Physics 560A

Midterm solutions

1) a) $f(\vec{x}+\vec{R}) = f(\vec{x}) \quad \forall \vec{R} \in BL$

$$f(\vec{x}) = \sum_{\vec{G}} f_{\vec{G}}\, e^{i\vec{G}\cdot\vec{x}}$$

$$f(\vec{x}+\vec{R}) = \sum_{\vec{G}} f_{\vec{G}}\, e^{i\vec{G}\cdot\vec{x}}\, e^{i\vec{G}\cdot\vec{R}}$$

$$\Rightarrow \boxed{e^{i\vec{G}\cdot\vec{R}} = 1 \quad \forall \vec{R} \in BL}$$

b) $\vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{b}\hat{y}$, $\vec{b}_3 = \frac{2\pi}{c}\hat{z}$

c) $|k_x| \le \frac{\pi}{a}$, $|k_y| \le \frac{\pi}{b}$

$|k_z| \le \frac{\pi}{c}$

2) $$C_V = \int_0^\infty d\varepsilon \; \varepsilon D(\varepsilon) \frac{\partial f}{\partial T}$$

$$f = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} \quad , \quad D(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$$

$$\frac{\partial f}{\partial T} = \frac{\varepsilon-\mu}{T}\left(-\frac{\partial f}{\partial \varepsilon}\right) = \frac{1}{k_B T^2} \frac{(\varepsilon-\mu)\, e^{\beta(\varepsilon-\mu)}}{\left(e^{\beta(\varepsilon-\mu)}+1\right)^2}$$

$$C_V = \frac{1}{k_B T^2}\int_0^\infty d\varepsilon \, \frac{\varepsilon D(\varepsilon)(\varepsilon-\mu)}{\left(e^{\frac{\beta(\varepsilon-\mu)}{2}} + e^{-\frac{\beta(\varepsilon-\mu)}{2}}\right)^2}$$

let $\beta(\varepsilon-\mu) = x$

$$C_V = k_B^{\,2} T \int_{-\beta\mu}^{\infty} dx \, \frac{\left(x^2+\beta\mu x\right) D\left(\mu + \frac{x}{\beta}\right)}{\left(e^{x/2}+e^{-x/2}\right)^2}$$

integrand is sharply peaked about $x=0$.

$\Rightarrow$ can extend lower limit to $-\infty$ with negligible error.

Also, we can pull $D(\varepsilon_F)$ outside the integral.

$$C_V \simeq \frac{k_B^2 T D(\varepsilon_F)}{4} \int_{-\infty}^{\infty} dx \; \frac{x^2 + \beta\mu x}{\cosh^2\left(\frac{x}{2}\right)}$$

$$\boxed{C_V \cong \frac{\pi^2}{3} k_B^2 T D(\varepsilon_F)}$$

(odd term integrates to zero).

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3) $$\langle x_n^2 \rangle = \frac{1}{L} \sum_{k,k'} \frac{\hbar}{2m\sqrt{\omega_k \omega_{k'}}}$$

$$\times \langle 0 | \left(a_k e^{ikna} + a_k^\dagger e^{-ikna}\right)\left(a_{k'} e^{ik'na} + a_{k'}^\dagger e^{-ik'na}\right)$$

$$\times |0\rangle$$

$$\langle x_n^2 \rangle = \frac{1}{L} \sum_k \frac{\hbar}{2m\omega_k} \langle 0 | a_k a_k^\dagger + a_k^\dagger a_k | 0 \rangle$$

$\langle 0 | a_k^\dagger a_k | 0 \rangle = 0 \qquad a_k a_k^\dagger = 1 + a_k^\dagger a_k$

$$\langle x_n^2 \rangle = \frac{1}{L} \sum_{\substack{k \\ k \neq 0}} \frac{\hbar}{2m\omega_k}$$

$$\langle x_n^2 \rangle = \frac{a}{2\pi} \int_{-\frac{\pi}{a}}^{\pi/a} dk \, \frac{\hbar}{2m\sqrt{\frac{4C}{m}} \left|\sin\left(\frac{ka}{2}\right)\right|}$$

$$\boxed{\langle x_n^2 \rangle = \frac{\hbar}{2\pi\sqrt{mC}} \int_0^{\pi/2} \frac{dx}{\sin x} \to \infty}$$

$\Rightarrow$ There is no possibility of crystalline order in 1D. This Hamiltonian describes a "harmonic fluid," not a 1D crystal.