

Week 1 Summary

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8/22/13



topics

- 1) Bandstructure review
- 2) Quantum confinement
- 3) Heterostructures
- 4) Counting states
- 5) Sums in k-space / integrals in energy space

wave equation

$$-\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \quad \Psi(\vec{r}, t) = \psi(\vec{r})e^{i\omega t}$$

free space, constant potential:

$$-\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) = E\psi(\vec{r}) \quad \psi(\vec{r}) = A e^{i\vec{k} \cdot \vec{r}} \quad k = \sqrt{2m_0 E} / \hbar$$

momentum: $\vec{p} = \hbar \vec{k}$

position: $\psi^*(\vec{r})\psi(\vec{r}) = |A|^2$

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electrons in crystals

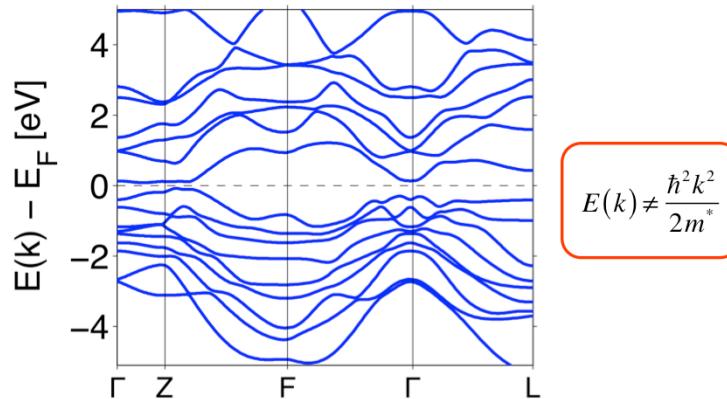
$$-\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + U_c(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) \quad U_c(\vec{r} + \vec{a}) = U_c(\vec{r})$$

$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \quad u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r}) \quad k: \text{Brillouin zone}$$

Bloch wave

$\vec{p} \neq \hbar\vec{k}$ but.... “crystal momentum”

bandstructure (dispersion)



DFT calculations of Bi_2Te_3 by Dr. J. Maassen, Purdue

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near-equilibrium, ballistic transport

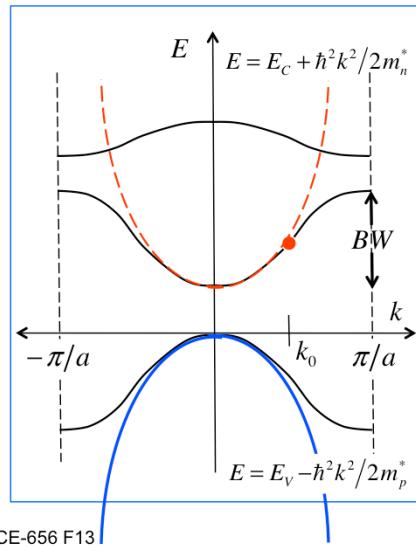
Electrons in a solid behave as both particles (quasi-particles) and as waves.

Electron waves are described by a “dispersion:”

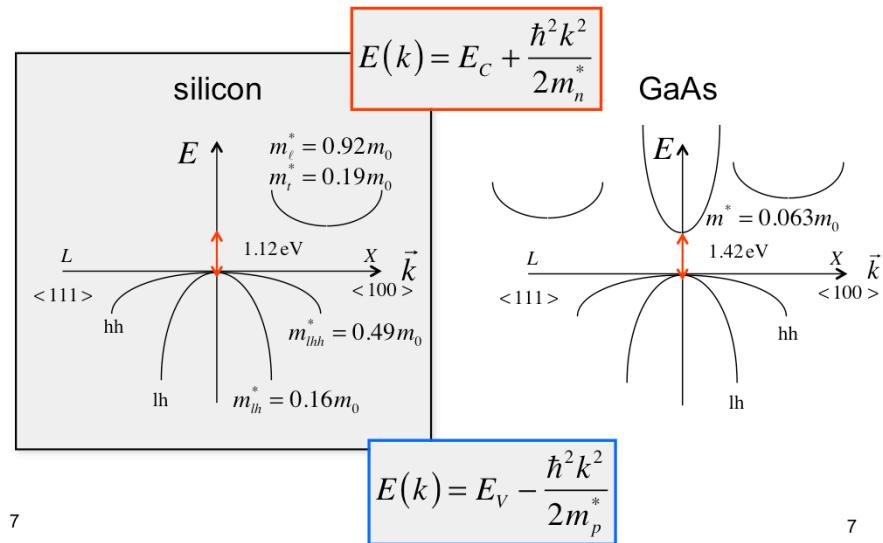
Because the crystal is periodic, the dispersion is periodic in k (Brillouin zone).

Particles described by a “wavepacket.”

The “group velocity” of a wavepacket is determined by the dispersion:



model bandstructure



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$E(k)$ for graphene

Recall:

$$v_g(\vec{k}) = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

For graphene:

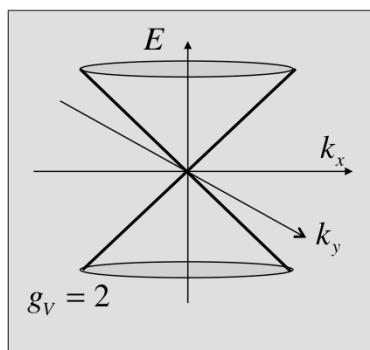
$$v_g(\vec{k}) = v_F$$

Also recall:

$$m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E(k)}{d^2 k} \right)^{-1}$$

For graphene:

$$m^* = ?$$



$$E(k) = \pm \hbar v_F \sqrt{k_x^2 + k_y^2} = \pm \hbar v_F k$$

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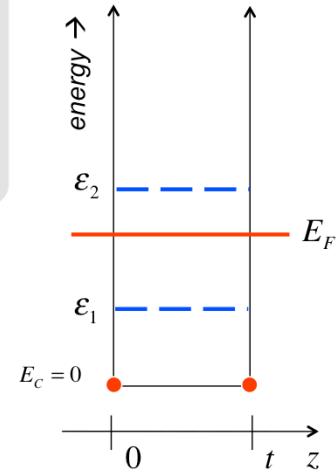
particle in a box

$$\frac{d^2\psi(z)}{dz^2} + k^2\psi = 0 \quad k^2 = \frac{2m^*(E - E_c(z))}{\hbar^2}$$

$$\psi(z) = \sin k_n z \quad k_n = \frac{n\pi}{t} \quad n = 1, 2, 3 \dots$$

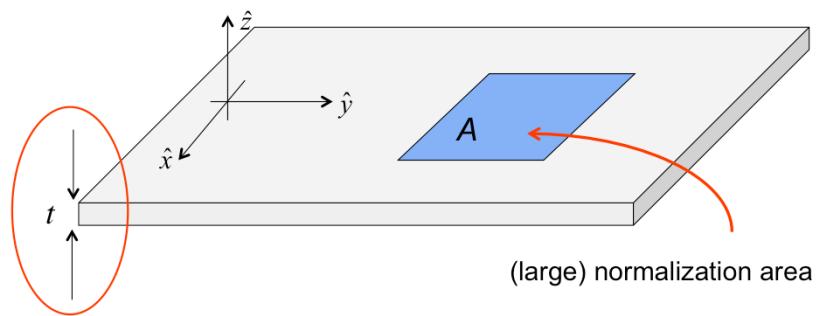
$$\epsilon_n = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 n^2 \pi^2}{2m^* t^2}$$

Light mass or narrow well \rightarrow high subband energy, but specifics depend on the shape of the well.



Note: electrons are free to move in the x-z plane. **2D electrons.**

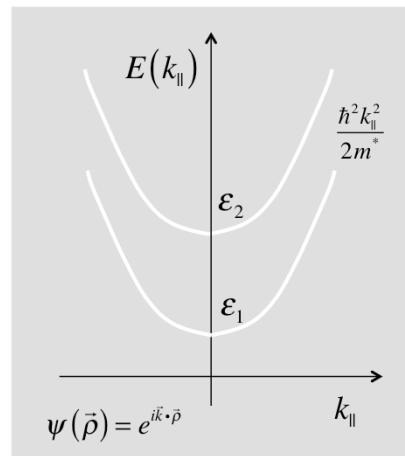
2D electrons



Semi-infinite in the x-y plane, but very thin in the z-direction.

$$\psi(\vec{r}) \sim e^{i\vec{k} \cdot \vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

“subbands”



$$\epsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* t^2}$$

$$k_{\parallel} = \sqrt{k_x^2 + k_y^2}$$

$$E = \epsilon_j + \frac{\hbar^2 k_{\parallel}^2}{2m^*}$$

ex. quantum confinement in Si cond. band.

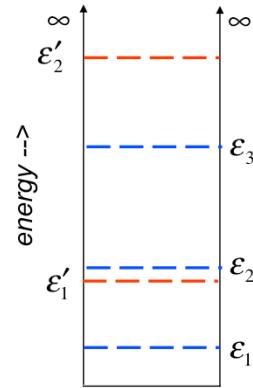
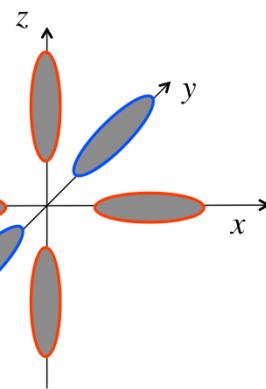
Si conduction band

$$m_\ell^* = 0.9m_0$$

$$m_t^* = 0.19m_0$$

$$\varepsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* t_{Si}^2}$$

$$m^* = ?$$

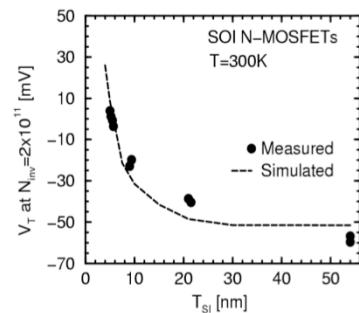
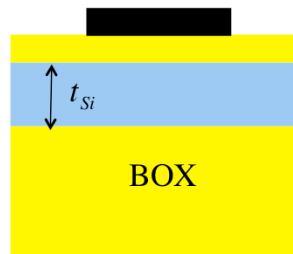


unprimed ladder: $m^* = m_\ell^*$ $g_V = 2$

primed ladder: $m^* = \frac{m_\ell^*}{m_t^*}$ from ECE 556 F13

quantum confinement in SOI

SOI



(D. Esseni et al. IEDM 2000 and TED 2001)

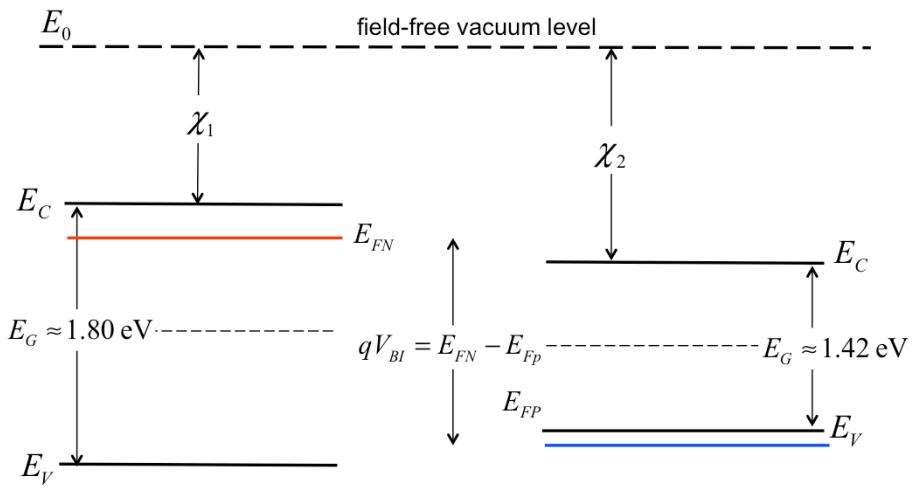
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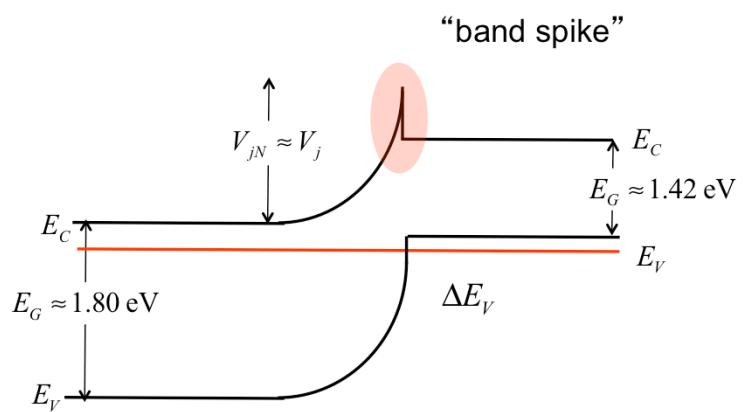
heterojunctions



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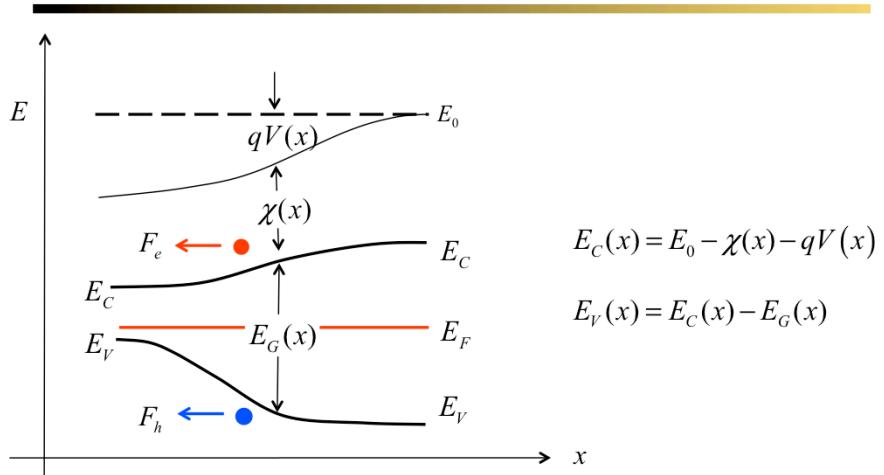
Type I HJ e-band



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general, graded heterostructure



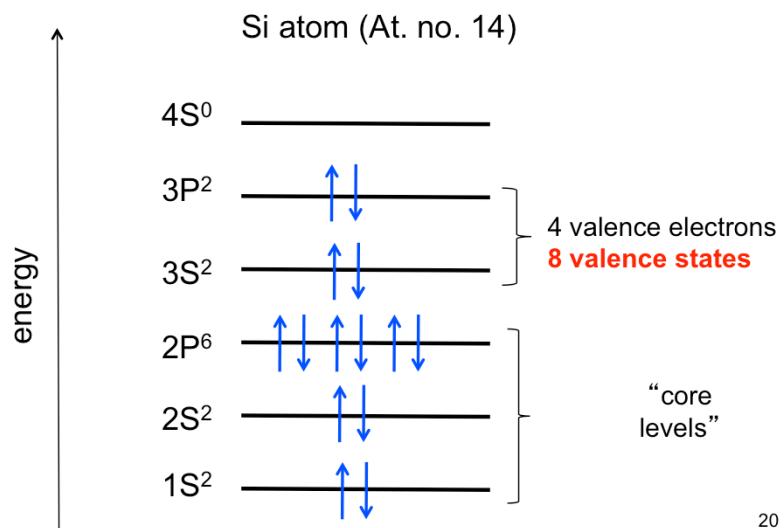
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topic

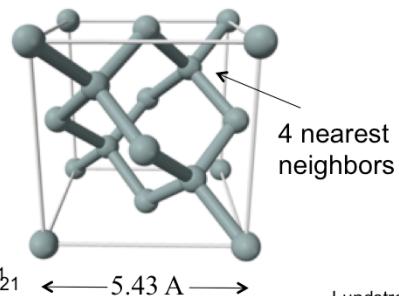
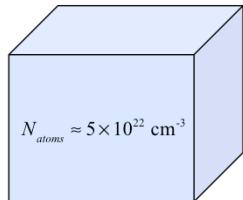
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energy levels in Si



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states in a Si crystal



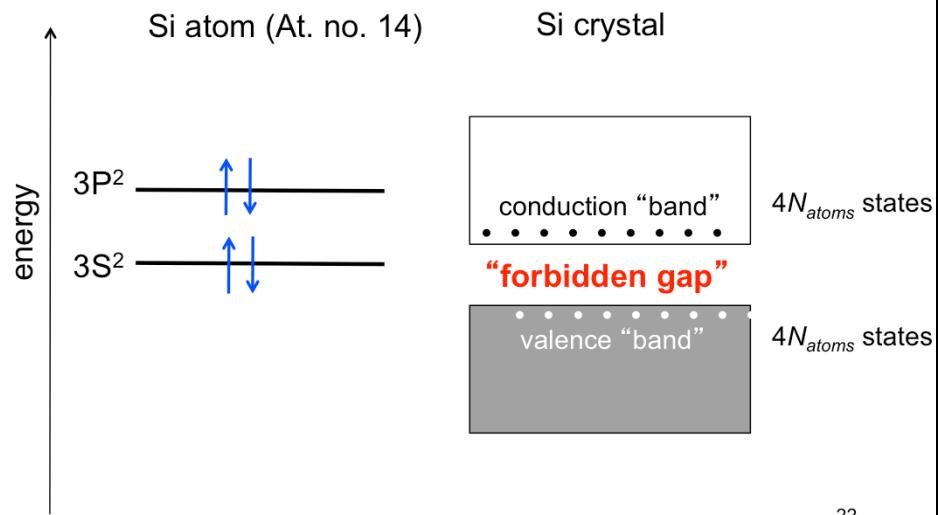
- Only the valence states are of interest to us.

- The 8 valence states give rise to $8N_{atoms}$ states per cm^3 in the solid.

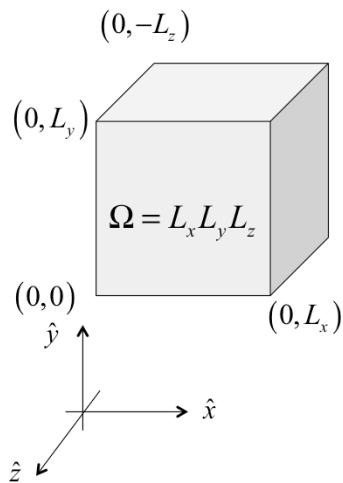
- But the interaction of the electron wavefunctions alters the discrete energy levels of the isolated Si atoms.

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energy levels → energy bands



states in a finite volume of semiconductor



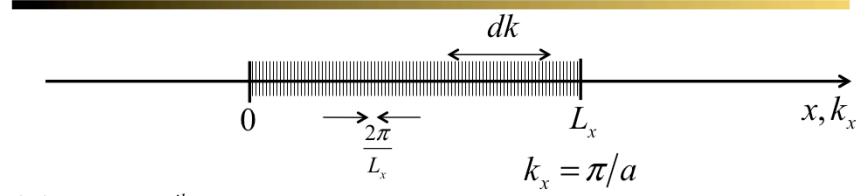
Finite volume, Ω
(part of an infinite volume)

Finite number of states

Periodic boundary conditions:

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x-direction



$$\psi(x) = u_k(x) e^{ik_x x}$$

$$\psi(0) = \psi(L_x) \rightarrow e^{ik_x L_x} = 1$$

$$k_x L_x = 2\pi j \quad j = 1, 2, 3, \dots$$

$$k_x = \frac{2\pi}{L_x} j$$

$$\# \text{ of states} = \frac{dk_x}{(2\pi/L_x)} \times 2 = N_k dk$$

$$N_k = \frac{L_x}{\pi} = \text{density of states in } k\text{-space}$$

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density-of-states in k-space

1D:

$$N_k = 2 \times \left(\frac{L}{2\pi} \right) = \frac{L}{\pi} \quad dk$$

2D:

$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \quad dk_x dk_y$$

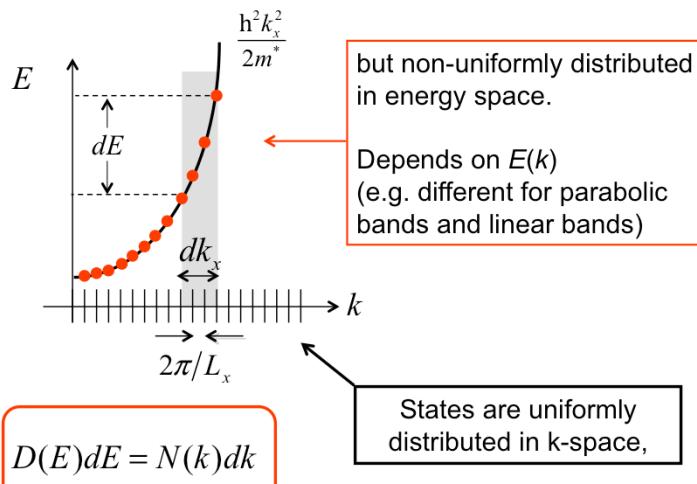
independent of $E(k)$

3D:

$$N_k = 2 \times \left(\frac{\Omega}{8\pi^2} \right) = \frac{\Omega}{4\pi^3} \quad dk_x dk_y dk_z$$

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DOS: k-space vs. energy space



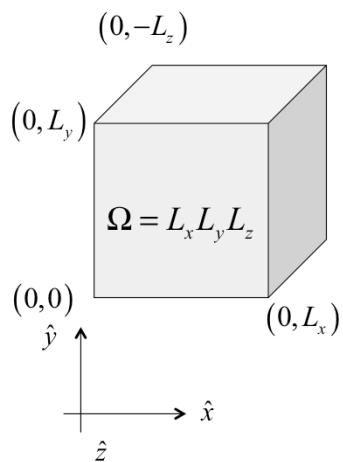
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sums in k-space



$$N = \sum_{\vec{k}} f_0(E_{\vec{k}}) \quad f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$n = \frac{1}{\Omega} \sum_{\vec{k}} f_0(E_{\vec{k}}) \text{ cm}^{-3}$$

$$n = \frac{1}{\Omega} \frac{\Omega}{4\pi^3} \int_{BZ} f_0(E_{\vec{k}}) d^3k \text{ cm}^{-3}$$

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continued

$$n = \frac{1}{4\pi^3} \int_{BZ} f_0(E_k) d^3k$$

Note: We extend the integral to infinity because we can usually assume that the higher energy states at large k have $E \gg E_F$, so they are not occupied.

$$n = \frac{1}{4\pi^3} \int_0^\infty \frac{4\pi k^2 dk}{1 + e^{(E-E_F)/k_B T}}$$

$$f_0 = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

$$E = E_C + E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}$$

continued

$$\eta_F = (E_F - E_C) / k_B T$$

$$n = \frac{1}{\Omega} \sum_{\vec{k}} f_0(E_k) \rightarrow N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}$$

$$N_C = \frac{1}{4} \left(\frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$E = E_C + E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}$$

$$\mathcal{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

k-space vs. energy space

$$n = \frac{1}{\Omega} \sum_{\vec{k}} f_0(E_k) \rightarrow N_c \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}$$

$$n = \int_{E_C}^{\infty} D_C(E) f_0(E) dE$$

$$D(E) = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} (E - E_C)^{1/2} \quad E = E_C + E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}$$

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