Homework 3 Answer

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1 Problem 1

Recall, Born-von Karman boundary condition, $\psi(\vec{r}) = \psi(\vec{r} + n_i\vec{a}_i)$. For momentum eigenstates, we need $e^{i\vec{k}_i \cdot \delta\vec{r}_i} = 1$. Where we define $\delta\vec{r}_i = n_i\vec{a}_i$ and $n_i \in [1, N_i]$.

To satisfy the condition, we need $(\vec{k}_i \cdot n_i\vec{a}_i) = 2\pi * m, \forall i \in \{x, y, z\}$, where $\vec{k}_i = h_i\vec{b}_i$. And $\vec{b}_i$, $\vec{a}_i$ are basis vector in the momentum and real space respectively and m is an integer.

Within the first Brillouin Zone, $m = 1$. We then have, $\vec{k}_i \cdot \vec{a}_i = 2\pi/n_i$. Recall $\vec{k}_i$ and $\vec{a}_i$ are parallel. We see $||\vec{k}_i|| = 2\pi/(||\vec{a}_i||n_i)$ where $n_i \in [1, N_i]$. We see now, $\vec{k}_i$ could take N_i different values.

The arguement above should be repeated in all three dimensions, in result $\sum_i \vec{k}_i$ could take $\prod_i N_i$ different results which is also the number of lattice points in real space.

2 Problem 2

Using $f(\vec{r}) = f(\vec{r} + \vec{R})$, let's sum up and take average $f(\vec{r} + \vec{R})$ with $\vec{R}$ range from all lattice points in our crystal. It should be equal to $f(\vec{r})$.

$$
\begin{aligned}
f(\vec{r}) &= \frac{1}{N_{crystal}} \sum_{R\in\{\vec{R}\}} f(\vec{r}+\vec{R}) \\
&= \frac{1}{N_{crystal}} \sum_{R\in\{\vec{R}\}} V \int \frac{d\vec{k}}{(2\pi)^3} f_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}+\vec{R})} \\
&= \frac{1}{N_{crystal}} V \int \frac{d\vec{k}}{(2\pi)^3} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \sum_{R\in\{\vec{R}\}} e^{i(\vec{k}\cdot\vec{R})} \\
&= \frac{1}{N_{crystal}} V \int \frac{d\vec{k}}{(2\pi)^3} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \frac{(2\pi)^3}{v} \delta(\vec{k}-\vec{G}) \\
&= \frac{1}{N_{crystal}} V/v \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \\
&= \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \quad \square
\end{aligned}
$$

where we have used in the last line, $V = v * N_{crystal}$. The total volume of the crystal is the number of unit cells multiplied by the unit cell volume.