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Summary so far

- Carriers in crystals can be treated as "free" particles w/ an effective mass in bands of conduction.
- We can grow layered crystal structures w/ monolayer precision combining various different materials.
- We can therefore engineer potentials in the growth direction, control carrier concentration by doping, and make a variety of devices.

Next ...

- Optical excitation can create electron-hole pairs in direct gap semiconductors.
- Selection rules allow for circularly polarized light to create spin polarized carriers.
- Spins in crystals behave like "free" spins w/ an effective g-factor.
- Carrier spins can interact w/ lattice spins.
- Devices, dots, lasers, etc...

Effective mass approx.

Suppose we add a perturbation to a perfect crystal, i.e. a QW, barrier, superlattice, goto potential, or impurity.

$$\left[\hat{H}_{per} + V_{imp}(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \qquad (1)$$

$\hat{H}_{per}$: perfect crystal; $V_{imp}(\vec{r})$: impurity

Lets go to 1D for simplicity:

$$\hat{H}_{per}\,\phi_{nk}(x) = \varepsilon_n(k)\,\phi_{nk}(x)$$

solutions form a complete set

Therefore:

$$\psi(x) = \sum_n \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\,\phi_{nk}(x)\,\frac{dk}{2\pi} \qquad (2)$$

$\sum_n$: sum over bands; $\int_{-\pi/a}^{\pi/a}$: integral over Brillouin zone; $\tilde{\chi}(k)$: expansion coeffs.

We need to make more approximations...

- Assume that more functions from only one band play a significant part. Thus, the summation over n is dropped.
- Assume that only a small region of k-space contributes significantly to the integral.

E.g. for a donor:
- the energy is near the CB
- k is around 0 or the bottom of the CB

$$\phi_{nk}(x) = u_{nk}(x)\,e^{ikx}$$

assume that this is slowly varying in k compared to e^{ikx}.

∴ for small regions of k-space:

$$\phi_{nk}(x) = u_{nk}(x)\, e^{ikx} \approx u_{n0}(x)\, e^{ikx} = \phi_{n0}(x)\, e^{ikx}$$

$$\phi_{nk}(x) \approx \phi_{n0}(x)\, e^{ikx} \qquad \text{for small } k$$

So (2) becomes:

$$\psi(x) \approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, e^{ikx}\, \frac{dk}{2\pi} = \phi_{n0}(x)\, \chi(x)$$

($\chi(x)$: envelope function; $\phi_{n0}(x)$: Bloch function; $\tilde{\chi}(k)$: Inverse F.T.)

Since we assumed that only a small range of k contributes to $\tilde{\chi}(k)$, $\chi(x)$ will vary slowly compared to the lattice.

Now we want an equation for $\chi(x)$. Put (2) into (1) with the single band reduction:

$$\hat{H}_{per}\, \psi(x) = \hat{H}_{per} \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, \phi_{nk}(x)\, \frac{dk}{2\pi} = \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, \varepsilon_n(k)\, \phi_{nk}(x)\, \frac{dk}{2\pi}$$

$$\hat{H}_{per}\, \psi(x) \approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, \varepsilon_n(k)\, e^{ikx}\, \frac{dk}{2\pi}$$

Expand energy as a power series: $\varepsilon_n(k) = \sum_m a_m k^m$

$$\hat{H}_{per}\, \psi(x) \approx \phi_{n0}(x) \sum_m a_m \underbrace{\int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, k^m\, e^{ikx}\, \frac{dk}{2\pi}}_{\text{Inverse F.T.}}$$

Recall integration by parts:

$$\int u \frac{dv}{dx}\, dx = uv - \int v \frac{du}{dx}\, dx$$

let $u = e^{-ikx}$

$v = \chi(x)$

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{d\psi(x)}{dx}\, dx = e^{-ikx}\psi(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi(x)\,(-ik)\, e^{-ikx}\, dx$$

$$\int_{-\infty}^{\infty} \frac{d\psi(x)}{dx}\, e^{-ikx}\, dx = ik \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx$$

$$\int_{-\infty}^{\infty} \left(-i\frac{d\psi(x)}{dx}\right) e^{-ikx}\, dx = k\,\tilde{\psi}(k)$$

F.T. of $\left(-i\frac{d\psi(x)}{dx}\right)$ is $k\,\tilde{\psi}(k)$

Inverse F.T. of $k\,\tilde{\psi}(k)$ is $\left(i\frac{d\psi(x)}{dx}\right)$.

Generalizing

$$\text{I.F.T.}$$

$$k\,\tilde{\psi}(k) \longrightarrow i\frac{d\psi(x)}{dx}$$

$$k\left[k\,\tilde{\psi}(k)\right] \longrightarrow i\frac{d}{dx}\left[i\frac{d\psi(x)}{dx}\right]$$

$$\vdots$$

$$k^n\,\tilde{\psi}(k) \longrightarrow \left(i\frac{d}{dx}\right)^n \psi(x)$$

Therefore:

$$\hat{H}_{par}\,\psi(x) \approx \phi_{n0}(x) \sum_n a_n \left(i\frac{d}{dx}\right)^n \psi(x)$$

$$\approx \phi_{n0}(x)\, \Sigma_n \left(-i\frac{d}{dx}\right) \psi(x)$$

→ expansion of derivatives

So the original Schrödinger Eq. (1) becomes:

$$\hat{H}_{per}\,\psi(x) + V_{imp}(x)\,\psi(x) = E\,\psi(x)$$

↳

$$\phi_{n0}(x)\,\Sigma_n\left(-i\frac{d}{dx}\right)\chi(x) + V_{imp}(x)\,\phi_{n0}(x)\,\chi(x) = E\,\phi_{n0}(x)\,\chi(x)$$

$$\left[\Sigma_n\left(-i\frac{d}{dx}\right) + V_{imp}(x)\right]\chi(x) = E\,\chi(x)$$

↳ Schrödinger equation for envelope function w/ effective Hamiltonian.

Still complex if we consider full band structure, but we simplify in a small region of k.

E.g. near Γ in GaAs (3D)

$$\Sigma_n(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m^*}$$

$$\Sigma_n\left(-i\vec{\nabla}\right) = E_c - \frac{\hbar^2\nabla^2}{2m^*}$$

$$\therefore \left[-\frac{\hbar^2}{2m^*}\nabla^2 + V_{imp}(\vec{R})\right]\chi(\vec{R}) = (E - E_c)\,\chi(\vec{R})$$

m^* ↳ eff. mass

energy measured from cond. band

For heterostructures the crystal changes $\Rightarrow$ therefore so does $m^* \Rightarrow E_c$.

IF interface btw. A & B occurs at $z=0$:

$$\psi(0_A) = \psi(0_B)$$ ← wavefunctions equal

$$\frac{1}{m_A^*}\frac{d\psi(z)}{dz} = \frac{1}{m_B^*}\frac{d\psi(z)}{dz}$$ ← momentum equal

2D Systems

Recall our Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{R})\right]\psi(\vec{R}) = E\psi(\vec{R})$$

Let's say $U(\vec{R}) = U(z)$

Confinement only in growth dir. z.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + U(z)\right]\psi(x,y,z) = E\psi(x,y,z)$$

Guess solution of the form:

$$\psi(x,y,z) = e^{ik_x x} e^{ik_y y} u(z)$$

End up w/:

$$\left[\frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} - \frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + U(z)\right]u(z) = E u(z)$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + U(z)\right]u(z) = \underbrace{\left(E - \frac{\hbar^2 k_x^2}{2m} - \frac{\hbar^2 k_y^2}{2m}\right)}_{\varepsilon} u(z)$$

Purely 1D Schrödinger equation.

$$\therefore \psi_{k_x,k_y,n}(x,y,z) = e^{ik_x x} e^{ik_y y} u_n(z)$$

$$E_n(k_x,k_y) = \varepsilon_n - \frac{\hbar^2 k_x^2}{2m^*} - \frac{\hbar^2 k_y^2}{2m^*}$$

or

$$\psi_{k_\perp,n}(\vec{R}) = e^{i\vec{k}_\perp\cdot\vec{R}} u_n(z)$$

$$E_n(\vec{k}_\perp) = \varepsilon_n + \frac{\hbar^2 \vec{k}_\perp^2}{2m^*}$$