1 Elastic Constants

Elastic[1].

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + V(\boldsymbol{q}_i) \tag{1}$$

$$\boldsymbol{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}, \quad \boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \tag{2}$$

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = \sum_\alpha a_{i\alpha} b_{j\alpha} = 2\pi\delta_{ij} \tag{3}$$

$$a_{11}b_{12} + a_{21}b_{22} + a_{31}b_{32} = a_{11}(a_{23}a_{31} - a_{21}a_{33}) + a_{21}(a_{33}a_{11} - a_{31}a_{13}) + a_{31}(a_{13}a_{21} - a_{11}a_{23}) \tag{4}$$

$$= 0 \tag{5}$$

$$a_{11}b_{11} + a_{21}b_{21} + a_{31}b_{31} = \frac{a_{11}(a_{22}a_{33} - a_{23}a_{32}) + a_{21}(a_{32}a_{13} - a_{33}a_{12}) + a_{31}(a_{12}a_{23} - a_{13}a_{22})}{V/2\pi} \tag{6}$$

$$= \frac{a_{11}(a_{22}a_{33} - a_{23}a_{32}) + a_{12}(a_{23}a_{31} - a_{21}a_{33}) + a_{13}(a_{21}a_{32} - a_{22}a_{31})}{V/2\pi} \tag{7}$$

$$= \frac{\mathbf{a_1} \cdot \mathbf{a_2} \times \mathbf{a_3}}{V/2\pi} \tag{8}$$

$$= 2\pi \tag{9}$$

$$\sum_i a_{i\alpha} b_{i\beta} = a_{i\alpha} a_{i\gamma} \times a_{i\alpha} = 2\pi\delta_{\alpha\beta} \tag{10}$$

$$\mathrm{b}_1 = 2\pi \frac{\mathrm{a}_2 \times \mathrm{a}_3}{V} = \frac{2\pi}{V} \begin{pmatrix} a_{22}a_{33} - a_{23}a_{32} \\ a_{23}a_{31} - a_{21}a_{33} \\ a_{21}a_{32} - a_{22}a_{31} \end{pmatrix} \tag{11}$$

$$\mathrm{b}_2 = 2\pi \frac{\mathrm{a}_3 \times \mathrm{a}_1}{V} \tag{12}$$

$$\mathrm{b}_3 = 2\pi \frac{\mathrm{a}_1 \times \mathrm{a}_2}{V} \tag{13}$$

$$\mathrm{H} = \begin{pmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \boldsymbol{a}_3 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \tag{14}$$

$$\mathrm{H}^{-1} = \frac{1}{2\pi} \begin{pmatrix} \boldsymbol{b}_1^T \\ \boldsymbol{b}_2^T \\ \boldsymbol{b}_3^T \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} \tag{15}$$

$$\tag{16}$$

$$
\begin{aligned}
\mathrm{H}^{-1}\mathrm{H} &= \frac{1}{2\pi}\begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}\begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} && (17) \\
&= \frac{1}{2\pi}\begin{pmatrix} \sum_\alpha b_{1\alpha}a_{1\alpha} & \sum_\alpha b_{1\alpha}a_{2\alpha} & \sum_\alpha b_{1\alpha}a_{3\alpha} \\ \sum_\alpha b_{2\alpha}a_{1\alpha} & \sum_\alpha b_{2\alpha}a_{2\alpha} & \sum_\alpha b_{2\alpha}a_{3\alpha} \\ \sum_\alpha b_{3\alpha}a_{1\alpha} & \sum_\alpha b_{3\alpha}a_{2\alpha} & \sum_\alpha b_{3\alpha}a_{3\alpha} \end{pmatrix} && (18) \\
&= \mathrm{I} && (19)
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{q} &= \mathrm{H}\boldsymbol{s} && (20) \\
&= \sum_i s_i \boldsymbol{a}_i && (21) \\
&= \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}\begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix} && (22) \\
\boldsymbol{p} &= (\mathrm{H}^{-1})^T \tilde{\boldsymbol{p}} && (23)
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{s} &= \mathrm{H}^{-1}\boldsymbol{q} && (24) \\
\tilde{\boldsymbol{p}} &= \mathrm{H}^T \boldsymbol{p} && (25)
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{H} &= \mathrm{H}_0 + \mathrm{dH} && (26) \\
\mathrm{H}^\mathrm{T}\mathrm{H} &= (\mathrm{H}_0 + \mathrm{dH})^\mathrm{T}(\mathrm{H}_0 + \mathrm{dH}) && (27) \\
&= \mathrm{H}_0^\mathrm{T}\mathrm{H}_0 + \mathrm{dH}^\mathrm{T}\mathrm{H}_0 + \mathrm{H}_0^\mathrm{T}\mathrm{dH} + \mathrm{dH}^\mathrm{T}\mathrm{dH} && (28) \\
&\approx \mathrm{H}_0^\mathrm{T}\mathrm{H}_0 + \mathrm{dH}^\mathrm{T}\mathrm{H}_0 + \mathrm{H}_0^\mathrm{T}\mathrm{dH} && (29) \\
&:= \mathrm{H}_0^\mathrm{T}\mathrm{H}_0 + 2\mathrm{H}_0^\mathrm{T}\mathrm{e}\mathrm{H}_0 && (30) \\
&= \mathrm{H}_0^\mathrm{T}(1 + 2\mathrm{e})\mathrm{H}_0 && (31) \\
\mathrm{e} &= \frac{1}{2}\left((\mathrm{H}_0^\mathrm{T})^{-1}\mathrm{H}^\mathrm{T}\mathrm{H}\mathrm{H}_0^{-1} - 1\right) && (32) \\
\mathrm{H}_0^{-\mathrm{T}} &:= (\mathrm{H}_0^\mathrm{T})^{-1} = (\mathrm{H}_0^{-1})^\mathrm{T} && (33)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial q_{i\alpha}}{\partial H_{\beta\gamma}} &= \frac{\partial}{\partial H_{\beta\gamma}} \sum_\sigma H_{\alpha\sigma}\mathrm{s}_\sigma && (34) \\
&= \sum_\sigma \delta_{\alpha\beta}\delta_{\sigma\gamma}s_\sigma && (35) \\
&= \delta_{\alpha\beta}s_\gamma && (36) \\
&= \delta_{\alpha\beta}(\mathrm{H}^{-1}\boldsymbol{q})_\gamma && (37) \\
&= \delta_{\alpha\beta}\sum_\sigma \mathrm{H}_{\gamma\sigma}^{-1}\boldsymbol{q}_\sigma && (38)
\end{aligned}
$$

$$\frac{\partial \tilde{p}_{i\alpha}}{\partial H_{\beta\gamma}} = \frac{\partial}{\partial H_{\beta\gamma}} \left(\mathrm{H}^T \mathbf{p_i}\right)_\alpha \tag{39}$$

$$0 = \frac{\partial}{\partial H_{\beta\gamma}} \sum_\sigma H^T_{\alpha\sigma} p_{i\sigma} \tag{40}$$

$$= \sum_\sigma \left(\frac{\partial H_{\sigma\alpha}}{\partial H_{\beta\gamma}} p_{i\sigma} + H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} \right) \tag{41}$$

$$= \sum_\sigma \left(\delta_{\sigma\beta}\delta_{\alpha\gamma} p_{i\sigma} + H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} \right) \tag{42}$$

$$= \delta_{\alpha\gamma} p_{i\beta} + \sum_\sigma H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} \tag{43}$$

$$\sum_\sigma H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -\delta_{\alpha\gamma} p_{i\beta} \tag{44}$$

$$\sum_\alpha H^{-1}_{\alpha\tau} \sum_\sigma H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -\sum_\alpha H^{-1}_{\alpha\tau} \delta_{\alpha\gamma} p_{i\beta} \tag{45}$$

$$\sum_\sigma \left(H H^{-1}\right)_{\sigma\tau} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -H^{-1}_{\gamma\tau} p_{i\beta} \tag{46}$$

$$\sum_\sigma \delta_{\sigma\tau} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -H^{-1}_{\gamma\tau} p_{i\beta} \tag{47}$$

$$\frac{\partial p_{i\tau}}{\partial H_{\beta\gamma}} = -H^{-1}_{\gamma\tau} p_{i\beta} \tag{48}$$

$$\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial H_{\beta\gamma}} = \sum_{i,\alpha} \left\{ \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial q_{i\alpha}} \frac{\partial q_{i\alpha}}{\partial H_{\beta\gamma}} + \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial p_{i\alpha}} \frac{\partial p_{i\alpha}}{\partial H_{\beta\gamma}} \right\} \tag{49}$$

$$= \sum_i \left\{ \sum_\alpha \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial q_{i\alpha}} \left(\delta_{\alpha\beta} \sum_\sigma \mathrm{H}^{-1}_{\gamma\sigma} q_{i\sigma} \right) + \sum_\alpha \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial p_{i\alpha}} \left(-H^{-1}_{\gamma\alpha} p_{i\beta} \right) \right\} \tag{50}$$

$$= \sum_i \left\{ \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial q_{i\beta}} \sum_\sigma \mathrm{H}^{-1}_{\gamma\sigma} q_{i\sigma} - p_{i\beta} \sum_\alpha H^{-1}_{\gamma\alpha} \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial p_{i\alpha}} \right\} \tag{51}$$

$$= \sum_i \left\{ \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial q_{i\beta}} \left(\mathrm{H}^{-1} q_i\right)_\gamma - p_{i\beta} \left(H^{-1} \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial \boldsymbol{p}_i} \right)_\gamma \right\} \tag{52}$$

$$\frac{\partial A}{\partial \mathrm{H}} = \sum_i \left\{ \frac{\partial A}{\partial \boldsymbol{q}_i} \otimes \left(\mathrm{H}^{-1} \boldsymbol{q}_i\right) - \boldsymbol{p}_i \otimes \left(\mathrm{H}^{-1} \frac{\partial A}{\partial \boldsymbol{p}_i} \right) \right\} \tag{53}$$

$$\frac{\partial \mathcal{H}}{\partial q_{i\alpha}} = \frac{\partial}{\partial q_{i\alpha}} \left(\sum_j \sum_\beta \frac{p^2_{j\beta}}{2m_j} + V\left(\{\boldsymbol{q}_j\}\right) \right) = \frac{\partial}{\partial q_{i\alpha}} V\left(\{\boldsymbol{q}_j\}\right) := V_{i\alpha} \tag{54}$$

$$\frac{\partial \mathcal{H}}{\partial p_{i\alpha}} = \frac{\partial}{\partial p_{i\alpha}} \left(\sum_j \sum_\beta \frac{p^2_{j\beta}}{2m_j} + V\left(\{\boldsymbol{q}_j\}\right) \right) = \frac{p_{i\alpha}}{m_i} \tag{55}$$

$$\frac{\partial \mathcal{H}}{\partial \boldsymbol{q}_i} = \boldsymbol{V}_i, \qquad \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}_i} = \frac{\boldsymbol{p}_i}{m_i} \tag{56}$$

$$
\begin{aligned}
\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}} &= \sum_i \left\{ \frac{\partial \mathcal{H}}{\partial q_{i\alpha}} \left(\mathrm{H}^{-1} q_i\right)_\beta - p_{i\alpha} \left(H^{-1} \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}_i} \right)_\beta \right\} && (57) \\
&= \sum_i \left\{ V_{i\alpha} \left(\mathrm{H}^{-1} q_i\right)_\beta - p_{i\alpha} \left(H^{-1} \frac{\boldsymbol{p}_i}{m_i} \right)_\beta \right\} && (58) \\
&= \sum_i \left\{ V_{i\alpha} \left(\mathrm{H}^{-1} q_i\right)_\beta - p_{i\alpha} \left(\frac{\boldsymbol{p}_i}{m_i} H^{-T} \right)_\beta \right\} && (59) \\
\frac{\partial \mathcal{H}}{\partial \mathrm{H}} &= \sum_i \left\{ \boldsymbol{V}_i \otimes \left(\mathrm{H}^{-1} \boldsymbol{q}_i\right) - \boldsymbol{p}_i \otimes \left(H^{-1} \frac{\boldsymbol{p}_i}{m_i} \right) \right\} && (60)
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{H}^{\mathrm{T}}\mathrm{H} &= \mathrm{H}_0^{\mathrm{T}}(1 + 2\mathrm{e})\mathrm{H}_0 && (61) \\
(\mathrm{H} + \mathrm{dH})^{\mathrm{T}}(\mathrm{H} + \mathrm{dH}) &= \mathrm{H}_0^{\mathrm{T}}(1 + 2(\mathrm{e} + \mathrm{de}))\mathrm{H}_0 && (62) \\
\mathrm{H}^{\mathrm{T}}\mathrm{dH} + \mathrm{dH}^{\mathrm{T}}\mathrm{H} + \mathrm{dH}^{\mathrm{T}}\mathrm{dH} &= 2\mathrm{H}_0^{\mathrm{T}}\mathrm{de}\mathrm{H}_0 && (63) \\
\mathrm{de} &= \frac{1}{2}\mathrm{H}_0{}^{-T}(\mathrm{dH}^{\mathrm{T}}\mathrm{H} + \mathrm{H}^{\mathrm{T}}\mathrm{dH})\mathrm{H}_0^{-1} && (64) \\
\mathrm{dw} &:= \frac{1}{2}\mathrm{H}_0{}^{-T}(\mathrm{dH}^{\mathrm{T}}\mathrm{H} - \mathrm{H}^{\mathrm{T}}\mathrm{dH})\mathrm{H}_0^{-1} && (65) \\
\mathrm{de} + \mathrm{dw} &= \mathrm{H}_0{}^{-T}\mathrm{dH}^{\mathrm{T}}\mathrm{H}\mathrm{H}_0^{-1} && (66) \\
\mathrm{de} - \mathrm{dw} &= \mathrm{H}_0{}^{-T}\mathrm{H}^{\mathrm{T}}\mathrm{dH}\mathrm{H}_0^{-1} && (67) \\
\mathrm{dH} &= \mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}(\mathrm{de} - \mathrm{dw})\mathrm{H}_0 && (68) \\
\mathrm{dH}^{T} &= \mathrm{H}_0^{\mathrm{T}}(\mathrm{de} + \mathrm{dw})\mathrm{H}_0\mathrm{H}^{-1} && (69) \\
& && (70)
\end{aligned}
$$

$$
\begin{aligned}
dA(\boldsymbol{q}_i, \boldsymbol{p}_i) &= \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} && (71) \\
&= \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH^{T}_{\beta\alpha} && (72) \\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}} \mathrm{dH}^{T} \right) && (73) \\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}} \left(\mathrm{H}_0^{\mathrm{T}}(\mathrm{de} + \mathrm{dw})\mathrm{H}_0\mathrm{H}^{-1} \right) \right) && (74) \\
&= \mathrm{Tr}\left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^{T}(\mathrm{de} + \mathrm{dw}) \right) && (75) \\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^{T} \right)_{\alpha\beta} (\mathrm{de} + \mathrm{dw})^{T}_{\alpha\beta} && (76) \\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^{T} \right)_{\alpha\beta} (\mathrm{de} - \mathrm{dw})_{\alpha\beta} && (77) \\
& && (78)
\end{aligned}
$$

$$
\begin{aligned}
dA(\boldsymbol{q}_i, \boldsymbol{p}_i) &= \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} && (79)\\
&= \sum_{\alpha,\beta} \frac{\partial A}{\partial H^T_{\beta\alpha}} dH_{\alpha\beta} && (80)\\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{dH}\right) && (81)\\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \left(\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}(\mathrm{de}-\mathrm{dw})\mathrm{H}_0\right)\right) && (82)\\
&= \mathrm{Tr}\left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T}\mathrm{H}_0^{T}(\mathrm{de}-\mathrm{dw})\right) && (83)\\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T}\mathrm{H}_0^{T}\right)_{\alpha\beta} (\mathrm{de}-\mathrm{dw})_{\beta\alpha} && (84)\\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T}\mathrm{H}_0^{T}\right)_{\alpha\beta} (\mathrm{de}+\mathrm{dw})_{\alpha\beta} && (85)\\
& && (86)
\end{aligned}
$$

$$
\mathrm{dA} = \sum_{\alpha\beta}\left(\frac{1}{2}\left(\mathrm{H}_0\mathrm{H}^{-1}\frac{\partial A}{\partial \mathrm{H}}\mathrm{H}_0^T + \mathrm{H}_0\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}}\mathrm{H}^{-T}\mathrm{H}_0^T\right)_{\alpha\beta}\mathrm{de}_{\alpha\beta} + \frac{1}{2}\left(\mathrm{H}_0\mathrm{H}^{-1}\frac{\partial A}{\partial \mathrm{H}}\mathrm{H}_0^T - \mathrm{H}_0\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}}\mathrm{H}^{-T}\mathrm{H}_0^T\right)_{\alpha\beta}\mathrm{dw}_{\alpha\beta}\right) \tag{87}
$$

$$
\begin{aligned}
\frac{\mathrm{dA}}{\mathrm{de}} &= \frac{1}{2}\left(\mathrm{H}_0\mathrm{H}^{-1}\frac{\partial A}{\partial \mathrm{H}}\mathrm{H}_0^T + \mathrm{H}_0\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}}\mathrm{H}^{-T}\mathrm{H}_0^T\right) && (88)\\
\frac{\partial A}{\partial e_{\alpha\sigma}} &= \frac{1}{2}\sum_i\sum_{\beta\gamma}\left(\left(\mathrm{H}_0\mathrm{H}^{-1}\right)_{\alpha\beta}\left\{\frac{\partial \mathrm{A}}{\partial q_{i\beta}}\left(\mathrm{H}^{-1}q_i\right)_\gamma - p_{i\beta}\left(H^{-1}\frac{\partial \mathrm{A}}{\partial \boldsymbol{p}_i}\right)_\gamma\right\}\mathrm{H}^T_{0\gamma\sigma}\right. && (89)\\
&\left.+\ \mathrm{H}_{0\alpha\beta}\left\{\left(\mathrm{H}^{-1}q_i\right)_\beta\frac{\partial \mathrm{A}}{\partial q_{i\gamma}} - \left(H^{-1}\frac{\partial \mathrm{A}}{\partial \boldsymbol{p}_i}\right)_\beta p_{i\gamma}\right\}\left(\mathrm{H}^{-T}\mathrm{H}_0^T\right)_{\gamma\sigma}\right) && (90)\\
& && (91)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial H_{\beta\gamma}} &= \sum_i\left\{\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial q_{i\beta}}\left(\mathrm{H}^{-1}q_i\right)_\gamma - p_{i\beta}\left(H^{-1}\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial \boldsymbol{p}_i}\right)_\gamma\right\} && (92)\\
\frac{\partial A}{\partial \mathrm{H}} &= \sum_i\left\{\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes\left(\mathrm{H}^{-1}\boldsymbol{q}_i\right) - \boldsymbol{p}_i\otimes\left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\right\} && (93)\\
\frac{\partial A}{\partial \mathrm{H}^T} &= \sum_i\left\{\left(\mathrm{H}^{-1}\boldsymbol{q}_i\right)\otimes\frac{\partial A}{\partial \boldsymbol{q}_i} - \left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes\boldsymbol{p}_i\right\} && (94)
\end{aligned}
$$

$$(A\,(b\otimes c))_{ik} = \sum_j A_{ij} b_j c_k = (Ab)_i c_k = (bA^T)_i c_k \tag{95}$$

$$= ((Ab)\otimes c)_{ik} \tag{96}$$

$$= \left((bA^T)\otimes c\right)_{ik} \tag{97}$$

$$((a\otimes b)C)_{ik} = \sum_j a_i b_j C_{jk} \tag{98}$$

$$= (a\otimes (bC))_{ik} \tag{99}$$

$$= \left(a\otimes\left(C^T b\right)\right)_{ik} \tag{100}$$

$$\mathrm{H}^{-1}\frac{\partial A}{\partial \mathrm{H}} + \frac{\partial A}{\partial \mathrm{H}^T}\mathrm{H}^{-T} = \mathrm{H}^{-1}\sum_i \left\{\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes\left(\mathrm{H}^{-1}\boldsymbol{q}_i\right) - \boldsymbol{p}_i\otimes\left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\right\} \tag{101}$$

$$+ \sum_i \left\{\left(\mathrm{H}^{-1}\boldsymbol{q}_i\right)\otimes\frac{\partial A}{\partial \boldsymbol{q}_i} - \left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes\boldsymbol{p}_i\right\}\mathrm{H}^{-T} \tag{102}$$

$$= \sum_i \left\{H^{-1}\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes H^{-1}\boldsymbol{q}_i - H^{-1}\boldsymbol{p}_i\otimes\left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\right. \tag{103}$$

$$\left. + \left(\mathrm{H}^{-1}\boldsymbol{q}_i\right)\otimes\frac{\partial A}{\partial \boldsymbol{q}_i}\mathrm{H}^{-T} - \left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes\boldsymbol{p}_i\mathrm{H}^{-T}\right\} \tag{104}$$

$$= \sum_i \left\{H^{-1}\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes\left(\boldsymbol{q}_i H^{-T}\right) - \left(H^{-1}\boldsymbol{p}_i\right)\otimes\left(\frac{\partial A}{\partial \boldsymbol{p}_i}\mathrm{H}^{-T}\right)\right. \tag{105}$$

$$\left. + \left(\mathrm{H}^{-1}\boldsymbol{q}_i\right)\otimes\frac{\partial A}{\partial \boldsymbol{q}_i}\mathrm{H}^{-T} - \left(\mathrm{H}^{-1}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes\left(\boldsymbol{p}_i\mathrm{H}^{-T}\right)\right\} \tag{106}$$

$$= \sum_i \mathrm{H}^{-1}\left\{\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes\boldsymbol{q}_i + \boldsymbol{q}_i\otimes\frac{\partial A}{\partial \boldsymbol{q}_i} - \boldsymbol{p}_i\otimes\frac{\partial A}{\partial \boldsymbol{p}_i} - \frac{\partial A}{\partial \boldsymbol{p}_i}\otimes\boldsymbol{p}_i\right\}\mathrm{H}^{-T} \tag{107}$$

$$:= \mathrm{H}^{-1}(\hat{D}A)\mathrm{H}^{-T} \tag{108}$$

$$\frac{1}{Z}\frac{\partial Z}{\partial H_{\alpha\beta}} = -\frac{1}{k_B T}\left\langle\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle \tag{109}$$

$$\frac{\partial\langle A\rangle}{\partial H_{\alpha\beta}} = \frac{\partial}{\partial H_{\alpha\beta}}\frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}A\exp(-\mathcal{H}/k_B T) \tag{110}$$

$$= -\frac{1}{Z^2}\frac{\partial Z}{\partial H_{\alpha\beta}}\int d\boldsymbol{q}d\boldsymbol{p}A\exp(-\mathcal{H}/k_B T) + \frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}\frac{\partial A}{\partial H_{\alpha\beta}}\exp(-\mathcal{H}/k_B T) \tag{111}$$

$$+ \frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}A\frac{\partial}{\partial H_{\alpha\beta}}\exp(-\mathcal{H}/k_B T) \tag{112}$$

$$= -\frac{1}{Z}\left(-\frac{1}{k_B T}\right)\left\langle\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle + \left\langle\frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{Z}\frac{1}{k_B T}\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle \tag{113}$$

$$= \left\langle\frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{k_B T}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle + \left\langle\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle\right) \tag{114}$$

$$= \left\langle\frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{k_B T}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle + \left\langle\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle\right) \tag{115}$$

$$\frac{\partial\langle A\rangle}{\partial H_{\alpha\beta}} = \left\langle\frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{k_B T}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle + \left\langle\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle\right) \tag{116}$$

$$
\begin{aligned}
\frac{\partial \langle A \rangle}{\partial e_{\alpha\beta}} &= \frac{1}{2} \left(\mathrm{H}_0 \mathrm{H}^{-1} \frac{\partial \langle A \rangle}{\partial \mathrm{H}} \mathrm{H}_0^T + \mathrm{H}_0 \frac{\partial \langle A \rangle}{\partial \mathrm{H}^T} \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} \right)_{\alpha\beta} && (117) \\
&= \frac{1}{2} \mathrm{H}_0 \left(\mathrm{H}^{-1} \frac{\partial \langle A \rangle}{\partial \mathrm{H}} + \frac{\partial \langle A \rangle}{\partial \mathrm{H}^T} \mathrm{H}^{-\mathrm{T}} \right) \mathrm{H}_0^{\mathrm{T}} && (118) \\
&= \frac{1}{2} \mathrm{H}_0 \left[\mathrm{H}^{-1} \left\{ \left\langle \frac{\partial A}{\partial \mathrm{H}} \right\rangle - \frac{1}{k_B T} \left(\left\langle A \frac{\partial \mathcal{H}}{\partial \mathrm{H}} \right\rangle + \left\langle \frac{\partial \mathcal{H}}{\partial \mathrm{H}} \right\rangle \langle A \rangle \right) \right\} \right. && (119) \\
&\left. + \left\{ \left\langle \frac{\partial A}{\partial \mathrm{H}^T} \right\rangle - \frac{1}{k_B T} \left(\left\langle A \frac{\partial \mathcal{H}}{\partial \mathrm{H}^T} \right\rangle + \left\langle \frac{\partial \mathcal{H}}{\partial \mathrm{H}^T} \right\rangle \langle A \rangle \right) \right\} \mathrm{H}^{-\mathrm{T}} \right] \mathrm{H}_0^{\mathrm{T}} && (120) \\
& && (121)
\end{aligned}
$$

$$
\begin{aligned}
F &= -k_B T \ln Z && (122) \\
\Omega\, t_{\alpha\beta} &= -\Omega \frac{\partial F}{\partial e_{\alpha\beta}} && (123) \\
&= k_B T Z^{-1} \frac{\partial Z}{\partial e_{\alpha\beta}} && (124) \\
&= \frac{1}{2} k_B T Z^{-1} \left(\mathrm{H}_0 \mathrm{H}^{-1} \frac{\partial Z}{\partial \mathrm{H}} \mathrm{H}_0^T + \mathrm{H}_0 \frac{\partial Z}{\partial \mathrm{H}^T} \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} \right)_{\alpha\beta} && (125) \\
&= \frac{1}{2} k_B T \left\{ \mathrm{H}_0 \mathrm{H}^{-1} \left(-\frac{1}{k_B T} \left\langle \frac{\partial \mathcal{H}}{\partial \mathrm{H}} \right\rangle \right) \mathrm{H}_0^T + \mathrm{H}_0 \left(-\frac{1}{k_B T} \left\langle \frac{\partial \mathcal{H}}{\partial \mathrm{H}^T} \right\rangle \right) \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} \right\}_{\alpha\beta} && (126) \\
&= -\frac{1}{2} \sum_i \left\{ \mathrm{H}_0 \mathrm{H}^{-1} \left\langle \boldsymbol{V}_i \otimes (\mathrm{H}^{-1} \boldsymbol{q}_i) - \boldsymbol{p}_i \otimes \left(\mathrm{H}^{-1} \frac{\boldsymbol{p}_i}{m_i} \right) \right\rangle \mathrm{H}_0^T \right. && (127) \\
&\left. + \mathrm{H}_0 \left\langle (\mathrm{H}^{-1} \boldsymbol{q}_i) \otimes \boldsymbol{V}_i - \left(\mathrm{H}^{-1} \frac{\boldsymbol{p}_i}{m_i} \right) \otimes \boldsymbol{p}_i \right\rangle \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} \right\}_{\alpha\beta} && (128) \\
&= -\frac{1}{2} \sum_i \left\{ \mathrm{H}_0 \mathrm{H}^{-1} \langle \boldsymbol{q}_i \otimes \boldsymbol{V}_i \rangle \mathrm{H}^{-T} \mathrm{H}_0^T - \mathrm{H}_0 \mathrm{H}^{-1} \left\langle \boldsymbol{p}_i \otimes \frac{\boldsymbol{p}_i}{m_i} \right\rangle \mathrm{H}^{-T} \mathrm{H}_0^T \right. && (129) \\
&\left. + \mathrm{H}_0 \mathrm{H}^{-1} \langle \boldsymbol{V}_i \otimes \boldsymbol{q}_i \rangle \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} - \mathrm{H}_0 \mathrm{H}^{-1} \left\langle \frac{\boldsymbol{p}_i}{m_i} \otimes \boldsymbol{p}_i \right\rangle \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} \right\}_{\alpha\beta} && (130) \\
&= -\frac{1}{2} \sum_i \mathrm{H}_0 \mathrm{H}^{-1} \left\{ \langle \boldsymbol{q}_i \otimes \boldsymbol{V}_i \rangle + \langle \boldsymbol{V}_i \otimes \boldsymbol{q}_i \rangle - \left\langle \boldsymbol{p}_i \otimes \frac{\boldsymbol{p}_i}{m_i} \right\rangle - \left\langle \frac{\boldsymbol{p}_i}{m_i} \otimes \boldsymbol{p}_i \right\rangle \right\} \mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} && (131) \\
&= \Omega \left\langle t_{\alpha\beta} \right\rangle && (132)
\end{aligned}
$$

$$
\frac{\partial \mathcal{H}}{\partial \mathrm{H}} = \sum_i \left\{ \boldsymbol{V}_i \otimes (\mathrm{H}^{-1} \boldsymbol{q}_i) - \boldsymbol{p}_i \otimes \left(\mathrm{H}^{-1} \frac{\boldsymbol{p}_i}{m_i} \right) \right\} \tag{133}
$$

$$
C_{\alpha\beta\gamma\sigma} = -\frac{\partial \left\langle t_{\alpha\beta} \right\rangle}{\partial e_{\gamma\sigma}} \tag{134}
$$

参考文献

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