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

1   Initial setup

1.1   Functional derivatives and independent variables

Here I assume all the components of $\underline{\underline{E}}$ are independent, except symmetry, and that $\underline{\underline{E}}$ and $\underline{\underline{E}}^*$ are independent as usual with Wirtinger derivatives. The reason for this is essentially as symmetry is easy to include, unlike the others which will be enforced for the dynamics using Lagrange multipliers, at least for now.

This can be achieved by a suitable choice of $\frac{\partial E_{ij}}{\partial E_{ab}}$ (and respectively for gradients), in the previous derivation I used $\delta_{ia}\delta_{jb}$. Here something of the form $\frac{\partial E_{ij}}{\partial E_{ab}} = \kappa(\delta_{ai}\delta_{bj} + \delta_{aj}\delta_{bi})$ seems like a logical choice, with κ being there due to the following problem.

This form however can't quite be made right for all i, j, a, b. Consider $i = j$, then the only non-zero choice for a, b is $a = b = i = j$, this then gets a contribution of 2κ, but it should be 1 as clearly $\frac{\partial E_{ii}}{\partial E_{ii}} = \frac{\partial x}{\partial x} = 1$ (no sums). Thus to get the $i = j$ terms right we would need $\kappa = \frac{1}{2}$.

However then for any $i \neq j$ we would get two non-zero options, either $a = i, b = j$ or $a = j, b = i$, for each of these the formula above gives κ. However for each of these we should get $\frac{\partial E_{ij}}{\partial E_{ij}} = \frac{\partial E_{ij}}{\partial E_{ij}} = 1$, this means κ would have to be 1.

Essentially the diagonal and off-didagonal elements of $\underline{\underline{E}}$ would have to be treated differently, all of this can be nicely summarized by table 1.

	11	22	33	12	21	13	31	23	32
11	1	0	0	0	0	0	0	0	0
22	0	1	0	0	0	0	0	0	0
33	0	0	1	0	0	0	0	0	0
12	0	0	0	1	1	0	0	0	0
21	0	0	0	1	1	0	0	0	0
13	0	0	0	0	0	1	1	0	0
31	0	0	0	0	0	1	1	0	0
23	0	0	0	0	0	0	0	1	1
32	0	0	0	0	0	0	0	1	1

Table 1: The results of $\frac{\partial E_{ij}}{\partial E_{ab}}$ for a symmetric $\underline{\underline{E}}$, rows and columns correspond to the ij and ab tuples and the table values to the partial derivative, clearly there is a difference between the $i = j$ and $i \neq j$ terms.

So in this work I adopt using $\frac{\partial E_{ij}}{\partial E_{ab}} = \kappa(\delta_{ai}\delta_{bj} + \delta_{aj}\delta_{bi})$ and $\frac{\partial E_{ij,k}}{\partial E_{abc}} = \kappa(\delta_{ai}\delta_{bj} + \delta_{aj}\delta_{bi})\delta_{kc}$ and leave κ unspecified, hoping that we can then set it to 1 or $\frac{1}{2}$ depending on if $i = j$ in $\frac{\delta F}{\delta E_{ij}^*}$

1.2 Free energies and projection operators

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

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

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

$$f_{\text{curv}} = \quad \ldots \quad \text{for later} \quad \ldots \tag{4}$$

$$\tag{5}$$

where

$$\underline{\underline{\Pi}} = \underline{N}\,\underline{N} \qquad \text{and} \qquad \underline{\underline{T}} = \underline{\underline{\delta}} - \underline{\underline{\Pi}} \tag{6}$$

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

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

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

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

2

2 $F_{\textbf{bulk}}$

2.1 Using κ

$$\frac{\delta F_{\text{bulk}}}{\delta E_{ij}^*} = \frac{A\kappa}{2}(E_{ij} + E_{ji}) + \frac{B\kappa}{4}2(E_{ab}E_{ab}^*)(E_{ij} + E_{ji}) \tag{9}$$

$$= \kappa(A + BE_{ab}E_{ab}^*)E_{ij} \quad \text{using symmetry of } \underline{\underline{E}} \tag{10}$$

2.2 Treating the $i = j$ and $i \neq j$ separately, as according to table 1

With **no sum on i**:

$$\frac{\delta F_{\text{bulk}}}{\delta E_{ii}^*} = \frac{A}{2}E_{ii} + \frac{B}{4}2(E_{ab}E_{ab}^*)E_{ii} \tag{11}$$

$$= (A + BE_{ab}E_{ab}^*)\frac{E_{ii}}{2} \tag{12}$$

and clearly

$$\frac{\delta F_{\text{bulk}}}{\delta E_{ij}^*} = (A + BE_{ab}E_{ab}^*)E_{ij} \tag{13}$$

3 F_{comp} using eq. (8)

(This lead to a symmetric result even without requiring symmetry of $\underline{\underline{E}}$, so this should lead to the same result)

To simplify use $s = \sqrt{\frac{d-1}{d}}$ to get

$$\Pi_{kl} = s(E_{ab}E_{ab})^{-\frac{1}{2}}E_{kl} - \frac{\delta_{kl}}{d} \quad \text{and recall} \quad f_{\text{comp}} = (b_1^{\parallel} - b_1^{\perp})\Pi_{kl}E_{ij,k}E_{ij,l}^* + b_1^{\perp}E_{ij,k}E_{ij,k}^* \tag{14}$$

So to get $\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*}$, the first term in the Euler-Lagrange equations will be 0 again as only gradients of $\underline{\underline{E}}$ appear directly in the form of f_{comp} and $\underline{\underline{\Pi}}$ only has non-conjugated elements of $\underline{\underline{E}}$ appear. Thus

$$\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*} = -\partial_k \frac{\partial f_{\text{comp}}}{\partial E_{ij,k}} = -\partial_k\Big((b_1^{\parallel} - b_1^{\perp})\Pi_{cd}E_{ab,c}\kappa(\delta_{ia}\delta_{jb} + \delta_{ib}\delta_{ja})\delta_{kd} + b_1^{\perp}E_{ab,c}\kappa(\delta_{ia}\delta_{jb} + \delta_{ib}\delta_{ja})\delta_{kc}\Big) \tag{15}$$

$$= -\kappa\partial_k\Big((b_1^{\parallel} - b_1^{\perp})\Pi_{ck}(E_{ij,c} + E_{ji,c}) + (E_{ij,k} + b_1^{\perp}E_{ji,k})\Big) \tag{16}$$

$$= -2\kappa\partial_k\Big((b_1^{\parallel} - b_1^{\perp})\Pi_{ck}E_{ij,c} + b_1^{\perp}E_{ij,k}\Big) \tag{17}$$

$$= -2\kappa\Big((b_1^{\parallel} - b_1^{\perp})\Pi_{ck,k}E_{ij,c} + (b_1^{\parallel} - b_1^{\perp})\Pi_{ck}E_{ij,ck} + b_1^{\perp}E_{ij,kk}\Big) \tag{18}$$

So we need

$$\Pi_{ck,k} = \partial_k\left(s(E_{ab}E_{ab})^{-\frac{1}{2}}E_{ck} - \frac{\delta_{ck}}{d}\right) = s\partial_k\Big((E_{ab}E_{ab})^{-\frac{1}{2}}E_{ck}\Big) \tag{19}$$

$$= s\left((E_{ab}E_{ab})^{-\frac{1}{2}}E_{ck,k} - \frac{1}{2}(E_{ab}E_{ab})^{-\frac{3}{2}}E_{ck}2E_{ab}E_{ab,k}\right) \tag{20}$$

$$= s\left((E_{ab}E_{ab})^{-\frac{1}{2}}E_{ck,k} - (E_{ab}E_{ab})^{-\frac{3}{2}}E_{ck}E_{ab}E_{ab,k}\right) \tag{21}$$

$$= \frac{s}{\sqrt{E_{ab}E_{ab}}}\left(E_{ck,k} - \frac{E_{ab}E_{ab,k}}{E_{ab}E_{ab}}E_{ck}\right) \tag{22}$$

so together we get

$$\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*} = -2\kappa\left(\frac{s(b_1^{\parallel} - b_1^{\perp})}{\sqrt{E_{ab}E_{ab}}}\left(E_{ck,k} - \frac{E_{ab}E_{ab,k}}{E_{ab}E_{ab}}E_{ck}\right)E_{ij,c} + (b_1^{\parallel} - b_1^{\perp})E_{ij,ck} + b_1^{\perp}E_{ij,kk}\right) \tag{23}$$

4 The extra term in F_{comp}

Should be easy so might as well

$$\frac{\delta}{\delta E_{ij}^*}\ b_1^d E_{ab,b}E_{ac,c}^* = b_1^d\partial_d E_{ab,b}\frac{\partial E_{ac,c}^*}{\partial E_{ij,d}^*} \tag{24}$$

$$= b_1^d \partial_d E_{ab,b} \kappa (\delta_{ia}\delta_{jc} + \delta_{ic}\delta_{ja})\delta_{cd} \tag{25}$$
$$= b_1^d \kappa \partial_d (E_{ib,b}\delta_{jc}\delta_{cd} + E_{jb,b}\delta_{ic}\delta_{cd}) \tag{26}$$
$$= b_1^d \kappa \partial_d (E_{ib,b}\delta_{jd} + E_{jb,b}\delta_{id}) \tag{27}$$
$$= b_1^d \kappa (E_{ib,bd}\delta_{jd} + E_{jb,bd}\delta_{id}) \tag{28}$$
$$= b_1^d \kappa (E_{ib,bj} + E_{jb,bi}) \tag{29}$$
$$\tag{30}$$

Agress with the result for unconstraint $\underline{\underline{E}}$ except κ, as expected.