1 Elastic Constants

Elastic[1].

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

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

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

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

$$= 0 \tag{5}$$

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

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

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

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

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

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

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

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

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

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

$$\tag{16}$$

$$\mathrm{H}^{1}\mathrm{H} = \frac{1}{2\pi}\begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}\begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \tag{17}$$

$$= \frac{1}{2\pi}\begin{pmatrix} \sum_\alpha b_{1\alpha}a_{1\alpha} & \sum_\alpha b_{1\alpha}a_{2\alpha} & \sum_\alpha b_{1\alpha}a_{3\alpha} \\ \sum_\alpha b_{2\alpha}a_{1\alpha} & \sum_\alpha b_{2\alpha}a_{2\alpha} & \sum_\alpha b_{2\alpha}a_{3\alpha} \\ \sum_\alpha b_{3\alpha}a_{1\alpha} & \sum_\alpha b_{3\alpha}a_{2\alpha} & \sum_\alpha b_{3\alpha}a_{3\alpha} \end{pmatrix} \tag{18}$$

$$= \mathrm{I} \tag{19}$$

$$\boldsymbol{q} = \mathrm{H}\boldsymbol{s} \tag{20}$$

$$= \sum_i s_i \boldsymbol{a}_i \tag{21}$$

$$= \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}\begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix} \tag{22}$$

$$\boldsymbol{p} = (\mathrm{H}^{-1})^{T}\boldsymbol{p} \tag{23}$$

$$\boldsymbol{s} = \mathrm{H}^{-1}\boldsymbol{q} \tag{24}$$

$$\boldsymbol{q} = \mathrm{H}^{T}\boldsymbol{p} \tag{25}$$

$$\mathrm{H} = \mathrm{H}_0 + \mathrm{dH} \tag{26}$$

$$\mathrm{H}^{\mathrm{T}}\mathrm{H} = (\mathrm{H}_0 + \mathrm{dH})^{\mathrm{T}}(\mathrm{H}_0 + \mathrm{dH}) \tag{27}$$

$$= \mathrm{H}_0^{\mathrm{T}}\mathrm{H}_0 + \mathrm{dH}^{\mathrm{T}}\mathrm{H}_0 + \mathrm{H}_0^{\mathrm{T}}\mathrm{dH} + \mathrm{dH}^{\mathrm{T}}\mathrm{dH} \tag{28}$$

$$\approx \mathrm{H}_0^{\mathrm{T}}\mathrm{H}_0 + \mathrm{dH}^{\mathrm{T}}\mathrm{H}_0 + \mathrm{H}_0^{\mathrm{T}}\mathrm{dH} \tag{29}$$

$$:= \mathrm{H}_0^{\mathrm{T}}\mathrm{H}_0 + 2\mathrm{H}_0^{\mathrm{T}}\mathrm{e}\mathrm{H}_0 \tag{30}$$

$$= \mathrm{H}_0^{\mathrm{T}}(1 + 2\mathrm{e})\mathrm{H}_0 \tag{31}$$

$$\mathrm{e} = \frac{1}{2}\left((\mathrm{H}_0^{\mathrm{T}})^{-1}\mathrm{H}^{\mathrm{T}}\mathrm{H}\mathrm{H}_0^{-1} - 1\right) \tag{32}$$

$$\mathrm{H}_0^{-\mathrm{T}} := (\mathrm{H}_0^{\mathrm{T}})^{-1} = (\mathrm{H}_0^{-1})^{\mathrm{T}} \tag{33}$$

$$\frac{\partial q_{i\alpha}}{\partial H_{\beta\gamma}} = \frac{\partial}{\partial a_{\beta\gamma}}\left(\sum_\sigma s_\sigma \mathbf{a}_\sigma\right)_\alpha \tag{34}$$

$$= \frac{\partial}{\partial a_{\beta\gamma}}\sum_\sigma a_{\sigma\alpha}s_\sigma \tag{35}$$

$$= \sum_\sigma \delta_{\beta\sigma}\delta_{\gamma\alpha}s_\sigma \tag{36}$$

$$= \delta_{\alpha\gamma}s_\beta \tag{37}$$

$$= \delta_{\alpha\gamma}(\mathrm{H}^{-1}\boldsymbol{q})_\beta \tag{38}$$

$$= \delta_{\alpha\gamma}\sum_\sigma \mathrm{H}^{-1}_{\beta\sigma}\boldsymbol{q}_\sigma \tag{39}$$

$$
\begin{aligned}
\frac{\partial}{\partial H_{\beta\gamma}}\tilde{p}_{i\alpha} &= \frac{\partial}{\partial H_{\beta\gamma}}\left(\mathrm{H}^T\mathbf{p_i}\right)_\alpha && (40)\\
0 &= \frac{\partial}{\partial H_{\beta\gamma}}\sum_\sigma H^T_{\alpha\sigma}p_{i\sigma} && (41)\\
&= \sum_\sigma\left(\frac{\partial H_{\sigma\alpha}}{\partial H_{\beta\gamma}}p_{i\sigma} + H_{\sigma\alpha}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}}\right) && (42)\\
&= \sum_\sigma\left(\delta_{\sigma\beta}\delta_{\alpha\gamma}p_{i\sigma} + H_{\sigma\alpha}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}}\right) && (43)\\
&= \delta_{\alpha\gamma}p_{i\beta} + \sum_\sigma H_{\sigma\alpha}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} && (44)\\
\sum_\sigma H_{\sigma\alpha}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} &= -\delta_{\alpha\gamma}p_{i\beta} && (45)\\
\sum_\alpha H^{-1}_{\alpha\tau}\sum_\sigma H_{\sigma\alpha}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} &= -\sum_\alpha H^{-1}_{\alpha\tau}\delta_{\alpha\gamma}p_{i\beta} && (46)\\
\sum_\sigma\left(HH^{-1}\right)_{\sigma\tau}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} &= -H^{-1}_{\gamma\tau}p_{i\beta} && (47)\\
\sum_\sigma\delta_{\sigma\tau}\frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} &= -H^{-1}_{\gamma\tau}p_{i\beta} && (48)\\
\frac{\partial p_{i\tau}}{\partial H_{\beta\gamma}} &= -H^{-1}_{\gamma\tau}p_{i\beta} && (49)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial H_{\beta\gamma}} &= \sum_{i,\alpha}\left\{\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial q_{i\alpha}}\frac{\partial q_{i\alpha}}{\partial H_{\beta\gamma}} + \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial p_{i\alpha}}\frac{\partial p_{i\alpha}}{\partial H_{\beta\gamma}}\right\} && (50)\\
&= \sum_i\left\{\sum_\alpha\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial q_{i\alpha}}\left(\delta_{\alpha\gamma}\sum_\sigma \mathrm{H}^{-1}_{\beta\sigma}q_{i\sigma}\right) + \sum_\alpha\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial p_{i\alpha}}\left(-H^{-1}_{\gamma\alpha}p_{i\beta}\right)\right\} && (51)\\
&= \sum_i\left\{\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial q_{i\gamma}}\sum_\sigma \mathrm{H}^{-1}_{\beta\sigma}q_{i\sigma} - p_{i\beta}\sum_\alpha H^{-1}_{\gamma\alpha}\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial p_{i\alpha}}\right\} && (52)\\
&= \sum_i\left\{\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial q_{i\gamma}}\left(\mathrm{H}^{-1}q_i\right)_\beta - p_{i\beta}\left(H^{-T}\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i,\boldsymbol{p}_i\})}{\partial \boldsymbol{p}_i}\right)_\gamma\right\} && (53)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial\mathcal{H}}{\partial q_{i\alpha}} &= \frac{\partial}{\partial q_{i\alpha}}\left(\sum_j\sum_\beta\frac{p^2_{j\beta}}{2m_j} + V\left(\{\boldsymbol{q}_j\}\right)\right) && (54)\\
&= \frac{\partial}{\partial q_{i\alpha}}V\left(\{\boldsymbol{q}_j\}\right) && (55)\\
&:= V_{i\alpha} && (56)\\
\frac{\partial\mathcal{H}}{\partial p_{i\alpha}} &= \frac{\partial}{\partial p_{i\alpha}}\left(\sum_j\sum_\beta\frac{p^2_{j\beta}}{2m_j} + V\left(\{\boldsymbol{q}_j\}\right)\right) && (57)\\
&= \frac{p_{i\alpha}}{m_i} && (58)
\end{aligned}
$$

$$\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}} = \sum_i \left\{ \frac{\partial \mathcal{H}}{\partial q_{i\beta}} \left(\mathrm{H}^{-1} q_i\right)_\alpha - p_{i\alpha} \left(H^{-T} \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}_i} \right)_\beta \right\} \tag{59}$$

$$= \sum_i \left\{ V_{i\beta} \left(\mathrm{H}^{-1} q_i\right)_\alpha - p_{i\alpha} \left(H^{-T} \frac{\boldsymbol{p}_i}{m_i} \right)_\beta \right\} \tag{60}$$

$$= \sum_i \left\{ V_{i\beta} \left(\mathrm{H}^{-1} q_i\right)_\alpha - p_{i\alpha} \left(\frac{\boldsymbol{p}_i}{m_i} H^{-1} \right)_\beta \right\} \tag{61}$$

$$\frac{\partial \mathcal{H}}{\partial \mathrm{H}} = \sum_i \left\{ \left(\mathrm{H}^{-1} \boldsymbol{q}_i\right) \otimes \boldsymbol{V}_i - \boldsymbol{p}_i \otimes \left(H^{-T} \frac{\boldsymbol{p}_i}{m_i} \right) \right\} \tag{62}$$

$$\mathrm{H}^{\mathrm{T}}\mathrm{H} = \mathrm{H}_0^{\mathrm{T}}(1 + 2\mathrm{e})\mathrm{H}_0 \tag{63}$$

$$(\mathrm{H} + \mathrm{dH})^{\mathrm{T}}(\mathrm{H} + \mathrm{dH}) = \mathrm{H}_0^{\mathrm{T}}(1 + 2(\mathrm{e} + \mathrm{de}))\mathrm{H}_0 \tag{64}$$

$$\mathrm{H}^{\mathrm{T}}\mathrm{dH} + \mathrm{dH}^{\mathrm{T}}\mathrm{H} + \mathrm{dH}^{\mathrm{T}}\mathrm{dH} = 2\mathrm{H}_0^{\mathrm{T}}\mathrm{de}\mathrm{H}_0 \tag{65}$$

$$\mathrm{de} = \frac{1}{2}\mathrm{H}_0{}^{-T}(\mathrm{dH}^{\mathrm{T}}\mathrm{H} + \mathrm{H}^{\mathrm{T}}\mathrm{dH})\mathrm{H}_0^{-1} \tag{66}$$

$$\mathrm{dw} := \frac{1}{2}\mathrm{H}_0{}^{-T}(\mathrm{dH}^{\mathrm{T}}\mathrm{H} - \mathrm{H}^{\mathrm{T}}\mathrm{dH})\mathrm{H}_0^{-1} \tag{67}$$

$$\mathrm{de} + \mathrm{dw} = \mathrm{H}_0{}^{-T}\mathrm{dH}^{\mathrm{T}}\mathrm{H}\mathrm{H}_0^{-1} \tag{68}$$

$$\mathrm{de} - \mathrm{dw} = \mathrm{H}_0{}^{-T}\mathrm{H}^{\mathrm{T}}\mathrm{dH}\mathrm{H}_0^{-1} \tag{69}$$

$$\mathrm{dH} = \mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}(\mathrm{de} - \mathrm{dw})\mathrm{H}_0 \tag{70}$$

$$\mathrm{dH}^T = \mathrm{H}_0^{\mathrm{T}}(\mathrm{de} + \mathrm{dw})\mathrm{H}_0\mathrm{H}^{-1} \tag{71}$$

$$\tag{72}$$

$$dA(\boldsymbol{q}_i, \boldsymbol{p}_i) = \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} \tag{73}$$

$$= \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH^T_{\beta\alpha} \tag{74}$$

$$= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}} \mathrm{dH}^T \right) \tag{75}$$

$$= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}} \left(\mathrm{H}_0^{\mathrm{T}}(\mathrm{de} + \mathrm{dw})\mathrm{H}_0\mathrm{H}^{-1} \right) \right) \tag{76}$$

$$= \mathrm{Tr}\left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T(\mathrm{de} + \mathrm{dw}) \right) \tag{77}$$

$$= \sum_{\alpha\beta} \left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T \right)_{\alpha\beta} (\mathrm{de} + \mathrm{dw})^T_{\alpha\beta} \tag{78}$$

$$= \sum_{\alpha\beta} \left(\mathrm{H}_0\mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T \right)_{\alpha\beta} (\mathrm{de} - \mathrm{dw})_{\alpha\beta} \tag{79}$$

$$\tag{80}$$

$$
\begin{aligned}
dA(\boldsymbol{q}_i, \boldsymbol{p}_i) &= \sum_{\alpha,\beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} && (81)\\
&= \sum_{\alpha,\beta} \frac{\partial A}{\partial H^T_{\beta\alpha}} dH_{\alpha\beta} && (82)\\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{dH}\right) && (83)\\
&= \mathrm{Tr}\left(\frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \left(\mathrm{H}^{-\mathrm{T}} \mathrm{H}_0^{\mathrm{T}} (\mathrm{de} - \mathrm{dw}) \mathrm{H}_0\right)\right) && (84)\\
&= \mathrm{Tr}\left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T (\mathrm{de} - \mathrm{dw})\right) && (85)\\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T\right)_{\alpha\beta} (\mathrm{de} - \mathrm{dw})_{\beta\alpha} && (86)\\
&= \sum_{\alpha\beta} \left(\mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T\right)_{\alpha\beta} (\mathrm{de} + \mathrm{dw})_{\alpha\beta} && (87)\\
& && (88)
\end{aligned}
$$

$$
\mathrm{dA} = \sum_{\alpha\beta} \left(\frac{1}{2} \left(\mathrm{H}_0 \mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T + \mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T\right)_{\alpha\beta} \mathrm{de}_{\alpha\beta} + \frac{1}{2} \left(\mathrm{H}_0 \mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T - \mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T\right)_{\alpha\beta} \mathrm{dw}_{\alpha\beta} \right) \tag{89}
$$

$$
\begin{aligned}
\frac{\mathrm{dA}}{\mathrm{de}} &= \frac{1}{2} \left(\mathrm{H}_0 \mathrm{H}^{-1} \frac{\partial A}{\partial \mathrm{H}} \mathrm{H}_0^T + \mathrm{H}_0 \frac{\partial A}{\partial \mathrm{H}^{\mathrm{T}}} \mathrm{H}^{-T} \mathrm{H}_0^T\right) && (90)\\
\frac{\partial A}{\partial e_{\alpha\sigma}} &= \frac{1}{2} \sum_i \sum_{\beta\gamma} \left(\left(\mathrm{H}_0 \mathrm{H}^{-1}\right)_{\alpha\beta} \left\{ \frac{\partial \mathrm{A}}{\partial q_{i\gamma}} \left(\mathrm{H}^{-1} q_i\right)_\beta - p_{i\beta} \left(H^{-T} \frac{\partial \mathrm{A}}{\partial \boldsymbol{p}_i}\right)_\gamma \right\} \mathrm{H}^T_{0\gamma\sigma} \right. && (91)\\
&\left. + \mathrm{H}_{0\alpha\beta} \left\{ \frac{\partial \mathrm{A}}{\partial q_{i\beta}} \left(\mathrm{H}^{-1} q_i\right)_\gamma - p_{i\gamma} \left(H^{-T} \frac{\partial \mathrm{A}}{\partial \boldsymbol{p}_i}\right)_\beta \right\} \left(\mathrm{H}^{-T} \mathrm{H}_0^T\right)_{\gamma\sigma} \right) && (92)\\
& && (93)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial H_{\beta\gamma}} &= \sum_i \left\{ \left(\mathrm{H}^{-1} q_i\right)_\beta \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial q_{i\gamma}} - p_{i\beta} \left(H^{-T} \frac{\partial \mathrm{A}(\{\boldsymbol{q}_i, \boldsymbol{p}_i\})}{\partial \boldsymbol{p}_i}\right)_\gamma \right\} && (94)\\
\frac{\partial A}{\partial \mathrm{H}} &= \sum_i \left\{ \left(\mathrm{H}^{-1} \boldsymbol{q}_i\right) \otimes \frac{\partial A}{\partial \boldsymbol{q}_i} - \boldsymbol{p}_i \otimes \left(\mathrm{H}^{-T} \frac{\partial A}{\partial \boldsymbol{p}_i}\right) \right\} && (95)\\
\frac{\partial A}{\partial \mathrm{H}^T} &= \sum_i \left\{ \frac{\partial A}{\partial \boldsymbol{q}_i} \otimes \left(\mathrm{H}^{-1} \boldsymbol{q}_i\right) - \left(\mathrm{H}^{-T} \frac{\partial A}{\partial \boldsymbol{p}_i}\right) \otimes \boldsymbol{p}_i \right\} && (96)
\end{aligned}
$$

$$
\begin{aligned}
(A\,(b\otimes c))_{ik} &= \sum_j A_{ij}b_jc_k = (Ab)_i c_k = (bA^T)_i c_k && (97)\\
&= ((Ab)\otimes c)_{ik} && (98)\\
&= \left((bA^T)\otimes c\right)_{ik} && (99)\\
((a\otimes b)C)_{ik} &= \sum_j a_i b_j C_{jk} && (100)\\
&= (a\otimes (bC))_{ik} && (101)\\
&= \left(a\otimes \left(C^T b\right)\right)_{ik} && (102)
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{H}^{-1}\frac{\partial A}{\partial \mathrm{H}} + \frac{\partial A}{\partial \mathrm{H}^T}\mathrm{H}^{-T} &= \mathrm{H}^{-1}\sum_i \left\{\left(\mathrm{H}^{-1}\boldsymbol{q}_i\right)\otimes \frac{\partial A}{\partial \boldsymbol{q}_i} - \boldsymbol{p}_i \otimes \left(\mathrm{H}^{-T}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\right\} && (103)\\
&+ \sum_i \left\{\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes \left(\mathrm{H}^{-1}\boldsymbol{q}_i\right) - \left(\mathrm{H}^{-T}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes \boldsymbol{p}_i\right\}\mathrm{H}^{-T} && (104)\\
&= \sum_i \left\{H^{-1}H^{-1}\boldsymbol{q}_i \otimes \frac{\partial A}{\partial \boldsymbol{q}_i} - H^{-1}\boldsymbol{p}_i \otimes \left(\mathrm{H}^{-T}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\right. && (105)\\
&+ \left.\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes \left(\mathrm{H}^{-1}\boldsymbol{q}_i\mathrm{H}^{-T}\right) - \left(\mathrm{H}^{-T}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes \boldsymbol{p}_i\mathrm{H}^{-T}\right\} && (106)\\
&= \sum_i \left\{\left(H^{-1}\boldsymbol{q}_iH^{-T}\right)\otimes \frac{\partial A}{\partial \boldsymbol{q}_i} - \left(H^{-1}\boldsymbol{p}_i\right)\otimes \left(\frac{\partial A}{\partial \boldsymbol{p}_i}\mathrm{H}^{-1}\right)\right. && (107)\\
&+ \left.\frac{\partial A}{\partial \boldsymbol{q}_i}\otimes \left(\mathrm{H}^{-1}\boldsymbol{q}_i\mathrm{H}^{-T}\right) - \left(\mathrm{H}^{-T}\frac{\partial A}{\partial \boldsymbol{p}_i}\right)\otimes \left(\boldsymbol{p}_i\mathrm{H}^{-T}\right)\right\} && (108)
\end{aligned}
$$

$$
\frac{1}{Z}\frac{\partial Z}{\partial H_{\alpha\beta}} = -\frac{1}{k_BT}\left\langle \frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle \qquad (109)
$$

$$
\begin{aligned}
\frac{\partial \langle A\rangle}{\partial H_{\alpha\beta}} &= \frac{\partial}{\partial H_{\alpha\beta}}\frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}A\exp(-\mathcal{H}/k_BT) && (110)\\
&= -\frac{1}{Z^2}\frac{\partial Z}{\partial H_{\alpha\beta}}\int d\boldsymbol{q}d\boldsymbol{p}A\exp(-\mathcal{H}/k_BT) + \frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}\frac{\partial A}{\partial H_{\alpha\beta}}\exp(-\mathcal{H}/k_BT) && (111)\\
&+ \frac{1}{Z}\int d\boldsymbol{q}d\boldsymbol{p}A\frac{\partial}{\partial H_{\alpha\beta}}\exp(-\mathcal{H}/k_BT) && (112)\\
&= -\frac{1}{Z}\left(-\frac{1}{k_BT}\right)\left\langle \frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle \langle A\rangle + \left\langle \frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{Z}\frac{1}{k_BT}\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle && (113)\\
&= \left\langle \frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{k_BT}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle + \left\langle \frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle\right) && (114)\\
&= \left\langle \frac{\partial A}{\partial H_{\alpha\beta}}\right\rangle - \frac{1}{k_BT}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle + \left\langle \frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}}\right\rangle\langle A\rangle\right) && (115)
\end{aligned}
$$

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

$$\frac{\partial \langle A \rangle}{\partial e_{\alpha\beta}} = \frac{1}{2}\left(\mathrm{H}_0\mathrm{H}^{-1}\frac{\partial \langle A \rangle}{\partial \mathrm{H}}\mathrm{H}_0^T + \mathrm{H}_0\frac{\partial \langle A \rangle}{\partial \mathrm{H}^T}\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}\right)_{\alpha\beta} \tag{117}$$

$$= \frac{1}{2}\mathrm{H}_0\left(\mathrm{H}^{-1}\frac{\partial \langle A \rangle}{\partial \mathrm{H}} + \frac{\partial \langle A \rangle}{\partial \mathrm{H}^T}\mathrm{H}^{-\mathrm{T}}\right)\mathrm{H}_0^{\mathrm{T}} \tag{118}$$

$$= \frac{1}{2}\mathrm{H}_0\left[\mathrm{H}^{-1}\left\{\left\langle\frac{\partial A}{\partial \mathrm{H}}\right\rangle - \frac{1}{k_B T}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial \mathrm{H}}\right\rangle + \left\langle\frac{\partial \mathcal{H}}{\partial \mathrm{H}}\right\rangle\langle A\rangle\right)\right\}\right. \tag{119}$$

$$\left. + \left\{\left\langle\frac{\partial A}{\partial \mathrm{H}^T}\right\rangle - \frac{1}{k_B T}\left(\left\langle A\frac{\partial \mathcal{H}}{\partial \mathrm{H}^T}\right\rangle + \left\langle\frac{\partial \mathcal{H}}{\partial \mathrm{H}^T}\right\rangle\langle A\rangle\right)\right\}\mathrm{H}^{-\mathrm{T}}\right]\mathrm{H}_0^{\mathrm{T}} \tag{120}$$

$$\tag{121}$$

$$F = -k_B T \ln Z \tag{122}$$

$$\Omega\, t_{\alpha\beta} = -\Omega\frac{\partial F}{\partial e_{\alpha\beta}} \tag{123}$$

$$= k_B T Z^{-1}\frac{\partial Z}{\partial e_{\alpha\beta}} \tag{124}$$

$$= \frac{1}{2}k_B T Z^{-1}\left(\mathrm{H}_0\mathrm{H}^{-1}\frac{\partial Z}{\partial \mathrm{H}}\mathrm{H}_0^T + \mathrm{H}_0\frac{\partial Z}{\partial \mathrm{H}^T}\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}\right)_{\alpha\beta} \tag{125}$$

$$= \frac{1}{2}k_B T\left\{\mathrm{H}_0\mathrm{H}^{-1}\left(-\frac{1}{k_B T}\left\langle\frac{\partial \mathcal{H}}{\partial \mathrm{H}}\right\rangle\right)\mathrm{H}_0^T + \mathrm{H}_0\left(-\frac{1}{k_B T}\left\langle\frac{\partial \mathcal{H}}{\partial \mathrm{H}^T}\right\rangle\right)\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}\right\}_{\alpha\beta} \tag{126}$$

$$= -\frac{1}{2}\sum_i\left\{\mathrm{H}_0\mathrm{H}^{-1}\left\langle(\mathrm{H}^{-1}\boldsymbol{q}_i)\otimes\boldsymbol{V}_i - \boldsymbol{p}_i\otimes\left(\mathrm{H}^{-T}\frac{\boldsymbol{p}_i}{m_i}\right)\right\rangle\mathrm{H}_0^T\right. \tag{127}$$

$$\left. + \mathrm{H}_0\left\langle\boldsymbol{V}_i\otimes(\mathrm{H}^{-1}\boldsymbol{q}_i) - \left(\mathrm{H}^{-T}\frac{\boldsymbol{p}_i}{m_i}\right)\otimes\boldsymbol{p}_i\right\rangle\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}\right\}_{\alpha\beta} \tag{128}$$

$$= -\frac{1}{2}\sum_i\left\{\mathrm{H}_0\mathrm{H}^{-1}\mathrm{H}^{-1}\langle\boldsymbol{q}_i\otimes\boldsymbol{V}_i\rangle\mathrm{H}_0^T - \mathrm{H}_0\mathrm{H}^{-1}\left\langle\boldsymbol{p}_i\otimes\frac{\boldsymbol{p}_i}{m_i}\right\rangle\mathrm{H}^{-1}\mathrm{H}_0^T\right. \tag{129}$$

$$\left. + \mathrm{H}_0\langle\boldsymbol{V}_i\otimes\boldsymbol{q}_i\rangle\mathrm{H}^{-T}\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}} - \mathrm{H}_0\mathrm{H}^{-T}\left\langle\frac{\boldsymbol{p}_i}{m_i}\otimes\boldsymbol{p}_i\right\rangle\mathrm{H}^{-\mathrm{T}}\mathrm{H}_0^{\mathrm{T}}\right\}_{\alpha\beta} \tag{130}$$

$$= \Omega\left\langle t_{\alpha\beta}\right\rangle \tag{131}$$

$$\frac{\partial \mathcal{H}}{\partial \mathrm{H}} = \sum_i\left\{(\mathrm{H}^{-1}\boldsymbol{q}_i)\otimes\boldsymbol{V}_i - \boldsymbol{p}_i\otimes\left(\mathrm{H}^{-T}\frac{\boldsymbol{p}_i}{m_i}\right)\right\} \tag{132}$$

$$C_{\alpha\beta\gamma\sigma} = -\frac{\partial\left\langle t_{\alpha\beta}\right\rangle}{\partial e_{\gamma\sigma}} \tag{133}$$

参考文献

[1] J F Lutsko. Generalized expressions for the calculation of elastic constants by computer simulation. *Journal of Applied Physics*, Vol. 65, No. 8, pp. 2991–2997, 1989.