Bloch Functions

Addendum to Problem 3 of Problem Set 2

Consider the form of a Bloch function in one dimension: $\psi_k(x) = e^{ikx}u_k(x)$, where $u_k(x)$ has the periodicity of the lattice $u_k(x+a) = u_k(x)$. Hence, $u_k(x)$ can be represented as a complex Fourier series:

$$u_k(x) = \sum_{n=-\infty}^{\infty} U_n(k) e^{2n\pi ix/a},$$

where the $U_n(k)$ are the Fourier coefficients of $u_k(x)$. We now introduce the notation used in the course notes: $G_n = 2n\pi/a$, in which case we can write

$$u_k(x) = \psi_k(x)e^{-ikx} = \sum_G U_G(k)e^{iGx}. \tag{1}$$

We now invoke the orthogonality property of the complex exponentials over the unit cell:

$$\int_0^a e^{iGx}e^{-iG'x}\,dx = \int_0^a \exp\left[\frac{2\pi i}{a}(n-n')x\right]dx = a\delta_{n,n'} = a\delta_{G,G'},$$

to project individual Fourier components in (1):

$$\begin{aligned}
\int_0^a \psi_k(x)e^{-ikx}e^{-iG'x}\,dx &= \int_0^a \psi_k(x)e^{i(k+G')x}\,dx \\
&= \int_0^a \left[\sum_G U_G(k)e^{iGx}\right]e^{-iG'x}\,dx \\
&= \sum_G U_G(k) \underbrace{\int_0^a e^{i(G-G')x}\,dx}_{a\delta_{G,G'}} \\
&= aU_{G'}(k) \\
&\equiv \tilde{u}(k+G'),
\end{aligned}$$

where in the last line we have redefined the Fourier coefficients to absorb the factor of a. Therefore, the Fourier representation of a Bloch function can be written as

$$\boxed{\psi_k(x) = e^{ikx}\sum_G \tilde{u}(k+G)e^{iGx} = \sum_G \tilde{u}(k+G)e^{i(k+G)x}.} \tag{2}$$

The same procedure can be used to obtain analogous expressions in higher dimensions:

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{G}} \tilde{u}(\boldsymbol{k}+\boldsymbol{G})e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{x}}.$$

The expansion in (2) has important consequences. Consider the operation of the momentum operator on a Bloch state:

$$\begin{aligned}
-i\hbar\frac{d\psi_k(x)}{dx} &= -i\hbar\frac{d}{dx}\left[\sum_G \tilde{u}(k+G)e^{i(k+G)x}\right] = -i\hbar\sum_G \tilde{u}(k+G)\frac{de^{i(k+G)x}}{dx} \\
&= k\sum_G \tilde{u}(k+G)e^{i(k+G)x} + \sum_G G\tilde{u}(k+G)e^{i(k+G)x} \\
&= k\psi_k(x) + \sum_G G\tilde{u}(k+G)e^{i(k+G)x}.
\end{aligned}$$

The first term on the right-hand side of this equation appears like a momentum eigenstate, but the second term includes contributions from other wave vectors, in effect, from the periodic lattice. In other words, the fact that an electron in a periodic lattice is not a momentum eigenstate is due to the fact that the lattice imposes a periodicity on the electron, so the momentum is characteristic of the electron-lattice system, rather than the electron alone. For this reason, k is called a **crystal momentum**.

As a second example of the utility of (2), we can immediately write

$$\psi_{k+G}(x) = \sum_{G'} \tilde{u}(k+G+G')e^{i(k+G+G')x}\,.$$

The summation index G' is a dummy variable whose range extends from minus to plus infinity. Thus, we can shift this variable by defining a new summation index $G'' = G+G'$, in which case we obtain

$$\psi_{k+G}(x) = \sum_{G''} \tilde{u}(k+G'')e^{i(k+G'')x} = \sum_{G} \tilde{u}(k+G)e^{i(k+G)x} = \psi_k(x)\,,$$

where we have again used the fact that G and G'' are both dummy variables. Hence,

$$\boxed{\psi_{k+G}(x) = \psi_k(x)\,.}$$

An immediate consequence of this result is obtained from the Schrödinger equations solved by $\psi_k(x)$ and $\psi_{k+G}(x)$. We have

$$\widehat{H}\psi_k(x) = E(k)\psi_k(x)\,,$$

where $\widehat{H}$ is the Hamiltonian operator and, by changing k to $k+G$,

$$\widehat{H}\psi_{k+G}(x) = E(k+G)\psi_{k+G}(x)\,,$$

which is the same as

$$\widehat{H}\psi_k(x) = E(k+G)\psi_k(x)\,.$$

This implies that

$$\boxed{E(k+G) = E(k)\,.}$$