Bloch states + energy levels.

Recall that for a particle in a periodic potential $V(\vec{r}) = V(\vec{r} + \vec{a})$ the energy eigenstates can always be expressed as:

$$\Psi_k(\vec{r}) = e^{i \vec{k} \cdot \vec{r}} u_k(\vec{r})$$  \hspace{1cm} (1)

where $\vec{k}$ is some wavevector and

$$u_k(\vec{r} + \vec{a}) = u_k(\vec{r})$$  \hspace{1cm} (2)

for every lattice vector. (Note label $E$.)

As an example we considered a one dimensional lattice with spacing $a$. If $V = 0$ we arrive at the empty lattice model, and we find that the energy eigenstates are described by two labels:

$n \sim \text{integer}$

$k \sim \text{real number}$.

The eigenstates are:

$$\Psi_{n,k}(x) = A e^{i k x} e^{i \frac{2n\pi x}{a}}$$  \hspace{1cm} (3)

with energy:

$$E_n(k) = \frac{\hbar^2}{2m} \left( k + \frac{2n\pi}{a} \right)^2$$  \hspace{1cm} (4)

where, at this stage, $k$ can take on any real value.
Recall that this is really equivalent to the conventional free particle eigenstate:

$$\psi(x) = Ae^{i k' x}$$

where

$$k' = k + \frac{2n\pi}{a}.$$ 

Now plotting (4) we see.

and clearly more than one combination of $n$ and $k$ give the same energy.

We now investigate this. What possible values of $k$ and $n$ result in the same energy $E_n$ eigenstates? How can we restrict $k$, or $n$ meaningfully.

The answer will come in two forms

i) we shall restrict $k$ according to properties of the crystal.

ii) we shall restrict $n$ so that it runs through the natural numbers $n=0,1,2,3,...$. 
Example: Consider $n=0$ and a fixed value of $k$. Determine $k'$ such that for $n=1$:

$$E_1(k') = E_0(k)$$

Then consider the wavefunctions, do they differ?

**Answer:** Need:

$$(k' + \frac{2\pi}{a})^2 = k^2$$

$$k' + \frac{2\pi}{a} = \pm k$$

$$\Rightarrow k' = \pm k - \frac{2\pi}{a}.$$

Then

$$\Psi_{1,k'} = A e^{\pm ikx} e^{-\frac{2\pi}{a}x} e^{\frac{2\pi}{a}x/a}$$

$$= A e^{\pm ikx}$$

$$= \Psi_{0,\pm k}.$$  

Thus for $k' = k - \frac{2\pi}{a}$ the wavefunctions are identical and for $k' = -k - \frac{2\pi}{a}$ the wavefunctions are not identical but the energies are. These are illustrated in the graph.

So clearly the following wavefunctions are identical:

<table>
<thead>
<tr>
<th>$n$</th>
<th>-2</th>
<th>-1</th>
<th>0</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>$k+\frac{4\pi}{a}$</td>
<td>$k+\frac{2\pi}{a}$</td>
<td>$k$</td>
<td>$k-\frac{2\pi}{a}$</td>
<td>$k-\frac{4\pi}{a}$</td>
</tr>
</tbody>
</table>
It follows that we can restrict the values of $k$ to a region of width $\frac{2\pi}{a}$. Beyond this we have multiple labels representing the same wavefunction. It is conventional to limit $k$ to $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$.

We can see that, by this construction, every value of $n$ and $k$ gives a unique wavefunction. A general proof is: Suppose that $n,k$ and $n',k'$ give the same wavefunction. Then:

$$e^{ik'x} e^{i2n'\pi x/a} = e^{ikx} e^{i2n\pi x/a}$$

for all $x$

$$e^{i(k'-k)x} = e^{i2(n-n')\pi x/a}$$

$$k'-k = 2(n-n')\frac{\pi}{a}.$$

If $n \neq n'$ then $|k'-k| \geq \frac{2\pi}{a}$ which is not allowed by the construction. If $n = n'$ then $k = k'$. This proves the result. Thus we can label the eigenstates with:

$n \sim \text{any integer}$

$k \sim \text{any real in range } -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$
General restrictions on $\mathbf{k}$.

In the one dimensional case you may recall that the basic reciprocal lattice vector has magnitude $2\pi/a$. Thus the reciprocal lattice is:

$$\begin{align*}
&-\frac{2\pi}{a}, \quad -\frac{\pi}{a}, \quad 0, \quad \frac{\pi}{a}, \quad \frac{2\pi}{a}, \quad \frac{3\pi}{a} \quad \text{etc.}
\end{align*}$$

The first Brillouin zone is the set of points that is closer to the origin than any other point. But this is exactly the range of $\mathbf{k}$ values for the Bloch states.

We now show that the restriction is constructed quite generally along the same lines as above. To do this we return to our original statement of the Bloch theorem, that the wavefunction can always be constructed so that

$$\Psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \Psi(\mathbf{r})$$

for some $\mathbf{k}$. Now suppose that $\mathbf{k}' = \mathbf{k} + \mathbf{R}$ where $\mathbf{R}$ is a reciprocal lattice vector. Then

$$\Psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}' \cdot \mathbf{r}} \Psi(\mathbf{r}) \quad \text{and} \quad \Psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{r}} \Psi(\mathbf{r})$$

for all lattice vectors $\mathbf{R}$ since $\mathbf{k} \cdot \mathbf{R}$ is an integer multiple of $2\pi$. Thus $\Psi(\mathbf{r})$ is equivalently described by $\mathbf{k}$ and $\mathbf{k}'$. Thus we can restrict possible values of $\mathbf{k}$ by:
If \( \mathbf{k}' = \mathbf{k} + \mathbf{k} \) where \( \mathbf{k} \) is a reciprocal lattice vector then \( \Psi_{\mathbf{k}'}(\mathbf{r}) \) and \( \Psi_{\mathbf{k}}(\mathbf{r}) \) describe the same wavefunction.

Billiard zones

Consider a two dimensional square lattice with separation \( a \).

In the \( k_x \)-\( k_y \) plane the reciprocal lattice points are as illustrated. The first BZ consists of all points that are closer to the origin than any other point. This can be done by bisecting as illustrated. Only values of \( \mathbf{k} \) within the first BZ contribute to distinct energy eigenstates. The second BZ consists of points which are closer to the origin than any other point (except for the four nearest neighbors to the origin).