Problem set 5.

Problem 1. The d-dimensional Debye model

State-counting: $\sum_{\vec{k}} = \underbrace{N}_{\text{number of lattice sites}} = \alpha \int_{1.BZ} = \alpha \cdot \underbrace{\Omega_r}_{\text{volume of reciprocal cell}} = \alpha \cdot \frac{(2\pi)^d}{\Omega} \mapsto \alpha = \frac{N}{\Omega_r} \mapsto \frac{1}{N}\sum_{\vec{k}} (\cdot) = \frac{1}{\Omega_r}\int_{1.BZ} (\cdot)$

$$\langle E\rangle = \sum_{\vec{k}} \underbrace{\langle E(\vec{k})\rangle}_{\text{energy of each } \vec{k}} = \frac{N}{\Omega_r}\int_{1.BZ} d\vec{k}\, \langle E(\vec{k})\rangle \overset{\text{int. over}}{\underset{\text{sphere}}{=}} \frac{N}{\Omega_r} A_d \cdot \int_0^{k_D} dk \cdot k^{d-1} \langle E(k)\rangle$$

Let $\varepsilon = \hbar\omega_s(\vec{k}) = \hbar v_s \cdot k$, $\varepsilon_D = \hbar\Omega_D = \hbar v_s k_D$

$$\langle E\rangle = \frac{N}{\Omega_r} A_d (\hbar v_s)^{-d} \int_0^{\varepsilon_D} d\varepsilon \cdot \varepsilon^{d-1} \langle E(\varepsilon)\rangle$$

density of state

$$f(\varepsilon') \propto \int_0^{\varepsilon_D} d\varepsilon \cdot \varepsilon^{d-1}\delta(\varepsilon-\varepsilon') = \begin{cases} \varepsilon'^{d-1}, & \varepsilon' \in (0, \varepsilon_D) \\ 0, & \text{otherwise} \end{cases} = \varepsilon'^{d-1}\Theta(\underset{\hbar\Omega_D = \hbar v_s k_D}{\varepsilon_D} - \varepsilon')$$

$\cancel{\langle E(\varepsilon)\rangle}$ $\langle E(\varepsilon)\rangle = \underset{\text{Dofs of HO}}{d} \cdot \langle \underset{\hbar\omega}{\varepsilon}(\hat{n}+\frac{1}{2})\rangle = d\cdot\varepsilon(n_{BE}(\beta)+\frac{1}{2})$, $\Omega_r = A_d\int_0^{k_D} dk \cdot k^{d-1} = A_d \frac{k_D^d}{d}$

$$\langle E\rangle = \frac{d\cdot N}{A_d \frac{k_D^d}{d}} \cdot A_d (\hbar v_s)^{-d} \int_0^{\varepsilon_D} d\varepsilon \frac{\varepsilon^d}{e^{\beta\varepsilon}-1} + ZPE, \quad \text{let } x = \beta\cdot\varepsilon,\ \varepsilon = k_B T x.$$

$$\frac{\langle E\rangle}{N} = d \cdot k_B T \frac{(k_B T)^d}{(\hbar v_s k_D)^d} \cdot d \int_0^x dx \frac{x^d}{e^x - 1} + ZPE$$

$$= d \cdot k_B T \underbrace{\left(\frac{T}{\Theta_D}\right)^d d\int_0^{x_D} dx \frac{x^d}{e^x-1}}_{\text{Debye function, } D_n(x) = \frac{n}{x^n}\int_0^x dt \frac{t^n}{e^t-1}} + ZPE, \quad \Theta_D = \frac{\hbar v_s k_D}{k_B},\ x_D = \frac{\hbar v_s k_D}{k_B T} = \frac{\Theta_D}{T}$$

If $x \to 0$, $t \to 0$, $T \to \infty$,

$$D_n(x) = \frac{n}{x^n}\int_0^x dt \frac{t^n}{1+t-1} = \frac{n}{x^n}\int_0^x dt \cdot t^{n-1} = \frac{n}{x^n}\frac{t^n}{n}\Big|_0^x = 1, \rightarrow \frac{\langle E\rangle}{N} \approx d k_B T \rightarrow \frac{\partial\langle E\rangle}{\partial T} \approx d N k_B$$

If $x \to \infty$, $T \to 0$

$$D_n(x) = \frac{n}{x^n}\int_0^x dt \frac{t^n}{e^t-1} = \frac{n}{x^n}\left(\int_0^x dt \cdot t^n \cdot \sum_{k=1}^\infty e^{-kt}\right) = \frac{n}{x^n}\sum_{k=1}^\infty \int_0^x dt \cdot t^n \cdot e^{-kt}.$$

$$= \frac{n}{x^n}\sum_{k=1}^\infty \frac{1}{k^{n+1}}\int_0^\infty dt \cdot t^n \cdot e^{-kt} = \frac{n}{x^n}\cdot\zeta(n+1)\Gamma(n+1).$$ $\zeta(n)$ converge when $n>1$

$$\frac{\langle E\rangle}{N} \propto d\, k_B T \cdot \left(\frac{T}{\Theta_D}\right)^d \rightarrow \frac{\partial\langle E\rangle/N}{\partial T} \propto T^d$$

Correction on Ex. 4

$\Gamma_{\vec{q}} = \frac{1}{2} \langle\langle (\vec{q}\cdot\vec{X}_j)^2 \rangle\rangle$, $\vec{X}_j = \frac{1}{\sqrt{N}} \sum_k \vec{\varepsilon}(\vec{k}) \sqrt{\frac{\hbar}{2m\omega(\vec{k})}} (a_k + a_{-k}^+) e^{i\vec{k}\cdot\vec{R}_j}$

$$\Gamma_{\vec{q}} = \frac{1}{2N} \sum_{kk'} (\vec{q}\cdot\vec{\varepsilon}(\vec{k}))(\vec{q}\cdot\vec{\varepsilon}(\vec{k}')) \frac{\hbar}{2m\sqrt{\omega(\vec{k})\omega(\vec{k}')}} e^{i(\vec{k}+\vec{k}')\cdot\vec{R}_j} \langle\langle (a_k + a_{-k}^+)(a_{k'} + a_{-k'}^+) \rangle\rangle$$

Using translational symmetry, $\langle\langle (\vec{q}\cdot\vec{X}_j)^2 \rangle\rangle = \frac{1}{N}\sum_j \langle\langle (\vec{q}\cdot\vec{X}_j)^2 \rangle\rangle$

$$\Gamma_{\vec{q}} = \frac{1}{2N^2} \sum_j \sum_{kk'} e^{i(\vec{k}+\vec{k}')\cdot\vec{R}_j} \boxed{\cdots\cdots} \quad , \quad \frac{1}{N}\sum_j e^{i(\vec{k}+\vec{k}')\cdot\vec{R}_j} = \delta(\vec{k}+\vec{k}')$$

$$= \frac{1}{2N} \sum_k (\vec{q}\cdot\vec{\varepsilon}(\vec{k}))^2 \frac{\hbar}{2m\omega(\vec{k})} \langle\langle (a_k + a_{-k}^+)(a_{-k} + a_k^+) \rangle\rangle$$

[assuming $\omega(\vec{k}) = \omega(-\vec{k})$, $\varepsilon(\vec{k}) = \varepsilon(-\vec{k})$]

$\langle\langle \cdots \rangle\rangle$ over $e^{-\beta H}/Z$, $\langle\langle a\,a \rangle\rangle = \langle\langle a^+ a^+ \rangle\rangle = 0$, $\langle\langle a_{-k}^+ a_{-k} + a_k a_k^+ \rangle\rangle = 2n_\beta(\omega(\vec{k})) + 1$

$$\Gamma_{\vec{q}} = \frac{1}{2N} \sum_k (\vec{q}\cdot\vec{\varepsilon}(\vec{k}))^2 \frac{\hbar}{2m\omega(\vec{k})} \coth\left(\frac{\beta\hbar\omega(\vec{k})}{2}\right)$$

Using $\frac{1}{N}\sum_k = \frac{1}{\Omega_r}\int_{1.BZ} \approx \frac{A_d}{\Omega_r}\int_0^{k_D} dk \cdot k^{d-1}$ and $\omega(\vec{k}) = \hbar v_s |\vec{k}|$

$$\Gamma_{\vec{q}} \propto \int_0^{k_D} dk\, k^{d-1-\alpha} \coth\left(\frac{\beta\hbar v_s k^\alpha}{2}\right) = \int_0^{k_D} dk\, k^{d-1-\alpha} \left(\frac{2}{e^{\beta\hbar v_s k^\alpha} - 1} + 1\right) .$$

When $\beta \to \infty$, $T \to 0$,

$$\Gamma_{\vec{q}} \propto \int_0^{k_D} dk \cdot k^{d-1-\alpha}$$

When β is finite

$$\Gamma_{\vec{q}} \propto \underbrace{F(k_D)}_{\text{finite}} - F(0^+) \quad , \quad F(0^+) \approx \int dk\, k^{d-1-2\alpha} \Big|_{k=0^+}$$

$F(k) = \int k^n dk$, $F(0^+)$ converge if $n > -1$, diverge if $n \leq -1$