$\boxed{\text{VACF}}$ to fit the friction coefficient

§1. Harmonic system

$$H = \sum_i \frac{p_i^2}{2M_i} + \frac{1}{2}\sum_{ii'} u_i \Phi_{ii'} u_{i'} \qquad (1)$$

$p_i = M_i \mathring{u}_i$, i - atom + Cartesian (DOF)

It is diagonalised with:

$$u_i(t) = \sum_\lambda q_\lambda(t) \frac{e_{i\lambda}}{\sqrt{M_i}} \qquad (2)$$

$$\mathring{u}_i(t) = \sum_\lambda \mathring{q}_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}} \; ; \; p_i(t) = \sum_\lambda \sqrt{M_i}\, \mathring{q}_\lambda e_{i\lambda} \qquad (3)$$

where

$$\sum_{i'} \underbrace{\Phi_{ii'} \frac{1}{\sqrt{M_i M_{i'}}}}_{\mathcal{D}_{ii'}} \cdot e_{i'\lambda} = \omega_\lambda^2 e_{i\lambda} \qquad (4)$$

Indeed,

$$H_{KE} = \sum_i \frac{1}{2M_i} \sum_{\lambda\lambda'} M_i \mathring{q}_\lambda \mathring{q}_{\lambda'} e_{i\lambda} e_{i\lambda'} = \frac{1}{2}\sum_{\lambda\lambda'} \mathring{q}_\lambda \mathring{q}_{\lambda'} \underbrace{\sum_i e_{i\lambda} e_{i\lambda'}}_{\delta_{\lambda\lambda'}} = \frac{1}{2}\sum_\lambda \mathring{q}_\lambda^2 \; ;$$

$$H_{PE} = \frac{1}{2}\sum_{ii'} \Phi_{ii'} \frac{1}{\sqrt{M_i M_{i'}}} \cdot \sum_\lambda q_\lambda q_{\lambda'} e_{i\lambda} e_{i'\lambda'} =$$

$$= \frac{1}{2}\sum_{\lambda\lambda'}\sum_i \left(\sum_{i'} \frac{\Phi_{ii'}}{\sqrt{M_i M_{i'}}} e_{i'\lambda'} \right) q_\lambda q_{\lambda'} e_{i\lambda} = \frac{1}{2}\sum_{\lambda\lambda'} \omega_{\lambda'}^2 \underbrace{\sum_i e_{i\lambda'} e_{i\lambda}}_{\delta_{\lambda\lambda'}} q_\lambda q_{\lambda'}$$

$$= \frac{1}{2}\sum_\lambda q_\lambda^2 \omega_\lambda^2$$

$$\boxed{p_\lambda = \mathring{q}_\lambda}$$

so that

$$H = \frac{1}{2}\sum_\lambda \left(\mathring{q}_\lambda^2 + \omega_\lambda^2 q_\lambda^2 \right) \equiv \frac{1}{2}\sum_\lambda \left(p_\lambda^2 + \omega_\lambda^2 q_\lambda^2 \right) \qquad (5)$$

is a sum of harmonic oscillators:

$$\boxed{v_i(t) = \sum_\lambda p_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}}}$$

$$q_\lambda(t) = A_\lambda e^{i\omega_\lambda t} + A_\lambda^* e^{-i\omega_\lambda t} \tag{6}$$

- Averages of normal modes.

$$f(u,p) = \frac{1}{Z} e^{-\beta H(u,p)} \quad , \beta = 1/k_B T \tag{7}$$

is the distribution function (Classical) w.r.t. initial positions and momenta.

$$Z = \int du \int dp \; e^{-\beta H} \tag{8}$$

The Jacobean

$$J = \frac{\partial(q_\lambda, p_\lambda)}{\partial(u,p)} = \begin{vmatrix} \frac{\partial q_\lambda}{\partial u_i} & \frac{\partial p_\lambda}{\partial u_i} \\ \frac{\partial q_\lambda}{\partial p_i} & \frac{\partial p_\lambda}{\partial p_i} \end{vmatrix} = \begin{vmatrix} \partial q_\lambda/\partial u_i & 0 \\ 0 & \partial p_\lambda/\partial p_i \end{vmatrix} \tag{9}$$

~~Here~~ f From (2), (3),

$$q_\lambda = \sum_i \sqrt{M_i}\, e_{i\lambda} u_i \tag{10}$$

$$\cancel{p_\lambda = \sum_i \frac{1}{\sqrt{M_i}} e_{i\lambda}} \quad p_i = M_i \dot{u}_i = \sum_\lambda \sqrt{M_i}\, \underbrace{\dot{q}_\lambda}_{p_\lambda} e_{i\lambda}$$

$$\hookrightarrow \quad p_\lambda = \sum_i \frac{1}{\sqrt{M_i}} e_{i\lambda} p_i \tag{11}$$

and hence

$$\frac{\partial q_\lambda}{\partial u_i} = \sqrt{M_i}\, e_{i\lambda} \quad , \quad \frac{\partial p_\lambda}{\partial p_i} = \frac{1}{\sqrt{M_i}} e_{i\lambda}$$

$$J = \begin{vmatrix} \sqrt{M_i}\, e_{i\lambda} & 0 \\ 0 & \frac{1}{\sqrt{M_i}} e_{i\lambda} \end{vmatrix} = \left| \sqrt{M_i}\, e_{i\lambda} \right| \cdot \left| \frac{1}{\sqrt{M_i}} e_{i\lambda} \right| =$$

$$= |M^{1/2} e| \, |M^{-1/2} e| = \underbrace{|M^{1/2}| |M^{-1/2}|}_{|E| = 1} \cdot \underbrace{|e|^2}_{=1} = 1$$

$\{e_{i\lambda}\}$ - is orthogonal matrix.

Therefore,

$$Z = \prod_\lambda \int dq_\lambda \int dp_\lambda \, e^{-\beta H_\lambda}, \quad H_\lambda = \frac{1}{2}(p_\lambda^2 + \omega_\lambda^2 q_\lambda^2)$$

$$Z = \prod_\lambda \int dq_\lambda \, e^{-\frac{\beta \omega_\lambda^2}{2} q_\lambda^2} \int dp_\lambda \, e^{-\frac{\beta}{2} p_\lambda^2}$$

$$= \prod_\lambda \sqrt{\frac{2\pi}{\beta \omega_\lambda^2}} \sqrt{\frac{2\pi}{\beta}} = \prod_\lambda \frac{2\pi}{\beta \omega_\lambda}, \quad Z_\lambda = \frac{2\pi}{\beta \omega_\lambda} \qquad (12)$$

• Next, calculate

$$\langle q_\lambda^2 \rangle = \frac{1}{Z_\lambda} \int q_\lambda^2 e^{-\frac{\beta \omega_\lambda^2}{2} q_\lambda^2} dq_\lambda \underbrace{\int e^{-\beta p_\lambda^2 / 2} dp_\lambda}_{\sqrt{\frac{2\pi}{\beta}}}$$

But

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = -\frac{\partial}{\partial \alpha} \int e^{-\alpha x^2} dx = -\frac{\partial}{\partial \alpha} \sqrt{\frac{\pi}{\alpha}} = -\sqrt{\pi}\left(-\frac{1}{2}\right) \alpha^{-3/2}$$

$$= \frac{\sqrt{\pi}}{2\alpha^{3/2}},$$

so that

$$\langle q_\lambda^2 \rangle = \frac{1}{Z_\lambda} \cdot \frac{\sqrt{\pi}}{2 \frac{\beta \omega_\lambda^2}{2} \sqrt{\frac{\beta \omega_\lambda^2}{2}}} * \sqrt{\frac{2\pi}{\beta}} = \frac{\beta \omega_\lambda}{2\pi} \cdot \frac{\pi}{\beta \omega_\lambda^2 \sqrt{\beta \omega_\lambda^2}}$$

$$= \frac{1}{2\omega_\lambda \sqrt{\beta \omega_\lambda^2}} = \frac{1}{2\beta \omega_\lambda^2},$$

$$\langle p_\lambda^2 \rangle = \frac{1}{Z_\lambda} \int e^{-\frac{\beta \omega_\lambda^2}{2} q_\lambda^2} dq \int p_\lambda^2 e^{-\beta p_\lambda^2 / 2} dp_\lambda =$$

$$\cancel{= \frac{\beta\omega_\lambda}{2\pi} \cdot \sqrt{\frac{2\pi}{\beta\omega_\lambda^2}} \cdot \frac{\sqrt{\pi}}{2\frac{\beta}{2}\sqrt{\frac{\beta}{2}}} = \frac{1}{2\beta}}$$

$$\langle q_\lambda^2\rangle = \underbrace{\frac{1}{Z_\lambda}}_{\frac{\beta\omega_\lambda}{2\pi}} \underbrace{\int q_\lambda^2 e^{-\left(\frac{\beta\omega_\lambda^2}{2}\right)q_\lambda^2} dq_\lambda}_{\frac{\sqrt{\pi}}{2\cdot\frac{\beta\omega_\lambda^2}{2}\cdot\sqrt{\frac{\beta\omega_\lambda^2}{2}}}} \underbrace{\int e^{-\left(\frac{\beta}{2}\right)p_\lambda^2} dp_\lambda}_{\sqrt{\frac{2\pi}{\beta}}}$$

$$= \cancel{\frac{\beta\omega_\lambda}{2\pi}} \cdot \sqrt{\frac{\cancel{2\pi}}{\beta\omega_\lambda^2}} \cdot \frac{1}{\cancel{\beta\omega_\lambda^2}} \cdot \sqrt{\frac{\cancel{2\pi}}{\beta}} = \frac{\cancel{\omega_\lambda}\,1}{\beta\omega_\lambda^2}\;; \qquad (13)$$

$$\langle p_\lambda^2\rangle = \underbrace{\frac{1}{Z_\lambda}}_{\frac{\beta\omega_\lambda}{2\pi}} \underbrace{\int e^{-\left(\frac{\beta\omega_\lambda^2}{2}\right)q_\lambda^2} dq_\lambda}_{\sqrt{\frac{2\pi}{\beta\omega_\lambda}}} \underbrace{\int p_\lambda^2 e^{-\left(\frac{\beta}{2}\right)p_\lambda^2} dp_\lambda}_{\frac{\sqrt{\pi}}{2\cdot\frac{\beta}{2}\sqrt{\frac{\beta}{2}}}}$$

$$= \cancel{\frac{\beta\omega_\lambda}{2\pi}} \cdot \sqrt{\frac{\cancel{2\pi}}{\beta\cancel{\omega_\lambda^2}}} \cdot \sqrt{\frac{\cancel{2\pi}}{\beta}}\,\frac{1}{\cancel{\beta}} = \frac{1}{\beta} \qquad (14)$$

Also,

$$\langle p_\lambda\rangle = \langle q_\lambda\rangle = \langle q_\lambda p_{\lambda'}\rangle = 0 \qquad (15)$$

§2. Time dependence

Since

$$q_\lambda(t) = A_\lambda e^{i\omega_\lambda t} + A_\lambda^* e^{-i\omega_\lambda t}, \qquad (16)$$

then

$$u_i(t) = \sum_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}}\left(A_\lambda e^{i\omega_\lambda t} + A_\lambda^* e^{-i\omega_\lambda t}\right), \qquad (17)$$

$$p_i(t) = \sum_\lambda \sqrt{M_i}\, e_{i\lambda}\, i\omega_\lambda \left(A_\lambda e^{i\omega_\lambda t} - A_\lambda^* e^{-i\omega_\lambda t}\right) \qquad (18)$$

These should allow us to express $u_i(t)$, $p_i(t)$ via their initial values:

$$u_i^\circ = \sum_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}}(A_\lambda + A_\lambda^*) \quad \to A_\lambda + A_\lambda^* = \sum_i u_i^\circ \sqrt{M_i}\, e_{i\lambda} \quad (19)$$

$$p_i^\circ = \sum_\lambda \sqrt{M_i}\, e_{i\lambda}\, i\omega_\lambda (A_\lambda - A_\lambda^*) \to i\omega_\lambda (A_\lambda - A_\lambda^*) = \sum_i \frac{1}{\sqrt{M_i}} e_{i\lambda} p_i^\circ \quad (20)$$

or

$$\begin{cases} A_\lambda + A_\lambda^* = \sum_i \sqrt{M_i}\, e_{i\lambda} u_i^\circ \\ A_\lambda - A_\lambda^* = \frac{1}{i\omega_\lambda} \sum_i \frac{e_{i\lambda}}{\sqrt{M_i}} p_i^\circ \end{cases} \quad (21)$$

$$A_\lambda = \frac{1}{2}\sum_i \left[\sqrt{M_i}\, e_{i\lambda} u_i^\circ + \frac{1}{i\omega_\lambda} \frac{e_{i\lambda}}{\sqrt{M_i}} p_i^\circ \right]$$

$$A_\lambda = \frac{1}{2}\sum_i e_{i\lambda} \left[\sqrt{M_i}\, u_i^\circ + \frac{1}{i\omega_\lambda \sqrt{M_i}} p_i^\circ \right] \quad (22)$$

(A_λ^* follows by $*$). Then, substituting into (17), (18):

$$u_i = \sum_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}} \left\{ \frac{1}{2} \sum_{i'} e_{i'\lambda} \left[\sqrt{M_{i'}}\, u_{i'}^\circ + \frac{p_{i'}^\circ}{i\omega_\lambda \sqrt{M_{i'}}} \right] e^{i\omega_\lambda t} + c.c. \right\}$$

$$= \sum_{i'} u_{i'}^\circ \left\{ \sum_\lambda \frac{e_{i\lambda} e_{i'\lambda}}{2} \sqrt{\frac{M_{i'}}{M_i}}\, e^{i\omega_\lambda t} + c.c. \right\}$$

$$+ \sum_{i'} p_{i'}^\circ \left\{ \sum_\lambda \frac{e_{i\lambda} e_{i'\lambda}}{2 i\omega_\lambda \sqrt{M_i M_{i'}}}\, e^{i\omega_\lambda t} + c.c. \right\} \quad (23) \oplus$$

and

$$p_i = \sum_\lambda \sqrt{M_i}\, e_{i\lambda} (i\omega_\lambda) \left\{ \frac{1}{2} \sum_{i'} e_{i'\lambda} \left[\sqrt{M_{i'}}\, u_{i'}^\circ + \frac{p_{i'}^\circ}{i\omega_\lambda \sqrt{M_{i'}}} \right] e^{i\omega_\lambda t} - c.c. \right\}$$

$$= \sum_{i'} u_{i'}^\circ \left\{ \frac{1}{2} \sum_\lambda i\omega_\lambda \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda}\, e^{i\omega_\lambda t} \underline{\underline{+}}\, c.c. \right\}$$

("+ cc" since $i\omega_\lambda$ was taken in)

$$+ \sum_{i'} p_{i'}^\circ \left\{ \frac{1}{2} \sum_\lambda \sqrt{\frac{M_i}{M_{i'}}}\, e_{i\lambda} e_{i'\lambda}\, e^{i\omega_\lambda t} \underline{\underline{+}}\, c.c. \right\} \quad (24)$$

- Calculate averages w.r.t. initial state:

$$\cancel{\langle u_i u_{i'} \rangle} =$$

$$u_i^\circ = \cancel{u_i(0)} = \sum_\lambda q_\lambda^\circ \frac{e_{i\lambda}}{\sqrt{M_i}}$$

$$\langle u_i^\circ u_{i'}^\circ \rangle = \sum_{\lambda\lambda'} \frac{e_{i\lambda}}{\sqrt{M_i}} \frac{e_{i'\lambda'}}{\sqrt{M_{i'}}} \langle q_\lambda^\circ q_{\lambda'}^\circ \rangle =$$

$$= \sum_{\lambda\lambda'} \frac{e_{i\lambda} e_{i'\lambda'}}{\sqrt{M_i M_{i'}}} \cdot \delta_{\lambda\lambda'} \frac{1}{\beta \omega_\lambda^2} = \frac{1}{\beta} \left(\sum_\lambda \frac{e_{i\lambda} e_{i'\lambda}}{\omega_\lambda^2} \right) \cdot \frac{1}{\sqrt{M_i M_{i'}}} \qquad (25)$$

$$\langle p_i^\circ p_{i'}^\circ \rangle = \sum_{\lambda\lambda'} \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda'} \langle p_\lambda^\circ p_{\lambda'}^\circ \rangle$$

$$= \sum_{\lambda\lambda'} \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda'} \delta_{\lambda\lambda'} \frac{1}{\beta} = \frac{1}{\beta} \sum_\lambda \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda}$$

$$= \frac{1}{\beta} \sqrt{M_i M_{i'}} \cdot \underbrace{\sum_\lambda e_{i\lambda} e_{i'\lambda}}_{\delta_{ii'}} = \frac{M_i}{\beta} \delta_{ii'} \qquad (26)$$

- Checking (23) and (24):

$$u_i^\circ = \cancel{\sum_\lambda \frac{e_{i\lambda}}{\sqrt{M_i}} \left\{ \frac{1}{2} \sum_{i'} \right.} \sum_{i'} \left[u_{i'}^\circ \sum_\lambda \frac{1}{2} e_{i\lambda} e_{i'\lambda} \sqrt{\frac{M_{i'}}{M_i}}\, 2 \right.$$

$$\left. + p_{i'}^\circ \sum_\lambda \underbrace{\left(\frac{1}{2} \frac{e_{i\lambda} e_{i'\lambda}}{i\omega_\lambda \sqrt{M_i M_{i'}}} - \text{the same} \right)}_{0} \right] = \sum_{i'} u_{i'}^\circ \overbrace{\left(\sum_\lambda e_{i\lambda} e_{i'\lambda} \right)}^{\delta_{ii'}} \sqrt{\frac{M_{i'}}{M_i}}$$

$$\equiv u_i^\circ ,$$

$$p_i^\circ = \sum_{i'} u_{i'}^\circ \frac{1}{2} \sum_\lambda \left\{ i\omega_\lambda \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda} \overset{0}{+} (-i\omega_\lambda) \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda} \right\}$$

$$+ \sum_{i'} p_{i'}^\circ \frac{1}{2} \sum_\lambda \left\{ \sqrt{\frac{M_i}{M_{i'}}}\, e_{i\lambda} e_{i'\lambda}\, 2 \right\} \equiv p_i^\circ$$

• Now calculating the VACF:

$$VACF(\Delta) = \left\langle \sum_i V_i(t)\, V_i(t+\Delta) \right\rangle = \sum_i \frac{1}{M_i^2} \left\langle P_i(t)\, P_i(t+\Delta) \right\rangle \quad (27)$$

We have:

$$P_i(t) = \sum_{i'} \left[u^0_{i'}\, B_{ii'}(t) + p^0_{i'}\, G_{ii'}(t) \right] \quad (28)$$

$$B_{ii'}(t) = \sum_\lambda i\omega_\lambda \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda} \underbrace{\left(e^{i\omega_\lambda t} - e^{-i\omega_\lambda t} \right)}_{2i \sin\omega_\lambda t} \frac{1}{2}$$

$$= -\sum_\lambda \omega_\lambda \sqrt{M_i M_{i'}}\, e_{i\lambda} e_{i'\lambda} \sin\omega_\lambda t \,, \quad \oplus \quad (29)$$

$$G_{ii'}(t) = \sum_\lambda \sqrt{\frac{M_i}{M_{i'}}}\, e_{i\lambda} e_{i'\lambda} \underbrace{\frac{1}{2}\left(e^{i\omega_\lambda t} + e^{-i\omega_\lambda t} \right)}_{\cos\omega_\lambda t}$$

$$= \sqrt{\frac{M_i}{M_{i'}}} \sum_\lambda e_{i\lambda} e_{i'\lambda} \cos\omega_\lambda t \quad (30)$$

Therefore,

$$\left\langle P_i(t)\, P_i(t+\Delta) \right\rangle = \sum_{jj'} \Big[B_{ij}(t)\, B_{ij'}(t+\Delta) \left\langle u^0_j u^0_{j'} \right\rangle$$

$$+ G_{ij}(t)\, G_{ij'}(t+\Delta) \left\langle p^0_j p^0_{j'} \right\rangle \Big]$$

$$= \sum_{jj'} \Big[B_{ij}(t)\, B_{ij'}(t+\Delta) \frac{1}{\beta\sqrt{M_j M_{j'}}} \sum_\lambda \frac{e_{j\lambda} e_{j'\lambda}}{\omega_\lambda^2} +$$

$$+ G_{ij}(t)\, G_{ij'}(t+\Delta)\, \delta_{jj'} \frac{M_j}{\beta} \Big] \quad \oplus$$

$$= \frac{1}{\beta}\sum_j G_{ij}(t)G_{ij}(t+\Delta)M_j + \frac{1}{\beta}\sum_\lambda\sum_{jj'}\frac{e_{j\lambda}e_{j'\lambda}}{\omega_\lambda^2}B_{ij}(t)B_{ij}(t+\Delta)\times$$

$$\times\frac{1}{\sqrt{M_jM_{j'}}} = I_1 + I_2 ;$$

$$I_1 = \frac{1}{\beta}\sum_j \cancel{\frac{M_i}{M_j}}\cdot \cancel{M_j}\cdot\sum_\lambda e_{i\lambda}e_{j\lambda}\cos\omega_\lambda t\sum_{\lambda'}e_{i\lambda'}e_{j\lambda'}\cos\omega_{\lambda'}(t+\Delta)$$

$$= \frac{M_i}{\beta}\sum_{\lambda\lambda'}\underbrace{\left(\sum_j e_{j\lambda}e_{j\lambda'}\right)}_{=\delta_{\lambda\lambda'}}e_{i\lambda}e_{i\lambda'}\cos\omega_\lambda t\cos\omega_{\lambda'}(t+\Delta)$$

$$= \cancel{M_i}\,\frac{M_i}{\beta}\sum_\lambda e_{i\lambda}e_{i\lambda}\cos\omega_\lambda t\cos\omega_\lambda(t+\Delta) . \qquad (31)\ \oplus$$

$$I_2 = \frac{1}{\beta}\sum_\lambda\sum_{jj'}\frac{1}{\cancel{\sqrt{M_jM_{j'}}}}\cdot\frac{e_{j\lambda}e_{j'\lambda}}{\omega_\lambda^2}\cdot\sum_{\lambda_1\lambda_2}\omega_{\lambda_1}\omega_{\lambda_2}\sqrt{M_i\cancel{M_j}}\sqrt{M_i\cancel{M_{j'}}}\times$$

$$\times e_{i\lambda_1}e_{j\lambda_1}e_{i\lambda_2}e_{j'\lambda_2}\sin\omega_{\lambda_1}t\sin\omega_{\lambda_2}(t+\Delta)$$

$$= \frac{M_i}{\beta}\sum_{\lambda\lambda_1\lambda_2}\left(\sum_{jj'}\frac{e_{j\lambda}e_{j'\lambda}}{\omega_\lambda^2}\omega_{\lambda_1}\omega_{\lambda_2}e_{i\lambda_1}e_{i\lambda_2}e_{j\lambda_1}e_{j'\lambda_2}\right)\sin\omega_{\lambda_1}t\sin\omega_{\lambda_2}(t+\Delta) \qquad (32)$$

$\to \delta_{\lambda\lambda_1}$

$\to \delta_{\lambda\lambda_2}$

Note that:

$$\sum_i I_1\frac{1}{M_i} = \frac{1}{\beta}\left(\sum_i\right)\sum_\lambda \overset{=1}{\boxed{e_{i\lambda}e_{i\lambda}}}\cos\omega_\lambda t\cos\omega_\lambda(t+\Delta)$$

$$= \frac{1}{\beta}\sum_\lambda\cos\omega_\lambda t\cos\omega_\lambda(t+\Delta) ; \qquad (33)$$

$$\sum_i\frac{1}{M_i}I_2 = \frac{1}{\beta}\sum_{\lambda\lambda_1\lambda_2}\sum_{jj'}\frac{e_{j\lambda}e_{j'\lambda}}{\omega_\lambda^2}\omega_{\lambda_1}\omega_{\lambda_2}\underbrace{\left(\sum_i e_{i\lambda_1}e_{i\lambda_2}\right)}_{=\delta_{\lambda_1\lambda_2}}e_{j\lambda_1}e_{j'\lambda_2}\times$$

$$\times\sin\omega_{\lambda_1}t\sin\omega_{\lambda_2}(t+\Delta) =$$

$$= \frac{1}{\beta} \sum_{\lambda\lambda_1} \underbrace{\sum_{j}}_{} \sum_{j'} \frac{e_{j\lambda} e_{j'\lambda} \omega_{\lambda_1}^2 e_{j\lambda_1} e_{j'\lambda_1}}{\omega_\lambda^2} \sin\omega_{\lambda_1} t \sin\omega_{\lambda_1}(t+\Delta)$$

$\delta_{\lambda\lambda_1}$ $\delta_{\lambda\lambda_1}$

$$= \frac{1}{\beta} \sum_{\lambda} \frac{1}{\cancel{\omega_\lambda^2}} \cancel{\omega_\lambda^2} \sin\omega_\lambda t \sin\omega_\lambda(t+\Delta)$$

$$= \frac{1}{\beta} \sum_{\lambda} \sin\omega_\lambda t \sin\omega_\lambda(t+\Delta) \qquad (34)$$

Therefore,

$$\sum_i \frac{1}{m_i} \langle p_i(t)\, p_i(t+\Delta) \rangle = \frac{1}{\beta} \sum_\lambda \Big[\cos\omega_\lambda t \cos\omega_\lambda(t+\Delta) +$$

$$+ \sin\omega_\lambda t \sin\omega_\lambda(t+\Delta) \Big] = \frac{1}{\beta} \sum_\lambda \cos\omega_\lambda\Delta \equiv f(\Delta).$$

$$f(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega\Delta} f(\Delta)\, d\Delta = \frac{1}{2\pi\beta} \sum_\lambda \frac{1}{2} \int_{-\infty}^{\infty} e^{i\omega\Delta} \left(e^{i\omega_\lambda\Delta} + e^{-i\omega_\lambda\Delta} \right) d\Delta$$

$$= \frac{1}{2\beta} \sum_\lambda \frac{1}{2\pi} \left[\int e^{i(\omega+\omega_\lambda)\Delta} d\Delta + \int e^{i(\omega-\omega_\lambda)\Delta} d\Delta \right]$$

$$= \frac{1}{2\beta} \sum_\lambda \left[\delta(\omega+\omega_\lambda) + \delta(\omega-\omega_\lambda) \right]$$

$$= \frac{1}{\beta} \sum_\lambda \delta(\omega^2 - \omega_\lambda^2)$$