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Topic- Condensed Matter (Bloch theorem)

Bloch Theorem

Let $T_{\mathbf{R}}$ be the translation operator of vector $\mathbf{R}$. $T_{\mathbf{R}}$ commutes with the Hamiltonian. Indeed, the kinetic energy is translationally invariant, and the potential energy is periodic:

$$[T_{\mathbf{R}}, V]f(\boldsymbol{r}) = T_{\mathbf{R}}V(\boldsymbol{r})f(\boldsymbol{r}) - V(\boldsymbol{r})T_{\mathbf{R}}f(\boldsymbol{r}) = V(\boldsymbol{r}+\mathbf{R})f(\boldsymbol{r}+\mathbf{R}) - V(\boldsymbol{r})f(\boldsymbol{r}+\mathbf{R}) = 0 \tag{1}$$

On the other hand, $[T_{\mathbf{R}}, T_{\mathbf{R}'}] = 0$. Thus, the Hamiltonian and all the translation operators of the crystal commute with each other. They possess, therefore, a common set of eigenstates.

Let us search then the eigenstates of the translation operators $T_{\mathbf{R}}$. For a general function satisfying the boundary conditions of the problem, one can write, after expanding the eigenstate on a plane wave basis, the eigenvalue equation as follows:

$$T_{\mathbf{R}}f(\boldsymbol{r}) = T_{\mathbf{R}}\sum_{\boldsymbol{q}} C_{\boldsymbol{q}}\, e^{i\mathbf{q}.\mathbf{r}} = \sum_{\boldsymbol{q}} C_{\boldsymbol{q}}\, e^{i\mathbf{q}.\mathbf{r}} e^{i\mathbf{q}.\mathbf{R}} = t_R \sum_{\boldsymbol{q}} C_{\boldsymbol{q}}\, e^{i\mathbf{q}.\mathbf{r}} \tag{2}$$

where we denoted the eigenvalue by t_R. In order for the above equality to be true, $e^{i\mathbf{q}.\mathbf{R}}$ must be a constant: $\mathbf{q}.\mathbf{R} = 2\pi n + \text{constant} \Rightarrow \mathbf{q} = \mathbf{k} + \mathbf{G}$ where $\mathbf{k}$ is an arbitrary vector and $\mathbf{G}$ is a **reciprocal lattice vector**: $\mathbf{G}.\mathbf{R} = 2\pi n$. The eigenvalue is therefore $t_R = e^{i\mathbf{k}.\mathbf{R}}$ and the eigenvector could be any plane wave of momentum $\mathbf{k} + \mathbf{G}$. The eigenvalue t_R being degenerate with respect to $\mathbf{k} + \mathbf{G}$, a general eigenvector associated with this eigenvalue can be written as:

$$f_{\mathbf{k}}(r) = \sum_G C_{\mathbf{k}+\mathbf{G}}\, e^{i(\mathbf{k}+\mathbf{G}).\mathbf{r}} = e^{i\mathbf{k}.\mathbf{r}} \sum_G C_{\mathbf{k}+\mathbf{G}}\, e^{i\mathbf{G}.\mathbf{r}} = e^{i\mathbf{k}.\mathbf{r}} u_{\mathbf{k}}(r) \qquad (3)$$

The arbitrary vector $\mathbf{k}$ labels thus different eigenvalues and eigenstates of translation operators. Furthermore, the above function is also eigenstate of all possible translation operators of the lattice. Note that the infinite sum over all possible momenta $\boldsymbol{q}$ is now reduced to a discrete (still infinite) sum over the reciprocal lattice vectors, and that is a great simplification in the problem. We can also notice that all states corresponding to $\mathbf{k}$ and any $\mathbf{k} + \mathbf{G}$ are equal, i.e. the function $f_{\mathbf{k}}$ is periodic in the reciprocal space $f_{\mathbf{k}} = f_{\mathbf{k}+\mathbf{G}}, \forall \mathbf{G}$. Due to the previously-mentioned commutation relation, $f_{\mathbf{k}}$ is also eigenstate of $\mathcal{H}$. To obtain its coefficients $C_{\mathbf{k}+\mathbf{G}}$, we just need to insert this wavefunction into the Schroedinger equation. The Hamiltonian matrix must therefore be diagonalized in the space of all plane waves of momentum $\mathbf{k}+\mathbf{G}$ for any vector $\mathbf{k}$ chosen in the first Brillouin zone. Indeed the periodicity of $f_{\mathbf{k}}$ in the reciprocal space implies that it is sufficient to chose the arbitrary vector $\mathbf{k}$ in the first Brillouin zone.

Let us finally state **Bloch's theorem:** The eigenstates $f_{\mathbf{k}}$ of a periodic Hamiltonian can be written as a product of a periodic function with a plane wave of momentum $\mathbf{k}$ restricted to be in the first Brillouin zone $f_{\mathbf{k}}(\boldsymbol{r}) = u_{\mathbf{k}}(\boldsymbol{r})e^{i\mathbf{k}.\mathbf{r}}$ (with $u_{\mathbf{k}}$ periodic in $\mathbf{k}$ and in $\boldsymbol{r}$) ; furthermore $f_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}.\mathbf{R}} f_{\mathbf{k}}(\mathbf{r})$.