

Derivation of $\frac{\delta F}{\delta E_{ij}^*}$ in terms of E_{ij} and its derivatives – Old version using $\frac{\delta E_{ij}}{\delta E_{ab}} = \delta_{ai}\delta_{bj}$, most probably wrong!

1 Initial setup

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

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

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

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

$$(5)$$

where

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

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

$$\underline{\underline{\Pi}} = \frac{d-1}{d-2} \left(\frac{\underline{E} \cdot \underline{E}^*}{\underline{E} : \underline{E}^*} - \frac{\underline{\underline{\delta}}}{d(d-1)} \right) \quad \text{or} \quad (7)$$

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

$\underline{\underline{T}}$ just being calculated from $\underline{\underline{\Pi}}$.

2 $\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*}$ using eq. (7) for $\underline{\underline{\Pi}}$ 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{E} so we can use the usual Euler-Lagrange expression for calculating the functional.

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

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

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

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

2.1 The first term

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

$$\frac{\partial \Pi_{kl}}{\partial E_{ij}^*} = p \left(\frac{E_{kc} \delta_{li} \delta_{cj}}{E_{ab} E_{ab}^*} - \frac{E_{kc} E_{lc}^*}{(E_{ab} E_{ab}^*)^2} E_{ab} \delta_{ai} \delta_{bj} \right) \quad (12)$$

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

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{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{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 $E_{ij} = X_{ij} + iY_{ij}$

$$\frac{\partial \Pi_{kl}}{\partial E_{ij}^*} = \frac{p}{2} \left(\frac{\partial}{\partial X_{ij}} + i \frac{\partial}{\partial Y_{ij}} \right) \frac{(X_{kc} + iY_{kc})(X_{lc} - iY_{lc})}{(X_{ab} + iY_{ab})(X_{ab} - iY_{ab})} \quad (14)$$

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

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

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

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

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

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

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

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

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

then we get

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

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

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

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

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

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

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 $\underline{\Pi}$ 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 $\underline{\Pi}$ and \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{E} and not on any of its derivatives we have

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

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

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

$$\partial_\alpha \Pi_{\beta\gamma} = p \partial_\alpha \frac{E_{\beta j} E_{\gamma j}^*}{E_{ij} E_{ij}^*} \quad (31)$$

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

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

which leads to

$$\partial_c \frac{\partial f_{\text{comp}}}{\partial (E_{ab,c}^*)} = \left(b_1^\parallel \Pi_{kc, c} E_{ab, k} - b_1^\perp \Pi_{kc, c} E_{ab, k} \right) + \left(b_1^\parallel \Pi_{kc} E_{ab, kc} + b_1^\perp (\delta_{kc} - \Pi_{kc}) E_{ab, kc} \right) \quad (34)$$

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

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

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

leading to

$$\partial_c \frac{\partial f_{\text{comp}}}{\partial (E_{ab,c}^*)} = p(b_1^{\parallel} - b_1^{\perp}) \left(\frac{Y_{kc,c}}{Y_{ii}} - \frac{Y_{kc}Y_{ii,c}}{Y_{ii}^2} \right) E_{ab,k} + (b_1^{\perp} E_{ab,cc} + (b_1^{\parallel} - b_1^{\perp}) \Pi_{kc} E_{ab,kc}) \quad (37)$$

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

2.3 Combining the terms

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

$$- \frac{p(b_1^{\parallel} - b_1^{\perp})}{Y_{aa}^2} (Y_{aa} Y_{kc,c} - Y_{kc} Y_{aa,c}) E_{ij,k} - (b_1^{\perp} E_{ij,cc} + (b_1^{\parallel} - b_1^{\perp}) \Pi_{kc} E_{ij,kc}) \quad (40)$$

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

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

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

$$- S_{ij} \quad (44)$$

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

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

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

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

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

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

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

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

$$- (b_1^{\perp} E_{ij,cc} + (b_1^{\parallel} - b_1^{\perp}) \Pi_{kc} E_{ij,kc}) \quad (53)$$

$$(54)$$

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, $\underline{\Pi}$ and Y_{aa} can readily be expressed in terms of \underline{E} for computation.

3 $\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*}$ using eq. (8) for $\underline{\Pi}$ 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.

So lets use

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

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

Note that this gives $\frac{\partial \Pi_{kl}}{\partial E_{ij}^*} = 0$ as $\underline{\Pi}$ is independent of the conjugated \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

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

so we need

$$\partial_c \Pi_{kc} = s \left(\frac{E_{kc,c}}{\sqrt{E_{ab}E_{ab}}} - \frac{E_{kc}(E_{ab,c}E_{ab} + E_{ab}E_{ab,c})}{2(E_{ab}E_{ab})^{\frac{3}{2}}} \right) \quad (57)$$

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}} \left(E_{kc,c} - \frac{E_{kc}E_{ab}E_{ab,c}}{E_{ab}E_{ab}} \right) \quad (58)$$

$$\quad (59)$$

giving

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

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 $\frac{\delta E_{ab}^*(\underline{r})}{\delta E_{ij}^*(\underline{r}')} = \delta_{ai} \delta_{bj} \delta(\underline{r} - \underline{r}')$ and it gave the same, so I don't present it.

$$\frac{\delta}{\delta E_{ij}^*} b_1^d E_{ab,b} E_{ac,c}^* = b_1^d \partial_d E_{ab,b} \delta_{ia} \delta_{jc} \delta_{dc} = b_1^d E_{ib,bj} \quad (61)$$