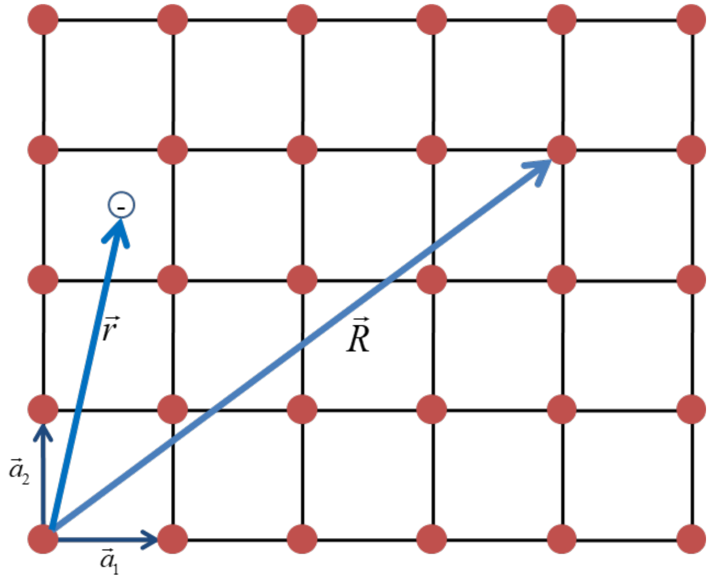
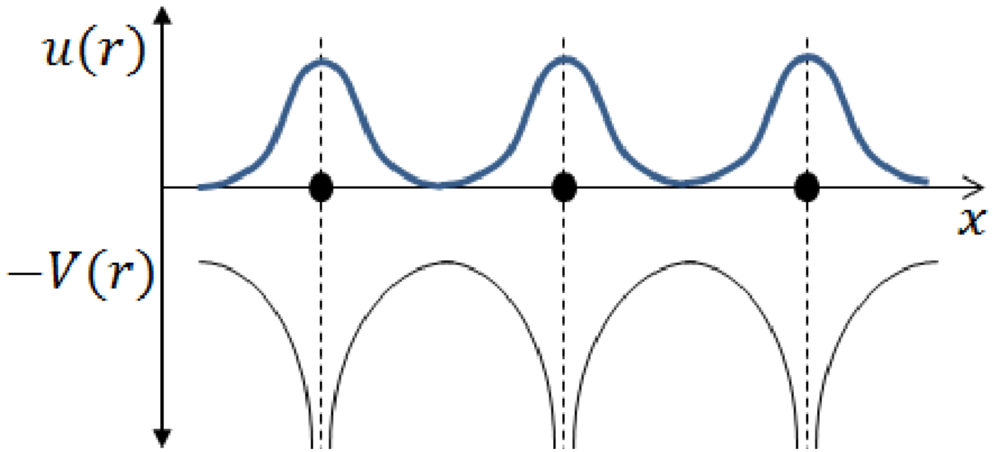
Hamiltonian with a translational symmetry



Translation Operator



- Now let us think of Hamiltonian with a periodic potential

$$V(\vec{r}+\vec{R}) = V(\vec{r})$$

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(\vec{r})$$

$$\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r})$$

Statements for symmetry

I. The Hamiltonian is invariant over the translation

II. The Hamiltonian commutes with the translation operator.

$$\left[\hat{H}, \hat{T}(\vec{R})\right] = 0 \quad , \hat{H}\hat{T} - \hat{T}\hat{H} = 0$$

$$\hat{T}^{-1}\hat{H}\hat{T} = \hat{H}$$

$$\hat{T}(\vec{R})\hat{H}(\vec{r})\psi(\vec{r}) = \hat{H}(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R}) = \hat{H}(\vec{r})\psi(\vec{r}+\vec{R}) = \hat{H}\hat{T}(\vec{R})\psi(\vec{r})$$

Good quantum number, stationary state

I. Once the operator commutes with the Hamiltonian, the eigenvalue of the operator can stay there stationary.

II. Say, at $t = 0$, we have the eigenstates for translation, $\hat{T}[\vec{R}]$, it keeps the same eigenvalue at $t > 0$.

$$\hat{T}(\vec{R})\left|\psi_{\vec{k}}(t=0)\right\rangle = e^{i\vec{k}\cdot\vec{R}}\left|\psi_{\vec{k}}(t=0)\right\rangle$$

$$\left|\psi_{\vec{k}}(t)\right\rangle = \exp[-i\frac{\hat{H}}{\hbar}t]\left|\psi_{\vec{k}}(t=0)\right\rangle$$

$$\hat{T}(\vec{R})\left|\psi_{\vec{k}}(t)\right\rangle = \hat{T}(\vec{R})\exp[-i\frac{\hat{H}}{\hbar}t]\left|\psi_{\vec{k}}(t=0)\right\rangle = \exp[-i\frac{\hat{H}}{\hbar}t]\hat{T}(\vec{R})\left|\psi_{\vec{k}}(t=0)\right\rangle = \exp[-i\frac{\hat{H}}{\hbar}t]e^{i\vec{k}\cdot\vec{R}}\left|\psi_{\vec{k}}(t=0)\right\rangle = e^{i\vec{k}\cdot\vec{R}}\exp[-i\frac{\hat{H}}{\hbar}t]\left|\psi_{\vec{k}}(t=0)\right\rangle$$

We have $\hat{T}(\vec{R})\left|\psi_{\vec{k}}(t)\right\rangle = e^{i\vec{k}\cdot\vec{R}}\exp[-i\frac{\hat{H}}{\hbar}t]\left|\psi_{\vec{k}}(t=0)\right\rangle$

Therefore, it is ...

Good quantum number, stationary state

I. To analyze the Hamiltonian spectrum, when the Hamiltonian has a symmetry, it is much convenient to search for the simultaneous eigenstates.

II. For simultaneous eigenstates for $\hat{T}[\vec{R}]$ with $\hat{H}$,

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(\vec{r})$$

$$\left(-\frac{1}{2}\nabla^2 + V(\vec{r})\right)e^{i\vec{k}\cdot\vec{r}}u(\vec{r}) = Ee^{i\vec{k}\cdot\vec{r}}u(\vec{r})$$

$$\left(\frac{1}{2}(-i\nabla + \vec{k})^2 + V(\vec{r})\right)u(\vec{r}) = Eu(\vec{r})$$

Differential equation eigenvalue problem.

I. We want to determine the eigenvalue and the eigenfunction.

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{\vec{k}}(\vec{r})=E(\vec{k})u_{\vec{k}}(\vec{r})$$

II. The label for the discrete eigenspectral

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\vec{k}}(\vec{r})=E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

III. Look up the math text : the operator and BC

Differential equation eigenvalue problem.

III. Look up the math text : the operator and BC

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\vec{k}}(\vec{r})=E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

$$u_{n,\vec{k}}(\vec{r}+\vec{R})=u_{n,\vec{k}}(\vec{r})$$

Question

- Suppose we have a cell-periodic charge density, say, $\rho(\vec{r}) = \rho(\vec{r} + \vec{R})$. Does the Coulomb potential have the same periodicity ?

$$V_H(\vec{r}) = \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3\vec{r}'$$

$$V_H(\vec{r}) = V_H(\vec{r} + \vec{R}) \quad ???$$