Санкт-Петербургский государственный университет
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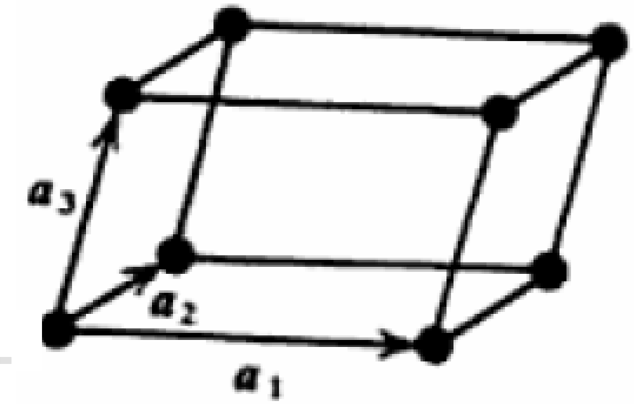
Лекция 3. Основы теории ядерного рассеяния нейтронов.

- Ядерное рассеяние в кристаллах
- Сечение когерентного рассеяния
- Фактор Дебая-Валлера

$$\mathbf{R}_j^{(0)} = j_1\mathbf{a}_1 + j_2\mathbf{a}_2 + j_3\mathbf{a}_3$$

$$\mathrm{v}_0 = \left|\mathbf{a}_1\left[\mathbf{a}_2 \times \mathbf{a}_3\right]\right|$$



$$\boldsymbol{\tau}_1 = \frac{2\pi}{\mathrm{v}_0}\left[\mathbf{a}_2 \times \mathbf{a}_3\right] \qquad \boldsymbol{\tau}_2 = \frac{2\pi}{\mathrm{v}_0}\left[\mathbf{a}_3 \times \mathbf{a}_1\right] \qquad \boldsymbol{\tau}_3 = \frac{2\pi}{\mathrm{v}_0}\left[\mathbf{a}_1 \times \mathbf{a}_2\right]$$

$$\boldsymbol{\tau}_1\left[\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3\right] = \frac{(2\pi)^3}{\mathrm{v}_0} \qquad \mathbf{a}_i\boldsymbol{\tau}_j = 2\pi\delta_{ij}$$

$$\mathbf{R}_j = \mathbf{R}_j^{(0)} + \mathbf{u}_j$$

$$\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(t)}\right\rangle = N\sum_n e^{i\mathbf{QR}_n^{(0)}}\left\langle e^{-i\mathbf{Qu}_0(0)}e^{i\mathbf{Qu}_n(t)}\right\rangle$$

$$\sum_{j}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_j(t)}\right\rangle = N\left\langle e^{-i\mathbf{Qu}_0(0)}e^{i\mathbf{Qu}_0(t)}\right\rangle$$

$$\boxed{\mathbf{R}_j(t) = \mathbf{R}_j^{(0)} + \mathbf{u}_j(t)}$$

Нормальные моды

$$\mathbf{u}_j = \sqrt{\frac{\hbar}{2MN}} \sum_{s=1}^{3} \sum_{\mathbf{q}} \frac{1}{\sqrt{\omega_s(\mathbf{q})}} \left(a_{\mathbf{q},s} \mathbf{e}_s(\mathbf{q}) e^{i\mathbf{q}\mathbf{R}_j^{(0)}} + a_{\mathbf{q},s}^{+} \mathbf{e}_s(\mathbf{q})^{*} e^{-i\mathbf{q}\mathbf{R}_j^{(0)}} \right)$$

$$\left[a_{\mathbf{q},s}, a_{\mathbf{q},s}^{+} \right] = a_{\mathbf{q},s} a_{\mathbf{q},s}^{+} - a_{\mathbf{q},s}^{+} a_{\mathbf{q},s} = 1$$

$$a_{\mathbf{q},s}(t) = e^{iHt/\hbar} a_{\mathbf{q},s} e^{-iHt/\hbar} = a_{\mathbf{q},s} e^{-i\omega_s(\mathbf{q})t}$$

$$a_{\mathbf{q},s}^{+}(t) = e^{iHt/\hbar} a_{\mathbf{q},s}^{+} e^{-iHt/\hbar} = a_{\mathbf{q},s}^{+} e^{i\omega_s(\mathbf{q})t}$$

$$H = \sum_{s=1}^{3} \sum_{\mathbf{q}} \hbar \omega_s(\mathbf{q}) \left(a_{\mathbf{q},s}^{+} a_{\mathbf{q},s} + \frac{1}{2} \right)$$

$$\mathbf{Q}\mathbf{u}_j(t) = \sqrt{\frac{\hbar}{2MN}} \sum_{s=1}^{3} \sum_{\mathbf{q}} \frac{1}{\sqrt{\omega_s(\mathbf{q})}} \left(a_{\mathbf{q},s} (\mathbf{Q}\mathbf{e}_s(\mathbf{q})) e^{i(\mathbf{q}\mathbf{R}_j^{(0)} - \omega_s(\mathbf{q})t)} + a_{\mathbf{q},s}^{+} (\mathbf{Q}\mathbf{e}_s(\mathbf{q})^{*}) e^{-i(\mathbf{q}\mathbf{R}_j^{(0)} - \omega_s(\mathbf{q})t)} \right)$$

Функция распределения вероятностей гармонического осциллятора

$$H\psi_\alpha(x) = E_\alpha \psi_\alpha(x)$$

$$f(x) = \sum_\alpha P_\alpha |\psi_\alpha(x)|^2 \qquad \int_{-\infty}^{\infty} f(x)dx = 1$$

$$P_\alpha = \frac{1}{Z} e^{-E_\alpha/(k_b T)}$$

$$Z = \sum_\alpha e^{-E_\alpha/(k_b T)}$$

$$\langle A(x) \rangle = \sum_\alpha P_\alpha \int_{-\infty}^{\infty} A(x) |\psi_\alpha(x)|^2 dx$$

$$= \int_{-\infty}^{\infty} A(x) \sum_\alpha P_\alpha |\psi_\alpha(x)|^2 dx = \int_{-\infty}^{\infty} A(x) f(x) dx$$

Функция распределения вероятностей гармонического осциллятора

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{1}{2m}\left(p^2 + m^2\omega^2x^2\right) \qquad \omega^2 = \frac{k}{m}$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \qquad \left[\hat{p}, x\right] = -i\hbar$$

$$a = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x + i\hat{p}\right) \qquad a^{+} = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x - i\hat{p}\right)$$

$$\left[a, a^{+}\right] = 1$$

$$H = \hbar\omega\left(a^{+}a + \frac{1}{2}\right) \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$a^{+}\psi_n = \sqrt{n+1}\,\psi_{n+1} \qquad a\psi_n = \sqrt{n}\,\psi_{n-1}$$

$$f(x) = \frac{1}{Z}\sum_n e^{-E_n/(k_b T)}\psi_n(x)^2$$

$$\frac{\partial f(x)}{\partial x} = \frac{2}{Z}\sum_n e^{-E_n/(k_b T)}\psi_n(x)\frac{\partial \psi_n(x)}{\partial x}$$

$$\frac{\partial}{\partial x} = \frac{i}{\hbar}\hat{p} = \sqrt{2m\hbar\omega}\left(a - a^+\right)$$

$$\psi_n(x)\frac{\partial \psi_n(x)}{\partial x} = \sqrt{\frac{m\omega}{2\hbar}}\left(\sqrt{n}\psi_n\psi_{n-1} - \sqrt{n+1}\psi_n\psi_{n+1}\right)$$

$$\frac{\partial f(x)}{\partial x} = -\sqrt{\frac{2m\omega}{\hbar}}\left(1 - e^{-\hbar\omega/(k_b T)}\right)\frac{1}{Z}\sum_n e^{-E_n/(k_b T)}\sqrt{n+1}\psi_n\psi_{n+1}$$

$$xf = \sqrt{\frac{\hbar}{2m\omega}}\left(1 + e^{-\hbar\omega/(k_b T)}\right)\frac{1}{Z}\sum_n e^{-E_n/(k_b T)}\sqrt{n+1}\psi_n\psi_{n+1}$$

$$\frac{\partial f(x)}{\partial x} = -\frac{1}{\sigma^2}xf \qquad \sigma^2 = \frac{\hbar}{2M\omega}\coth\left(\frac{\hbar\omega}{2k_B T}\right)$$

Функция распределения вероятностей гармонического осциллятора

$$f(x)=\frac{1}{\sqrt{2\pi\sigma}}e^{-x^2/2\sigma^2}$$

$$\sigma^2=\frac{\hbar}{2M\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right)$$

$$x\to\frac{p}{\omega}$$

$$f(p)=\frac{1}{\sqrt{2\pi\sigma}}e^{-p^2/2\omega^2\sigma^2}$$

$$\sigma^2=\frac{\hbar}{2M\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right)$$

$$\langle x\rangle=0$$

$$\langle x^2\rangle=\sigma^2$$

$$\langle e^x\rangle=e^{\frac{1}{2}\sigma^2}=e^{\frac{1}{2}\langle x^2\rangle}$$

$$\langle p\rangle=0$$

$$\langle p^2\rangle=\omega^2\sigma^2$$

$$\langle e^p\rangle=e^{\frac{1}{2}\omega^2\sigma^2}=e^{\frac{1}{2}\langle p^2\rangle}$$

$$\left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\text{coh}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\frac{N}{2\pi\hbar}\sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}}\int_{-\infty}^{\infty}\left\langle e^U e^V \right\rangle e^{-i\omega t}\,dt$$

$$U = -i\mathbf{Q}\mathbf{u}_0(0) = -i\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(g_s(\mathbf{q})a_{\mathbf{q},s} + g_s^*(\mathbf{q})a_{\mathbf{q},s}^+\right)$$

$$V = i\mathbf{Q}\mathbf{u}_j(t) = i\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(h_s(\mathbf{q})a_{\mathbf{q},s} + h_s^*(\mathbf{q})a_{\mathbf{q},s}^+\right)$$

$$g_s(\mathbf{q}) = \sqrt{\frac{\hbar}{2MN}}\frac{(\mathbf{Q}\mathbf{e}_s(\mathbf{q}))}{\sqrt{\omega_s(\mathbf{q})}}$$

$$h_s(\mathbf{q}) = \sqrt{\frac{\hbar}{2MN}}\frac{(\mathbf{Q}\mathbf{e}_s(\mathbf{q}))}{\sqrt{\omega_s(\mathbf{q})}}e^{i(\mathbf{q}\mathbf{R}_j^{(0)} - \omega_s(\mathbf{q})t)}$$

$$[A,B]=c$$

$$e^{A}e^{B}=e^{A+B}e^{c/2}$$

$$UV-VU=\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(g_{s}(\mathbf{q})a_{\mathbf{q},s}+g_{s}^{*}(\mathbf{q})a_{\mathbf{q},s}^{+}\right)\sum_{s'=1}^{3}\sum_{\mathbf{q}'}\left(h_{s'}(\mathbf{q}')a_{\mathbf{q}',s'}+h_{s'}^{*}(\mathbf{q}')a_{\mathbf{q}',s'}^{+}\right)$$

$$-\sum_{s'=1}^{3}\sum_{\mathbf{q}'}\left(h_{s'}(\mathbf{q}')a_{\mathbf{q}',s'}+h_{s'}^{*}(\mathbf{q}')a_{\mathbf{q}',s'}^{+}\right)\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(g_{s}(\mathbf{q})a_{\mathbf{q},s}+g_{s}^{*}(\mathbf{q})a_{\mathbf{q},s}^{+}\right)$$

$$=\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(g_{s}(\mathbf{q})h_{s}^{*}(\mathbf{q})-g_{s}^{*}(\mathbf{q})h_{s}(\mathbf{q})\right)\left(a_{\mathbf{q},s}a_{\mathbf{q},s}^{+}-a_{\mathbf{q},s}^{+}a_{\mathbf{q},s}\right)$$

$$=\sum_{s=1}^{3}\sum_{\mathbf{q}}\left(g_{s}(\mathbf{q})h_{s}^{*}(\mathbf{q})-g_{s}^{*}(\mathbf{q})h_{s}(\mathbf{q})\right)$$

Сечение когерентного рассеяния

$$\left\langle e^{U} e^{V} \right\rangle = \left\langle e^{U+V} \right\rangle e^{\frac{1}{2}(UV-VU)}$$

$$\left\langle e^{U+V} \right\rangle = e^{\frac{1}{2}\left\langle (U+V)^2 \right\rangle}$$

$$\left\langle e^{U} e^{V} \right\rangle = e^{\frac{1}{2}\left\langle (U+V)^2 \right\rangle} e^{\frac{1}{2}(UV-VU)} = e^{\frac{1}{2}\left\langle U^2+V^2+UV+VU+UV-VU \right\rangle}$$

$$= e^{\frac{1}{2}\left\langle U^2+V^2 \right\rangle} e^{\left\langle UV \right\rangle} = e^{\left\langle U^2 \right\rangle} e^{\left\langle UV \right\rangle}$$

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f} \right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi} \frac{k_f}{k_i} \frac{N}{2\pi\hbar} e^{\left\langle U^2 \right\rangle} \sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}} \int_{-\infty}^{\infty} e^{\left\langle UV \right\rangle} e^{-i\omega t} dt$$

Сечение когерентного упругого рассеяния

$$e^{\langle UV\rangle} = 1 + \langle UV\rangle + \frac{1}{2}\langle UV\rangle^2 + \ldots + \frac{1}{n!}\langle UV\rangle^n + \ldots$$

$$\left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\text{coh,el}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\frac{N}{2\pi\hbar} e^{\langle U^2\rangle} \sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}} \int_{-\infty}^{\infty} e^{-i\omega t}\, dt$$

$$\int_{-\infty}^{\infty} e^{-i\omega t}\, dt = 2\pi\delta(\omega) = 2\pi\hbar\delta(\hbar\omega)$$

$$k_i = k_f$$

$$\left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\text{coh,el}} = \frac{\sigma_{\text{coh}}}{4\pi} e^{\langle U^2\rangle} N \sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}} \delta(\hbar\omega)$$

Сечение когерентного упругого рассеяния

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{coh,el}} = \int_0^\infty \left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\text{coh,el}} dE_f = \frac{\sigma_{\text{coh}}}{4\pi} e^{\langle U^2 \rangle} N \sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}}$$

$$\sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}} = \frac{(2\pi)^3}{\text{v}_0} \sum_{\boldsymbol{\tau}} \delta(\mathbf{Q}-\boldsymbol{\tau})$$

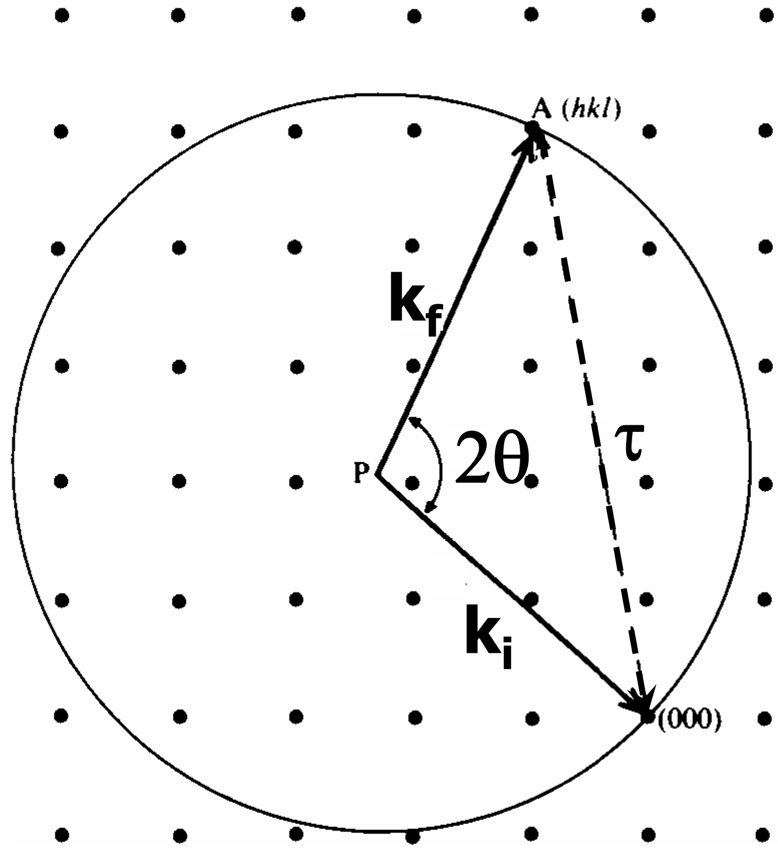
$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{coh,el}} = \frac{\sigma_{\text{coh}}}{4\pi} e^{-2W} N \frac{(2\pi)^3}{\text{v}_0} \sum_{\boldsymbol{\tau}} \delta(\mathbf{Q}-\boldsymbol{\tau})$$

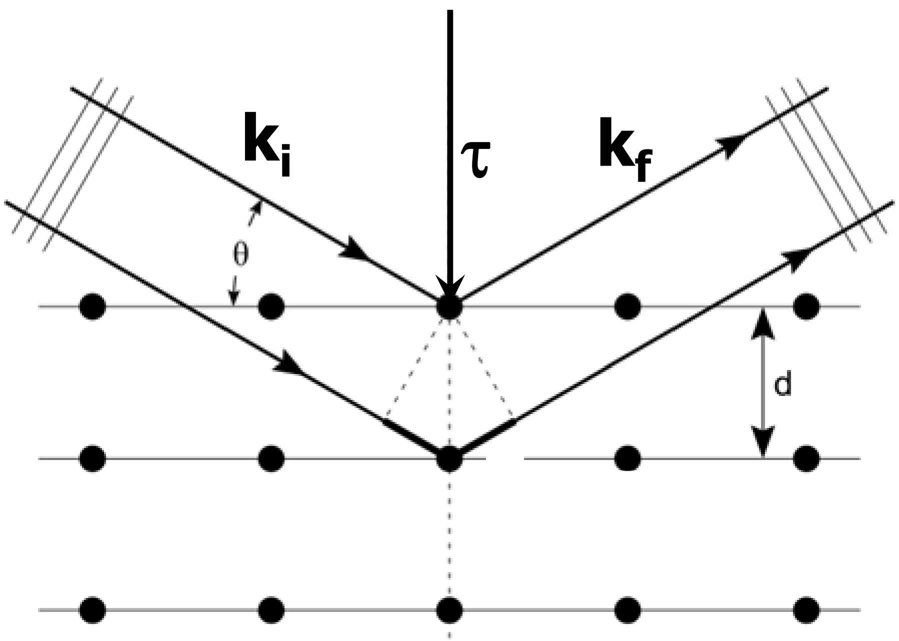
$$2W = -\langle U^2 \rangle$$

Закон Брэгга

$$\mathbf{k}_i - \mathbf{k}_f = \boldsymbol{\tau}$$

$$\tau = 2k \sin\theta$$





$$\tau = n\frac{2\pi}{d} \qquad k = \frac{2\pi}{\lambda}$$

$$n\lambda = 2d\sin\theta$$

Фактор Дебая-Валлера

$$2W = -\left\langle U^2 \right\rangle =$$

$$= \sum_{\alpha} P_{\alpha} \sum_{s=1}^{3} \sum_{\mathbf{q}} \sum_{s'=1}^{3} \sum_{\mathbf{q}'} \left\langle \alpha \left| \left(g_s(\mathbf{q}) a_{\mathbf{q},s} + g_s^*(\mathbf{q}) a_{\mathbf{q},s}^{+} \right) \left(g_{s'}(\mathbf{q}') a_{\mathbf{q}',s'} + g_{s'}^*(\mathbf{q}') a_{\mathbf{q}',s'}^{+} \right) \right| \alpha \right\rangle$$

$$= \sum_{\alpha} P_{\alpha} \sum_{s=1}^{3} \sum_{\mathbf{q}} \left| g_s(\mathbf{q}) \right|^2 \left\langle \alpha \left| \left(a_{\mathbf{q},s} a_{\mathbf{q},s}^{+} + a_{\mathbf{q},s}^{+} a_{\mathbf{q},s} \right) \right| \alpha \right\rangle$$

$$\left\langle \alpha \left| \left(a_{\mathbf{q},s} a_{\mathbf{q},s}^{+} + a_{\mathbf{q},s}^{+} a_{\mathbf{q},s} \right) \right| \alpha \right\rangle = 2n_{\mathbf{q},s} + 1$$

$$2W = \frac{\hbar}{2MN} \sum_{s=1}^{3} \sum_{\mathbf{q}} \frac{|\mathbf{Q}\mathbf{e}_s(\mathbf{q})|^2}{\omega_s(\mathbf{q})} \left\langle 2n_{\mathbf{q},s} + 1 \right\rangle$$

$$\left\langle n_{\mathbf{q},s} \right\rangle = \frac{1}{e^{\hbar\omega_s(\mathbf{q})/(k_B T)} - 1}$$

$$\left\langle 2n_{\mathbf{q},s} + 1 \right\rangle = \frac{e^{\hbar\omega_s(\mathbf{q})/(k_B T)} + 1}{e^{\hbar\omega_s(\mathbf{q})/(k_B T)} - 1} = \frac{e^{\hbar\omega_s(\mathbf{q})/(2k_B T)} + e^{-\hbar\omega_s(\mathbf{q})/(2k_B T)}}{e^{\hbar\omega_s(\mathbf{q})/(2k_B T)} - e^{-\hbar\omega_s(\mathbf{q})/(2k_B T)}} = \coth\left(\frac{\hbar\omega_s(\mathbf{q})}{2k_B T} \right)$$

Фактор Дебая-Валлера

$$e^{-2W}$$

$$2W = \frac{\hbar}{2MN}\sum_{s=1}^{3}\sum_{\mathbf{q}}\frac{|\mathbf{Q}\mathbf{e}_s(\mathbf{q})|^2}{\omega_s(\mathbf{q})}\coth\left(\frac{\hbar\omega_s(\mathbf{q})}{2k_BT}\right)$$

Кубические кристаллы

$$2W = \frac{\hbar}{2MN}\sum_{\mathbf{q}}\frac{Q_x^2 + Q_y^2 + Q_z^2}{\omega(\mathbf{q})}\coth\left(\frac{\hbar\omega(\mathbf{q})}{2k_BT}\right)$$

$$= \frac{\hbar Q^2}{2M}\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{\omega(\mathbf{q})}\coth\left(\frac{\hbar\omega(\mathbf{q})}{2k_BT}\right)$$

$$\omega_1(\mathbf{q}) = \omega_2(\mathbf{q}) = \omega_3(\mathbf{q}) = \omega(\mathbf{q})$$

$$2W = \frac{\hbar Q^2}{2M}\int_0^\infty Z(\omega)\frac{1}{\omega}\coth\left(\frac{\hbar\omega}{2k_BT}\right)d\omega$$