Bloch's Theorem

Bloch's theorem is a simple application of group theory ("irreducible representation"). Here without going into the full group theory we can derive Bloch's theorem using step 2, which happens to hold for the translation symmetry.

Step 1: *Fundamental Theorem of Quantum-Mechanics/Group-Theory: If Hamiltonian H commutes with an operator X, then X is block-diagonal with respect to eigen-states of H. States that belong to any given block share the same H eigenvalue.* Proof: Consider an eigenstate |p> of H, satisfying H|p> = E|p>. HX = XH means HX|p>=XH|p>, i.e. HX|p> = EX|p>, i.e. H|p'>=E|p'> where |p'>=X|p>. QED.

Step 2: *Corollary: If Hamiltonian H commutes with an operator X, and if eigen-states of X form a complete basis (note that X is commonly Unitary, and NOT Hermitian), then it is possible to choose eigen-states of H, so that each eigen-state of H is also an eigen-state of X.* Proof: Start from the complete basis that diagonalizes X. By the above theorem, H is block-diagonal in this basis. Now, each block is also a hermitian matrix, which is thus diagonalizable. This procedure gives simultaneous eigen-states of X and H. QED.

Step 3: Consider the specific case where X is the crystal translation operator, which we define as $T_{\mathbf{R}}$: for an arbitrary function f(**x**), $T_{\mathbf{R}}$ f(**x**) = f(**x**+**R**), where **R** is <u>a lattice vector</u>. Bloch's theorem is none other than the application of the above corollary to $T_{\mathbf{R}}$. Note that $T_{\mathbf{R}}$ does have the property that it can be diagonalized (trivially) with a complete basis, which is the plane wave basis. We have to remember however that due to the <u>discrete</u> crystal translation symmetry, plane waves whose wave vectors are the same modulo reciprocal lattice vectors **G** have the same eigen-value for $T_{\mathbf{R}}$. I.e. the most general form of eigenstates of $T_{\mathbf{R}}$ is $\sum_{\mathbf{G}} C(\mathbf{G}) \exp\left(i(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}\right)$, where $C(\mathbf{G})$'s are complex numbers, and the eigenvalue of $T_{\mathbf{R}}$ is $\exp(i\mathbf{k}\cdot\mathbf{R})$. Let's factor out $\exp\left(i\mathbf{k}\cdot\mathbf{x}\right)$ and write this function as $\exp(i\mathbf{k}\cdot\mathbf{x})\, u_{\mathbf{k}}(\mathbf{x})$, where $u_{\mathbf{k}}(\mathbf{x}) \equiv \sum_{\mathbf{G}} C(\mathbf{G}) \exp\left(i\mathbf{G}\cdot\mathbf{x}\right)$. Note that $u_{\mathbf{k}}(\mathbf{x})$ is invariant under $T_{\mathbf{R}}$. The above corollary means that any eigenstate of H can be written in this form, and this is Bloch's theorem.

Bloch's theorem (form 1):

The eigenstates of a periodic Hamiltonian can be chosen so that each eigenstate $\psi(\mathbf{x})$ satisfies:

$$\psi(\mathbf{x}) = \exp(i\mathbf{k}\cdot\mathbf{x})\, u_{\mathrm{n}\mathbf{k}}(\mathbf{x}),$$

where $u_{\mathrm{n}\mathbf{k}}(\mathbf{x})$ has the same periodicity as the Hamiltonian, i.e.

$$u_{\mathrm{n}\mathbf{k}}(\mathbf{x}+\mathbf{R}) = u_{\mathrm{n}\mathbf{k}}(\mathbf{x})$$

for any lattice vector $\mathbf{R}$ of the Hamiltonian. ($\hbar\mathbf{k}$ is crystal momentum – NOT true momentum – and n is symbol for all other quantum numbers – e.g. phonon branch in the case of phonons and band index, spin in the case of electrons)

Bloch's theorem (form 2):

The eigenstates of a periodic Hamiltonian can be chosen so that each eigenstate $\psi(\mathbf{x})$ satisfies:

$$\psi(\mathbf{x}+\mathbf{R}) = \exp(i\mathbf{k}\cdot\mathbf{R})\, \psi(\mathbf{x})$$

for any lattice vector $\mathbf{R}$ of the Hamiltonian.