Derivation of $\frac{\delta F}{\delta E^*_{ij}}$ in terms of $\underline{\underline{E}}$, $\underline{\underline{\Pi}}$ and their derivatives

1 Final comments on how it is done here

So after a lot of deliberation, I am pretty confident that there are a couple ways to get the functional derivatives, but the general rule is based on simply $\frac{\delta E_{ij}}{\delta E_{ab}} = \delta_{ia}\delta_{jb}$. If one is to symmetrize it, a factor of $\frac{1}{2}$ should be used and the result should be equivalent to simply symmetrizing the possibly asymmetric result, doing $\frac{\delta F}{\delta E_{ij}} + \frac{\delta F}{\delta E_{ji}}$. When it comes to the second order gradient "symmetry", essentially the same applies, when using the "integral/delta function" method, the problem doesn't come up and equaling the two gives something along the lines of $\frac{\partial \psi_{,ij}}{\partial \psi_{,ab}} = \delta_{ia}\delta_{jb}$, though if one uses the symmetrized version with a $\frac{1}{2}$ factor, it gives the same result.

Next about the asymmetries that seem to occur in our F, they would come up anywhere where there is a term with $E^*_{ij,\ldots}$ without a matching $E_{ij,\ldots}$ in the term. Notably, this doesn't happen in any of the terms used by Jack, or the expression for $\underline{\underline{\Pi}}$ that he used, however the other $\underline{\underline{\Pi}}$ expression which has $\underline{\underline{E}}^*$ occuring does have this happen, thus it leads to asymmetries that would need to be fixed.

In this document I will only use the square root version of $\underline{\underline{\Pi}}$ and so we do not need to worry about asymmetry there, this document is meant as a reference for the code implementation without too much commentary, just correct results, split in smaller terms.

2 Final, cheatsheet

$$\Pi_{kl} = \frac{sE_{kl}}{\sqrt{E_{ab}E_{ab}}} + \frac{\delta_{kl}}{d} \tag{1}$$

$$\Pi_{kl,m} = \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,m} - \frac{E_{kl}E_{cd}E_{cd,m}}{E_{ab}E_{ab}}\right) \tag{2}$$

$$\Pi_{kl,mn} = \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl,m}E_{cd}E_{cd,n} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}}\right. \tag{3}$$

$$\left. + 3\frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right) \tag{4}$$

$$f_{\text{bulk}} = \frac{A}{2}E_{ij}E^*_{ij} + \frac{C}{4}(E_{ij}E^*_{ij})^2 \tag{5}$$

$$f_{\text{comp}} = b_1^{\|}\Pi_{kl}E_{ij,k}E^*_{ij,l} + b_1^{\perp}T_{kl}E_{ij,k}E^*_{ij,l} \tag{6}$$

$$f_{\text{curv}} = b_2^{\|}\Pi_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm} + b_2^{\perp}T_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} + b_2^{\|\perp}(\Pi_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} + T_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm}) \tag{7}$$

$$\frac{\delta F_{\text{bulk}}}{\delta E^*_{ij}} = \frac{1}{2}(A + CE_{ab}E^*_{ab})E_{ij} \tag{8}$$

$$\frac{\delta F_{\text{comp}}}{\delta E^*_{ij}} = -(b_1^{\|} - b_1^{\perp})(\Pi_{kl,l}E_{ij,k} + \Pi_{kl}E_{ij,kl}) - b_1^{\perp}E_{ij,kk} \tag{9}$$

$$\begin{aligned}\frac{\delta F_{\text{curv}}}{\delta E^*_{ij}} = {} & (b_2^{\|} + b_2^{\perp} - 2b_2^{\|\perp})\Big((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \\ & \qquad + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo}\Big) \\ & + (b_2^{\|\perp} - b_2^{\perp})\Big(\Pi_{po,po}E_{ij,kk} + \Pi_{kl,oo}E_{ij,lk} \\ & \qquad + 2\Pi_{po,o}E_{ij,kkp} + 2\Pi_{kl,o}E_{ij,lko} + 2\Pi_{kl}E_{ij,lkoo}\Big) \\ & + b_2^{\perp}E_{ij,kkoo}\end{aligned} \tag{10}$$

Brief derivations are below

3 Gradients of $\underline{\underline{\Pi}}$

$$\underline{\underline{\Pi}} = \sqrt{\frac{d-1}{d\underline{\underline{E}} : \underline{\underline{E}}}}\underline{\underline{E}} + \frac{\underline{\underline{\delta}}}{d} \quad \text{or} \quad \Pi_{kl} = \frac{sE_{kl}}{\sqrt{E_{ab}E_{ab}}} + \frac{\delta_{kl}}{d} \tag{11}$$

gives

$$\Pi_{kl,m} = \frac{sE_{kl,m}}{\sqrt{E_{ab}E_{ab}}} - \frac{sE_{kl}E_{cd}E_{cd,m}}{(E_{ab}E_{ab})^{\frac{3}{2}}} = \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,m} - \frac{E_{kl}E_{cd}E_{cd,m}}{E_{ab}E_{ab}}\right) \tag{12}$$

$$\Pi_{kl,mn} = \frac{sE_{kl,mn}}{\sqrt{E_{ab}E_{ab}}} - \frac{sE_{kl,m}E_{cd}E_{cd,n}}{(E_{ab}E_{ab})^{\frac{3}{2}}} - \frac{s(E_{kl,n}E_{cd}E_{cd,m} + E_{kl}E_{cd,n}E_{cd,m} + E_{kl}E_{cd}E_{cd,mn})}{(E_{ab}E_{ab})^{\frac{3}{2}}} \tag{13}$$

$$+ \frac{3sE_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^{\frac{5}{2}}}$$

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,mn} - \frac{E_{kl,m}E_{cd}E_{cd,n} + E_{kl,n}E_{cd}E_{cd,m} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}}\right. \tag{14}$$

$$\left. + 3\frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right)$$

or, to check, also do

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl}E_{cd,n}E_{cd,m} + E_{kl}E_{cd}E_{cd,mn}}{E_{ab}E_{ab}} + 2\frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right) \tag{15}$$

$$- \frac{sE_{gh}E_{gh,n}}{(E_{ab}E_{ab})^{\frac{3}{2}}}\left(E_{kl,m} - \frac{E_{kl}E_{cd}E_{cd,m}}{E_{ab}E_{ab}}\right)$$

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl}E_{cd,n}E_{cd,m} + E_{kl}E_{cd}E_{cd,mn}}{E_{ab}E_{ab}} + 2\frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right. \tag{16}$$

$$\left. - \frac{E_{kl,m}E_{cd}E_{cd,n}}{E_{ab}E_{ab}} + \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right)$$

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl,m}E_{cd}E_{cd,n} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}}\right. \tag{17}$$

$$\left. + 3\frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2}\right) \quad \text{which is the same as above – yay}$$

4 Free energies and their functional derivatives

We start from the following terms, though quickly reorganize them in terms of $\underline{\underline{\Pi}}$ only

$$F = \int f_{\text{bulk}} + f_{\text{comp}} + f_{\text{curv}} \,\mathrm{d}V = F_{\text{bulk}} + F_{\text{comp}} + F_{\text{curv}} \tag{18}$$

$$f_{\text{bulk}} = \frac{A}{2} E_{ij} E^*_{ij} + \frac{C}{4} (E_{ij} E^*_{ij})^2 \tag{19}$$

$$f_{\text{comp}} = b_1^{\|} \Pi_{kl} E_{ij,k} E^*_{ij,l} + b_1^{\perp} T_{kl} E_{ij,k} E^*_{ij,l} \quad \text{maybe try adding} \quad b_1^d E_{ij,j} E^*_{ik,k} \quad \text{later too} \tag{20}$$

$$f_{\text{curv}} = b_2^{\|} \Pi_{kl} E_{ij,lk} \Pi_{mn} E^*_{ij,nm} + b_2^{\perp} T_{kl} E_{ij,lk} T_{mn} E^*_{ij,nm} + b_2^{\|\perp} (\Pi_{kl} E_{ij,lk} T_{mn} E^*_{ij,nm} + T_{kl} E_{ij,lk} \Pi_{mn} E^*_{ij,nm}) \tag{21}$$

leading to

$$f_{\text{comp}} = (b_1^{\|} - b_1^{\perp}) \Pi_{kl} E_{ij,k} E^*_{ij,l} + b_1^{\perp} E_{ij,k} E^*_{ij,k} \tag{22}$$

and

$$\begin{aligned} f_{\text{curv}} = \; & (b_2^{\|} + b_2^{\perp} - 2 b_2^{\|\perp}) \Pi_{kl} E_{ij,lk} \Pi_{mn} E^*_{ij,nm} \\ & + (b_2^{\|\perp} - b_2^{\perp}) (\Pi_{mn} E_{ij,kk} E^*_{ij,nm} + \Pi_{kl} E_{ij,lk} E^*_{ij,mm}) \\ & + b_2^{\perp} E_{ij,kk} E^*_{ij,mm} \end{aligned} \tag{23}$$

4.1 F_{bulk}

$$\frac{\delta}{\delta E^*_{ij}} \left(\frac{A}{2} E_{ab} E^*_{ab} + \frac{C}{4} (E_{ab} E^*_{ab})^2 \right) = \left(\frac{A}{2} + \frac{C}{2} E_{ab} E^*_{ab} \right) E_{ij} \tag{24}$$

(doesn't need symmetrizing, and using the symmetric functional derivative gives the same)

4.2 F_{comp} terms

$$\frac{\delta}{\delta E^*_{ij}} \Pi_{kl} E_{ab,k} E^*_{ab,l} = -\partial_m \Pi_{km} E_{ij,k} = -\Pi_{kl,l} E_{ij,k} - \Pi_{kl} E_{ij,kl} \tag{25}$$

(note that $\underline{\underline{\Pi}}$ only directly depends on $\underline{\underline{E}}$ meaning any derivatives wrt to $\underline{\underline{E}}^*$ are 0. This was also checked using the "integral/delta function" method, and again needs no symmetrizing and agrees with the previous, more detailed work)

$$\frac{\delta}{\delta E^*_{ij}} E_{ab,k} E^*_{ab,k} = -\partial_l E_{ij,l} = -E_{ij,kk} \tag{26}$$

(symmetric and agrees with previous) so

$$\frac{\delta F_{\text{comp}}}{\delta E^*_{ij}} = -(b_1^{\|} - b_1^{\perp}) (\Pi_{kl,l} E_{ij,k} + \Pi_{kl} E_{ij,kl}) - b_1^{\perp} E_{ij,kk} \tag{27}$$

4.3 $F_{\mathbf{curv}}$ terms

$$\frac{\delta}{\delta E^*_{ij}}\Pi_{kl}E_{ab,lk}\Pi_{mn}E^*_{ab,nm} = \partial_o\partial_p\Pi_{kl}E_{ij,lk}\Pi_{po} \tag{28}$$

$$= \partial_o(\Pi_{kl,p}E_{ij,lk}\Pi_{po} + \Pi_{kl}E_{ij,lkp}\Pi_{po} + \Pi_{kl}E_{ij,lk}\Pi_{po,p}) \tag{29}$$

$$\begin{aligned} = {} & \Pi_{kl,po}E_{ij,lk}\Pi_{po} + \Pi_{kl,o}E_{ij,lkp}\Pi_{po} + \Pi_{kl,o}E_{ij,lk}\Pi_{po,p} \\ & + \Pi_{kl,p}E_{ij,lko}\Pi_{po} + \Pi_{kl}E_{ij,lkpo}\Pi_{po} + \Pi_{kl}E_{ij,lko}\Pi_{po,p} \\ & + \Pi_{kl,p}E_{ij,lk}\Pi_{po,o} + \Pi_{kl}E_{ij,lkp}\Pi_{po,o} + \Pi_{kl}E_{ij,lk}\Pi_{po,po} \end{aligned} \tag{30}$$

$$\begin{aligned} = {} & (\Pi_{kl}\Pi_{po,po} + \Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,p}\Pi_{po,o} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \\ & + (\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + (\Pi_{kl,p}\Pi_{po} + \Pi_{kl}\Pi_{po,p})E_{ij,lko} \\ & + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \quad \text{next step uses symmetry of } \underline{\underline{\Pi}} \end{aligned} \tag{31}$$

$$\begin{aligned} = {} & (\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \\ & + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} \\ & + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \end{aligned} \tag{32}$$

(same result as previously, the only thing that makes me worried at all is using the symmetry of $\underline{\underline{\Pi}}$, but I think it's ok)

$$\frac{\delta}{\delta E^*_{ij}}\Pi_{mn}E_{ab,kk}E^*_{ab,nm} = \partial_o\partial_p\Pi_{po}E_{ij,kk} \tag{33}$$

$$= \Pi_{po,po}E_{ij,kk} + \Pi_{po,p}E_{ij,kko} + \Pi_{po,o}E_{ij,kkp} + \Pi_{po}E_{ij,kkpo} \tag{34}$$

$$= \Pi_{po,po}E_{ij,kk} + 2\Pi_{po,o}E_{ij,kkp} + \Pi_{po}E_{ij,kkpo} \tag{35}$$

$$\frac{\delta}{\delta E^*_{ij}}\Pi_{kl}E_{ab,lk}E^*_{ab,mm} = \partial_o\partial_p\Pi_{kl}E_{ij,lk}\delta_{po} \tag{36}$$

$$= \partial_o\partial_o\Pi_{kl}E_{ij,lk} \tag{37}$$

$$= \Pi_{kl,oo}E_{ij,lk} + 2\Pi_{kl,o}E_{ij,lko} + \Pi_{kl}E_{ij,lkoo} \tag{38}$$

$$\frac{\delta}{\delta E^*_{ij}}E_{ab,kk}E^*_{ab,mm} = \partial_o\partial_oE_{ij,kk} = E_{ij,kkoo} \tag{39}$$

giving overall

$$\begin{aligned}
\frac{\delta F_{\mathrm{curv}}}{\delta E^*_{ij}} = \; & (b_2^{\|} + b_2^{\perp} - 2b_2^{\|\perp})\Big((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \\
& \qquad\qquad + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo}\Big) \\
& + (b_2^{\|\perp} - b_2^{\perp})\Big(\Pi_{po,po}E_{ij,kk} + 2\Pi_{po,o}E_{ij,kkp} + \Pi_{po}E_{ij,kkpo} \\
& \qquad\qquad + \Pi_{kl,oo}E_{ij,lk} + 2\Pi_{kl,o}E_{ij,lko} + \Pi_{kl}E_{ij,lkoo}\Big) \\
& + b_2^{\perp}E_{ij,kkoo}
\end{aligned} \tag{40}$$

after one more simplification from symmetry

$$\begin{aligned}
= \; & (b_2^{\|} + b_2^{\perp} - 2b_2^{\|\perp})\Big((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \\
& \qquad\qquad + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo}\Big) \\
& + (b_2^{\|\perp} - b_2^{\perp})\Big(\Pi_{po,po}E_{ij,kk} + \Pi_{kl,oo}E_{ij,lk} \\
& \qquad\qquad + 2\Pi_{po,o}E_{ij,kkp} + 2\Pi_{kl,o}E_{ij,lko} + 2\Pi_{kl}E_{ij,lkoo}\Big) \\
& + b_2^{\perp}E_{ij,kkoo}
\end{aligned} \tag{41}$$