

1 Elastic Constants

Elastic[1].

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

$$\mathbf{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}, \quad \mathbf{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \quad (2)$$

$$\mathbf{a}_i \cdot \mathbf{b}_j = \sum_{\alpha} a_{i\alpha} b_{j\alpha} = 2\pi \delta_{ij} \quad (3)$$

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

$$= 0 \quad (5)$$

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

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

$$= \frac{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}{V/2\pi} \quad (8)$$

$$= 2\pi \quad (9)$$

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

$$b_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V} = \frac{2\pi}{V} \begin{pmatrix} a_{22}a_{33} - a_{23}a_{32} \\ a_{23}a_{31} - a_{21}a_{33} \\ a_{21}a_{32} - a_{22}a_{31} \end{pmatrix} \quad (11)$$

$$b_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V} \quad (12)$$

$$b_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V} \quad (13)$$

$$\mathbf{H} = (\mathbf{a}_1 \quad \mathbf{a}_2 \quad \mathbf{a}_3) = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \quad (14)$$

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

$$(16)$$

$$\mathbf{H}^{-1}\mathbf{H} = \frac{1}{2\pi} \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \quad (17)$$

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

$$= \mathbf{I} \quad (19)$$

$$\mathbf{q} = \mathbf{H}\mathbf{s} \quad (20)$$

$$= \sum_i s_i \mathbf{a}_i \quad (21)$$

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

$$\mathbf{p} = (\mathbf{H}^{-1})^T \tilde{\mathbf{p}} \quad (23)$$

$$\mathbf{s} = \mathbf{H}^{-1} \mathbf{q} \quad (24)$$

$$\tilde{\mathbf{p}} = \mathbf{H}^T \mathbf{p} \quad (25)$$

$$\mathbf{H} = \mathbf{H}_0 + d\mathbf{H} \quad (26)$$

$$\mathbf{H}^T \mathbf{H} = (\mathbf{H}_0 + d\mathbf{H})^T (\mathbf{H}_0 + d\mathbf{H}) \quad (27)$$

$$= \mathbf{H}_0^T \mathbf{H}_0 + d\mathbf{H}^T \mathbf{H}_0 + \mathbf{H}_0^T d\mathbf{H} + d\mathbf{H}^T d\mathbf{H} \quad (28)$$

$$\approx \mathbf{H}_0^T \mathbf{H}_0 + d\mathbf{H}^T \mathbf{H}_0 + \mathbf{H}_0^T d\mathbf{H} \quad (29)$$

$$:= \mathbf{H}_0^T \mathbf{H}_0 + 2\mathbf{H}_0^T e\mathbf{H}_0 \quad (30)$$

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

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

$$\mathbf{H}_0^{-T} := (\mathbf{H}_0^T)^{-1} = (\mathbf{H}_0^{-1})^T \quad (33)$$

$$\frac{\partial q_{i\alpha}}{\partial H_{\beta\gamma}} = \frac{\partial}{\partial H_{\beta\gamma}} \sum_{\sigma} H_{\alpha\sigma} \mathbf{s}_{\sigma} \quad (34)$$

$$= \sum_{\sigma} \delta_{\alpha\beta} \delta_{\sigma\gamma} s_{\sigma} \quad (35)$$

$$= \delta_{\alpha\beta} s_{\gamma} \quad (36)$$

$$= \delta_{\alpha\beta} (\mathbf{H}^{-1} \mathbf{q})_{\gamma} \quad (37)$$

$$= \delta_{\alpha\beta} \sum_{\sigma} \mathbf{H}_{\gamma\sigma}^{-1} q_{\sigma} \quad (38)$$

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

$$0 = \frac{\partial}{\partial H_{\beta\gamma}} \sum_{\sigma} H_{\alpha\sigma}^T p_{i\sigma} \quad (40)$$

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

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

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

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

$$\sum_{\alpha} H_{\alpha\tau}^{-1} \sum_{\sigma} H_{\sigma\alpha} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -\sum_{\alpha} H_{\alpha\tau}^{-1} \delta_{\alpha\gamma} p_{i\beta} \quad (45)$$

$$\sum_{\sigma} (HH^{-1})_{\sigma\tau} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -H_{\gamma\tau}^{-1} p_{i\beta} \quad (46)$$

$$\sum_{\sigma} \delta_{\sigma\tau} \frac{\partial p_{i\sigma}}{\partial H_{\beta\gamma}} = -H_{\gamma\tau}^{-1} p_{i\beta} \quad (47)$$

$$\frac{\partial p_{i\tau}}{\partial H_{\beta\gamma}} = -H_{\gamma\tau}^{-1} p_{i\beta} \quad (48)$$

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

$$= \sum_i \left\{ \sum_{\alpha} \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial q_{i\alpha}} \left(\delta_{\alpha\beta} \sum_{\sigma} H_{\gamma\sigma}^{-1} q_{i\sigma} \right) + \sum_{\alpha} \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial p_{i\alpha}} \left(-H_{\gamma\alpha}^{-1} p_{i\beta} \right) \right\} \quad (50)$$

$$= \sum_i \left\{ \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial q_{i\beta}} \sum_{\sigma} H_{\gamma\sigma}^{-1} q_{i\sigma} - p_{i\beta} \sum_{\alpha} H_{\gamma\alpha}^{-1} \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial p_{i\alpha}} \right\} \quad (51)$$

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

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

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

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

$$\frac{\partial \mathcal{H}}{\partial \mathbf{q}_i} = \mathbf{V}_i, \quad \frac{\partial \mathcal{H}}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m_i} \quad (56)$$

$$\frac{\partial \mathcal{H}}{\partial H_{\alpha\beta}} = \sum_i \left\{ \frac{\partial \mathcal{H}}{\partial q_{i\alpha}} (H^{-1} q_i)_\beta - p_{i\alpha} \left(H^{-1} \frac{\partial \mathcal{H}}{\partial p_i} \right)_\beta \right\} \quad (57)$$

$$= \sum_i \left\{ V_{i\alpha} (H^{-1} q_i)_\beta - p_{i\alpha} \left(H^{-1} \frac{p_i}{m_i} \right)_\beta \right\} \quad (58)$$

$$= \sum_i \left\{ V_{i\alpha} (H^{-1} q_i)_\beta - p_{i\alpha} \left(\frac{p_i}{m_i} H^{-T} \right)_\beta \right\} \quad (59)$$

$$\frac{\partial \mathcal{H}}{\partial H} = \sum_i \left\{ \mathbf{V}_i \otimes (H^{-1} \mathbf{q}_i) - \mathbf{p}_i \otimes \left(H^{-1} \frac{\mathbf{p}_i}{m_i} \right) \right\} \quad (60)$$

$$H^T H = H_0^T (1 + 2e) H_0 \quad (61)$$

$$(H + dH)^T (H + dH) = H_0^T (1 + 2(e + de)) H_0 \quad (62)$$

$$H^T dH + dH^T H + dH^T dH = 2H_0^T de H_0 \quad (63)$$

$$de = \frac{1}{2} H_0^{-T} (dH^T H + H^T dH) H_0^{-1} \quad (64)$$

$$dw := \frac{1}{2} H_0^{-T} (dH^T H - H^T dH) H_0^{-1} \quad (65)$$

$$de + dw = H_0^{-T} dH^T H H_0^{-1} \quad (66)$$

$$de - dw = H_0^{-T} H^T dH H_0^{-1} \quad (67)$$

$$dH = H^{-T} H_0^T (de - dw) H_0 \quad (68)$$

$$dH^T = H_0^T (de + dw) H_0 H^{-1} \quad (69)$$

$$(70)$$

$$dA(q_i, p_i) = \sum_{\alpha, \beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} \quad (71)$$

$$= \sum_{\alpha, \beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\beta\alpha}^T \quad (72)$$

$$= \text{Tr} \left(\frac{\partial A}{\partial H} dH^T \right) \quad (73)$$

$$= \text{Tr} \left(\frac{\partial A}{\partial H} \left(H_0^T (de + dw) H_0 H^{-1} \right) \right) \quad (74)$$

$$= \text{Tr} \left(H_0 H^{-1} \frac{\partial A}{\partial H} H_0^T (de + dw) \right) \quad (75)$$

$$= \sum_{\alpha\beta} \left(H_0 H^{-1} \frac{\partial A}{\partial H} H_0^T \right)_{\alpha\beta} (de + dw)_{\alpha\beta}^T \quad (76)$$

$$= \sum_{\alpha\beta} \left(H_0 H^{-1} \frac{\partial A}{\partial H} H_0^T \right)_{\alpha\beta} (de - dw)_{\alpha\beta} \quad (77)$$

$$(78)$$

$$dA(\mathbf{q}_i, \mathbf{p}_i) = \sum_{\alpha, \beta} \frac{\partial A}{\partial H_{\alpha\beta}} dH_{\alpha\beta} \quad (79)$$

$$= \sum_{\alpha, \beta} \frac{\partial A}{\partial H_{\beta\alpha}^T} dH_{\alpha\beta} \quad (80)$$

$$= \text{Tr} \left(\frac{\partial A}{\partial \mathbf{H}^T} d\mathbf{H} \right) \quad (81)$$

$$= \text{Tr} \left(\frac{\partial A}{\partial \mathbf{H}^T} \left(\mathbf{H}^{-T} \mathbf{H}_0^T (\text{de} - \text{dw}) \mathbf{H}_0 \right) \right) \quad (82)$$

$$= \text{Tr} \left(\mathbf{H}_0 \frac{\partial A}{\partial \mathbf{H}^T} \mathbf{H}^{-T} \mathbf{H}_0^T (\text{de} - \text{dw}) \right) \quad (83)$$

$$= \sum_{\alpha\beta} \left(\mathbf{H}_0 \frac{\partial A}{\partial \mathbf{H}^T} \mathbf{H}^{-T} \mathbf{H}_0^T \right)_{\alpha\beta} (\text{de} - \text{dw})_{\beta\alpha} \quad (84)$$

$$= \sum_{\alpha\beta} \left(\mathbf{H}_0 \frac{\partial A}{\partial \mathbf{H}^T} \mathbf{H}^{-T} \mathbf{H}_0^T \right)_{\alpha\beta} (\text{de} + \text{dw})_{\alpha\beta} \quad (85)$$

$$(86)$$

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

$$\frac{dA}{\text{de}} = \frac{1}{2} \left(\mathbf{H}_0 \mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{H}} \mathbf{H}_0^T + \mathbf{H}_0 \frac{\partial A}{\partial \mathbf{H}^T} \mathbf{H}^{-T} \mathbf{H}_0^T \right) \quad (88)$$

$$\frac{\partial A}{\partial e_{\alpha\sigma}} = \frac{1}{2} \sum_i \sum_{\beta\gamma} \left((\mathbf{H}_0 \mathbf{H}^{-1})_{\alpha\beta} \left\{ \frac{\partial A}{\partial q_{i\beta}} (\mathbf{H}^{-1} \mathbf{q}_i)_\gamma - p_{i\beta} \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right)_\gamma \right\} \mathbf{H}_{0\gamma\sigma}^T \right) \quad (89)$$

$$+ \mathbf{H}_{0\alpha\beta} \left\{ (\mathbf{H}^{-1} \mathbf{q}_i)_\beta \frac{\partial A}{\partial q_{i\gamma}} - \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right)_\beta p_{i\gamma} \right\} (\mathbf{H}^{-T} \mathbf{H}_0^T)_{\gamma\sigma} \quad (90)$$

$$(91)$$

$$\frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial H_{\beta\gamma}} = \sum_i \left\{ \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial q_{i\beta}} (\mathbf{H}^{-1} \mathbf{q}_i)_\gamma - p_{i\beta} \left(\mathbf{H}^{-1} \frac{\partial A(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial \mathbf{p}_i} \right)_\gamma \right\} \quad (92)$$

$$\frac{\partial A}{\partial \mathbf{H}} = \sum_i \left\{ \frac{\partial A}{\partial \mathbf{q}_i} \otimes (\mathbf{H}^{-1} \mathbf{q}_i) - \mathbf{p}_i \otimes \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right) \right\} \quad (93)$$

$$\frac{\partial A}{\partial \mathbf{H}^T} = \sum_i \left\{ (\mathbf{H}^{-1} \mathbf{q}_i) \otimes \frac{\partial A}{\partial \mathbf{q}_i} - \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right) \otimes \mathbf{p}_i \right\} \quad (94)$$

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

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

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

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

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

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

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

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

$$= \sum_i \left\{ \mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{q}_i} \otimes \mathbf{H}^{-1} \mathbf{q}_i - \mathbf{H}^{-1} \mathbf{p}_i \otimes \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right) \right\} \quad (103)$$

$$+ (\mathbf{H}^{-1} \mathbf{q}_i) \otimes \frac{\partial A}{\partial \mathbf{q}_i} \mathbf{H}^{-T} - \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right) \otimes \mathbf{p}_i \mathbf{H}^{-T} \quad (104)$$

$$= \sum_i \left\{ \mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{q}_i} \otimes (\mathbf{q}_i \mathbf{H}^{-T}) - (\mathbf{H}^{-1} \mathbf{p}_i) \otimes \left(\frac{\partial A}{\partial \mathbf{p}_i} \mathbf{H}^{-T} \right) \right\} \quad (105)$$

$$+ (\mathbf{H}^{-1} \mathbf{q}_i) \otimes \frac{\partial A}{\partial \mathbf{q}_i} \mathbf{H}^{-T} - \left(\mathbf{H}^{-1} \frac{\partial A}{\partial \mathbf{p}_i} \right) \otimes (\mathbf{p}_i \mathbf{H}^{-T}) \quad (106)$$

$$= \sum_i \mathbf{H}^{-1} \left\{ \frac{\partial A}{\partial \mathbf{q}_i} \otimes \mathbf{q}_i + \mathbf{q}_i \otimes \frac{\partial A}{\partial \mathbf{q}_i} - \mathbf{p}_i \otimes \frac{\partial A}{\partial \mathbf{p}_i} - \frac{\partial A}{\partial \mathbf{p}_i} \otimes \mathbf{p}_i \right\} \mathbf{H}^{-T} \quad (107)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$(121)$$

$$F = -k_B T \ln Z \quad (122)$$

$$\Omega t_{\alpha\beta} = -\Omega \frac{\partial F}{\partial e_{\alpha\beta}} \quad (123)$$

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

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

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

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

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

$$= -\frac{1}{2} \sum_i \left\{ \mathbf{H}_0 \mathbf{H}^{-1} \langle \mathbf{q}_i \otimes \mathbf{V}_i \rangle \mathbf{H}^{-T} \mathbf{H}_0^T - \mathbf{H}_0 \mathbf{H}^{-1} \left\langle \mathbf{p}_i \otimes \frac{\mathbf{p}_i}{m_i} \right\rangle \mathbf{H}^{-T} \mathbf{H}_0^T \right. \quad (129)$$

$$\left. + \mathbf{H}_0 \mathbf{H}^{-1} \langle \mathbf{V}_i \otimes \mathbf{q}_i \rangle \mathbf{H}^{-T} \mathbf{H}_0^T - \mathbf{H}_0 \mathbf{H}^{-1} \left\langle \frac{\mathbf{p}_i}{m_i} \otimes \mathbf{p}_i \right\rangle \mathbf{H}^{-T} \mathbf{H}_0^T \right\}_{\alpha\beta} \quad (130)$$

$$= -\frac{1}{2} \sum_i \mathbf{H}_0 \mathbf{H}^{-1} \left\{ \langle \mathbf{q}_i \otimes \mathbf{V}_i \rangle + \langle \mathbf{V}_i \otimes \mathbf{q}_i \rangle - \left\langle \mathbf{p}_i \otimes \frac{\mathbf{p}_i}{m_i} \right\rangle - \left\langle \frac{\mathbf{p}_i}{m_i} \otimes \mathbf{p}_i \right\rangle \right\} \mathbf{H}^{-T} \mathbf{H}_0^T \quad (131)$$

$$:= -\frac{1}{2} \langle \hat{D}' H \rangle \quad (132)$$

$$:= \Omega \langle t_{\alpha\beta} \rangle \quad (133)$$

$$\frac{\partial \mathcal{H}}{\partial \mathbf{H}} = \sum_i \left\{ \mathbf{V}_i \otimes (\mathbf{H}^{-1} \mathbf{q}_i) - \mathbf{p}_i \otimes \left(\mathbf{H}^{-1} \frac{\mathbf{p}_i}{m_i} \right) \right\} \quad (134)$$

$$C_{\alpha\beta\gamma\sigma} = -\frac{\partial \langle t_{\alpha\beta} \rangle}{\partial e_{\gamma\sigma}} \quad (135)$$

参考文献

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