Derivation of $\frac{\delta F}{\delta E_{ij}^*}$ in terms of E_{ij} and its derivatives

1 Initial setup

$$F = \int f_{\text{bulk}} + f_{\text{comp}} + f_{\text{curv}} \, dV = F_{\text{bulk}} + F_{\text{comp}} + F_{\text{curv}}$$
(1)

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

$$f_{\text{comp}} = b_1^{\parallel} \Pi_{kl} E_{ij,k} E_{ij,l}^* + b_1^{\perp} T_{kl} E_{ij,k} E_{ij,l}^* \quad \text{maybe try adding} \quad b_1^d E_{ij,j} E_{ik,k}^* \quad \text{later too}$$
 (3)

$$f_{\rm curv} = \dots$$
 for later \dots (4)

(5)

where

$$\underline{\Pi} = \underline{N}\underline{N}$$
 and $\underline{T} = \underline{\delta} - \underline{\Pi}$ (6)

are the projection operators. We need to express these using $\underline{\underline{E}}$ as well, there are 2 options which I quote here

$$\underline{\underline{\Pi}} = \frac{d-1}{d-2} \left(\underbrace{\underline{\underline{E}} \cdot \underline{\underline{E}}^*}_{\underline{\underline{E}} : \underline{\underline{E}}^*} - \underbrace{\frac{\delta}{d(d-1)}}_{0} \right) \quad \text{or}$$

$$\tag{7}$$

$$\underline{\underline{\Pi}} = \sqrt{\frac{d-1}{d\underline{E}}} \underline{\underline{E}} - \frac{\underline{\delta}}{\underline{d}} \quad \text{which has a complex square root}$$
 (8)

<u>T</u> just being calculated from $\underline{\Pi}$.

2 $\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*}$ using eq. (7) for $\underline{\underline{\parallel}}$ and the Euler-Lagrange derivative

As $\frac{\delta F_{\text{bulk}}}{\delta E_{ij}^*}$ has been calculated before and it is the easier one, I move straight to the compression contribution. There the function in the integral only depends on the first derivatives of $\underline{\underline{E}}$ so we can use the usual Euler-Lagrange expression for calculating the functional.

$$\frac{\delta}{\delta\phi} \int f(\phi, \nabla\phi) \, dV = \frac{\partial f}{\partial\phi} - \nabla \cdot \frac{\partial f}{\partial(\nabla\phi)} \quad \text{or for us}$$
 (9)

$$\frac{\delta}{\delta E_{ij}^*} \int f_{\text{comp}}(\underline{\underline{\Pi}}(\underline{\underline{E}}, \underline{\underline{E}}^*), \mathbf{\nabla}\underline{\underline{E}}, \mathbf{\nabla}\underline{\underline{E}}^*) \, dV = \frac{\partial f_{\text{comp}}}{\partial E_{ij}^*} - \mathbf{\nabla} \cdot \frac{\partial f_{\text{comp}}}{\partial (\mathbf{\nabla}E_{ij}^*)}$$
(10)

Here I use eq. (7) as the expression for $\underline{\underline{\Pi}}$ further using $p = \frac{d-1}{d-2}$ and $q = \frac{1}{d(d-1)}$ as shorthands. I repeat the equations here for convenience

$$\Pi_{kl} = p \left(\frac{E_{kj} E_{lj}^*}{E_{ij} E_{ij}^*} - q \delta_{kl} \right) \quad \text{and} \quad f_{\text{comp}} = b_1^{\parallel} \Pi_{kl} E_{ij,k} E_{ij,l}^* + b_1^{\perp} (\delta_{kl} - \Pi_{kl}) E_{ij,k} E_{ij,l}^*$$
(11)

2.1 The first term

Noticing that the only dependence that f_{comp} only depends on \underline{E} through $\underline{\Pi}$ lets first get

$$\frac{\partial \Pi_{kl}}{\partial E_{ij}^*} = p \left(\frac{E_{kc} \delta_{li} \delta_{cj}}{E_{ab} E_{ab}^*} - \frac{E_{kc} E_{lc}^*}{(E_{ab} E_{ab}^*)^2} E_{ab} \delta_{ai} \delta_{bj} \right)$$

$$\tag{12}$$

$$= p \left(\frac{E_{kj} \delta_{li}}{E_{ab} E_{ab}^*} - \frac{E_{kc} E_{lc}^* E_{ij}}{(E_{ab} E_{ab}^*)^2} \right)$$
 (13)

Okay so here it got a little sketchy - the problem is that I always do $\frac{\partial E^*_{ij}}{\partial E^*_{ab}} = \delta_{ia}\delta_{jb}$, but I'm not sure this is compatible with $\underline{\underline{E}}$ being symmetric - then we should really have $\frac{\partial E^*_{ij}}{\partial E^*_{ab}} = \delta_{ia}\delta_{jb} + \delta_{ib}\delta_{ja}$ right? HOWEVER, I'm pretty sure we want to treat the different components of $\underline{\underline{E}}$ as independent, just "coincidentally" having the same values everywhere (and so also gradients), which is maintained by the Lagrange multiplier. Lets also try to do this using the real components of $E_{ij} = X_{ij} + iY_{ij}$

$$\frac{\partial \Pi_{kl}}{\partial E_{ij}^*} = \frac{p}{2} \left(\frac{\partial}{\partial X_{ij}} + i \frac{\partial}{\partial Y_{ij}} \right) \frac{(X_{kc} + iY_{kc})(X_{lc} - iY_{lc})}{(X_{ab} + iY_{ab})(X_{ab} - iY_{ab})}$$

$$\tag{14}$$

$$= \frac{p}{2} \left(\left(\frac{\delta_{ki}\delta_{cj}(X_{lc} - iY_{lc}) + (X_{kc} + iY_{kc})\delta_{li}\delta_{cj}}{E_{ab}E_{ab}^*} + \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} \delta_{ai}\delta_{bj}((X_{ab} - iY_{ab}) + (X_{ab} + iY_{ab})) \right)$$
(15)

$$+i\left(\frac{i\delta_{ki}\delta_{cj}(X_{lc}-iY_{lc})-i(X_{kc}+iY_{kc})\delta_{li}\delta_{cj}}{E_{ab}E_{ab}^{*}}+\frac{E_{kc}E_{lc}^{*}}{(E_{ab}E_{ab}^{*})^{2}}\delta_{ai}\delta_{bj}(i(X_{ab}-iY_{ab})-i(X_{ab}+iY_{ab}))\right)\right) (16)$$

$$= \frac{p}{2} \left(\left(\frac{\delta_{ki} (X_{lj} - iY_{lj}) + (X_{kj} + iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*} + \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} 2X_{ij} \right)$$
(17)

$$+ \left(\frac{-\delta_{ki}(X_{lj} - iY_{lj}) + (X_{kj} + iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*} - \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} (-2iY_{ij}) \right)$$
(18)

$$= \frac{p}{2} \left(\frac{\delta_{ki}(X_{lj} - iY_{lj}) + (X_{kj} + iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*} + 2X_{ij} \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} \right)$$
(19)

$$+\frac{-\delta_{ki}(X_{lj}-iY_{lj})+(X_{kj}+iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*}+2iY_{ij}\frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2}\right)$$
(20)

$$= \frac{p}{2} \left(\frac{2(X_{kj} + iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*} + 2(X_{ij} + iY_{ij}) \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} \right)$$
 (21)

$$= p \left(\frac{(X_{kj} + iY_{kj})\delta_{li}}{E_{ab}E_{ab}^*} + (X_{ij} + iY_{ij}) \frac{E_{kc}E_{lc}^*}{(E_{ab}E_{ab}^*)^2} \right) = p \left(\frac{E_{kj}\delta_{li}}{E_{ab}E_{ab}^*} + \frac{E_{kc}E_{lc}^*E_{ij}}{(E_{ab}E_{ab}^*)^2} \right)$$
(22)

omg, so it's actually the same...okay I'm pretty sure this is correct then

then we get

$$\frac{\partial f_{\text{comp}}}{\partial E_{ij}^*} = b_1^{\parallel} \frac{\partial \Pi_{kl}}{\partial E_{ij}^*} E_{\alpha\beta,k} E_{\alpha\beta,l}^* - b_1^{\perp} \frac{\partial \Pi_{kl}}{\partial E_{ij}^*} E_{\alpha\beta,k} E_{\alpha\beta,l}^*$$
(23)

$$= (b_1^{\parallel} - b_1^{\perp}) \frac{\partial \Pi_{kl}}{\partial E_{ij}^*} E_{\alpha\beta,k} E_{\alpha\beta,l}^* \tag{24}$$

$$= p(b_1^{\parallel} - b_1^{\perp}) \left(\frac{E_{kj} \delta_{li}}{E_{ab} E_{ab}^*} - \frac{E_{kc} E_{lc}^* E_{ij}}{(E_{ab} E_{ab}^*)^2} \right) E_{\alpha\beta,k} E_{\alpha\beta,l}^*$$
(25)

$$= p(b_1^{\parallel} - b_1^{\perp}) \left(\frac{E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^*}{E_{ab} E_{ab}^*} - \frac{E_{kc} E_{lc}^* E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^*}{(E_{ab} E_{ab}^*)^2} \right)$$
(26)

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{(E_{ab}E_{ab}^*)^2} \left(E_{ab}E_{ab}^* E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - E_{kc}E_{lc}^* E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^* \right)$$
(27)

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} \left(Y_{aa} E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - Y_{kl} E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^* \right) \quad \text{with} \quad Y_{ij} = E_{ik} E_{jk}^*$$
 (28)

which is suspicious to me as it's the first thing I encountered that is not symmetric. I also tried to first substitute in to $\underline{\underline{\Pi}}$ and then do the derivative and I got the same result, I think it is correct. Coming back to eq. (13) the first term there really encapsulates the problem, on the LHS both $\underline{\underline{\Pi}}$ and $\underline{\underline{E}}$ are symmetric but the first term on the RHS is not invariant under switching i and j or k and l. I am currently hoping that maybe it cancels with a part of the second term

2.2 The second term

Let's start working on the second term of eq. (10), firstly as the projection operators only depend on the $\underline{\underline{E}}$ and not on any of its derivatives we have

$$\frac{\partial f_{\text{comp}}}{\partial (E_{ab,c}^*)} = b_1^{\parallel} \Pi_{kl} E_{ij,k} \delta_{ia} \delta_{jb} \delta_{lc} + b_1^{\perp} T_{kl} E_{ij,k} \delta_{ia} \delta_{jb} \delta_{lc}$$
(29)

$$=b_1^{\parallel}\Pi_{kc}E_{ab,k} + b_1^{\perp}(\delta_{kc} - \Pi_{kc})E_{ab,k}$$
(30)

As the next step is to take a divergence of the above, lets first calculate

$$\partial_{\alpha} \Pi_{\beta\gamma} = p \,\partial_{\alpha} \, \frac{E_{\beta j} E_{\gamma j}^{*}}{E_{ij} E_{ij}^{*}} \tag{31}$$

$$= p \left(\frac{E_{\beta j,\alpha} E_{\gamma j}^*}{E_{ij} E_{ij}^*} + \frac{E_{\beta j} E_{\gamma j,\alpha}^*}{E_{ij} E_{ij}^*} - \frac{E_{\beta j} E_{\gamma j}^*}{(E_{ij} E_{ij}^*)^2} (E_{ij,\alpha} E_{ij}^* + E_{ij} E_{ij,\alpha}^*) \right)$$
 or (32)

$$\partial_{\alpha} \Pi_{\beta\gamma} = p \left(\frac{Y_{\beta\gamma,\alpha}}{Y_{ii}} - \frac{Y_{\beta\gamma}Y_{ii,\alpha}}{Y_{ii}^2} \right) \quad \text{using} \quad Y_{ij} = E_{ik}E_{jk}^*$$
 (33)

which leads to

$$\partial_{c} \frac{\partial f_{\text{comp}}}{\partial (E_{ab,c}^{*})} = \left(b_{1}^{\parallel} \Pi_{kc,c} E_{ab,k} - b_{1}^{\perp} \Pi_{kc,c} E_{ab,k} \right) + \left(b_{1}^{\parallel} \Pi_{kc} E_{ab,kc} + b_{1}^{\perp} (\delta_{kc} - \Pi_{kc}) E_{ab,kc} \right)$$
(34)

$$= \left(b_1^{\parallel} - b_1^{\perp}\right) \Pi_{kc,c} E_{ab,k} + \left(b_1^{\perp} E_{ab,cc} + \left(b_1^{\parallel} - b_1^{\perp}\right) \Pi_{kc} E_{ab,kc}\right)$$
(35)

bracketing to separate the first and second order derivatives. Turns out we only need

$$\Pi_{\alpha\beta,\beta} = \partial_{\beta}\Pi_{\alpha\beta} = p \left(\frac{Y_{\alpha\beta,\beta}}{Y_{ii}} - \frac{Y_{\alpha\beta}Y_{ii,\beta}}{Y_{ii}^2} \right)$$
(36)

leading to

$$\partial_{c} \frac{\partial f_{\text{comp}}}{\partial (E_{ab,c}^{*})} = p \left(b_{1}^{\parallel} - b_{1}^{\perp} \right) \left(\frac{Y_{kc,c}}{Y_{ii}} - \frac{Y_{kc}Y_{ii,c}}{Y_{ii}^{2}} \right) E_{ab,k} + \left(b_{1}^{\perp} E_{ab,cc} + \left(b_{1}^{\parallel} - b_{1}^{\perp} \right) \Pi_{kc} E_{ab,kc} \right)$$
(37)

$$= \frac{p\left(b_1^{\parallel} - b_1^{\perp}\right)}{Y_{ii}^2} (Y_{ii}Y_{kc,c} - Y_{kc}Y_{ii,c})E_{ab,k} + \left(b_1^{\perp}E_{ab,cc} + \left(b_1^{\parallel} - b_1^{\perp}\right)\Pi_{kc}E_{ab,kc}\right)$$
(38)

2.3 Combining the terms

$$\frac{\delta f_{\text{comp}}}{\delta E_{ij}^*} = \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} (Y_{aa} E_{kj} E_{\alpha\beta, k} E_{\alpha\beta, i}^* - Y_{kl} E_{ij} E_{\alpha\beta, k} E_{\alpha\beta, l}^*)$$
(39)

$$-\frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} (Y_{aa}Y_{kc,c} - Y_{kc}Y_{aa,c}) E_{ij,k} - (b_1^{\perp}E_{ij,cc} + (b_1^{\parallel} - b_1^{\perp})\Pi_{kc}E_{ij,kc})$$

$$(40)$$

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} \left(Y_{aa} E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - Y_{kl} E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^* + (Y_{kc} Y_{aa,c} - Y_{aa} Y_{kc,c}) E_{ij,k} \right)$$
(41)

$$-S_{ij} \quad \text{with} \quad S_{ij} = (b_1^{\perp} E_{ij,cc} + (b_1^{\parallel} - b_1^{\perp}) \Pi_{kc} E_{ij,kc}) \quad \text{containing the second order terms}$$
 (42)

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} \left(Y_{aa}(E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - Y_{kc,c} E_{ij,k}) + Y_{kl}(Y_{aa,l} E_{ij,k} - E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^*) \right)$$
(43)

$$-S_{ij} \tag{44}$$

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{cc}^2} \Big(Y_{aa}(E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - (E_{kd,c} E_{cd}^* + E_{kd} E_{cd,c}^*) E_{ij,k})$$
(45)

$$+Y_{kl}((E_{ad,l}E_{ad}^* + E_{ad}E_{ad,l}^*)E_{ij,k} - E_{ij}E_{\alpha\beta,k}E_{\alpha\beta,l}^*))$$
(46)

$$-S_{ij}$$
 (47)

$$= \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} \Big(Y_{aa} (E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - E_{cd}^* E_{ij,k} E_{kd,c} - E_{kd} E_{ij,k} E_{cd,c}^*)$$
(48)

$$+Y_{kl}(E_{ad}^*E_{ij,k}E_{ad,l} + E_{ad}E_{ij,k}E_{ad,l}^* - E_{ij}E_{\alpha\beta,k}E_{\alpha\beta,l}^*))$$
(49)

$$-S_{ij} (50)$$

$$\frac{\delta f_{\text{comp}}}{\delta E_{ij}^*} = \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} \Big(E_{af} E_{af}^* (E_{kj} E_{\alpha\beta,k} E_{\alpha\beta,i}^* - E_{cd}^* E_{ij,k} E_{kd,c} - E_{kd} E_{ij,k} E_{cd,c}^*)$$
(51)

$$+ E_{kf} E_{lf}^* \left(E_{ad}^* E_{ij,k} E_{ad,l} + E_{ad} E_{ij,k} E_{ad,l}^* - E_{ij} E_{\alpha\beta,k} E_{\alpha\beta,l}^* \right)$$
 (52)

$$-\left(b_{1}^{\perp}E_{ij,cc} + (b_{1}^{\parallel} - b_{1}^{\perp})\Pi_{kc}E_{ij,kc}\right) \tag{53}$$

(54)

I don't see any nicer or more intuitive way to write this as of now, also I do not see it being symmetric in exchanging i and j as I thought it would. For now I am leaving this as it is, $\underline{\underline{\Pi}}$ and Y_{aa} can readily be expressed in terms of $\underline{\underline{E}}$ for computation.

3 $\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*}$ using eq. (8) for $\underline{\underline{\parallel}}$ and the Euler-Lagrange derivative

We can still use the Euler-Lagrange version of the functional derivative as before, the only additional thing to consider is how to deal with the root – I will essentially ignore any problems with branch cuts etc. until the end, and just treat it like a real root until then. Also, the results here are surprisingly simple – making me question that treating E_{ij} and E_{ij}^* as completely independent is correct – I take that from the properties of Wirtinger derivatives.

So lets use

$$\Pi_{kl} = s\sqrt{E_{ab}E_{ab}}E_{kl} - \frac{\delta_{kl}}{d} \quad \text{and} \quad f_{\text{comp}} = b_1^{\parallel}\Pi_{kl}E_{ij,k}E_{ij,l}^* + b_1^{\perp}(\delta_{kl} - \Pi_{kl})E_{ij,k}E_{ij,l}^*$$
 (55)

with
$$s = \sqrt{\frac{d-1}{d}}$$

Note that this gives $\frac{\partial \Pi_{kl}}{\partial E^*_{ij}} = 0$ as $\underline{\underline{\Pi}}$ is independent of the conjugated $\underline{\underline{E}}$! This means that reusing eq. (23) we get that the first term of the Euler-Lagrange like expression (eq. (10)) is 0. So lets get the second term, for that we can reuse eq. (35) to get

$$\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*} = -\partial_c \frac{\partial f_{\text{comp}}}{\partial E_{ij,c}^*} = -\left(b_1^{\parallel} - b_1^{\perp}\right) \Pi_{kc,c} E_{ij,k} - \left(b_1^{\perp} E_{ij,cc} + \left(b_1^{\parallel} - b_1^{\perp}\right) \Pi_{kc} E_{ij,kc}\right)$$
(56)

so we need

$$\partial_c \Pi_{kc} = s \left(\sqrt{E_{ab} E_{ab}} E_{kc,c} + E_{kc} \partial_c \sqrt{E_{ab} E_{ab}} \right) \tag{57}$$

$$= s \left(\sqrt{E_{ab}E_{ab}} E_{kc,c} + \frac{E_{kc} 2E_{ab,c} E_{ab}}{2\sqrt{E_{ab}E_{ab}}} \right)$$

$$\tag{58}$$

$$= s \left(\sqrt{E_{ab}E_{ab}} E_{kc,c} + \frac{E_{ab,c}E_{ab}}{\sqrt{E_{ab}E_{ab}}} E_{kc} \right)$$

$$\tag{59}$$

giving

$$\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*} = -s \left(b_1^{\parallel} - b_1^{\perp} \right) \left(\sqrt{E_{ab} E_{ab}} E_{kc,c} + \frac{E_{ab,c} E_{ab}}{\sqrt{E_{ab} E_{ab}}} E_{kc} \right) E_{ij,k} - \left(b_1^{\perp} E_{ij,cc} + \left(b_1^{\parallel} - b_1^{\perp} \right) \Pi_{kc} E_{ij,kc} \right)$$
(60)

4 The divergence term of f_{comp}

This turned out a lot simpler. I do this using the Euler-Lagrange functional derivative (eq. (10)) again, though here I was a little unsure when taking the grad of a Kronecker delta, so I also tried acting it directly on the derivative and using $\frac{\delta E_{ab}^*(\underline{r})}{\delta E_{ii}^*(\underline{r}')} = \delta_{ai}\delta_{bj}\delta(\underline{r} - \underline{r}')$ and it gave the same, so I don't present it.

$$\frac{\delta}{\delta E_{ij}^*} b_1^d E_{ab,b} E_{ac,c}^* = b_1^d \partial_d E_{ab,b} \delta_{ia} \delta_{jc} \delta_{dc} = b_1^d E_{ib,bj}$$

$$\tag{61}$$