J. Effective Mass Theory: Revisited for its Validity

- Motivation: When does $\underbrace{\left[\underbrace{-\frac{\hbar^2}{2m^*}\nabla^2}_{V(\vec{r})\text{ handled}} + \underbrace{W_{extra}(\vec{r})}_{\text{beyond } V(\vec{r}) \text{ (e.g. impurity)}}\right]}_{\text{Hydrogen-like problem (easy)}}\psi = \varepsilon\psi$ work?

<u>Is it that easy?</u>

$V(\vec{r})$ in $\hat{H}_0 \rightarrow E_n(\vec{k}) \longrightarrow$ Take $E_n(\vec{k}) \rightarrow E_n(-i\vec{\nabla})$ OK!

But can we use $E_n(\vec{k}) = E_n(0) + \frac{\hbar^2}{2m^*}(-i\vec{\nabla})^2$ and stop there?

ignore $\underbrace{\text{higher terms}}_{\text{higher derivatives in } \underbrace{\psi}_{\text{impurity states?}}}$ in expansion?

so as to make use of m^* to make the equation simple

Back to an exact point (Eq. (49)):

$$\hat{H}_T \psi = \sum_n \left[E_n(-i\vec{\nabla}) + W\right] \left(\sum_{\vec{k}\in B.Z.} C_{n\vec{k}}(t)\, \psi_{n\vec{k}}(\vec{r})\right) = i\hbar \frac{\partial}{\partial t} \underbrace{\psi}_{\sum_n \sum_{\vec{k}} C_{n\vec{k}}(t)\, \psi_{n\vec{k}}(\vec{r})} \qquad (58) \qquad \text{(exact)}$$

(i) W not strong enough to induce band-to-band transitions (no interband transitions)

- No W, $\psi_{n\vec{k}}(\vec{r})$ [Bloch states] are eigenstate
  $\Rightarrow$ if electron in $\psi_{n\vec{k}}$ at time 0, stays there forever
- $W \neq 0$, W may take $\psi_{n\vec{k}}(\vec{r})$ to some other states
  $\therefore$ resulting wavefunction (wave packet) $\psi(\vec{r},t) = \sum_{n'\vec{k}'} C_{n'\vec{k}'}(t)\, \psi_{n'\vec{k}'}(\vec{r})$
  is describing this scenario and
  $|C_{n'\vec{k}'}(t)|^2$ = prob. of system in $\psi_{n'\vec{k}'}(\vec{r})$ at time t
- No interband transitions $\Rightarrow$ $\psi \approx \sum_{\vec{k}\in BZ} C_{n\vec{k}}(t)\, \psi_{n\vec{k}}(\vec{r})$ (only $\psi_{n\vec{k}}$ in band n)

Then, $$\left[E_{\underset{\uparrow}{n}}(-i\vec{\nabla}) + W\right]\left(\sum_{\vec{k}\in B.Z.} C_{\underset{\uparrow}{n\vec{k}}}(t)\,\psi_{\underset{\uparrow}{n\vec{k}}}(\vec{r})\right) = i\hbar\frac{\partial \overset{\swarrow \sum_{\vec{k}\in B.Z.} C_{n\vec{k}}(t)\psi_{n\vec{k}}(\vec{r})}{\psi}}{\partial t} \qquad (52)$$

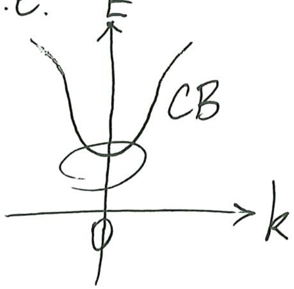
$\uparrow$ p. VI-(62)

- involves band n only
- Keep Eq. (58) in mind, when we need to involve a few bands (not all, but not only one either), we can retain in $\sum_{n}(\cdots)$ for $\sum\limits_{n \text{ over a few bands}}(\cdots)$ (a few VB's, for example)

(ii) But $E_n(-i\vec{\nabla})$ can be complicated as $E_n(\vec{k})$ is complicated for $\vec{k}$ over whole B.Z.

- Want to make use of simplicity near band edge, i.e.

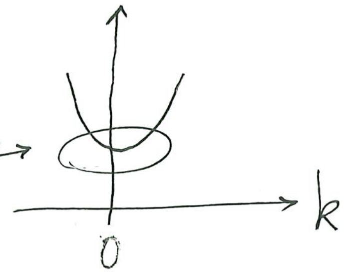
$$E_c(\vec{k}) \approx E_c(0) + \underbrace{\frac{\hbar^2 k^2}{2m_e^*}}_{-\frac{\hbar^2}{2m_e^*}\nabla^2} \quad \underbrace{(\text{stop here})}_{\text{neglect higher derivatives}}$$



But $\underbrace{\sum_{\vec{k}\in B.Z.}} C_{\underset{\sim}{n\vec{k}}}(t)\,\psi_{\underset{\sim}{n\vec{k}}}(\vec{r})$ includes $\vec{k}$ in whole B.Z.

How to make things consistent?

Consider →



- $\frac{\hbar^2 k^2}{2m_e^*}$ is good near minimum at $\vec{k}=0$

- Form wave packet only using $\vec{k}\approx 0$ Bloch functions (an approximation)

ψ in $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) + W\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$ (the original problem to solve)

is approximated by

$$\psi(\vec{r},t) \cong \sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\,\psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})$$

$$\approx \sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}}\, \underbrace{u_{n0}(\vec{r})}_{\text{assume } u_{n\vec{k}\approx 0}(\vec{r}) \,\approx\, u_{n0}(\vec{r})} \qquad (59)$$

(a further approximation)

[$u_{n\vec{k}}(\vec{r})$ varies rapidly in $\vec{r}$, no doubt, as it is periodic in atomic scale. Here, the approximation is about the $\vec{k}$-dependence, $u_{n\vec{k}\approx 0}(\vec{r})$ is not very different from $u_{n0}(\vec{r})$.]

$$\psi(\vec{r},t) \approx \sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\, \overbrace{e^{i\vec{k}\cdot\vec{r}}\, u_{n0}(\vec{r})}^{\text{Luttinger basis}}$$

$$= \left(\sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}}\right) \underbrace{\underbrace{e^{i\overset{\vec{k}=0}{\vec{0}}\cdot\vec{r}}}_{\text{“1”}}\, u_{n0}(\vec{r})}_{\psi_{n0}(\vec{r})}$$

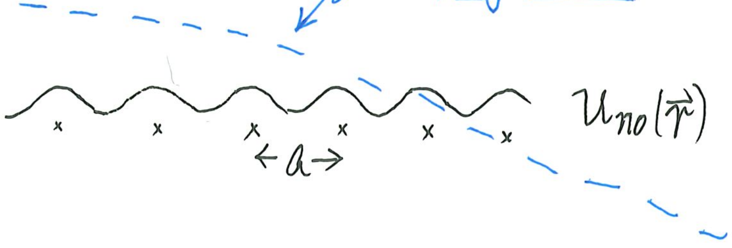
$$= \underbrace{\left(\sum_{\vec{k}\approx 0} C_{n\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}}\right)}_{F_n(\vec{r},t)\ \text{[Envelope Function]}} \cdot \underbrace{\psi_{n0}(\vec{r})}_{\underbrace{\text{rapidly varying in } \vec{r}\text{-space}}_{\text{atomic-scale}}\ [u_{n0}(\vec{r}) \text{ is periodic}]} \qquad (60)$$

Key Concept in Effective Mass Theory → [Envelope Function]

$F(\vec{r},t)$ involves $\underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\uparrow}$ for $\underbrace{\vec{k}\approx 0}$ long wavelengths

slowly varying on atomic scale

Envelope function is slowly varying



$$\therefore \quad \boxed{\psi(\vec{r},t) = \underbrace{F_n(\vec{r},t)}\cdot\psi_{n0}(\vec{r})} \qquad (61)$$

$F_n(\vec{r},t)$
↑
band n

Q: What is the equation governing $F_n(\vec{r},t)$?

Noting that $E_n(-i\vec{\nabla})\psi = E_n(-i\vec{\nabla})F_n(\vec{r},t)\psi_{n0}(\vec{r})$ ↙ just $u_{n0}(\vec{r})$

$u_{n0}(\vec{r}+\vec{R}) = u_{n0}(\vec{r})$

$$= \left(\sum_{\vec{R}} E_{n\vec{R}}\, e^{\vec{R}\cdot\vec{\nabla}}\right)F_n(\vec{r},t)\,\psi_{n0}(\vec{r}) = \sum_{\vec{R}} E_{n\vec{R}}\, F_n(\vec{r}+\vec{R},t)\,\overbrace{\psi_{n0}(\vec{r})}$$

$$= \psi_{n0}(\vec{r})\left(\sum_{\vec{R}} E_{n\vec{R}}\, e^{\vec{R}\cdot\vec{\nabla}}\right)F_n(\vec{r},t)$$

$$= \psi_{n0}(\vec{r})\,E_n(-i\vec{\nabla})\,F_n(\vec{r},t) \qquad (62)$$

$\therefore$ $[\hat{H}_0 + W]\psi = i\hbar\frac{\partial\psi}{\partial t}$ becomes

($\psi_{n0}(\vec{r})$ moved through and cancelled on both sides)

$$\boxed{[E_n(-i\vec{\nabla}) + W]\, F_n(\vec{r},t) = i\hbar\frac{\partial F_n(\vec{r},t)}{\partial t}}$$

Since quantities involved are those $\vec{k}\approx 0$ ones, $E_n(-i\vec{\nabla})$ becomes

$$\boxed{\left[-\frac{\hbar^2}{2m_e^*}\nabla^2 + W\right] F_n(\vec{r},t) = i\hbar\frac{\partial F_n(\vec{r},t)}{\partial t}} \quad (62a) \quad \text{if } E_n(\vec{k}) = \frac{\hbar^2 k^2}{2m_e^*}$$

OR

$$\boxed{\left[E_n(0) - \frac{\hbar^2}{2m_e^*}\nabla^2 + W\right] F_n(\vec{r},t) = i\hbar\frac{\partial F_n(\vec{r},t)}{\partial t}} \quad (62b) \quad \text{if } E_n(\vec{k}\approx 0) = E_n(0) + \frac{\hbar^2 k^2}{2m_e^*}$$

- The simple-looking Effective Mass Approximation is about solving for the slowly varying Envelope Function. (Key concept)

For $W = W(\vec r)$ only (e.g. impurity), then impurity state is governed by the effective TISE

$$\left[-\frac{\hbar^2}{2m_e^*}\nabla^2 + W(\vec r)\right] F_n(\vec r) = \left(E - E_n(0)\right) F_n(\vec r) \qquad (63)$$

This is the problem behind (Eq. (53)) the Donor impurity problem (see p. VI-(63))
(now properly stated/understood)

Ground state (impurity state): $F_n(r) \sim e^{-r/a_B^*}$

where $$\underset{\gg a_B}{a_B^*} = \underset{\sim 0.5\text{Å}}{a_B} \cdot \underbrace{\frac{\varepsilon_r}{\left(\frac{m_e^*}{m_e}\right)}}_{\gg 1}$$

ε_r ← dielectric constant (≈ 10)

m_e^*/m_e ← effective mass ($\approx$ 6%-7%)

(GaAs: $a_B^* \approx 90$Å for donor impurity)

dies off from impurity

$F_c(r)$ spreads out, $\psi \approx$ (spread out $F_c(r)$) $\cdot\, u_{n0}(\vec r)$

GaAs: Impurity ground state energy (see p. VI-(65))

$$\sim (-13.6\,\mathrm{eV}) \cdot \underbrace{\left(\frac{m_e^*}{m}\right)}_{\sim 7\%} \left(\frac{1}{\underset{\overset{\uparrow}{\varepsilon_r \sim 12}}{\varepsilon_r}}\right) \approx \underbrace{-6.6\ \mathrm{meV}}_{\text{only } -6.6\ \mathrm{meV} \text{ below bottom of CB}}$$

$\underbrace{\text{only } -6.6\ \mathrm{meV} \text{ below bottom of CB}}$

or only needs 6.6 meV to set free the bounded electron to the CB

Weakly bounded electron justifies the attractive potential $\underbrace{\text{is weak}}_{\text{screened out by } \varepsilon_r}$

So, the effective mass approximation as applied to impurity states (donors) in GaAs is consistent with the assumptions behind the approach.

Validity

- Effective Mass Approximation works for describing

$$\boxed{\text{electrons in the vicinity of band edges in weak slowly varying fields}}$$

effective mass description works (bottom of CB, top of VB)

$\Downarrow$

giving Schrödinger-like equation with "k.e." term replaced by $E_n(-i\vec{\nabla}) \rightarrow \frac{-\hbar^2}{2m^*}\vec{\nabla}$

↑ No interband processes

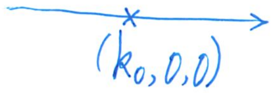
$u_{n0}(\vec{r})$ can be pulled out

($\psi_{n0}(\vec{r})$ can be pulled out)

Summary

- In solving impurity states using Eqs. (62), (63), we invoked the Envelope Function, which is slowly varying over $\vec{r}$-space
- Popular technique in doping physics (donor/acceptor)
- Can generalize to retain a few bands
- Can generalize to anisotropic band minimum (e.g. Si, Ge)

$\vec{k}_0$ = band minimum, axes along principal axes

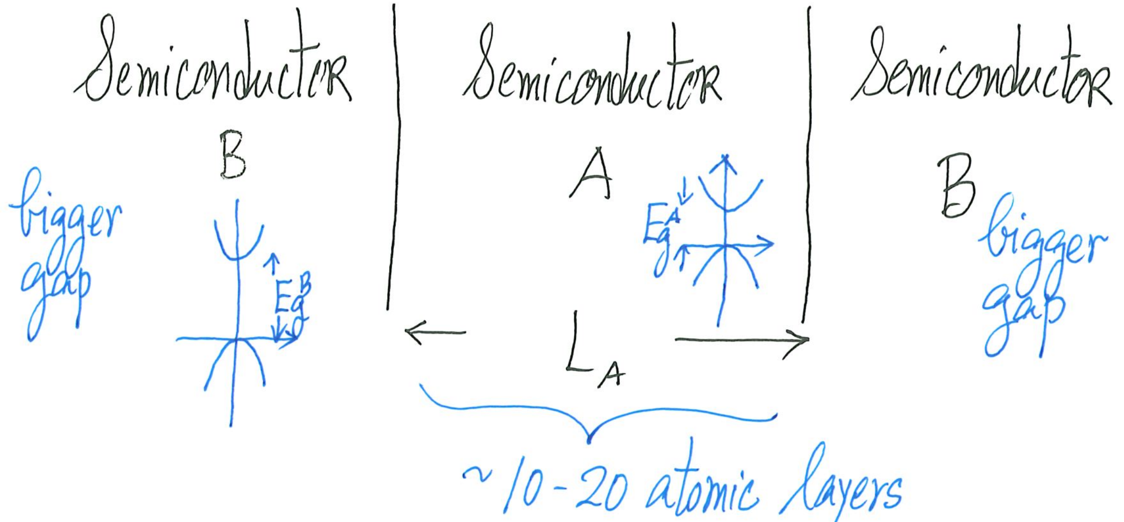


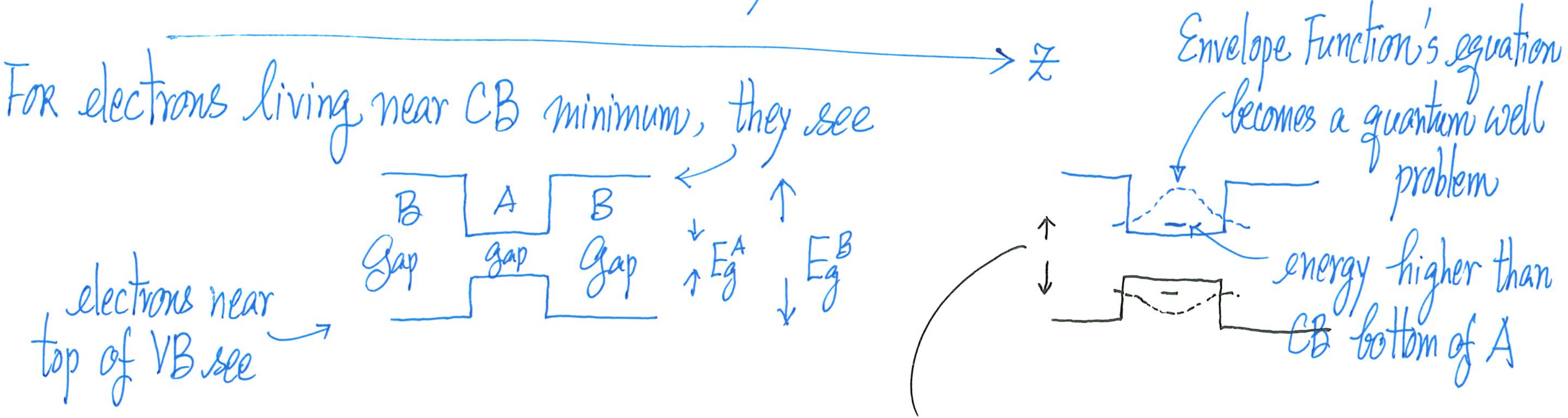
$$\left[-\frac{\hbar^2}{2m_\ell^*}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_t^*}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r r}\right]F(\vec{r}) = E\,F(\vec{r})$$

around one CB minimum with $\vec{k}$ measured from the minimum.

- This is the theory untold in Ch.5 of Balkanski and Wallis

- The Envelope Function Approximation is also applied to understand the physics of semiconductor heterostructures†





New Gap depends on L_A and what B is!
(a way of tuning band gap!)

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† G. Bastard, "Wave mechanics applied to semiconductor heterostructures"

References

- Ch. 3, Ch. 4, (part of Ch. 5) of Balkanski and Wallis
- Madelung, "Introduction to Solid State Theory"
- Ketterson, "The Physics of Solids"
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  - Kohn, Phys. Rev. 105, 509 (1957)
  - Luttinger and Kohn, Phys. Rev. 97, 869 (1955)
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