

Bloch Theorem

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Bloch theorem states a symmetry principle of crystal, and therefore is a group theoretical property. Fortunately, however, we do not need to know the full group theory to prove it. [If you are interested in group theory applied to physics, you may look up books such as Tinkham “Group theory and quantum mechanics”.] It is because step 2 holds for all translation operators with a common basis set (plane waves), which makes it very simple to discuss the translation operators.

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 $|p\rangle$ of H , satisfying $H|p\rangle = E|p\rangle$. $HX = XH$ means $HX|p\rangle = XH|p\rangle$, i.e. $HX|p\rangle = EX|p\rangle$, i.e. $H|p'\rangle = E|p'\rangle$ where $|p'\rangle = X|p\rangle$. QED.

Step 2 Corollary: If Hamiltonian H commutes with an operator X , and if eigen-states of X form a complete basis, 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: [Note that the roles of X and H are swapped here, compare to the above theorem. This is done on purpose!] Start from the complete basis that diagonalizes X . By the above theorem at step 1, 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 $X = T_{\vec{R}}$ ($\vec{R} \in$ Bravais lattice), a Bravais lattice translation operator: for an arbitrary function $f(x)$, $T_{\vec{R}}f(\vec{x}) \equiv f(\vec{x} + \vec{R})$.

Bloch theorem is simply the application of the above corollary to $T_{\vec{R}}$.

Note that $T_{\vec{R}}$ does have the property that, *regardless of the value of \vec{R}* , can be diagonalized (trivially) with a complete basis, which is simply the plane wave basis. We have to remember however that due to the discrete Bravais lattice translation symmetry, plane waves whose wave vectors are the same modulo reciprocal lattice vectors \vec{G} (i.e. those with the same crystal momentum value) have the same eigen-value for $T_{\vec{R}}$. That is, the most general form of eigenstates of $T_{\vec{R}}$ is $\sum_{\vec{G}} C(\vec{k} + \vec{G}) \exp(i(\vec{k} + \vec{G}) \cdot \vec{x})$, where $C(\vec{k} + \vec{G})$'s are complex numbers. This eigenstate is characterized by the crystal momentum $\hbar\vec{k}$ and the eigenvalue of $T_{\vec{R}}$, $\exp(i\vec{k} \cdot \vec{R})$. The above corollary means that any eigenstate of H can be written in this form, and this is Bloch theorem. There are many equivalent forms of Bloch theorem, which are listed now. [It is not hard to see that these forms are all equivalent. You may ask why should we care about different forms, if there is only one theorem. It is because they capture different physical connotations of the theorem and one form is more useful than the other in different applications. Below, $\psi_{n\vec{k}}(\vec{x})$ means an eigenstate of H with crystal momentum \vec{k} and “band” index n (recall that there can be more than one solutions for a given \vec{k} ; n is the group index for {branch (acoustic or optical), polarization} in the case of phonons; in general n is the group index for any quantum numbers other than the crystal momentum)]

Form 1 of Bloch Theorem [Modulated plane wave; Nearly free electron]

$$\psi_{n\vec{k}}(\vec{x}) = \exp(i\vec{k} \cdot \vec{x}) u_{n\vec{k}}(\vec{x}) \text{ where } u_{n\vec{k}}(\vec{x} + \vec{R}) = u_{n\vec{k}}(\vec{x}) \text{ for any } \vec{R} \in \text{BL.}$$

Form 2 of Bloch Theorem [BL translation eigenstate, Crystal momentum eigenstate]

$$\psi_{n\vec{k}}(\vec{x} + \vec{R}) = \exp(i\vec{k} \cdot \vec{R}) \psi_{n\vec{k}}(\vec{x}) \text{ for any } \vec{R} \in \text{BL.}$$

Form 3 of Bloch Theorem [Bragg diffraction of plane wave; Nearly free electron]

$$\psi_{n\vec{k}}(\vec{x}) = \sum_{\vec{G}} C_n(\vec{k} + \vec{G}) \exp[i(\vec{k} + \vec{G}) \cdot \vec{x}]$$

Form 4 of Bloch Theorem [Modulated local wave function; phonon or tight-binding electron]

$$\psi_{n\vec{k}}(\vec{x}) = \sum_{\vec{R}} \exp(i\vec{k} \cdot \vec{R}) \phi_n(\vec{x} - \vec{R})$$