

Derivation of $\frac{\delta F}{\delta E_{ij}^*}$ in terms of \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 equating 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 $E_{ij,\dots}^*$ without a matching $E_{ij,\dots}$ 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{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

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

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

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

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

$$f_{\text{bulk}} = AE_{ij}E_{ij}^* + \frac{C}{2}(E_{ij}E_{ij}^*)^2 \quad (5)$$

$$f_{\text{comp}} = b_1^{\parallel} \Pi_{kl} E_{ij,k} E_{ij,l}^* + b_1^{\perp} T_{kl} E_{ij,k} E_{ij,l}^* \quad (6)$$

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

$$\frac{\delta F_{\text{bulk}}}{\delta E_{ij}^*} = (A + CE_{ab}E_{ab}^*)E_{ij} \quad (8)$$

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

$$\frac{\delta F_{\text{curv}}}{\delta E_{ij}^*} = (b_2^{\parallel} + b_2^{\perp} - 2b_2^{\parallel\perp}) \left((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \right. \quad (10)$$

$$\begin{aligned} &+ 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \Big) \\ &+ (b_2^{\parallel\perp} - b_2^{\perp}) \left(\Pi_{po,po}E_{ij,kk} + \Pi_{kl,oo}E_{ij,lk} \right. \\ &\quad \left. + 2\Pi_{po,o}E_{ij,kkp} + 2\Pi_{kl,o}E_{ij,lko} + 2\Pi_{kl}E_{ij,lkoo} \right) \\ &+ b_2^{\perp} E_{ij,kkoo} \end{aligned}$$

Brief derivations are below

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

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

gives

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

$$\begin{aligned} \Pi_{kl,mn} &= \frac{sE_{kl,mn}}{\sqrt{E_{ab}E_{ab}}} - \frac{sE_{kl,m}E_{cd}E_{cd,n}}{(E_{ab}E_{ab})^{\frac{3}{2}}} - \frac{s(E_{kl,n}E_{cd}E_{cd,m} + E_{kl}E_{cd,n}E_{cd,m} + E_{kl}E_{cd}E_{cd,mn})}{(E_{ab}E_{ab})^{\frac{3}{2}}} \\ &\quad + \frac{3sE_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^{\frac{5}{2}}} \end{aligned} \quad (13)$$

$$\begin{aligned} &= \frac{s}{\sqrt{E_{ab}E_{ab}}} \left(E_{kl,mn} - \frac{E_{kl,m}E_{cd}E_{cd,n} + E_{kl,n}E_{cd}E_{cd,m} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}} \right. \\ &\quad \left. + 3 \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2} \right) \end{aligned} \quad (14)$$

or, to check, also do

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

$$\begin{aligned} &- \frac{sE_{gh}E_{gh,n}}{(E_{ab}E_{ab})^{\frac{3}{2}}} \left(E_{kl,m} - \frac{E_{kl}E_{cd}E_{cd,m}}{E_{ab}E_{ab}} \right) \\ &= \frac{s}{\sqrt{E_{ab}E_{ab}}} \left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl}E_{cd,n}E_{cd,m} + E_{kl}E_{cd}E_{cd,mn}}{E_{ab}E_{ab}} + 2 \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2} \right. \end{aligned} \quad (16)$$

$$\begin{aligned} &\quad \left. - \frac{E_{kl,m}E_{cd}E_{cd,n}}{E_{ab}E_{ab}} + \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2} \right) \\ &= \frac{s}{\sqrt{E_{ab}E_{ab}}} \left(E_{kl,mn} - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl,m}E_{cd}E_{cd,n} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}} \right. \\ &\quad \left. + 3 \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2} \right) \quad \text{which is the same as above – yay} \end{aligned} \quad (17)$$

4 Free energies and their functional derivatives

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

$$F = \int f_{\text{bulk}} + f_{\text{comp}} + f_{\text{curv}} dV = F_{\text{bulk}} + F_{\text{comp}} + F_{\text{curv}} \quad (18)$$

$$f_{\text{bulk}} = AE_{ij}E_{ij}^* + \frac{C}{2}(E_{ij}E_{ij}^*)^2 \quad (19)$$

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

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

leading to

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

and

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

4.1 F_{bulk}

$$\frac{\delta}{\delta E_{ij}^*} \left(AE_{ab}E_{ab}^* + \frac{C}{2}(E_{ab}E_{ab}^*)^2 \right) = (A + CE_{ab}E_{ab}^*)E_{ij} \quad (24)$$

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

4.2 F_{comp} terms

$$\frac{\delta}{\delta E_{ij}^*} \Pi_{kl} E_{ab,k} E_{ab,l}^* = -\partial_m \Pi_{km} E_{ij,k} = -\Pi_{kl,l} E_{ij,k} - \Pi_{kl} E_{ij,kl} \quad (25)$$

(note that $\underline{\Pi}$ only directly depends on \underline{E} meaning any derivatives wrt to \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)

$$\frac{\delta}{\delta E_{ij}^*} E_{ab,k} E_{ab,k}^* = -\partial_l E_{ij,l} = -E_{ij,kk} \quad (26)$$

(symmetric and agrees with previous) so

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

4.3 F_{curv} terms

$$\frac{\delta}{\delta E_{ij}^*} \Pi_{kl} E_{ab,lk} \Pi_{mn} E_{ab,nm}^* = \partial_o \partial_p \Pi_{kl} E_{ij,lk} \Pi_{po} \quad (28)$$

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

$$= \Pi_{kl,po} E_{ij,lk} \Pi_{po} + \Pi_{kl,o} E_{ij,lkp} \Pi_{po} + \Pi_{kl,o} E_{ij,lk} \Pi_{po,p} \quad (30)$$

$$\begin{aligned} &+ \Pi_{kl,p} E_{ij,lko} \Pi_{po} + \Pi_{kl} E_{ij,lkpo} \Pi_{po} + \Pi_{kl} E_{ij,lko} \Pi_{po,p} \\ &+ \Pi_{kl,p} E_{ij,lk} \Pi_{po,o} + \Pi_{kl} E_{ij,lkp} \Pi_{po,o} + \Pi_{kl} E_{ij,lk} \Pi_{po,po} \end{aligned} \quad (31)$$

$$\begin{aligned} &= (\Pi_{kl} \Pi_{po,po} + \Pi_{kl,o} \Pi_{po,p} + \Pi_{kl,p} \Pi_{po,o} + \Pi_{kl,po} \Pi_{po}) E_{ij,lk} \\ &+ (\Pi_{kl,o} \Pi_{po} + \Pi_{kl} \Pi_{po,o}) E_{ij,lkp} + (\Pi_{kl,p} \Pi_{po} + \Pi_{kl} \Pi_{po,p}) E_{ij,lko} \\ &+ \Pi_{kl} \Pi_{po} E_{ij,lkpo} \quad \text{next step uses symmetry of } \underline{\Pi} \\ &= (\Pi_{kl} \Pi_{po,po} + 2\Pi_{kl,o} \Pi_{po,p} + \Pi_{kl,po} \Pi_{po}) E_{ij,lk} \\ &+ 2(\Pi_{kl,o} \Pi_{po} + \Pi_{kl} \Pi_{po,o}) E_{ij,lkp} \\ &+ \Pi_{kl} \Pi_{po} E_{ij,lkpo} \end{aligned} \quad (32)$$

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

$$\frac{\delta}{\delta E_{ij}^*} \Pi_{mn} E_{ab,kk} E_{ab,nm}^* = \partial_o \partial_p \Pi_{po} E_{ij,kk} \quad (33)$$

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

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

$$\frac{\delta}{\delta E_{ij}^*} \Pi_{kl} E_{ab,lk} E_{ab,mm}^* = \partial_o \partial_p \Pi_{kl} E_{ij,lk} \delta_{po} \quad (36)$$

$$= \partial_o \partial_o \Pi_{kl} E_{ij,lk} \quad (37)$$

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

$$\frac{\delta}{\delta E_{ij}^*} E_{ab,kk} E_{ab,mm}^* = \partial_o \partial_o E_{ij,kk} = E_{ij,kkoo} \quad (39)$$

giving overall

$$\frac{\delta F_{\text{curv}}}{\delta E_{ij}^*} = (b_2^{\parallel} + b_2^{\perp} - 2b_2^{\parallel\perp}) \left((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \right. \quad (40)$$

$$\begin{aligned} & \left. + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \right) \\ & + (b_2^{\parallel\perp} - b_2^{\perp}) \left(\Pi_{po,po}E_{ij,kk} + 2\Pi_{po,o}E_{ij,kkp} + \Pi_{po}E_{ij,kkpo} \right. \\ & \left. + \Pi_{kl,oo}E_{ij,lk} + 2\Pi_{kl,o}E_{ij,lko} + \Pi_{kl}E_{ij,lkoo} \right) \\ & + b_2^{\perp}E_{ij,kkoo} \end{aligned}$$

after one more simplification from symmetry

$$\begin{aligned} = & (b_2^{\parallel} + b_2^{\perp} - 2b_2^{\parallel\perp}) \left((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \right. \quad (41) \\ & \left. + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \right) \\ & + (b_2^{\parallel\perp} - b_2^{\perp}) \left(\Pi_{po,po}E_{ij,kk} + \Pi_{kl,oo}E_{ij,lk} \right. \\ & \left. + 2\Pi_{po,o}E_{ij,kkp} + 2\Pi_{kl,o}E_{ij,lko} + 2\Pi_{kl}E_{ij,lkoo} \right) \\ & + b_2^{\perp}E_{ij,kkoo} \end{aligned}$$