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HW 5 Solution.

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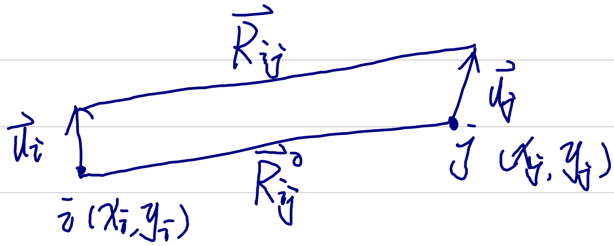
Problem 1:



$$\vec{R}_{ij} = -\vec{u}_i + \vec{R}_{ij}^{\,0} + \vec{u}_j$$

$$\Rightarrow |\vec{R}_{ij}|^2 = |\vec{u}_i|^2 + |\vec{u}_j|^2 + |\vec{R}_{ij}^{\,0}|^2 - 2\vec{u}_i \cdot \vec{R}_{ij}^{\,0} + 2\vec{u}_j \cdot \vec{R}_{ij}^{\,0} - 2\vec{u}_i \cdot \vec{u}_j$$

If we assume $|\vec{u}_i|, |\vec{u}_j|$ very small.

second order $\Rightarrow 0$

$$\Rightarrow |\vec{R}_{ij}|^2 = |\vec{R}_{ij}^{\,0}|^2 - 2\vec{R}_{ij}^{\,0} \cdot (\vec{u}_j - \vec{u}_i)$$

$$|\vec{R}_{ij}| = \sqrt{|\vec{R}_{ij}^{\,0}|^2 - 2\vec{R}_{ij}^{\,0} \cdot (\vec{u}_j - \vec{u}_i)}$$

$$= |\vec{R}_{ij}^{\,0}|^2 \sqrt{1 - \frac{2\vec{R}_{ij}^{\,0}}{|\vec{R}_{ij}^{\,0}|^2} \cdot (\vec{u}_j - \vec{u}_i)}$$

$$\sqrt{1-x} = 1 - \frac{1}{2}x$$

$$\Rightarrow |\vec{R}_{ij}| = |\vec{R}_{ij}^{\,0}| \left(1 - \frac{\vec{R}_{ij}^{\,0}}{|\vec{R}_{ij}^{\,0}|^2} (\vec{u}_j - \vec{u}_i)\right.$$

$$\Rightarrow \delta_{ij} = |\vec{R}_{ij}| - |\vec{R}_{ij}^{\,0}| = \frac{\vec{R}_{ij}^{\,0}}{|\vec{R}_{ij}^{\,0}|} (\vec{u}_i - \vec{u}_j)$$

Problem 2.

$$\hat{a}(q) = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega(q)}\,\hat{Q}(q) + \frac{i}{\sqrt{\omega(q)}}\hat{P}(q)\right) \qquad \omega(q) = \omega(-q)$$

$$\hat{a}^{+}(q) = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega(q)}\,\hat{Q}^{*}(q) - \frac{i}{\sqrt{\omega(q)}}\hat{P}^{*}(q)\right)$$

$$\hat{a}^{+}(-q) = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega(q)}\,\hat{Q}^{*}(-q) - \frac{i}{\sqrt{\omega(q)}}\hat{P}^{*}(-q)\right) \qquad \hat{Q}^{*}(-q) = \hat{Q}(q)$$

$$= \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega(q)}\,\hat{Q}(q) - \frac{i}{\sqrt{\omega(q)}}\hat{P}^{*}(-q)\right)$$

$$\Rightarrow \hat{Q}_j(q) = \sqrt{\frac{\hbar}{2\omega_j(q)}}\left(\hat{a}_j(q) + \hat{a}_j^{+}(-q)\right)$$

Matrix element

$$\langle n'(q';j')|\,\hat{Q}_j(q)\,|n_j(q)\rangle$$

$$\hat{Q}_j(q)|n_j(q)\rangle = \sqrt{\frac{\hbar}{2\omega_j(q)}}\left(\hat{a}_j(q) + \hat{a}_j^{+}(-q)\right)|n_j(q)\rangle$$

$$\hat{a}_j(q)|n_j(q)\rangle = \sqrt{n_j(q)}\,|n_j(q)-1\rangle$$

$$\hat{a}_j^{+}(-q)|n_j(q)\rangle = \hat{a}_j^{+}(-q)\frac{1}{\sqrt{n_j(q)!}}\hat{a}_j^{+n}(q)|0\rangle = \frac{1}{\sqrt{n_j(q)!}}\hat{a}_j^{+}(-q)\,\hat{a}_j^{+n}(q)|0\rangle$$

$$\left[\hat{a}_j^{+}(-q),\ \hat{a}_j^{+}(q)\right] = 0$$

$$\Rightarrow \hat{a}_j^{+}(-q)|n_j(q)\rangle = \frac{1}{\sqrt{n_j(q)!}}\hat{a}_j^{+n}(q)\,\hat{a}_j^{+}(-q)|0\rangle$$

$$= \frac{1}{\sqrt{n_j(q)!}}\hat{a}_j^{+n}(q)|1(-q)\rangle$$

$$= |n_j(q)\,1_j(-q)\rangle$$

$$\Rightarrow \langle n'(q',j')|\hat{Q}_j(q)|n_j(q)\rangle = \sqrt{n_j(q)}\,\langle n'(q',j')|n_j(q)-1\rangle$$

$$+ \langle n_j'(q')|n_j(q);1_j(-q)\rangle$$

$$= \sqrt{n}\,\delta_{qq'}\delta_{jj'}\delta_{n'n-1} + \delta_{jj'}\delta_{n',n+1}\delta_{q',0}\delta_{q,0}$$

if $n = n'$ $\Rightarrow$ Matrix element $= 0$

Problem 3. Harmonic Oscillator energy.

$(n_j + \frac{1}{2})\hbar\omega_j$

Considering probability of each eigen-energy

$$\Rightarrow \bar{E}_j = \frac{1}{2}\hbar\omega_j + \frac{\sum_{n_j} n_j\hbar\omega_j e^{-n_j\hbar\omega_j/k_BT}}{\sum_{n_j} e^{-n_j\hbar\omega_j/k_BT}} = \frac{1}{2}\hbar\omega_j - \frac{\partial}{\partial\beta}\ln\sum_{n_j} e^{-n_j\hbar\omega_j\beta}$$

$\beta = \frac{1}{k_BT}$

Simplify it using $\sum_n x^n = \frac{1}{1-x}$

$$\Rightarrow \bar{E}_j(T) = \frac{1}{2}\hbar\omega_j + \frac{\hbar\omega_j}{e^{\beta\hbar\omega_j}-1}$$

$$\Rightarrow \bar{E} = \sum_j \left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_j}-1}\right)\hbar\omega_j$$

$$\sum_j \rightarrow V\int d\omega\, D(\omega)$$

$\hookrightarrow$ density of states

$$\Rightarrow \bar{E} = V\int d\omega\, D(\omega)\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right)\hbar$$

$$C_V = \frac{\partial\bar{E}}{\partial T} = V\int d\omega\, D(\omega)\left(\frac{\partial}{\partial T}\frac{1}{e^{\beta\hbar\omega}-1}\right)\hbar\omega$$

Problem 4. Check Einstein Model