Proof of Bloch's theorem

$\hat{T}_n \quad \psi(\vec{r}) = \psi(\vec{r} + \vec{T}_n)$ ← translation operator action

$\vec{T}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ $\qquad \vec{a}_i$ = lattice vectors

n_i = integers

$\hat{T}_n \quad \psi(\vec{r}) = \psi(\vec{r} + \hat{A}\vec{n})$

$\hat{A} = (\vec{a}_1, \vec{a}_2, \vec{a}_3) \qquad \vec{n} = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$

•) Hypothesis: mean periodic potential

$$U(\vec{r} + \vec{T}_n) = U(\vec{r})$$

•) Hypothesis: electron-electron interaction negligible

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\vec{r})$$

Translation invariance $\Rightarrow \quad [\hat{H}, \hat{T}_n] = 0$

$\hat{H}$ and $\hat{T}_n$ have a common set of eigenfunctions.

$\hat{T}_n \quad \psi(\vec{r}) = \lambda_{\vec{n}} \psi(\vec{r})$

$\hat{T}_n$ is additive $\Rightarrow \hat{T}_{n_1} \hat{T}_{n_2} \psi(\vec{r}) = \psi(\vec{r} + \hat{A}\vec{n}_1 + \hat{A}\vec{n}_2) =$

$= \hat{T}_{n_1+n_2} \psi(\vec{r})$

$\Rightarrow \lambda_{\vec{n}_1} \lambda_{\vec{n}_2} = \lambda_{\vec{n}_1 + \vec{n}_2}$ which is true for $\lambda_{\vec{n}} = e^{\vec{s} \cdot \hat{A}\vec{n}}$ with

$s_i \in \mathbb{C} \qquad 1 = \int_V |\psi(\vec{r})|^2 d^3\vec{r} = \int_V |\hat{T}_n \psi(\vec{r})|^2 d^3\vec{r} = |\lambda_{\vec{n}}|^2 \int_V \psi(\vec{r}) d^3\vec{r}$

$|\lambda_{\vec{n}}|^2 = 1$ $\Rightarrow$ normalization condition over a primitive cell of volume V

$s_i = i k_i$ with $k_i \in \mathbb{R}$

$$\hat{T}_n \, \psi(\vec{r}) = \psi(\vec{r} + \hat{A} \cdot \vec{n}) = e^{i\vec{k}\cdot \hat{A}\vec{n}} \psi(\vec{r}) = e^{i\vec{k}\cdot\vec{T}_n} \psi(\vec{r})$$

This is true for a Bloch wave i.e.

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \, U_{\vec{k}}(\vec{r}) \quad \text{with } U_{\vec{k}}(\vec{r}) = U_{\vec{k}}(\vec{r} + \hat{A}\vec{n})$$

In 1-dim

$$\hat{T}_n \psi(x) = e^{ik\vec{n}\cdot\vec{a}} \psi(x)$$
$$= e^{ik\vec{n}\cdot\hat{A}} \psi(x)$$

where $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ have only 1 component now $\Rightarrow$ $(a_1, a_2, a_3) = \hat{A}$