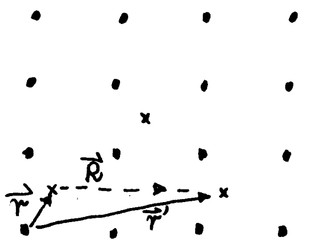
Appendix A: Fourier Analysis of Periodic function

- **Why are $\vec{G}$'s (reciprocal lattice vectors) important?**

Here, we illustrate the usefulness by considering the Fourier Analysis of a periodic function.



x are equivalent points

Consider a crystal, due to the periodicity, we expect that physical quantities such as electron density[+] should be the same at equivalent points in the lattice.

These equivalent points are related by lattice vectors.

e.g. $\vec{r}' = \vec{r} + \vec{R}$

where $\vec{R}$ is a lattice vector (in direct lattice)

i.e. $\vec{R} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$

In fact, points related by $\vec{R}$ are equivalent.

- Let $n(\vec{r})$ be, say, the electron concentration (number density) at $\vec{r}$, due to periodicity, we have[+]

$$n(\vec{r}) = n(\vec{r} + \vec{R}),$$

i.e. $n(\vec{r})$ is periodic with the same periodicity of the underlying lattice.

- Another example is to consider the potential energy function $V(\vec{r})$ that enters into the Schrödinger equation. Due to periodicity, we have

$$\boxed{V(\vec{r}) = V(\vec{r} + \vec{R})}$$ periodic potential energy function

i.e. the QM problem in solid state physics is to study the Schrödinger equation with a periodic $V(\vec{r})$.

- In short, we encounter many periodic functions in SSP. The periodicity reflects the discrete translational symmetry.

[+] It is important to note that we are considering $n(\vec{r})$ here. From Quantum Mechanics, $n(\vec{r}) \propto |\psi(\vec{r})|^2$. Hence we have $|\psi(\vec{r})|^2 = |\psi(\vec{r}+\vec{R})|^2$. However, it does not imply $\psi(\vec{r}) = \psi(\vec{r}+\vec{R})$. In fact, $\psi(\vec{r}) \neq \psi(\vec{r}+\vec{R})$. They differ by a phase factor (see Bloch's theorem

- For ANY FUNCTION of $\vec{r}$, $f(\vec{r})$, we can write down a Fourier expansion in general as:

$$f(\vec{r}) = \sum_{\vec{k}} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

where $\vec{k}$ goes over all possible vectors

- What if $f(\vec{r})$ is periodic?

An important theorem:

If $f(\vec{r})$ is periodic, then the Fourier expansion has contributions only from Fourier components corresponding to reciprocal lattice vectors $\vec{G}$, i.e.,

$$\underset{\text{periodic}}{f(\vec{r})} = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

where the sum is over all reciprocal lattice vectors $\vec{G}$

Appreciation: Compared with the general form, it means that many (in fact most) of the coefficients $f_{\vec{k}}$ are zero due to periodicity, and only $f_{\vec{G}}$ survive. Geometrically, it means that only plane waves $e^{i\vec{G}\cdot\vec{r}}$ are needed to construct a spatially periodic function.

Why? In general, $f(\vec{r}) = \sum_{\vec{k}} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$

For periodic function: $f(\vec{r}) = f(\vec{r}+\vec{R})$

$$f(\vec{r}+\vec{R}) = \sum_{\vec{k}} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{R}} = f(\vec{r}) = \sum_{\vec{k}} f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

This can be achieved only if:

$e^{i\vec{k}\cdot\vec{R}} = 1$ for all lattice vectors $\vec{R}$

OR $\vec{k}\cdot\vec{R} = 2\pi \cdot \text{integer}$

$\therefore$ $\vec{k}$ can only take on $\vec{G}$

$$\therefore \boxed{f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \quad \text{if } f(\vec{r}) \text{ is periodic.}}$$

e.g. electron concentration $n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$

potential energy function $V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$

$n_{\vec{G}}$, $V_{\vec{G}}$ can be found by an integral of $n(\vec{r})$, $V(\vec{r})$ over a volume Ω_c.