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Band Theory of Solids

- Electrons interact with each other and in a real solid atoms are vibrating causing time dependent variations in the potential energy.

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi(\vec{r}) = E \psi(\vec{r})$$
- The wavefunctions for the electron must satisfy Bloch's theorem

$$\psi(\vec{r}) = \psi_{n,k}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{n,k}(\vec{r})$$

$$\psi_{n,k}(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} \psi_{n,k}(\vec{r})$$

$$u_{n,k}(\vec{r} + \vec{R}) = u_{n,k}(\vec{r})$$
- There are two main categories of realistic band structure calculation for semiconductors:
 - Methods which describe the entire valence and conduction bands.
 - Methods which describe near band-edge band structures.

(a)

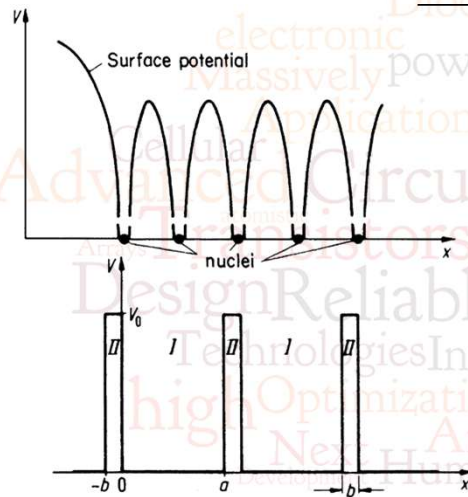
(b)

Tight Binding Methods, pseudopotential methods

K.P methods

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Krönig-Penney Model



$$\frac{d^2\psi(\vec{r})}{dx^2} + \frac{2m}{\hbar^2} E\psi(\vec{r}) = 0$$

$$\frac{d^2\psi(\vec{r})}{dx^2} + \frac{2m}{\hbar^2} (E - V_0)\psi(\vec{r}) = 0$$