,j)\mathrm{T}} \right) \left(V_{b_{n_2}}^{(a_{n_2})} L_m^{(i,j)\mathrm{T}} \right)}{2\,\alpha_m^{(i,j)}}$$

and if k_m is odd, one additional term of the form

$$\frac{\left(V_{b_{n_3}}^{a_{n_3}} L_m^{(i,j)\mathrm{T}} \right) p_m^{(i,j)}}{2\,\alpha_m^{(i,j)}}$$

and generically if we add up over all the appropriate m, the first of these turns into things of the form

$$\left(V^{(a_{n_1})}\, \Sigma^{(i,j)}\; V^{(a_{n_2})} \right)_{b_{n_1}\, b_{n_2}}$$

and the latter becomes

$$\left(V^{(a_{n_3})}\, \rho^{(i,j)} \right)_{b_{n_3}}$$

We might worry that we aren't adding over the correct set of m, but this fear is alleviated by considering that the μ_n weight the permutations appropriately once we consider the sum over s

This is tedious to show, but it becomes clear at least for the no momentum case when looking back at that 4th order integration from the Watson term

The other way to see this is to note that μ_0 always provides the number of partitions of the k_m elements into pairs

General Integral Form

Finally, the sign of the contribution will clearly depend on how many momentum terms we have, e.g. in the d=2 case we had

$$\left(V^{(1)} \Sigma^{(i,j)} V^{(2)} \right)_{nm} - \left(V^{(1)} \rho^{(i,j)} \right)_n \left(V^{(2)} \rho^{(i,j)} \right)_m$$

and similarly in the d=3 case by this argument we get

$$
\begin{aligned}
&\left(V^{(1)}\Sigma^{(i,j)}\,V^{(2)}\right)_{nm}\left(V^{(3)}\rho^{(i,j)}\right)_{l}\\
&\quad+\left(V^{(1)}\Sigma^{(i,j)}\,V^{(3)}\right)_{nl}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\\
&\quad+\left(V^{(2)}\Sigma^{(i,j)}\,V^{(3)}\right)_{ml}\left(V^{(3)}\rho^{(i,j)}\right)_{n}\\
&\quad-\left(V^{(1)}\rho\right)_{n}\left(V^{(2)}\,\rho\right)_{m}\left(V^{(3)}\rho^{(i,j)}\right)_{l}
\end{aligned}
$$

which matches up with the form

In[337]:=

```
testMk[3]
```

Out[337]=

```
{3, -1}
```

and in the 4th order case we'll expect

In[338]:=

```
testMk[4]
```

Out[338]=

```
{3, -6, 1}
```

and when we enumerate this we get

$$
\begin{aligned}
&\left(V^{(1)}\Sigma^{(i,j)}\,V^{(2)}\right)_{nm}\left(V^{(3)}\Sigma^{(i,j)}\,V^{(4)}\right)_{uv}\\
&\quad+\left(V^{(1)}\Sigma^{(i,j)}\,V^{(3)}\right)_{nu}\left(V^{(2)}\Sigma^{(i,j)}\,V^{(4)}\right)_{mv}\\
&\quad+\left(V^{(1)}\Sigma^{(i,j)}\,V^{(4)}\right)_{nv}\left(V^{(2)}\Sigma^{(i,j)}\,V^{(3)}\right)_{mu}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}\,V^{(2)}\right)_{nm}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}\,V^{(3)}\right)_{nu}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}\,V^{(4)}\right)_{nv}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\\
&\quad-\left(V^{(2)}\Sigma^{(i,j)}\,V^{(3)}\right)_{mu}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(2)}\Sigma^{(i,j)}\,V^{(4)}\right)_{mv}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\\
&\quad-\left(V^{(3)}\Sigma^{(i,j)}\,V^{(4)}\right)_{uv}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\\
&\quad+\left(V^{(1)}\rho\right)_{n}\left(V^{(2)}\,\rho\right)_{m}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\left(V^{(4)}\rho^{(i,j)}\right)_{v}
\end{aligned}
$$

Generic Algorithm

Take all integer partitions of d with maximum element at most 2

In[339]:=

```
Select[IntegerPartitions[4], Max[#] ≤ 2 &]
```

Out[339]=

```
{{2, 2}, {2, 1, 1}, {1, 1, 1, 1}}
```

The sign of the contribution will depend on the length of the partition

These will be our "bucket sizes", we'll split the indices we have into these buckets

Finally, we'll do successive swaps between the buckets to get unique permutations. This final step is a bit tricky, but for $d \leq 6$ we can do it quickly as there are only $6! = 720$ possible permutations to filter over.

Implementation

Cubic Terms

Tests

Tensor Expression Generator

We need the ability to build expressions involving φ and γ, including Watson-term expressions

Setup

Differentiate

Evaluate

Tests

Matrix Elements

Overlaps

Dealt with above

Kinetic Terms

Term Setup

Test

Simplification

The first simplification is a classic

$$\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(j)^{-1}}\right) = -\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \tag{7}$$

For the real component of the moment terms, we start with

$$\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)}\right)_m^2 + 2\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)}\right)J_m^{(j)} + \left(J_m^{(j)}\right)^2 = \left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J_m^{(j)}\right)^2$$

then we can get the symmetry from this by noting that

$$\begin{aligned}\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)} &= J^{(i,j)} - \Sigma^{(i)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)} \\ &= \Sigma^{(i)^{-1}}\,\Sigma^{(c)}\,J^{(j,i)} + J^{(i)}\end{aligned}$$

and so to put this in an explicitly symmetric form we'll write this as

$$\frac{1}{2}\left(J^{(i)}+J^{(j)} + \left({\Sigma^{(j)}}^{-1}-{\Sigma^{(i)}}^{-1}\right)\Sigma^{(c)}\,J^{(i,j)}\right)$$

The complex portion is given by

$$\Delta_m^{(i,j)}\left({\Sigma^{(j)}}^{-1}\,\Sigma^{(c)}\,J^{(i,j)}\right)_m + \Delta_m^{(i,j)}\left(J^{(j)}\right)_m = \Delta_m^{(i,j)}\left({\Sigma^{(j)}}^{-1}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)}\right)_m$$

and for exactly the same reason as above this will be anti-symmetric, since Δ is

So in total, letting

$$J^{+} = \frac{1}{2}\left(J^{(i)}+J^{(j)}+\left({\Sigma^{(j)}}^{-1}-{\Sigma^{(i)}}^{-1}\right)\Sigma^{(c)}\,J^{(i,j)}\right)$$
$$\Sigma^{+} = \left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}$$

we get

$$T = -\frac{1}{2}\sum_k \frac{1}{m_k}\left((\Sigma^{+}\Delta\xi)_k^2 - {\Sigma^{+}}_{kk} - {J_k^{+}}^2 - i(\Sigma^{+}\Delta\xi)_k\,J_k^{+}\right)$$

Automated Redo

In[650]:=

```
evaledKTerms /. {
    giMatEl[{Σ[j], Σ[j]}, {x_, y_}] ⧴
     giBaseEl[{Σ[j]}, {x, y}] - giBaseEl[{Γ[d]}, {x, y}],
    giBaseEl[{J[j]}, {y_}] ⧴ (
      giBaseEl[{J["+"]}, {y}] - giMomEl[{Σ[j]}, {y}]
     )
   } // Expand // simpIntPrint
```

$\Delta_m^2 - {J^{(+)}}^2_m - \Sigma^{(+)}_{m\,m} - 2\,i\,\Delta_m\,J^{(+)}_m$

Coriolis

Computer Assisted Expressions

Simplification

Real Terms

We'll reduce this bit by bit, here's our set of terms to reduce over

```
GroupBy[jPTerms,
    Cases[#, _giMomEl, Infinity] &, Simplify@*Total] // Values //
  ReplaceAll[d → "+"] // Scan[intPrint]
```

$-\left(\left[\xi^{(c)}\right]_m\left[\xi^{(c)}\right]_n+\left[\Sigma^{(c)}\right]_{n\,m}\right)\left[J^{(+)}\right]_u\left[J^{(+)}\right]_v$

$$\left(\left(\left[\Sigma^{(+)}\,\Delta\right]_v\,\left[\xi^{(c)}\right]_n-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{v\,n}\right)\,\left[J^{(+)}\right]_u+\left(\left[\Sigma^{(+)}\,\Delta\right]_u\,\left[\xi^{(c)}\right]_n+\left[\Sigma^{(c)}\,\Sigma^{(j)\,-1}\right]_{n\,u}\right)\,\left[J^{(+)}\right]_v\right)\,\left[\rho^{(c)}\right]_m$$

$$\left(\left(\left[\Sigma^{(+)}\,\Delta\right]_v\,\left[\xi^{(c)}\right]_m-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{v\,m}\right)\,\left[J^{(+)}\right]_u+\right.$$
$$\left.\left(\left[\Sigma^{(+)}\,\Delta\right]_u\,\left[\xi^{(c)}\right]_m-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{u\,m}\right)\,\left[J^{(+)}\right]_v+[\mathrm{I}]_{u\,m}\,\left[J^{(+)}\right]_v\right)\,\left[\rho^{(c)}\right]_n$$

$$\left(-\left[\Sigma^{(+)}\,\Delta\right]_u\,\left[\Sigma^{(+)}\,\Delta\right]_v+\left[J^{(+)}\right]_u\,\left[J^{(+)}\right]_v+\left[\Sigma^{(+)}\right]_{u\,v}\right)\,\left[\rho^{(c)}\right]_m\,\left[\rho^{(c)}\right]_n$$

Simps

Redone with Color

In[1269]:=

```
cleanJPReal = (
    jPTerms /. {
      giMatEl[{Σ[j], Ị | I}, {n, u}] ⧴ giMatEl[{Σ[i], Ị}, {u, n}],
      giMatEl[{Σ[j], Ị | I}, {m, v}] ⧴ giMatEl[{Σ[i], Ị}, {v, m}],
      giMatEl[{Ị | I, Σ[j]}, {e_, f_}] ⧴ giMatEl[{Σ[j], Ị}, {f, e}],
      giBaseEl[{Ị | I}, {e_, f_}] ⧴ (
        giMatEl[{Σ[j], Ị}, {e, f}] + giMatEl[{Σ[i], Ị}, {e, f}]
       )

      (*giMatEl[{Ị|I,Σ[j]},{m_,v_}]⧴-giMatEl[{Σ[i], Ị}, {v, m}],
      giMatEl[{Ị|I,Σ[j]},{v,m}]⧴giMatEl[{Σ[i], Ị}, {v, m}],

      giMatEl[{Σ[j], Ị|I}, {m, v}]→giMatEl[{Σ[i], Ị}, {v, m}],
      giMatEl[{Σ[j], Ị|I}, {v, m}]→-giMatEl[{Σ[i], Ị}, {v, m}]*)
     }
   ) //. {
    giMatEl[{Σ[i], Ị}, {u, n}] → -giMatEl[{Σ[j], Ị}, {u, n}]
   };
```

In[1270]:=

```
cleanJPReal // GroupBy[#, Cases[#, _giMomEl, Infinity] &, Simplify@*Total] & //
  Scan[Scan[simpIntPrint]@*Apply[List]@*Distribute]
```

Terms

$$-J_u^{(+)}\,J_v^{(+)}(\xi_m\,\xi_n+\Sigma_{n\,m})$$

$$\left(J_u^{(+)}\,J_v^{(+)}+\Sigma_{u\,v}^{(+)}-\Delta_u\,\Delta_v\right)\rho_m\,\rho_n$$

$$\left(\Delta_u\,J_v^{(+)}+\Delta_v\,J_u^{(+)}\right)(\xi_n\,\rho_m+\xi_m\,\rho_n)$$

$$\left(\left[\Sigma^{(i)\,-1}\,\Sigma\right]_{u\,m}\rho_n-\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{u\,n}\,\rho_m\right)\,J_v^{(+)}\;+\;\left(\left[\Sigma^{(i)\,-1}\,\Sigma\right]_{v\,m}\rho_n-\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{v\,n}\rho_m\right)\,J_u^{(+)}$$

where notably the $\Delta_u\,\Delta_v(\xi_m\,\xi_n+\Sigma_{n\,m})$ term is missing since it's already in the no-momentum expression

Final Term Redo

We can do the trick from below in the no-momentum case for the final term above, replacing the terms involving $J_u^{(+)}$ to get

$$\left(\left[\Sigma^{(i)-1}\,\Sigma\right]_{u\,m}\rho_n-\left[\Sigma^{(j)-1}\,\Sigma\right]_{u\,n}\,\rho_m\right)J_v^{(+)}+\left(\left[\Sigma^{(i)-1}\,\Sigma\right]_{u\,n}\,\rho_m-\left[\Sigma^{(j)-1}\,\Sigma\right]_{u\,m}\rho_n\right)J_v^{(+)}$$

which condenses down to

$$\left(\Sigma^{(i)-1}-\Sigma^{(j)-1}\right)_u(\Sigma_m\,\rho_n+\Sigma_n\,\rho_m)\,J_v^{(+)}$$

So in total we have

$$-J_u^{(+)}\,J_v^{(+)}(\xi_m\,\xi_n+\Sigma_{n\,m})$$

$$\left(J_u^{(+)}\,J_v^{(+)}+\Sigma_{u\,v}^{(+)}-\Delta_u\,\Delta_v\right)\rho_m\,\rho_n$$

$$\left(\Delta_u\,J_v^{(+)}+\Delta_v\,J_u^{(+)}\right)(\xi_n\,\rho_m+\xi_m\,\rho_n)$$

$$\left(\Sigma^{(i)-1}-\Sigma^{(j)-1}\right)_u(\Sigma_m\,\rho_n+\Sigma_n\,\rho_m)\,J_v^{(+)}$$

Test

In[4284]:=

```
testExprsReal = {
   - ( ξI[m] * ξI[n] + ΣI[n, m]) * (JI[u] * JI[v]),
   - (ρI[m] * ρI[n]) (ΔI[u] * ΔI[v] - JI[u] * JI[v] - ΣpI[u, v]),
   (ξI[n] * ρI[m] + ξI[m] * ρI[n]) (ΔI[u] * JI[v] + ΔI[v] * JI[u]),
   (
    (ΓI[i][v, m] * ρI[n] - ΓI[j][v, n] * ρI[m]) * JI[u]
     + (ΓI[i][u, m] * ρI[n] - ΓI[j][u, n] * ρI[m]) * JI[v]
   )
  };
```

No-Momentum Terms

Just for the fun of it, we'll redo the no momentum terms to build a full real-term expression

In[4319]:=

```
cleanJPNonMomTerms = (
   jPNonMomTerms /. {
     giMatEl[{Σ[j], I | I}, {n, u}] :> giMatEl[{Σ[i], I}, {u, n}],
     giMatEl[{Σ[j], I | I}, {m, v}] :> giMatEl[{Σ[i], I}, {v, m}],
     giMatEl[{I | I, Σ[j]}, {e_, f_}] :> giMatEl[{Σ[j], I}, {f, e}],
     giBaseEl[{I | I}, {e_, f_}] :> (
       giMatEl[{Σ[j], I}, {e, f}] + giMatEl[{Σ[i], I}, {e, f}]
      )

     (*giMatEl[{I|I,Σ[j]},{m_,v_}]:>-giMatEl[{Σ[i], I}, {v, m}],
     giMatEl[{I|I,Σ[j]},{v,m}]:>giMatEl[{Σ[i], I}, {v, m}],

     giMatEl[{Σ[j], I|I}, {m, v}]→giMatEl[{Σ[i], I}, {v, m}],
     giMatEl[{Σ[j], I|I}, {v, m}]→-giMatEl[{Σ[i], I}, {v, m}]*)
    }
   ) //. {
   giMatEl[{Σ[i], I}, {u, n}] → -giMatEl[{Σ[j], I}, {u, n}]
   };
```

In[4320]:=

```
cleanJPNonMomTerms //
  GroupBy[#, Cases[#, _giMomEl, Infinity] &, Simplify@*Total] & //
 Scan[Scan[simpIntPrint]@*Apply[List]@*Distribute]
```

$(\xi_m\,\xi_n+\Sigma_{n\,m})\,(\Delta_v\,\Delta_u-\Sigma^{(+)}_{u\,v})$

$-([\Sigma^{(i)\,-1}\,\Sigma]_{v\,m}\,[\Sigma^{(j)\,-1}\,\Sigma]_{u\,n}+[\Sigma^{(i)\,-1}\,\Sigma]_{u\,m}\,[\Sigma^{(j)\,-1}\,\Sigma]_{v\,n})$

$(\xi_n\,[\Sigma^{(i)\,-1}\,\Sigma]_{v\,m}-\xi_m\,[\Sigma^{(j)\,-1}\,\Sigma]_{v\,n})\,\Delta_u$

$(\xi_n\,[\Sigma^{(i)\,-1}\,\Sigma]_{u\,m}-\xi_m\,[\Sigma^{(j)\,-1}\,\Sigma]_{u\,n})\,\Delta_v$

we could do the extra trick from the previous version where we noted that we're summing over every possible version of these indices, so there will *also* be a term where $n\leftrightarrow m$ and $u\leftrightarrow v$

And by doing that swap only on the terms involving Δ_u we get

$(\xi_m\,[\Sigma^{(i)-1}\,\Sigma]_{u\,n}-\xi_n\,[\Sigma^{(j)-1}\,\Sigma]_{u\,m})\,\Delta_v$

$(\xi_n\,[\Sigma^{(i)\,-1}\,\Sigma]_{u\,m}-\xi_m\,[\Sigma^{(j)\,-1}\,\Sigma]_{u\,n})\,\Delta_v$

which can be condensed down to

$(\Sigma^{(i)\,-1}-\Sigma^{(j)-1})_u\,(\Sigma_m\,\xi_n+\Sigma_n\,\xi_m)\,\Delta_v$

Giving us, as expected

$(\xi_m\, \xi_n + \Sigma_{n\, m}) \left(\Delta_v\, \Delta_u - \Sigma^{(+)}_{u\, v}\right)$

$-\left(\left[\Sigma^{(i)\,-1}\, \Sigma\right]_{v\, m} \left[\Sigma^{(j)\,-1}\, \Sigma\right]_{u\, n} + \left[\Sigma^{(i)\,-1}\, \Sigma\right]_{u\, m} \left[\Sigma^{(j)\,-1}\, \Sigma\right]_{v\, n}\right)$

$\left(\Sigma^{(i)\,-1} - \Sigma^{(j)-1}\right)_u (\Sigma_m\, \xi_n + \Sigma_n\, \xi_m)\, \Delta_v$

Complex Terms

We'll automate two of the simplifications from before

In[1271]:=

```
cleanJP = (imagJPTerms /. {
      giMatEl[{I̦ | I, Σ[j]}, {n, u}] :→ giMatEl[{Σ[i], I̦}, {n, u}],
      giMatEl[{I̦ | I, Σ[j]}, {m, v}] :→ giMatEl[{Σ[i], I̦}, {m, v}],
      giMatEl[{I̦ | I, Σ[j]}, {e_, f_}] :→ giMatEl[{Σ[j], I̦}, {f, e}],
      giBaseEl[{I̦ | I}, {e_, f_}] :→ (
        giMatEl[{Σ[j], I̦}, {e, f}] + giMatEl[{Σ[i], I̦}, {e, f}]
       )

      (*giMatEl[{I̦|I,Σ[j]},{m_,v_}]:→-giMatEl[{Σ[i], I̦}, {v, m}],
      giMatEl[{I̦|I,Σ[j]},{v,m}]:→giMatEl[{Σ[i], I̦}, {v, m}],

      giMatEl[{Σ[j], I̦|I}, {m, v}]→giMatEl[{Σ[i], I̦}, {v, m}],
      giMatEl[{Σ[j], I̦|I}, {v, m}]→-giMatEl[{Σ[i], I̦}, {v, m}]*)
     }) //. {
    giMatEl[{Σ[i], I̦}, {n, u}] → giMatEl[{Σ[j], I̦}, {u, n}],
    giMatEl[{Σ[i], I̦}, {m, v}] → -giMatEl[{Σ[i], I̦}, {v, m}]
   };
```

In[1272]:=

```
cleanJP // GroupBy[#, Cases[#, _giMomEl, Infinity] &, Simplify@*Total] & //
 Scan[Scan[simpIntPrint]@*Apply[List]@*Distribute]
```

Terms Redo

We start with

$i\, (\rho_m\, \rho_n - \xi_m\, \xi_n - \Sigma_{n\, m}) \left(\Delta_u\, J^{(+)}_v + \Delta_v\, J^{(+)}_u\right)$

$i\, (\xi_n\, \rho_m + \xi_m\, \rho_n) \left(\Delta_u\, \Delta_v - J^{(+)}_u\, J^{(+)}_v - \Sigma^{(+)}_{u\, v}\right)$

$-i\, \left(\left(\xi_n\left[\Sigma^{(i)\,-1}\, \Sigma\right]_{u\, m} - \xi_m\left[\Sigma^{(j)\,-1}\, \Sigma\right]_{u\, n}\right) J^{(+)}_v + \left(\xi_n\left[\Sigma^{(i)\,-1}\, \Sigma\right]_{v\, m} - \xi_m\left[\Sigma^{(j)\,-1}\, \Sigma\right]_{v\, n}\right) J^{(+)}_u\right)$

$i\, \left(\left(\left[\Sigma^{(i)\,-1}\, \Sigma\right]_{v\, m} \rho_n - \left[\Sigma^{(j)\,-1}\, \Sigma\right]_{v\, n} \rho_m\right) \Delta_u + \left(\left[\Sigma^{(i)\,-1}\, \Sigma\right]_{u\, m} \rho_n - \left[\Sigma^{(j)\,-1}\, \Sigma\right]_{u\, n} \rho_m\right) \Delta_v\right)$

and now we'll do the same trick from above to replace the $J^{(+)}_u$ and Δ_u terms to get the final set as

$\mathbb{i}(\rho_m\, \rho_n - \xi_m\, \xi_n - \Sigma_{n\,m})\left(\Delta_u\, J^{(+)}_v + \Delta_v\, J^{(+)}_u\right)$

$\mathbb{i}(\xi_n\, \rho_m + \xi_m\, \rho_n)\left(\Delta_u\, \Delta_v - J^{(+)}_u\, J^{(+)}_v - \Sigma^{(+)}_{u\,v}\right)$

$-\mathbb{i}\left(\Sigma^{(i)\,-1} - \Sigma^{(j)-1}\right)_u (\Sigma_m\, \xi_n + \Sigma_n\, \xi_m)\, J^{(+)}_v$

$\mathbb{i}\left(\Sigma^{(i)\,-1} - \Sigma^{(j)-1}\right)_u (\Sigma_m\, \rho_n + \Sigma_n\, \rho_m)\, \Delta_v$

Terms

Test

Rephasing

Generically, if we want to have real matrix elements, we will choose some linear combination of basis functions like

$$\begin{aligned}\varphi^{(i)+} &= \exp\left(-\frac{1}{2}\left(q - \xi^{(i)}\right)\Sigma^{(i)-1}\left(q - \xi^{(i)}\right) + \mathbb{i}\, J^{(i)}\, q\right)\\ \varphi^{(i)-} &= \exp\left(-\frac{1}{2}\left(q - \xi^{(i)}\right)\Sigma^{(i)-1}\left(q - \xi^{(i)}\right) - \mathbb{i}\, J^{(i)}\, q\right)\end{aligned}$$

and then we'll let

$$\varphi^{(i)} = \frac{1}{2}\left(\varphi^{(i)+} + \varphi^{(i)-}\right)$$

Then when we evaluate integrals involving a linear operator $\mathcal{L}$ (involving derivatives, polynomials, multiplicative factors, etc.) we will have

$$\int \varphi^{(i)}\, \mathcal{L}\varphi^{(j)*}\, dq = \frac{1}{4}\left(\int \varphi^{(i)+}\, \mathcal{L}\varphi^{(j)+*} + \int \varphi^{(i)+}\, \mathcal{L}\varphi^{(j)-*} + \int \varphi^{(i)-}\, \mathcal{L}\varphi^{(j)+*} + \int \varphi^{(i)-}\, \mathcal{L}\varphi^{(j)-*}\right)$$

and considering a generic polynomial of order n to start, the standard form of these integrals will be

$$\int \varphi^{(i)\pm}\, \mathcal{L}\varphi^{(j)\pm*} = X_0^{(i,j)}\left(\mathbb{i}^n \sum_{x \in \mathcal{P}(n)} c_x \prod_k \rho_k^{x_k}\right)$$

where $\mathcal{P}(n)$ is the set of permutations of integer partitions of n, $o(x)$ is the order of the permutation and c_x is the appropriate coefficient from the polynomial $\mathcal{L}$, and $\rho = \Sigma^{(i,j)} J^{(i,j)}$

Then recalling that

$$X_0^{(i,j)} = \sqrt{\pi^d \left|\Sigma^{(i,j)}\right|}\, \exp\left(-\frac{1}{2}\, J^{(i,j)}\, \Sigma^{(i,j)}\, J^{(i,j)\mathrm{T}}\right) \exp\left(-\mathbb{i}\xi^{(i,j)} \cdot J^{(i,j)}\right)$$

We will now consider first just the pair

$$\int \varphi^{(i)+}\, \mathcal{L}\varphi^{(j)+*} + \int \varphi^{(i)-}\, \mathcal{L}\varphi^{(j)-*}$$

and note that this is equivalent to considering replacing $J^{(i,j)}$ with $-J^{(i,j)}$

Doing that, letting $v = \xi^{(i,j)} \cdot J^{(i,j)}$, we'll consider that

$$\begin{aligned} \exp(-\mathbb{i}\, v) &= \cos(v) - \mathbb{i}\sin(v) \\ \exp(\mathbb{i}\, v) &= \cos(v) + \mathbb{i}\sin(v) \end{aligned}$$

so splitting this into cases, first the cos terms come out to

$$\begin{aligned} \frac{\left[\int \varphi^{(i)+}\, \mathcal{L}\varphi^{(j)+*} + \varphi^{(i)-}\, \mathcal{L}\varphi^{(j)-*}\right]^{(\cos)}}{\cos(v)} &= \mathbb{i}^n \sum_{x \in \mathcal{P}(n)} c_x \left(\prod_k \rho_k^{x_k} + \prod_k (-1)^{x_k}\, \rho_k^{x_k}\right) \\ &= \mathbb{i}^n \sum_{x \in \mathcal{P}(n)} c_x \left(\prod_k \rho_k^{x_k} + (-1)^n \prod_k \rho_k^{x_k}\right) \\ &= (1 + (-1)^n)\, \mathbb{i}^n \sum_{x \in \mathcal{P}(n)} c_x \left(\prod_k \rho_k^{x_k}\right) \end{aligned}$$

by the fact that, being an integer partition permutation, the x_k add up to n, and so this vanishes for odd n. By a directly analogous argument, the sin terms vanish for even n, and the imaginary prefactor gets multiplied by the extra $\mathbb{i}$ from the $\mathbb{i}\sin(\mathrm{v})$ term

This was applied for the $\varphi^{(i)+}\, \varphi^{(j)+*}$ and $\varphi^{(i)-}\, \varphi^{(j)-*}$, but it should be clear the same argument applies to $\varphi^{(i)+}\, \varphi^{(j)-*}$ and $\varphi^{(i)-}\, \varphi^{(j)+*}$ although the terms will differ in value

Generically, then we can write

$$\frac{1}{2} \int \varphi^{(i)+}\, \mathcal{L}\varphi^{(j)+*} + \varphi^{(i)-}\, \mathcal{L}\varphi^{(j)-*} = (-1)^n \sum_{x \in \mathcal{P}(n)} c_x \left(\prod_k \rho_k^{x_k}\right) \begin{cases} \sin(v) & n \text{ odd} \\ \cos(v) & n \text{ even} \end{cases}$$

A similar argument may be applied to the Coriolis and kinetic terms. There the relevant expansion is in both ρ and $J^{(+)}$, but noting that

$$J^{(+)} = \frac{1}{2} \left(J^{(i)} + J^{(j)} + \left(\Sigma^{(j)^{-1}} - \Sigma^{(i)^{-1}}\right) \Sigma^{(c)}\, J^{(i,j)}\right)$$

$J^{(+)}$ will clearly flip sign when both $J^{(i)}$and $J^{(j)}$ flip

Note that this means we need a slightly different normalization, as now

$$\int \varphi^{(i)}\, \mathcal{L}\varphi^{(i)*}\, d q = \frac{1}{2} \left(1 + \cos\left(2\, \xi^{(i)} \cdot J^{(i)}\right) \exp\left(-J^{(i)}\, \Sigma^{(i)}\, J^{(i)\mathrm{T}}\right)\right)$$

and so we need to divide out the square root of this term in the normalization

A Note on Polynomial Evaluation

A Note on Alpha Choice

Evaluation of Properties

Our final wavefunctions are expressed as a linear combination of the DGB functions

$$\psi_n(\boldsymbol{x}) = \sum_i c_i^{(n)} \varphi_i(\boldsymbol{x})$$

Meaning we can apply the same ideas to evaluating properties that we used for integrating the potential.

Projections

Standard Basis

If we want to integrate out a DOF we have

$$\begin{aligned}
\int \psi_n(\boldsymbol{x})\, dx_k &= \sum_i c_i^{(n)} \int \varphi_i(\boldsymbol{x})\, dx_k \\
&= \sum_i c_i^{(n)} \varphi_i(\boldsymbol{y}) \int \phi_i(x_k)\, dx_k \\
&= \sum_i \sqrt{\frac{2}{N(\alpha_i)}}\; c_i^{(n)} \varphi_i(\boldsymbol{y})
\end{aligned}$$

and so if we have K degrees of freedom $\{k_m\}$to project out we end up with

$$\psi_n(\boldsymbol{y}) = \sum_i \left(\sqrt{\frac{2}{N(\alpha_i)}}\right)^K c_i^{(n)} \varphi_i(\boldsymbol{y})$$

Rotated Basis

If we want to apply projections in the rotated basis, we still have

$$\int \psi_n(\boldsymbol{x})\, dx_k = \sum_i c_i^{(n)} \int \varphi_i(\boldsymbol{x})\, dx_k$$

but now

$$\varphi_i(\boldsymbol{x}) = \phi\left(x,\, \xi^{(i)},\, \Sigma^{(i)}\right) = N\left(\Sigma^{(i)}\right) e^{-\frac{1}{2}\left(\Sigma^{-1} \odot \left(x-\xi^{(i)}\right)^2\right)}$$

But here we can once again take a page from probability people and note that integrating out some set of degrees of freedom is called taking the *marginal* probability distribution, and it's well known in that community that if we have a projected space A and its complement B

$$\Sigma_{\text{new}} = \Sigma_A$$
$$\xi^{(i)}_{\text{new}} = \xi^{(i)}_A$$

where we just get to throw out all the extraneous info. Admittedly we do need to scale our values a bit, since the normalization of the marginal Gaussian is different from the normalization of the full Gaussian.

The bigger problem of course is that we really want ${\Sigma_A}^{-1}$ for how we evaluate these things, and in particular we want the eigensystem of ${\Sigma_A}^{-1}$. Unfortunately that's not trivial to compute, so we'll construct

$$\Sigma = L^T \Lambda L$$

and then diagonalize Σ_A as the same eigensystem (mostly) works

Complex Phase

To handle projections with a complex phase, we note that we start with a function of the form

$$\exp\left(-\frac{1}{2}\,\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot q\right)$$

and since we can easily do projections with a proper quadratic form we'll note that

$$\begin{aligned}-\frac{1}{2}\,\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot q &= .-\frac{1}{2}\,\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot(q-\mu) + \mathbb{i}\,p\cdot\mu \\ &= -\frac{1}{2}\,\Sigma^{-1}\odot(q-(\mu+\mathbb{i}\Sigma p))^2 - \frac{1}{2}\,\Sigma\odot p^2 + \mathbb{i}\,p\cdot\mu\end{aligned}$$

which is of course the source of the prefactors we see in the integrals

Then we can integrate d.o.fs out from this like a normal Gaussian because of the surprising fact that Gaussian integrals are independent of the mean being complex (this can be seen by taking limits of contour integrals that converge to the real line), giving us

$$\int_B \exp\left(-\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot q\right) = S_B \exp\left(-\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-(\mu+\mathbb{i}\Sigma p)_A)^2\right)$$

where

$$S_B = \sqrt{\pi^d\,|\Sigma|}\,\exp\left(-\frac{1}{2}\,\Sigma\odot p^2\right)\exp(\mathbb{i}\,p\cdot\mu)$$

is the standard norm contribution in B space

And the interior term may be reexpanded as

$$-\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-\mu_A-\mathbb{i}(\Sigma p)_A)^2 = -\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-\mu_A)^2 + \mathbb{i}(\Sigma_A)^{-1}\,(\Sigma p)_A\,(q-\mu) + \frac{1}{2}(\Sigma_A)\odot(\Sigma p)_A{}^2$$

where $(\Sigma_A)^{-1}\,(\Sigma(p-\mu))_A = (\Sigma_A)^{-1}\,\Sigma_{A:}(p-\mu)$ is the product of the inverse of the A subblock of Σ and the A rows of Σ, giving

$$\int_B \exp\!\left(-\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot q\right) =$$

$$S_B\exp\!\left(-\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-\mu_A)^2 + \mathbb{i}(\Sigma_A)^{-1}\,(\Sigma p)_A\right)\exp\!\left(\frac{1}{2}(\Sigma_A)\odot(\Sigma p)_A{}^2\right)\exp\!\left(-\mathbb{i}(\Sigma_A)^{-1}\,(\Sigma p)_A\cdot\mu_A\right)$$

and the last pieces there come directly out of the norm of $\exp\!\left(-\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-\mu_A)^2 + \mathbb{i}(\Sigma_A)^{-1}\,(\Sigma p)_A\right)$ and so we end up with

$$\int_B \exp\!\left(-\Sigma^{-1}\odot(q-\mu)^2 + \mathbb{i}\,p\cdot q\right) = S_B\,S_A{}^{-1}\exp\!\left(-\frac{1}{2}\,(\Sigma_A)^{-1}\odot(q_A-\mu_A)^2 + \mathbb{i}(\Sigma_A)^{-1}\,(\Sigma p)_A\right)$$

which, with the exception of the $(\Sigma_A)^{-1}\,\Sigma_{A:}$ is identical to the no-momentum case, but tells us we just need to adjust our momentum and everything else is as normal

---

Normal Mode Gaussians

Subindices in A Rotated Basis

Initializing Runs

A common thing we'll want to do is put some amount of vibrational energy into the different normal modes to start a calculation. Given that these modes are linear combinations of the various internals, it's not entirely obvious how to do this.

Assume we're given some energy partition, $\{E_i\}$, dictating how much kinetic energy to put into the modes, and a transformation from the Cartesian coordinates to the normal modes L. First off, we know classically that

$$T = \frac{1}{2}\sum_{k=1}^{3N} m_k v_k{}^2$$

which we can view in matrix form as

$$T = \frac{1}{2}\,v^{\mathrm{T}} M\,v$$

use L to express this in terms of our vibrational coordinates as

$$2T = (Lv)^{\mathrm{T}}\left(LML^{\mathrm{T}}\right)(Lv)$$

and now our *goal* is to be able to put a certain amount of energy into each vibration specifically. The difficulty is that $G = LML^{\mathrm{T}}$ is not necessarily diagonal, and so we can a few things

Case 1: ignore all coupling between vibrational modes

This corresponds to just treating G as diagonal and using these diagonal elements as effective masses. To get the correct total energy, though, we need to account for what's missing. This means we will calculate the kinetic deficit,

$$2T_{\mathrm{def}} = (Lv)^{\mathrm{T}} G_{\mathrm{off}}(Lv)$$

and then we want a new set of velocities, u, so that

$$2T = (Lu)^{\mathrm{T}} G(Lu)$$

gives us our target total energy and we want the relative energies per mode to follow the same distribution as before, therefore we'll have

$$(Lu)^{\mathrm{T}} G(Lu) = (Lv)^{\mathrm{T}} G(Lv) - (Lv)^{\mathrm{T}} G_{\mathrm{off}}(Lv)$$

which can be handled like case (2) by diagonalizing G to get a transformation Q, and a set of effective masses γ, and with that we get

$$\sum_{j=1}^{3N-6} \gamma_j (\mathrm{QL}u)_j{}^2 = \sum_{j=1}^{3N-6} g_{jj}(Lv)_j{}^2$$

and assuming we've maximized the similarity between our new and old modes, we'll get...

Case 2: diagonalize G

We will then that put the appropriate amount of kinetic energy into the modes most closely resembles our mode of interest.

In terms of minimizing the surprise factor, (2) is likely the best option, and so by diagonalizing G we get a transformation Q, and a set of effective masses g, and with that, writing $u = QLv$, we have

$$2T = \sum_{j=1}^{3N-6} g_j u_j{}^2$$

Multi-Harmonic Basis

Polynomial Augmentation

Mass-Weighted Transformation

Morse Fits

Reduced Integrations

Multivariate Gaussian Quadrature

We start from the idea that we want to reduce an integral of the form

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\,\Sigma^{-1}\,\boldsymbol{x}\right)}\, d\boldsymbol{x}$$

and want to express it as

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\,\Sigma^{-1}\,\boldsymbol{x}\right)}\, d\boldsymbol{x} = N \int V(r)\, e^{-(\ldots)}\, d?$$

For this, we will note that we can write

$$r = \sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}$$

and therefore letting $\delta_c = c_1-c_2$, we get what we want with

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\,\Sigma^{-1}\,\boldsymbol{x}\right)}\, d\boldsymbol{x} = N \int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^T\,\Sigma_\delta^{-1}\,\boldsymbol{\delta}\right)}\, d\boldsymbol{\delta}$$

and to do this, we just need to let

$$A = \begin{pmatrix} A_\delta \\ A_P \end{pmatrix}$$

where, e.g. in 3D

$$\begin{aligned} (A_\delta)_1 &= (1\ \ 0\ \ 0\ \ {-1}\ \ 0\ \ 0) \\ (A_P)_1 &= (1\ \ 0\ \ 0\ \ 1\ \ 0\ \ 0) \end{aligned}$$

Using this transformation we have

$$A^T\,\Sigma A = \begin{pmatrix} \Sigma_\delta & C \\ C^T & \Sigma_P \end{pmatrix}$$

Then we can integrate out the dependence on $\boldsymbol{p}$, writing

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\,\Sigma^{-1}\,\boldsymbol{x}\right)}\, d\boldsymbol{x} = \int V(r)\, e^{-\frac{1}{2}\left([\boldsymbol{\delta}\ \ \boldsymbol{p}]^T\left(A^T\,\Sigma A\right)^{-1}\,[\boldsymbol{\delta}\ \ \boldsymbol{p}]\right)}\, d\boldsymbol{\delta}\, d\boldsymbol{p}$$

But this is just equivalent to taking the marginal distribution in $\boldsymbol{\delta}$ and multiplying by the integral over the $\boldsymbol{p}$ coordinates, which in fact means we only need to compute ${\Sigma_\delta}^{-1}$ and (once all normalization factors are accounted for) we get

$$\begin{aligned}\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\,\Sigma^{-1}\,\boldsymbol{x}\right)}\, d\boldsymbol{x} &= \sqrt{\frac{|2\pi\Sigma|}{|\pi\Sigma_\delta|}}\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^T\,{\Sigma_\delta}^{-1}\boldsymbol{\delta}\right)}\, d\boldsymbol{\delta} \\ &= \left(\sqrt{\pi^{(d-k)}\,\frac{|\Sigma|}{|\Sigma_\delta|}}\right)\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^T\,{\Sigma_\delta}^{-1}\boldsymbol{\delta}\right)}\, d\boldsymbol{\delta}\end{aligned}$$

When Factoring out the Overlap Element

Tests

Dealing with Watson Modes

When working with Gaussians constructed from Cartesian-displacement normal modes the approach above won't work as specified, since even though we have proper Gaussians in $(3N-6)$-dimensional normal modes space, we don't have them in proper $3N$ space as that would require a singular covariance matrix

The difficulty is then to figure out how many modes we can construct that *don't* change the bond length, this is equivalent to finding the set of solutions W such that

$$(L\,W_P)_1 = (L\,W_P)_2$$

where $(L\,W_P)_1$ is the $3{\times}(3N{-}6)$ matrix encoding how the Cartesian coordinates of atom 1 change and L_2 is the corresponding matrix for atom 2

This implies that

$$(L\,W_P)_1 - (L\,W_P)_2 = 0$$

but we also know that (using the A_δ from above)

$$\begin{aligned}(L\,W_P)_1 - (L\,W_P)_2 &= A_\delta\, L\, W_P \\ &= 0\end{aligned}$$

therefore W_P is simply a basis for the nullspace of $A_\delta\, L$ and the total transformation W_P we are truly interested

We can recognize now that this is equivalent to computing the SVD of $A_\delta\, L$ as

$$V\,S\,W = A_\delta\, L$$

where we will have k (up to 3) non-zero singular values corresponding to the columns of A that change the bond length (W_δ) and $3N{-}6{-}k$ columns of A that correspond to the dimensions that do not change the bond length (W_P)

Moreover, to actually determine how the bond lengths change, given a set of k displacements along these new modes, $\boldsymbol{q}$, we can note that we'll have an initial set of δ coordinates given by

$$\boldsymbol{\delta}_0 = A_\delta \boldsymbol{c}$$

where $\boldsymbol{c}$ is the vector of $3N$ coordinates and to get the change in these coordinates we simply note that the unit change is given by $A_\delta\, L W_\delta$ and so in total we have

$$r = |\boldsymbol{\delta}_0 + A_\delta\, L W_\delta \boldsymbol{q}|$$

and then to get derivatives with respect to the normal modes we start by writing $\boldsymbol{\delta} = A_\delta\, L W_\delta \boldsymbol{q}$ because we already have formulae for $\nabla_{\boldsymbol{\delta}^n} r$, and so we know

$$\begin{aligned}\nabla_{q^n} r &= \nabla_q \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= (A_\delta\, L W_\delta)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r\end{aligned}$$

and then to get back to the normal mode derivatives we can write

$$\begin{aligned}\nabla_{l^n} r &= \nabla_L \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= \nabla_L q\, \nabla_q \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= W_\delta^{-1} (A_\delta\, L W_\delta)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= (A_\delta\, L)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r\end{aligned}$$

which is actually something we could have known without needing the W_δ step but oh well...

Then to get what we really need,

$$\nabla_{l^n} f(r) = T([\nabla_l r, \nabla_{l^2} r, \ldots], [\nabla_r f, \nabla_{r^2} f, \ldots])$$

where T is just a standard tensor derivative conversion obtained by mapping out all of the necessary transformations

Alternate Derivative Issues

We really have

$$A_\delta\, L = \nabla_\delta q$$

but can we say

Angles

Angles are given by

$$\theta_{ijk} = \tan^{-1}\left(\frac{|a \times b|}{|a|\,|b|}, \frac{a \cdot b}{|a|\,|b|}\right) \text{ where } a = x_j - x_i \text{ and } b = x_k - x_i$$

Therefore to get a change we either need a change in $\hat{a}$ or $\hat{b}$, which means to *avoid* changing the bond length we need to either shift every coordinate by the same amount or we need to displace along $\hat{a}$ or $\hat{b}$, we can set up a simple basis for this by taking every possible vector we can think of that doesn't change the angle and orthogonalizing this, leading in general to a basis of about 5 vectors that don't change the angle

We can then project this basis *out* of the normal modes and compute the nullspace for this to find both the proper angle-changing modes and the corresponding complement

Generic Form

Tests

Complex Phase Quadrature

We know from the work on projections that we can reduce the integrals down to the form

$$\int V(\delta)\,\exp\!\left(-\frac{1}{2}\,(\Sigma_\delta)^{-1}\odot(q_\delta-\mu_\delta)^2 + \mathbb{i}(\Sigma_\delta p)\cdot q_\delta\right)$$

and by expanding the product (and doing some shifts by μ) we get

$$\int V(\delta)\,\exp\!\left(-\frac{1}{2}\,(\Sigma_\delta)^{-1}\odot(q_\delta-\mu_\delta)^2 + \mathbb{i}(\Sigma_\delta p)\cdot q_\delta\right) = \int V(\delta+\mu)\,\exp(\mathbb{i}(\Sigma_\delta p)\cdot(\delta+\mu))\,\exp\!\left(-\frac{1}{2}\,(\Sigma_\delta)^{-1}\odot\delta^2\right)$$

where can evaluate the inner integral by Gauss Hermite quadrature, although we will first diagonalize Σ_δ and use the transformation to write $y_k = L_k(q-\mu)$

$$\int V(\delta-\mu)\,\exp(\mathbb{i}(\Sigma_\delta p)\cdot\delta)\,\exp\!\left(-(\Sigma_\delta)^{-1}\odot\delta^2\right) = \int V(\delta)\,\prod_k \exp(\mathbb{i}(\Sigma_\delta p)\cdot(L^{\mathrm{T}}y)_k)\,\exp\!\left(-\alpha_k\,{y_k}^2\right)$$

taking the appropriate direct product of 1D quadrature points and weights to get (for vector x)

$$\begin{aligned}\int V(\delta)\,\exp(\mathbb{i}(\Sigma_\delta p)\cdot\delta)\,\exp\!\left(-(\Sigma_\delta)^{-1}\odot(\delta-\mu_\delta)^2\right) &= \sum_x w_x\,V(x)\,\exp(\mathbb{i}(\Sigma_\delta p)\cdot(x-\mu)) \\ &= \sum_x w_x\,V(x)\,(\cos((\Sigma_\delta p)\cdot x) + \mathbb{i}\,\sin((\Sigma_\delta p)\cdot x))\end{aligned}$$

and upon rephasing, we will take the ± combinations of the $\mathbb{i}\sin((\Sigma_\delta p)\cdot x))$ terms to recover entirely real eigenvalues, and therefore can omit those terms in the calculations

---

Gram-Schmidt Orthogonalized Gaussians

Given two distributed Gaussians, ϕ_1, ϕ_2 we can obviously orthogonalize this system by writing

$$\varphi_2 = \phi_2 - \langle\phi_1|\phi_2\rangle\,\phi_1$$

which has corresponding norm

$$\langle\varphi_2|\varphi_2\rangle = \langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_1|\phi_2\rangle + \langle\phi_1|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_1|\phi_1\rangle$$

$$= 1 - \langle \phi_1 | \phi_2 \rangle^2$$

and then if we want to introduce a third Gaussian, ϕ_3, we can orthogonalize this relative to the initial set of Gaussians by writing

$$\varphi_3 = \phi_3 - \langle \phi_1 | \phi_3 \rangle \phi_1 - \langle \phi_2 | \phi_3 \rangle \phi_2$$

or we can oronalize relative the the new set by

$$\varphi_3 = \phi_3 - \langle \phi_1 | \phi_3 \rangle \phi_1 - \frac{\langle \varphi_2 | \phi_3 \rangle}{\langle \varphi_2 | \varphi_2 \rangle} \varphi_2$$

Partial Orthog Reduction

which almost orthogonal to φ_2, that being a simple linear combination of ϕ_1 and ϕ_2, therefore this has a norm given by (reduction done as I went)

$$\langle \varphi_3 | \varphi_3 \rangle = 1 - \langle \phi_1 | \phi_3 \rangle^2 - \langle \phi_2 | \phi_3 \rangle^2 + 2 \langle \phi_1 | \phi_3 \rangle \langle \phi_2 | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle$$

and introducing a n-th function, the orthogonalization is obvious but the normalization comes out to

$$\langle \varphi_3 | \varphi_3 \rangle = 1 - \sum_{i<4} \langle \phi_i | \phi_4 \rangle^2 + \sum_{j<4} \langle \phi_i | \phi_4 \rangle \sum_{i<4\neq j} \langle \phi_j | \phi_4 \rangle \langle \phi_i | \phi_j \rangle$$

Full Orthog Reduction

and generically we can write this as

$$\varphi_k = \phi_k - \sum_{i=1}^{k-1} \langle \overline{\varphi_i} | \phi_k \rangle \varphi_i$$

$$\langle \overline{\varphi_i} | \phi_k \rangle = \frac{\langle \varphi_i | \phi_k \rangle}{\langle \varphi_i | \varphi_i \rangle}$$

which inductively is

$$\begin{aligned}
\varphi_1 &= \phi_1 \\
\varphi_2 &= \phi_2 - \langle \phi_1 | \phi_2 \rangle \phi_1 \\
\varphi_3 &= \phi_3 - \langle \phi_1 | \phi_3 \rangle \phi_1 - \langle \overline{\varphi_2} | \phi_3 \rangle \varphi_2 \\
&= \phi_3 - \langle \phi_1 | \phi_3 \rangle \phi_1 - \langle \overline{\varphi_2} | \phi_3 \rangle \phi_2 + \langle \overline{\varphi_2} | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle \phi_1 \\
&= \phi_3 - \left(\langle \phi_1 | \phi_3 \rangle + \langle \overline{\varphi_2} | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle \right) \phi_1 - \langle \overline{\varphi_2} | \phi_3 \rangle \phi_2 \\
\varphi_4 &= \phi_4 - \langle \phi_1 | \phi_4 \rangle \phi_1 - \langle \overline{\varphi_2} | \phi_4 \rangle \varphi_2 - \langle \overline{\varphi_3} | \phi_4 \rangle \varphi_3 \\
&= \phi_4 - \left(\langle \phi_1 | \phi_3 \rangle + \langle \overline{\varphi_2} | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle \right) \phi_1 - \langle \overline{\varphi_2} | \phi_3 \rangle \phi_2 \\
&\qquad - \langle \overline{\varphi_3} | \phi_4 \rangle \left(\phi_3 - \left(\langle \phi_1 | \phi_3 \rangle + \langle \overline{\varphi_2} | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle \right) \phi_1 - \langle \overline{\varphi_2} | \phi_3 \rangle \phi_2 \right)
\end{aligned}$$

we'll note that we can also write

$$
\begin{aligned}
\Gamma_k &= \phi_k - \sum_{i=1}^{k-1} \left\langle \phi_i \middle| \phi_k \right\rangle \phi_i \\
\varphi_k &= \Gamma_k - \sum_{i=1}^{k-1} \left\langle \overline{\Gamma_i} \middle| \phi_k \right\rangle \Gamma_i \\
&= \phi_k - \sum_{i=1}^{k-1} \left\langle \phi_i \middle| \phi_k \right\rangle \phi_i
\end{aligned}
$$

Tests

Interpolations

The simplest treatment for the interpolation of the potential is the inverse-distance weighted interpolation, given by

$$
V(x) = \frac{\sum_i V\left(\xi^{(i)}\right) \left| x - \xi^{(i)} \right|^{-p}}{\sum_i \left| x - \xi^{(i)} \right|^{-p}}
$$

We will take advantage of the fact, however, that at every point we have a local quadratic expansion, i.e. we can write

$$
V\left(x;\, \xi^{(i)}\right) = V\left(\xi^{(i)}\right) + \nabla_x V\left(\xi^{(i)}\right) \odot \left(x - \xi^{(i)}\right) + \frac{1}{2} \nabla_x V\left(\xi^{(i)}\right) \odot \left(x - \xi^{(i)}\right)^2
$$

where $\odot$ is a total contraction and $\left(x - \xi^{(i)}\right)^2$ is the outer product of $\left(x - \xi^{(i)}\right)$ with itself.

Now we can do an inverse distance weighting of these Taylor series to give

$$
V(x) = \frac{\sum_i V\left(x;\, \xi^{(i)}\right) \left| x - \xi^{(i)} \right|^{-p}}{\sum_i \left| x - \xi^{(i)} \right|^{-p}}
$$

Derivatives

Unfortunately, derivatives of this interpolation are formally quite messy as we have

$$
\nabla_x V(x) = \sum_i \left(\nabla_x V\left(x;\, \xi^{(i)}\right) w^{(i)} + V\left(x;\, \xi^{(i)}\right) \nabla_x w^{(i)} \right)
$$

where

$$\nabla_x w^{(i)} = \frac{\nabla_x |x-\xi^{(i)}|^{-p}}{\sum_j \left|x-\xi^{(j)}\right|^{-p}} + \left|x-\xi^{(i)}\right|^{-p} \nabla_x \left(\sum_j \left|x-\xi^{(j)}\right|^{-p}\right)^{-1}$$

For later convenience, we will write

$$\begin{aligned} d\left(x,\ \xi^{(i)},\ m\right) &= \left(\left(x-\xi^{(i)}\right)\cdot\left(x-\xi^{(i)}\right)\right)^{-m} \\ &= \left|\left(x-\xi^{(i)}\right)\right|^{-2m} \end{aligned}$$

and so we have

$$\begin{aligned} \nabla_x |x-\xi^{(i)}|^{-p} &= \nabla_x\, d\left(x,\ \xi^{(i)},\ p/2\right) \\ &= p\ \left(x-\xi^{(i)}\right) d\left(x,\ \xi^{(i)},\ p/2+1\right) \end{aligned}$$

which is becomes poorly behaved when distances are small

Then we also have

$$\begin{aligned} \nabla_x \left(\sum_j \left|x-\xi^{(j)}\right|^{-p}\right)^{-1} &= -\left(\sum_j \left|x-\xi^{(j)}\right|^{-p}\right)^{-2} \sum_j \nabla_x |x-\xi^{(j)}|^{-p} \\ &= -\left(\sum_j \left|x-\xi^{(j)}\right|^{-p}\right)^{-2} \sum_j p\ \left(x-\xi^{(j)}\right)\ d\left(x,\ \xi^{(j)},\ p/2+1\right) \end{aligned}$$

giving us

$$\begin{aligned} \nabla_x w^{(i)} &= \left(x-\xi^{(i)}\right) \frac{p\ \ d\left(x,\ \xi^{(i)},\ p/2+1\right)}{\sum_j \left|x-\xi^{(i)}\right|^{-p}} - \frac{\left|x-\xi^{(i)}\right|^{-p}}{\left(\sum_j \left|x-\xi^{(i)}\right|^{-p}\right)^2} \sum_j p\ \left(x-\xi^{(j)}\right)\ d\left(x,\ \xi^{(j)},\ p/2+1\right) \\ &= \frac{1}{\sum_j \left|x-\xi^{(i)}\right|^{-p}} \left(\left(x-\xi^{(i)}\right) p\ \ d\left(x,\ \xi^{(i)},\ p/2+1\right) - w^{(i)} \sum_j p\ \left(x-\xi^{(j)}\right)\ d\left(x,\ \xi^{(j)},\ p/2+1\right)\ \right) \\ &= \sum_k \left(x-\xi^{(j)}\right) \left(\delta_{ki}-w^{(i)}\right) p\ \frac{d\left(x,\ \xi^{(j)},\ p/2+1\right)}{\sum_j d\left(x,\ \xi^{(j)},\ p/2\right)} \end{aligned}$$

then biting the bullet and doing this one more time we have

$$\nabla_{x^2} w^{(i)} = \nabla_x \left(\sum_j \left(x-\xi^{(j)}\right) \left(\delta_{ji}-w^{(i)}\right) p\ \frac{d\left(x,\ \xi^{(j)},\ p/2+1\right)}{\sum_k d\left(x,\ \xi^{(k)},\ p/2\right)}\right)$$

which has three terms, the first two of which are simple

$$\left(\nabla_x\left(x-\xi^{(j)}\right)\right)\ldots = I\ldots$$
$$\left(x-\xi^{(j)}\right)\nabla_x\left(\delta_{ji}-w^{(i)}\right)\ldots = -\left(x-\xi^{(j)}\right)\otimes\nabla_x w^{(i)}$$

and the last of which is a bit nastier, but is really just a redo of the previous stuff

$$\nabla_x\frac{d\left(x,\ \xi^{(j)},\ p/2+1\right)}{\sum_j d\left(x,\ \xi^{(j)},\ p/2\right)}=\sum_k\left(x-\xi^{(k)}\right)(p+2)\left(\delta_{kj}-\frac{d\left(x,\ \xi^{(j)},\ p/2+1\right)}{\sum_j d\left(x,\ \xi^{(j)},\ p/2\right)}\right)\frac{d\left(x,\ \xi^{(j)},\ p/2+2\right)}{\sum_j d\left(x,\ \xi^{(j)},\ p/2\right)}$$

Now we can generalize fully, letting

$$\Gamma^{(i)}(p,n) = \frac{d\left(x,\ \xi^{(j)},\ p/2+n\right)}{\sum_j d\left(x,\ \xi^{(j)},\ p/2\right)}$$
$$=\frac{\left|x-\xi^{(i)}\right|^{-(p+2n)}}{\sum_j\left|x-\xi^{(i)}\right|^{-p}}$$

We have

$$V(x) = \sum_i V\left(x;\ \xi^{(i)}\right)\Gamma^{(i)}(p,n)$$
$$\nabla_x\Gamma^{(i)}(p,n) =\sum_j\left(x-\xi^{(j)}\right)(p+n+1)\left(\delta_{ij}-\Gamma^{(i)}(p,n)\right)\Gamma^{(j)}(p,n+1)$$

which gives a generic way to build the derivatives if we wanted, for now, we'll just write

$$\nabla_x V(x) =\sum_i \nabla_x V\left(x;\ \xi^{(i)}\right)w^{(i)} + V\left(x;\ \xi^{(i)}\right)\nabla_x w^{(i)}$$
$$\nabla_{x^2} V(x) = \sum_i \nabla_{x^2} V\left(x;\ \xi^{(i)}\right)w^{(i)} + \left(\nabla_x V\left(x;\ \xi^{(i)}\right)\otimes\nabla_x w^{(i)}\right)^T + \left(\nabla_x V\left(x;\ \xi^{(i)}\right)\otimes\nabla_x w^{(i)}\right)$$
$$+ V\left(x;\ \xi^{(i)}\right)\nabla_{x^2} w^{(i)}$$

where

$$\nabla_x w^{(i)} = (p+1)\sum_j\left(x-\xi^{(j)}\right)\left(\delta_{ij}-w^{(i)}\right)\Gamma^{(i)}(p,1)$$
$$\nabla_{x^2} w^{(i)} = (p+1)\sum_j I\left(\delta_{ij}-w^{(i)}\right)\Gamma^{(i)}(p,1) - \left(x-\xi^{(j)}\right)\otimes\left(\nabla_x w^{(i)}\right)\Gamma^{(i)}(p,1)$$
$$+ (p+2)\left(\delta_{ij}-w^{(i)}\right)\sum_k\left(x-\xi^{(j)}\right)\otimes\left(x-\xi^{(k)}\right)\left(\delta_{jk}-\Gamma^{(j)}(p,1)\right)\Gamma^{(j)}(p,2)$$

Shifting to a full tensor algebra form, letting $\Gamma(p,n) = \left\{\Gamma^{(i)}(p,n)\right\}_i$, $\Delta=\left\{\left(x-\xi^{(i)}\right)\right\}$ we have

$$\nabla_x\Gamma(p,n) = (p+n+1)\left(\operatorname{diag}(\Gamma(p,n)) - \Gamma(p,n)\otimes\Gamma(p,n+1)\right)\Delta)$$

and then we'll note that

$$\nabla_x \mathrm{diag}(\Gamma(p,n)) = \mathrm{diag}(\nabla_x \Gamma(p,n))$$

and so quite simply we have (roughly...I didn't bother to get everything clean)

$$\begin{aligned}\nabla_{x^2}\Gamma(p,n) = (p+n+1)\,&(\mathrm{diag}(\nabla_x\Gamma(p,n)) - \nabla_x(\Gamma(p,n)\otimes\Gamma(p,n+1)))\,\Delta \\ &+ (\mathrm{diag}(\Gamma(p,n)) - \Gamma(p,n)\otimes\Gamma(p,n+1))\otimes\mathrm{diag}(I\ldots))\end{aligned}$$

$$\begin{aligned}\nabla_x(AB) &= \nabla_x A\ B + A\,\nabla_x B^{n\to 1} \\ \nabla_x() &= \end{aligned}$$

$$\nabla_Q(A\,\langle\alpha,\,\beta\rangle\,B) = \nabla_Q A\,\langle\alpha+1,\,\beta\rangle\,B + \left(A\,\langle\alpha,\,\beta+1\rangle\,\nabla_Q B\right)^{n\to 1}$$

In[635]:=

```
Grad[ConstantArray[{x, y, z}, 15], {x, y, z}] // Transpose[#,
    {2, 3, 1}
   ] & // Dimensions
```

Out[635]=

```
{3, 15, 3}
```

In[636]:=

```
Clear[DM, prod, transp, rank];
prod[A_, B_] := prod[A, B, rank[A], 1];
DM[prod[A_, B_, n_, m_]] :=
  transp[prod[DM[A], B, n + 1, m], 1, 1] +
   transp[prod[A, DM[B], n, m + 1], rank[A], 1];
DM[DM[x_, k_]] := DM[x, k + 1];
DM[transp[A_, n_, k_]] := transp[DM[A], n + 1, k + 1];
DM[HoldPattern[Plus][x___]] := Plus @@ Map[DM, {x}];
prod[HoldPattern[Plus][x___], B_, n_, k_] :=
  Plus @@ Map[prod[#, B, n, k] &, {x}];
prod[A_, HoldPattern[Plus][x___], n_, k_] :=
  Plus @@ Map[prod[A, #, n, k] &, {x}];
transp[HoldPattern[Plus][x___], n_, k_] :=
  Plus @@ Map[transp[#, n, k] &, {x}];
transp[A_, {n1_, k1_, r__}] :=
  Fold[transp[#, #2[[1]], #2[[2]]] &, A, Partition[{n1, k1, r}, 2]];
DMSimp[expr_] := expr //. {
    DM[s_Symbol] :> DM[s, 1],
    DM[DM[s_, k_]] :> DM[s, k + 1],
    rank[DM[x_, k_]] :> rank[x] + k
   };
DMFormat[expr_] :=
 Interpretation[
  Style[
   expr //. {
     DM[A_] :> Row@{Subscript["∇", "x"], A},
     DM[A_, k_] :> Row@{Subscript["∇", Superscript["x", k]], A},
     transp[x_, a_, b_] :> Superscript[Row@{"(", x, ")"}, Row@{a, "→", b}],
     prod[A_, B_, n_, k_] :> Row@{A, "〈", n, ",", k, "〉", B},
     rank[A_] :> Subscript["n", A]
    },
   18,
   ShowStringCharacters → False
  ],
  expr
 ]
```

In[626]:=

```
Ordering[#, -1] & /@ Permutations[{1, 0, 0, 0}]
```

In[624]:=

```
Ordering[#, -2] & /@ Permutations[{1, 1, 0, 0, 0}]
```

Out[624]=

```
{{1, 2}, {1, 3}, {1, 4}, {1, 5}, {2, 3}, {2, 4}, {2, 5}, {3, 4}, {3, 5}, {4, 5}}
```

In[627]:=

```
Ordering[#, -1] & /@ Permutations[{1, 0, 0, 0, 0}]
```

Out[627]=

```
{{1}, {2}, {3}, {4}, {5}}
```

In[648]:=

```
DM[DM[prod[A, B, a, b]]] // DMSimp // Apply[List] // Map[DMFormat] // Column
```

Out[648]=

$$((\mathrm{A}\langle \mathrm{a},2+\mathrm{b}\rangle \nabla_{\mathrm{x}^2}\mathrm{B})^{\mathrm{n_A}\to 1})^{1+\mathrm{n_A}\to 2}$$
$$((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1+\mathrm{a},1+\mathrm{b}\rangle \nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2}$$
$$((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1+\mathrm{a},1+\mathrm{b}\rangle \nabla_{\mathrm{x}^1}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2}$$
$$((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2+\mathrm{a},\mathrm{b}\rangle \mathrm{B})^{1\to 1})^{2\to 2}$$

In[492]:=

```
DM[DM[DM[prod[A, B, a, b]]]] // DMSimp // Apply[List] // Map[DMFormat] // Column
```

Out[492]=

$$(((\mathrm{A}\langle \mathrm{a},3+\mathrm{b}\rangle \nabla_{\mathrm{x}^3}\mathrm{B})^{\mathrm{n_A}\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1+\mathrm{a},2+\mathrm{b}\rangle \nabla_{\mathrm{x}^2}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1+\mathrm{a},2+\mathrm{b}\rangle \nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1+\mathrm{a},2+\mathrm{b}\rangle \nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2+\mathrm{a},1+\mathrm{b}\rangle \nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2+\mathrm{a},1+\mathrm{b}\rangle \nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2+\mathrm{a},1+\mathrm{b}\rangle \nabla_{\mathrm{x}^1}\mathrm{B})^{2+\mathrm{n_A}\to 1})^{2\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3+\mathrm{a},\mathrm{b}\rangle \mathrm{B})^{1\to 1})^{2\to 2})^{3\to 3}$$

In[619]:=

```
matDerivPerms[A_, B_, a_, b_, o_, s_] :=
  With[
   {
    base = prod[If[s == 0, A, DM[A, s]], If[s == o, B, DM[B, o - s]], a + s, b + (o - s)],
    nAPos =
     Ordering[#, -(o - s)] & /@
      Permutations@Join[ConstantArray[1, o - s], ConstantArray[0, s]],
    nAs = rank[A] + Range[(o - s)]
   },
   transp[
      base,
      Flatten@Transpose[{
         ReplacePart[Range[o], Thread[# → nAs]],
         Range[o]
        }]
     ] & /@ nAPos
  ];
matProdDeriv[prod[A_, B_, a_, b_], o_] :=
 Table[
  matDerivPerms[A, B, a, b, o, s],
  {s, 0, o}
 ]
```

In[629]:=

```
Binomial[6, 2]
```

Out[629]=

```
15
```

In[622]:=

```
matProdDeriv[prod[A, B, a, b], 4] // Flatten // Map[DMFormat] // Column
```

Out[622]=

$$((((\mathrm{A}\langle \mathrm{a},4 + \mathrm{b}\rangle\nabla_{\mathrm{x}^4}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3+\mathrm{n_A}\to 3})^{4+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},3 + \mathrm{b}\rangle\nabla_{\mathrm{x}^3}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3+\mathrm{n_A}\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},3 + \mathrm{b}\rangle\nabla_{\mathrm{x}^3}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3})^{3+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},3 + \mathrm{b}\rangle\nabla_{\mathrm{x}^3}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3})^{3+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},3 + \mathrm{b}\rangle\nabla_{\mathrm{x}^3}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3})^{3+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{3\to 3})^{2+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{3\to 3})^{2+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1\to 1})^{2\to 2})^{1+\mathrm{n_A}\to 3})^{2+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{3\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{3\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2\to 2})^{1+\mathrm{n_A}\to 3})^{4\to 4}$$
$$((((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2\to 2})^{3\to 3})^{1+\mathrm{n_A}\to 4}$$
$$((((\nabla_{\mathrm{x}^4}\mathrm{A}\langle 4 + \mathrm{a},\mathrm{b}\rangle\mathrm{B})^{1\to 1})^{2\to 2})^{3\to 3})^{4\to 4}$$

In[615]:=

```
Nest[DM, prod[A, B, a, b], 3] // DMSimp // Apply[List] // Map[DMFormat] // Column
```

Out[615]=

$$(((\mathrm{A}\langle \mathrm{a},3 + \mathrm{b}\rangle\nabla_{\mathrm{x}^3}\mathrm{B})^{\mathrm{n_A}\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1\to 1})^{1+\mathrm{n_A}\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^1}\mathrm{A}\langle 1 + \mathrm{a},2 + \mathrm{b}\rangle\nabla_{\mathrm{x}^2}\mathrm{B})^{1+\mathrm{n_A}\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2\to 2})^{2+\mathrm{n_A}\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{1\to 1})^{2+\mathrm{n_A}\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^2}\mathrm{A}\langle 2 + \mathrm{a},1 + \mathrm{b}\rangle\nabla_{\mathrm{x}^1}\mathrm{B})^{2+\mathrm{n_A}\to 1})^{2\to 2})^{3\to 3}$$
$$(((\nabla_{\mathrm{x}^3}\mathrm{A}\langle 3 + \mathrm{a},\mathrm{b}\rangle\mathrm{B})^{1\to 1})^{2\to 2})^{3\to 3}$$

and so

$$\nabla_x V(x) = \nabla_x V\big(x;\, \xi^{(.)}\big)\odot w^{(.)} + \nabla_x w^{(.)}\odot V\big(x;\, \xi^{(.)}\big)$$
$$\nabla_x V\,(x) = \nabla_x V\big(x;\, \xi^{(.)}\big)\odot w^{(.)}$$

3rd Derivative Estimation

We can assume a Morse-like expansion along each mode to estimate the 3rd derivative at each interpolation point