Part II. Surface Motion with Application to Molecular Solvation, Cell Shapes, and Cell Dynamics

[Part I: Continuum Electrostatics]

References: [1] Differential Geometry by E. Kreyszig, Dover, 1991

[2] Differential Geometry of Curves and Surfaces, by M. P. DoCarmo, Prentice-Hall, 1976.

[3] Surface Evolution Equations A Level Set Approach, by Y. Giga, Birkhäuser, 2006.

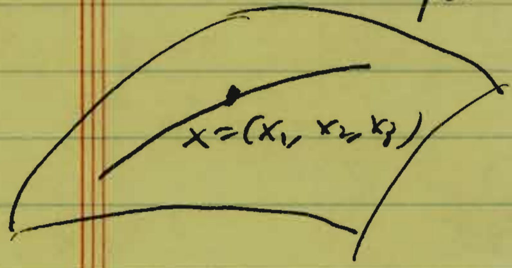
[4] Notes on Differential Geometry, by N. J. Hicks, Van Nostrand Reinhold, Co. 1965.

Plan:
- Basics
- Variations of surface and volume integrals
- Level set approach.
- The mean curvature flow.
- Hadwiger's Theorem. application to the calculation of solvation free energy of nonpolar systems
- ~~Discu~~
- Willmore flow. bending energy
- New models of cell shapes and cell dynamics
- Discussions
- The level-set method

Surface description. basic definition

parametric representation:

$$\vec{x} = \vec{x}(u^1, u^2) = (x_1(u^1,u^2), x_2(u^1,u^2), x_3(u^1,u^2))$$



$$\vec{x}_\alpha = \frac{\partial \vec{x}}{\partial u^\alpha} \qquad \alpha = 1, 2.$$

$$\vec{x}_{\alpha\beta} = \frac{\partial^2 \vec{x}}{\partial u^\alpha \partial u^\beta}, \qquad \alpha, \beta = 1, 2$$

Jacobian

$$J = \frac{\partial \vec{x}}{\partial u} \qquad J = \begin{bmatrix} \frac{\partial x_1}{\partial u^1} & \frac{\partial x_1}{\partial u^2} \\ \frac{\partial x_2}{\partial u^1} & \frac{\partial x_2}{\partial u^2} \\ \frac{\partial x_3}{\partial u^1} & \frac{\partial x_3}{\partial u^2} \end{bmatrix} = \begin{bmatrix} \vec{x}_1 & \vec{x}_2 \end{bmatrix} = \begin{bmatrix} \frac{\partial \vec{x}}{\partial u^1} & \frac{\partial \vec{x}}{\partial u^2} \end{bmatrix}$$

Assume: J is full-rank everywhere of a (u^1, u^2) region. i.e. $\frac{\partial \vec{x}}{\partial u^1}$, $\frac{\partial \vec{x}}{\partial u^2}$ are not parallel. or $\frac{\partial \vec{x}}{\partial u^1} \times \frac{\partial \vec{x}}{\partial u^2} \neq 0$.

a curve on a surface $\begin{cases} u^1 = u^1(t) \\ u^2 = u^2(t) \end{cases}$

$$\vec{x} = (x_1(u^1(t), u^2(t)), x_2(u^1(t), u^2(t)), x_3(u^1(t), u^2(t)))$$

First fundamental form

curve on a surface as above.

arc length element: ds

$$\begin{aligned} ds^2 &= d\vec{x} \cdot d\vec{x} \\ &= \left(\frac{\partial \vec{x}}{\partial u^1} du^1 + \frac{\partial \vec{x}}{\partial u^2} du^2\right) \cdot \left(\frac{\partial \vec{x}}{\partial u^1} du^1 + \frac{\partial \vec{x}}{\partial u^2} du^2\right) \\ &= \left(\frac{\partial \vec{x}}{\partial u^1} \cdot \frac{\partial \vec{x}}{\partial u^1}\right)(du^1)^2 + 2 \frac{\partial \vec{x}}{\partial u^1} \cdot \frac{\partial \vec{x}}{\partial u^2} du^1 du^2 + \frac{\partial \vec{x}}{\partial u^2} \cdot \frac{\partial \vec{x}}{\partial u^2} (du^2)^2 \\ &= (\vec{x}_1 \cdot \vec{x}_1)(du^1)^2 + 2 \vec{x}_1 \cdot \vec{x}_2 du^1 du^2 + (\vec{x}_2 \cdot \vec{x}_2)(du^2)^2 \end{aligned}$$

Denote $g_{\alpha\beta} = \vec{x}_\alpha \cdot \vec{x}_\beta = \dfrac{\partial \vec{x}}{\partial u^\alpha} \cdot \dfrac{\partial \vec{x}}{\partial u^\beta} \quad (\alpha, \beta = 1, 2)$

$g = \det(g_{\alpha\beta}) = g_{11} g_{22} - g_{12}^2$

Note: $g_{12} = g_{21}$

Easy to verify: $g = |\vec{x}_1 \times \vec{x}_2|^2$

$$\left[\begin{aligned} |\vec{x}_1 \times \vec{x}_2|^2 &= |\vec{x}_1|^2 |\vec{x}_2|^2 \sin^2\alpha \\ &= g_{11} g_{22} (1 - \cos^2\alpha) \\ &= g_{11} \cdot g_{22} - (\vec{x}_1 \cdot \vec{x}_2)^2 = g \end{aligned}\right]$$

The 1st fundamental form:

$$ds^2 = g_{11} (du^1)^2 + 2 g_{12}\, du^1 du^2 + g_{22} (du^2)^2$$

Gauss's notation

$$ds^2 = E (du^1)^2 + 2F\, du^1 du^2 + G (du^2)^2$$

$$E = g_{11}, \quad F = g_{12} = g_{21}, \quad G = g_{22}.$$

Always positive definite!

or: by Lagrange's identy

$$\begin{aligned} |\vec{x}_1 \times \vec{x}_2|^2 &= (\vec{x}_1 \times \vec{x}_2) \cdot (\vec{x}_1 \times \vec{x}_2) \\ &= (\vec{x}_1 \cdot \vec{x}_1)(\vec{x}_2 \cdot \vec{x}_2) - (\vec{x}_1 \cdot \vec{x}_2)^2 \\ &= g_{11} g_{12} - g_{12}^2 = g. \end{aligned}$$

change of coordinates:

$u^\alpha = u^\alpha(\bar{u}^1, \bar{u}^2), \quad \alpha = 1, 2$

Inverse: $\bar{u}^\mu = \bar{u}^\mu(u^1, u^2), \quad \mu = 1, 2$

Relations: $(\bar{g}_{\mu\nu}) = (g_{\alpha\beta}) \dfrac{\partial u}{\partial \bar{u}} \cdot \dfrac{\partial u}{\partial \bar{u}}$

$u = \begin{pmatrix} u^1 \\ u^2 \end{pmatrix}$

i.e. $\bar{g}_{\mu\nu} = \sum_{\alpha,\beta=1}^{2} g_{\alpha\beta} \dfrac{\partial u^\alpha}{\partial \bar{u}^\mu} \cdot \dfrac{\partial u^\beta}{\partial \bar{u}^\nu}$.

Similarly, $g_{\alpha\beta} = \sum_{\mu,\nu=1}^{2} \bar{g}_{\mu\nu} \dfrac{\partial \bar{u}^\mu}{\partial u^\alpha} \dfrac{\partial \bar{u}^\nu}{\partial v^\beta}$.

Also, $\bar{g} = D^2 g, \quad g = \bar{D}^2 g$.

where $\bar{g} = \det(\bar{g}_{\mu\nu}), \quad g = \det(g_{\alpha\beta})$

$D = \dfrac{\partial(u^1, u^2)}{\partial(\bar{u}^1, \bar{u}^2)}, \quad \bar{D} = \dfrac{\partial(\bar{u}^1, \bar{u}^2)}{\partial(u^1, u^2)}.$

Unit normal to a surface

$$\vec{n} = \frac{\vec{x}_1 \times \vec{x}_2}{|\vec{x}_1 \times \vec{x}_2|} = \frac{\vec{x}_1 \times \vec{x}_2}{\sqrt{g}}.$$

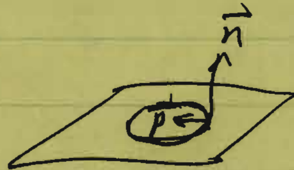
length of a curve $u^1 = u^1(t)$, $u^2 = u^2(t)$
on a surface $\vec{x} = \vec{x}(u^1, u^2)$.

$$s = \int_{t_0}^{t_1} |\vec{x}'(t)|\,dt = \int_{t_0}^{t_1} \sqrt{\sum_{\alpha,\beta=1}^{2} \frac{du^\alpha}{dt}\cdot\frac{du^\beta}{dt}\,\vec{x}_\alpha\cdot\vec{x}_\beta}\,dt.$$
$$= \int_{t_0}^{t_1} \sqrt{\sum_{\alpha\beta=1}^{2} g_{\alpha\beta}\,\dot{u}^\alpha \dot{u}^\beta}\,dt$$

surface area

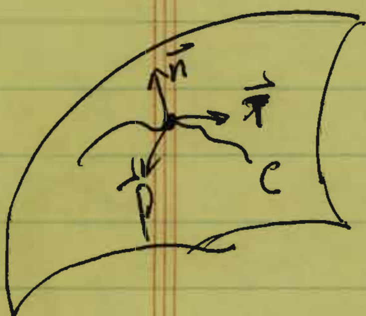
$$A = \int_U \sqrt{g}\,du^1du^2.$$

surface element: $dA = \sqrt{g}\,du^1du^2$



Second fundamental form **Curvatures**

unit tangent vector $\vec{t}(s) = \dot{\vec{x}}(s)$.



principal normal vector

$$\vec{p} = \frac{\vec{t}'(s)}{|\dot{\vec{t}}(s)|} = \frac{\ddot{\vec{x}}}{\kappa}$$

curvature: $\kappa = |\dot{\vec{t}}(s)|$.

$$\vec{p}\cdot\vec{n} = \frac{1}{\kappa}\,\ddot{\vec{x}}\cdot\vec{n} = \cos\gamma.$$

s: arc length
$\kappa\vec{p} = \dot{\vec{t}} = \ddot{\vec{x}}$
(by Frenet's)

($\dot{}$: arc length ~~time~~ derivative)

~~Notation~~ $\dot{\vec{x}} = \sum_{\alpha=1,2} \vec{x}_\alpha \dot{u}^\alpha$

$\vec{x}_\alpha\cdot\vec{n} = 0.$ $\Longrightarrow$ $\ddot{\vec{x}}\cdot n = \sum_{\alpha,\beta}(\vec{x}_{\alpha\beta}\cdot n)\,\dot{u}^\alpha \dot{u}^\beta$

Notation $\boxed{b_{\alpha\beta} = \vec{x}_{\alpha\beta}\cdot\vec{n}}$

Formulas of Frenet

$$\begin{bmatrix}\dot{\vec{t}}\\ \dot{\vec{p}}\\ \dot{\vec{b}}\end{bmatrix} = \begin{bmatrix}0 & \kappa & 0\\ -\kappa & 0 & \tau\\ 0 & -\tau & 0\end{bmatrix}\begin{bmatrix}\vec{t}\\ \vec{p}\\ \vec{b}\end{bmatrix}$$

$\vec{b}$ – binormal vector
$\vec{b} \equiv \vec{t}\times\vec{p}$.

The second fundamental form

$$b_{11}(du^1)^2 + 2b_{12}\,du^1 du^2 + b_{22}(du^2)^2$$

$$L = b_{11}, \qquad M = b_{12} \qquad N = b_{22}$$

$$L(du^1)^2 + 2M\,du^1du^2 + N(du^2)^2$$

$$\vec{x}_\alpha\cdot\vec{n} = 0 \xRightarrow{\frac{\partial}{\partial u^\beta}} \vec{x}_{\alpha\beta}\cdot\vec{n} + \vec{x}_\alpha\cdot\vec{n}_\beta = 0$$

$$\Rightarrow \boxed{b_{\alpha\beta} = -\vec{x}_\alpha\cdot\vec{n}_\beta}$$

$$\Rightarrow \boxed{\sum_{\alpha,\beta=1}^{2} b_{\alpha\beta}\,du^\alpha du^\beta = -d\vec{x}\cdot d\vec{n}.}$$

Also

$$b_{\alpha\beta} = \vec{x}_{\alpha\beta}\cdot\vec{n} = \vec{x}_{\alpha\beta}\cdot\frac{\vec{x}_1\times\vec{x}_2}{\sqrt{g}}$$

$$\boxed{b_{\alpha\beta} = \frac{1}{\sqrt{g}}\left|\vec{x}_1\ \vec{x}_2\ \vec{x}_{\alpha\beta}\right|}$$

using $s = s(t)$:

$$\dot{u}^\alpha = \frac{du^\alpha}{ds} = \frac{\frac{du^\alpha}{dt}}{\frac{ds}{dt}}$$

<u>Normal curvature</u>

$$k_n = \frac{\sum_{\alpha,\beta=1}^{2} b_{\alpha\beta}\,du^\alpha du^\beta}{\sum_{\alpha,\beta=1}^{2} g_{\alpha\beta}\,du^\alpha du^\beta}$$

$$\Rightarrow \ddot{\vec{x}}\cdot\vec{n} = \sum_{\alpha,\beta}(\vec{x}_{\alpha\beta}\cdot n)\dot{u}^\alpha\dot{u}^\beta = \frac{\sum_{\alpha,\beta} b_{\alpha\beta}\,du^\alpha du^\beta}{(ds)^2}$$

$\gamma = \langle\vec{p},\vec{n}\rangle$ ....angle.

$$k_n = k\cos\gamma = \ddot{\vec{x}}\cdot\vec{n} = k\,\vec{p}\cdot\vec{n}$$

[Depends on the curve under consideration.]

Which directions lead to max. and min. values of k_n?

$$\sum_{\alpha,\beta=1}^{2}\left(b_{\alpha\beta}-\kappa_n g_{\alpha\beta}\right) l^\alpha l^\beta = 0$$

where $l^\alpha = du^\alpha$. $(\alpha = 1, 2)$

Differentiate it w.r.t. l^γ, treating κ_n as a constant (since $d\kappa_n = 0$ is ~~the~~ necessary condition for κ_n to be extremal.)

$\sum_{\alpha,\beta=1}^{2}$

$$\frac{\partial}{\partial l^\gamma}\left(a_{\alpha\beta} l^\alpha l^\beta\right) = a_{\alpha\beta}\left(\frac{\partial l^\alpha}{\partial l^\gamma} l^\beta + l^\alpha \frac{\partial l^\beta}{\partial l^\gamma}\right)$$

$$= a_{\alpha\beta}\left(\delta^\alpha_\gamma l^\beta - l^\alpha \delta^\beta_\gamma\right) = \left(a_{\gamma\beta} + a_{\alpha\gamma}\right) l^\alpha$$

~~Symmetry~~ $\cancel{a_{\gamma\alpha} = a_{\alpha\gamma}}$

By the symmetry: $a_{\gamma\alpha} = a_{\alpha\gamma}$.

$$\sum_{\alpha=1,2}\left(b_{\alpha\gamma} - \kappa_n g_{\alpha\gamma}\right) l^\alpha = 0 \qquad \gamma = 1, 2.$$

$$Bl = \kappa_n G l \iff \begin{cases} (b_{11} - \kappa_n g_{11}) l^1 + (b_{21} - \kappa_n g_{21}) l^2 = 0 \\ (b_{12} - \kappa_n g_{12}) l^1 + (b_{22} - \kappa_n g_{22}) l^2 = 0 \end{cases} \iff \det(B - \kappa_n G) = $$

$B = (b_{\alpha\beta})$, $G = (g_{\alpha\beta})$

κ_n = eigenvalues

Eliminate κ_n:

$$\begin{vmatrix} \sum_{\alpha=1,2} g_{1\alpha} du^\alpha & \sum_{\beta=1,2} b_{1\beta} du^\beta \\ \sum_{\alpha=1,2} g_{2\alpha} du^\alpha & \sum_{\beta=1,2} b_{2\beta} du^\beta \end{vmatrix} = 0.$$

$$\iff \boxed{\begin{vmatrix} (du^2)^2 & -du^1 du^2 & (du^1)^2 \\ g_{11} & g_{12} & g_{22} \\ b_{11} & b_{12} & b_{22} \end{vmatrix} = 0.}$$

~~direction~~ $\Longrightarrow$ principal direction of normal curvature.

(or: curvature directions).

Thm. Roots are real. the principal directions are orthogonal.

$G^{-1}B\,l = \kappa_n l, \quad l = (l^1, l^2) \neq 0.$

$$\boxed{\kappa_n^2 - \left(\sum_{\alpha,\beta=1}^{2} b_{\alpha\beta}\, g^{\alpha\beta}\right)\kappa_n + \frac{b}{g} = 0} \qquad (g^{\alpha\beta}) = (g_{\alpha\beta})^{-1}.$$

$\Longrightarrow$ $\kappa_n = \kappa_1, \kappa_2$ the principal curvatures.

where $b = \det(b_{\alpha\beta}) = b_{11}b_{22} - b_{12}^2$.

<u>Definition</u>. Mean curvature

$$H = \frac{1}{2}(\kappa_1 + \kappa_2) = \frac{1}{2}\sum_{\alpha,\beta=1}^{2} b_{\alpha\beta}\, g^{\alpha\beta} = \frac{1}{2}\,\mathrm{trace}(G^{-1}B) = \frac{1}{2}\, G^{-1} : B.$$

Gaussian curvature (or total curvature)

$$K = \kappa_1 \kappa_2 = \frac{b}{g}.$$

<u>Euler's Thm</u> Let α = angle between the direction at a point and the principal dir. for κ_1. Then

$$\kappa_n = \kappa_1 \cos^2\alpha + \kappa_1 \sin^2\alpha$$

[Need to add some good examples of H, K, etc.
For instance, the surface is a (patch) of
~~shape~~ sphere, cylinder, ...]

Some parameterizations of surfaces

1. Monge (graph) parameterization

$$x_3 = h(x_1, x_2).$$

$$\vec{x} = (x_1, x_2, h(x_1, x_2)) \qquad u^1 = x_1,\ u^2 = x_2.$$

$$\vec{x}_1 = \frac{\partial \vec{x}}{\partial x_1} = (1, 0, h_1), \quad \vec{x}_2 = \frac{\partial \vec{x}}{\partial x_2} = (0, 1, h_2)$$

$$h_\alpha = \frac{\partial h}{\partial x_\alpha}, \quad h_{\alpha\beta} = \frac{\partial^2 h}{\partial x_\alpha \partial x_\beta}$$

$$(g_{\alpha\beta}) = (\vec{x}_\alpha \cdot \vec{x}_\beta) = \begin{pmatrix} 1+h_1^2 & h_1 h_2 \\ h_1 h_2 & 1+h_2^2 \end{pmatrix}$$

$$g = \det(g_{\alpha\beta}) = 1 + h_1^2 + h_2^2$$

$$G^{-1} = (g_{\alpha\beta})^{-1} = (g^{\alpha\beta}) = \frac{1}{1+h_1^2+h_2^2}\begin{pmatrix} 1+h_2^2 & -h_1 h_2 \\ -h_1 h_2 & 1+h_1^2 \end{pmatrix}$$

$$\vec{x}_1 \times \vec{x}_2 = \begin{pmatrix} -h_1 \\ -h_2 \\ 1 \end{pmatrix}$$

$$\vec{n} = \frac{\vec{x}_1 \times \vec{x}_2}{\sqrt{g}} = \frac{1}{\sqrt{1+h_1^2+h_2^2}}\begin{pmatrix} -h_1 \\ -h_2 \\ 1 \end{pmatrix}$$

$$B = (b_{\alpha\beta}) = (\vec{x}_{\alpha\beta} \cdot \vec{n}) = \frac{1}{\sqrt{1+h_1^2+h_2^2}} \underbrace{\begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix}}_{\text{Hessian of } h}.$$

Mean curvature

$$H = \frac{1}{2} G^{-1} : B = \frac{1}{2(1+h_1^2+h_2^2)^{3/2}}\left[h_{11}(1+h_2^2) + h_{22}(1+h_1^2) - 2 h_1 h_2 \cancel{h_{12}}\, h_{12} \right]$$

$$H = \frac{1}{2} \nabla \cdot \left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}} \right).$$

Gaussian curvature

$$K = \frac{b}{g} = \frac{h_{11} h_{22} - h_{12}^2}{(1+h_1^2+h_2^2)^2}.$$

Linearization around a flat surface

$h = h_0 + \varepsilon \tilde{h}(x_1, x_2) + \cdots \qquad |\varepsilon| << 1. \quad h_0 = \text{const}.$

$h_\alpha = \varepsilon \tilde{h}_\alpha + \cdots \qquad . \quad h_{\alpha\beta} = \varepsilon \tilde{h}_{\alpha\beta} + \cdots$

$H = H(h) = ?$

$1 + h_1^2 + h_2^2 = 1 + O(\varepsilon^2)$

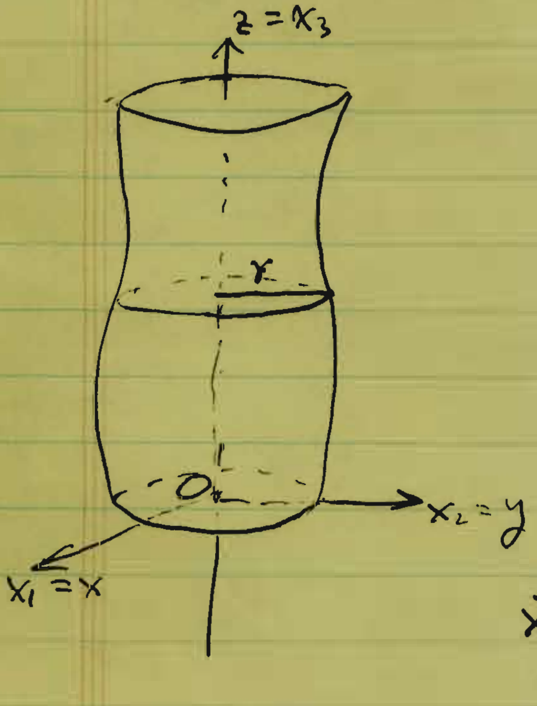
$h_\alpha^2 = O(\varepsilon^2).$

$h_\alpha h_\beta h_{12} = O(\varepsilon) O(\varepsilon) h_{12} = O(\varepsilon^2).$

$$\underline{H = \frac{1}{2}\left(\tilde{h}_{11} + \tilde{h}_{22}\right) = \frac{1}{2} \Delta \tilde{h}}.$$

$K = O(\varepsilon^2).$

2. Cylindrically symmetric surfaces



$\cancel{\vec{x} = \vec{x}(r, \theta, x_3) = \vec{x}(r, \theta, z)}.$

$$\vec{x} = \vec{x}(\theta, z) = \begin{bmatrix} r(z)\cos\theta \\ r(z)\sin\theta \\ z \end{bmatrix}$$

$u^1 = \theta, \; u^2 = z$

$$\vec{x}_1 = \begin{bmatrix} -r(z)\sin\theta \\ r(z)\cos\theta \\ 0 \end{bmatrix}$$

$$\vec{x}_2 = \begin{bmatrix} r'(z)\cos\theta \\ r'(z)\sin\theta \\ 1 \end{bmatrix}$$

$$\vec{x}_1 \times \vec{x}_2 = \begin{bmatrix} r\cos\theta \\ r\sin\theta \\ -rr' \end{bmatrix}$$

$$|\vec{x}_1 \times \vec{x}_2| = \sqrt{r^2(1+r'^2)} = r\sqrt{1+r'^2}$$

$$\vec{n} = \frac{1}{r\sqrt{1+r'^2}}\begin{bmatrix} r\cos\theta \\ r\sin\theta \\ -rr' \end{bmatrix} = \frac{1}{\sqrt{1+r'^2}}\begin{bmatrix} \cos\theta \\ \sin\theta \\ -r' \end{bmatrix}$$

$$G = (g_{\alpha\beta}) = \begin{bmatrix} r^2 & 0 \\ 0 & 1+r'^2 \end{bmatrix}$$

$$\vec{x}_{11} = \begin{bmatrix} -r\cos\theta \\ -r\sin\theta \\ 0 \end{bmatrix} \qquad \vec{x}_{22} = \begin{bmatrix} r''\cos\theta \\ r''\sin\theta \\ 0 \end{bmatrix}$$

$$\vec{x}_{12} = \begin{bmatrix} -r'\sin\theta \\ r'\cos\theta \\ 0 \end{bmatrix}.$$

$$B = (b_{\alpha\beta}) = (\vec{x}_{\alpha\beta}\cdot\vec{n}) = \frac{1}{\sqrt{1+r'^2}}\begin{bmatrix} -r & 0 \\ 0 & r'' \end{bmatrix}$$

$$G^{-1} = \begin{bmatrix} \frac{1}{r^2} & 0 \\ 0 \; \cancel{\frac{1}{\sqrt{1+r'^2}}} & \frac{1}{1+r'^2} \end{bmatrix}$$

$$H = \frac{1}{2}G^{-1}:B = \frac{1}{2\sqrt{1+r'^2}}\left(-\frac{1}{r} + \frac{r''}{1+r'^2}\right)$$

$$H = \frac{1}{2\sqrt{1+r'^2}}\left(\frac{r''}{1+r'^2} - \frac{1}{r}\right)$$

$$K = \det G^{-1}\cdot\det B = \cancel{\frac{r^2(1+r'^2)(-r)r''}{\sqrt{1+r'^2}}} \cancel{= -r^3\sqrt{1+r'^2}\,r''}.$$

$$= -\frac{r''}{r(1+r'^2)^{3/2}}.$$