Shape derivative of the energy functional with respect to a change in the surface parametrization

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Consider the magnetic energy functional

$$E := \frac{1}{2}\int_V B^2 dV, \tag{1}$$

where V is the three-dimensional volume bounded by $S = \partial V$, and where B can be expressed in term of the magnetic scalar potential $\mathbf{B} \equiv G\nabla(\omega + \phi)$. G is a surface dependance constant which depends on the surface parametrization. Both ω and the toroidal angle ϕ have to verify, as a consequence of $\nabla \cdot \mathbf{B}$, the Laplace equation $\Delta\omega = \Delta\phi = 0$ inside V. Moreover we require $\mathbf{B} \cdot \mathbf{n} = 0$ on S. Since E depends on B^2 integrated inside V, E is a functional of the surface S and hence depends on its parametrization. Let us parametrize S as follows:

$$S := \Big\{\boldsymbol{\sigma}(s,t) \in \mathbb{R}^3 : (s,t) \in \Omega\Big\}, \tag{2}$$

where $\Omega \subset \mathbb{R}^2$ is a bounded connected domain. We can then write the energy functional as follows:

$$E = \frac{1}{2}\int_V G^2 \nabla(\omega + \phi) \cdot \nabla(\omega + \phi). \tag{3}$$

We're interested in how the energy functional changes with a variation in the surface parametrization $\delta\boldsymbol{\sigma}$ so we want to express $\delta E[\delta\boldsymbol{\sigma}]$. According to the transport theorem for a volume functional such that the volume itself depends on the varied parameter, the shape derivative of energy can be written as

$$\begin{aligned}
\delta E[\delta\boldsymbol{\sigma}] &= \frac{1}{2}\int_V \delta\Big(G\nabla(\omega+\phi)\Big)^2 dV + \frac{1}{2}\int_{S=\partial V} (\delta\boldsymbol{\sigma}\cdot\boldsymbol{n})\Big(G\nabla(\omega+\phi)\Big)^2 dS \\
&= \frac{1}{2}\int_V \left[\delta\Big(G\nabla(\omega+\phi)\Big)^2 + \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\right] dV \\
&= \frac{1}{2}\int_V \left[2\delta\Big(G\nabla(\omega+\phi)\Big)\cdot\Big(G\nabla(\omega+\phi)\Big) + \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\right] dV \\
&= \frac{1}{2}\int_V \left[2\Big\{\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi) + G\nabla\delta\omega[\delta\boldsymbol{\sigma}]\Big\}\cdot G\nabla(\omega+\phi) + \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\right] dV,
\end{aligned} \tag{4}$$

where from the first to the second line, we used the scalar property of $\{G\nabla(\omega+\phi)\}^2$ to integrate over the volume. We might want to see if the above expression for $\delta E[\delta\boldsymbol{\sigma}]$ can be further reduced. Let us try to introduce the coordinates system $\{x^i\}_{i=1,2,3}$, and develop the above expression in tensor notation.

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Let us focus first on the term coming from the surface integral, that $\nabla \cdot \Big(\{G\nabla(\omega+\phi)\} \Big)^2$. Using that

$$\begin{aligned} \{G\nabla(\omega+\phi)\}^2 &= G^2\nabla(\omega+\phi)\cdot\nabla(\omega+\phi) \\ &= G^2\frac{\partial}{\partial x^i}(\omega+\phi)g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi), \end{aligned} \tag{5}$$

we can express the divergence in this coordinates system

$$\begin{aligned} \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big) =& \nabla_{\mathbf{x}}\cdot\Big[G^2\frac{\partial}{\partial x^i}(\omega+\phi)g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi)\delta\boldsymbol{\sigma}\Big] \\ =& \frac{\partial}{\partial x^l}\Big[G^2\frac{\partial}{\partial x^i}(\omega+\phi)g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi)\delta\sigma^l\Big] \\ =& 2\Big(\frac{\partial G}{\partial x^l}\Big)G\frac{\partial}{\partial x^i}(\omega+\phi)g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi)\delta\sigma^l \\ &+ G^2\Big[\frac{\partial^2}{\partial x^l\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi)+\frac{\partial^2}{\partial x^l\partial x^j}(\omega+\phi)\frac{\partial}{\partial x^i}(\omega+\phi)\Big]g^{ij}\delta\sigma^l \\ =& 2\left[\Big(\frac{\partial G}{\partial x^l}\Big)G\frac{\partial}{\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi)+G^2\frac{\partial^2}{\partial x^l\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi)\right]g^{ij}\delta\sigma^l \end{aligned} \tag{6}$$

where we assumed for the last line that the metric tensor g^{ij} is symmetric, as it can be the case on a stellarator field period. The first term in the integral from Eq.(4) can also be expressed in terms of coordinates. From the previous part, we already have the term $2G\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi)\cdot\nabla(\omega+\phi)$:

$$2G\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi)\cdot\nabla(\omega+\phi) = 2G\delta G[\delta\boldsymbol{\sigma}]\frac{\partial}{\partial x^i}(\omega+\phi)g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi), \tag{7}$$

and the same way, we derive the term

$$2G^2\nabla\delta\omega[\delta\boldsymbol{\sigma}] = 2G^2\frac{\partial}{\partial x^i}\delta\omega[\delta\boldsymbol{\sigma}]g^{ij}\frac{\partial}{\partial x^j}(\omega+\phi). \tag{8}$$

So if we combine all the previous terms, we get for the shape derivative of the energy functional

$$\begin{aligned} \delta E[\delta\boldsymbol{\sigma}] =& \frac{1}{2}\int_V\left[2\Big\{\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi)+G\nabla\delta\omega[\delta\boldsymbol{\sigma}]\Big\}\cdot G\nabla(\omega+\phi)+\nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\right]dV \\ =& \int_V dx^1dx^2dx^3g^{ij}\Bigg\{G^2\frac{\partial}{\partial x^i}\delta\omega[\delta\boldsymbol{\sigma}]\frac{\partial}{\partial x^j}(\omega+\phi)+G\delta G[\delta\boldsymbol{\sigma}]\frac{\partial}{\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi) \\ &+\left[\Big(\frac{\partial G}{\partial x^l}\Big)G\frac{\partial}{\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi)+G^2\frac{\partial^2}{\partial x^l\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^j}(\omega+\phi)\right]\delta\sigma^l\Bigg\} \end{aligned} \tag{9}$$

Remark: Note that in the case where the coordinate system $\{x^i\}$ is orthogonal, $g^{ij}=0$ for $i\neq j$ and Eq.(9) reduces to:

$$
\begin{aligned}
\delta E[\delta\boldsymbol{\sigma}] =& \frac{1}{2}\int_V \Bigg[2\Big\{\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi) + G\nabla\delta\omega[\delta\boldsymbol{\sigma}]\Big\}\cdot G\nabla(\omega+\phi) + \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\Bigg]dV \\
=& \int_V dx^1dx^2dx^3g^{ii}\Bigg\{G^2\frac{\partial}{\partial x^i}\delta\omega[\delta\boldsymbol{\sigma}]\frac{\partial}{\partial x^i}(\omega+\phi) + G\delta G[\delta\boldsymbol{\sigma}]\Big(\frac{\partial}{\partial x^i}(\omega+\phi)\Big)^2 \\
&+ \Bigg[\Big(\frac{\partial G}{\partial x^l}\Big)G\Big(\frac{\partial}{\partial x^i}(\omega+\phi)\Big)^2 + \frac{\partial^2}{\partial x^l\partial x^i}(\omega+\phi)\frac{\partial}{\partial x^i}(\omega+\phi)\Bigg]\delta\sigma^l\Bigg\}
\end{aligned}
\tag{10}
$$

Now, remains to express $\delta G[\delta\boldsymbol{\sigma}]$, and try to transform Eq.(9) in a surface integral. For that, we might want to try and write the term

$$
2\Big\{\delta G[\delta\boldsymbol{\sigma}]\nabla(\omega+\phi) + G\nabla\delta\omega[\delta\boldsymbol{\sigma}]\Big\}\cdot G\nabla(\omega+\phi) \tag{11}
$$

in the form of a divergence term as $\nabla\cdot(f\mathbf{u})$ $(\vee,+)$ $\nabla\cdot\mathbf{A}\mathbf{v}$ where $\mathbf{u},\mathbf{v}$ are two vectors, $\mathbf{A}$ some operator matrix and f a real valued function. Alternatively, we can start from the scalar potential $\varPhi$.

$$
\begin{aligned}
\delta(\mathbf{B}\cdot\mathbf{B}) =& 2\delta\mathbf{B}\cdot\mathbf{B} \\
=& 2\nabla\delta\varPhi\cdot\nabla\varPhi
\end{aligned}
\tag{12}
$$

We can thus use Eq.(12) to rewrite the shape derivative of E. Starting again from Eq.(1):

$$
\begin{aligned}
\delta\int_V \mathbf{B}\cdot\mathbf{B}dV &= \int_V \delta(\mathbf{B}\cdot\mathbf{B})dV + \int_S(\mathbf{B}\cdot\mathbf{B})\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \int_V 2\delta\mathbf{B}\cdot\mathbf{B}dV + \int_S(\mathbf{B}\cdot\mathbf{B})\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \int_V 2\delta\nabla\varPhi\cdot\nabla\varPhi dV + \int_S(\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \int_V \Delta(\varPhi\delta\varPhi) - \delta\varPhi\Delta\varPhi - \varPhi\Delta\delta\varPhi dV + \int_S(\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS,
\end{aligned}
\tag{13}
$$

we use now that $\nabla\cdot\mathbf{B}=0$ implies that the scalar potential has to satisfy $\Delta\varPhi=0$ in V and hence, so does its variation $\delta\varPhi[\delta\boldsymbol{\sigma}]$. Thus, we are left with the term

$$
\delta\int_V \mathbf{B}\cdot\mathbf{B}dV = \int_V \Delta(\varPhi\delta\varPhi)dV + \int_S(\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS, \tag{14}
$$

enabling to write the shape derivative as follows

$$
\begin{aligned}
\delta E[\delta\boldsymbol{\sigma}] &= \frac{1}{2}\int_V \delta(\mathbf{B}\cdot\mathbf{B})dV + \frac{1}{2}\int_S(\mathbf{B}\cdot\mathbf{B})\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \frac{1}{2}\int_V \Delta(\varPhi\delta\varPhi)dV + \frac{1}{2}\int_S(\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \frac{1}{2}\int_V \nabla\cdot\nabla(\varPhi\delta\varPhi)dV + \frac{1}{2}\int_S(\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\cdot\mathbf{n}dS \\
&= \frac{1}{2}\int_S \Bigg[\nabla(\varPhi\delta\varPhi) + (\nabla\varPhi\cdot\nabla\varPhi)\delta\boldsymbol{\sigma}\Bigg]\cdot\mathbf{n}dS.
\end{aligned}
\tag{15}
$$

We can now express the scalar potential in terms of ω and ϕ as we did previously:

$$\Phi = G(\omega+\phi) \implies \delta\Phi = \delta G(\omega+\phi) + G\delta\omega, \tag{16}$$

and hence the first term in the integrand of Eq.(15) reads

$$\begin{aligned}\nabla(\Phi\delta\Phi) &= \nabla\Big(G(\omega+\phi)\Big\{\delta G(\omega+\phi)+G\delta\omega\Big\}\Big)\\ &= \nabla\Big(G^2(\omega+\phi)\delta\omega + (\omega+\phi)^2 G\delta G\Big)\\ &= G^2\nabla(\omega+\phi)\delta\omega + G^2(\omega+\phi)\nabla\delta\omega + 2(\omega+\phi)\nabla(\omega+\phi)G\delta G.\end{aligned} \tag{17}$$

This way, we can rewrite Eq.(4) in the form of a surface integral:

$$\delta E[\delta\boldsymbol{\sigma}] = \frac{1}{2}\int_S \Bigg[G^2\nabla(\omega+\phi)\delta\omega + G^2(\omega+\phi)\nabla\delta\omega + 2(\omega+\phi)\nabla(\omega+\phi)G\delta G + \{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Bigg]\cdot\mathbf{n}dS \tag{18}$$

As a verification, let us take integrate the divergence of the all terms but the last in the integrand of Eq.(18):

$$\begin{aligned}&\int_V \nabla\cdot\Big(G^2\nabla(\omega+\phi)\delta\omega + G^2(\omega+\phi)\nabla\delta\omega + 2(\omega+\phi)\nabla(\omega+\phi)G\delta G\Big)dV\\ &= \int_V \Bigg[G^2\nabla(\omega+\phi)\cdot\nabla\delta\omega + G^2\Delta(\omega+\phi)\delta\omega\\ &\quad + G^2\nabla(\omega+\phi)\cdot\nabla\delta\omega + G^2\nabla(\omega+\phi)\Delta\delta\omega\\ &\quad + \Big(\nabla(\omega+\phi)\cdot\nabla(\omega+\phi) + (\omega+\phi)\Delta(\omega+\phi)\Big)2G\delta G\Bigg]dV\\ &= \int_V \Bigg[2G^2\nabla(\omega+\phi)\cdot\delta\nabla(\omega+\phi) + \big(\nabla(\omega+\phi)\cdot\nabla(\omega+\phi)\big)\delta(G^2)\Bigg]dV\\ &= \int_V \delta\Big(G\nabla(\omega+\phi)\cdot G\nabla(\omega+\phi)\Big)dV\\ &= \int_V \delta\Big(\mathbf{B}\cdot\mathbf{B}\Big)dV,\end{aligned} \tag{19}$$

where from the second to the third line we used that $\Delta\delta\omega = \Delta\omega = \Delta\phi = 0$ in V and $\delta\nabla(\omega+\phi) = \nabla\delta\omega$. To sum things up, we have that the shape derivative of E with respect to a change in the boundary can be expressed as a volume integral as well as a surface one and we get the following identity:

$$\begin{aligned}\delta E[\delta\boldsymbol{\sigma}] =& \frac{1}{2}\int_V \Bigg[2\Big\{\delta G\nabla(\omega+\phi) + G\nabla\delta\omega\Big\}\cdot G\nabla(\omega+\phi) + \nabla\cdot\Big(\{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Big)\Bigg]dV\\ =& \frac{1}{2}\int_S \Bigg[G^2\nabla(\omega+\phi)\delta\omega + G^2(\omega+\phi)\nabla\delta\omega + 2(\omega+\phi)\nabla(\omega+\phi)G\delta G + \{G\nabla(\omega+\phi)\}^2\delta\boldsymbol{\sigma}\Bigg]\cdot\mathbf{n}dS.\end{aligned} \tag{20}$$

As we did for the volume integral case, we can introduce a coordinate system on Ω to compute explicitly the surface integral of Eq.(20). Now we want to address the subject of the variation of G and ω and the way they can be related. For that, we start from the expression of $\mathbf{B}$ in terms of the magnetic scalar potential:

$$\mathbf{B} = G\nabla(\omega + \phi). \tag{21}$$

Thus, making use of Ampere's law, we can relate G and ω as follows:

$$\oiint_{\Sigma} \nabla \times \mathbf{B} \cdot \mathbf{n} dS = \oiint_{\Sigma} \mu_0 \mathbf{j} \cdot \mathbf{n} dS = \oint_{\partial\Sigma} \mathbf{B} \cdot \mathbf{dl} = G \oint_{\partial\Sigma} \nabla(\omega + \phi) \cdot \mathbf{dl} \tag{22}$$

so we can write G the following way:

$$G = \left(\oiint_{\Sigma} \mu_0 \mathbf{j} \cdot \mathbf{n} dS \right) \left(\oint_{\partial\Sigma} \nabla(\omega + \phi) \cdot \mathbf{dl} \right)^{-1} \tag{23}$$

where Σ is a closed surface with boundary $\partial\Sigma$ containing the hole of the torus.