

ECE-656: Fall 2009

Lecture 2: Sums in k-space / Integrals in energy space

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two things to do

1) send me an e-mail: **lundstro@purdue.edu**

- name (first name, last name)
- preferred e-mail address
- background (ECE-494N?, ECE-606, ECE -659
Phys. 545, Phys, 550, etc.)
- 1 or two sentences on why you are taking the course and what you hope to get out of it
- if you are auditing the course, let me know

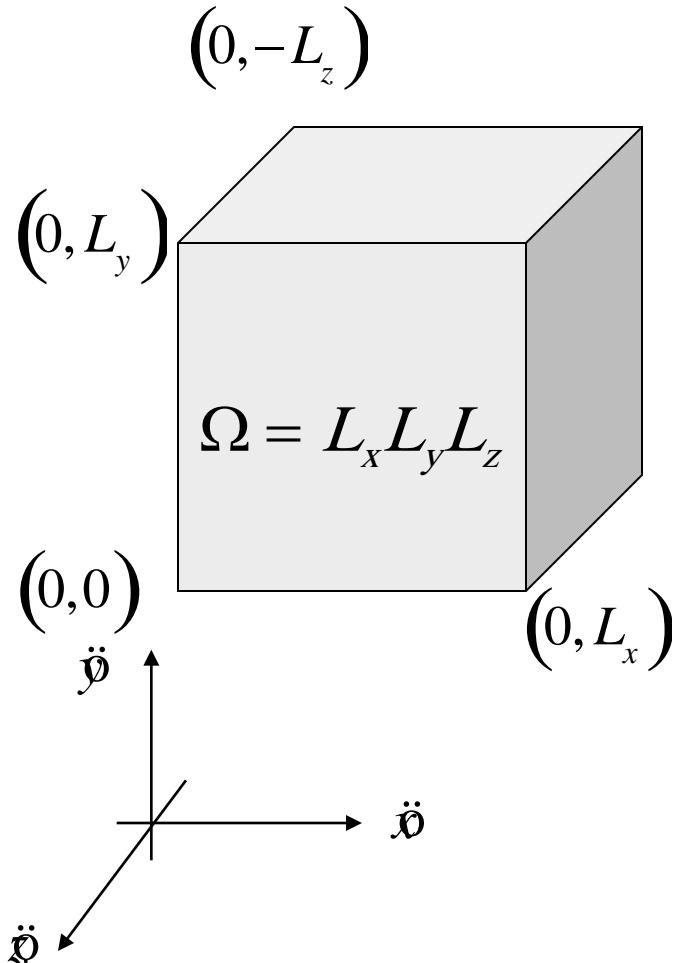
2) Visit the course web site and download HW1 and 2

<http://cobweb.ecn.purdue.edu/~ee656>

outline

- 1) Density of states in k-space
- 2) Example
- 3) Working in energy space
- 4) Discussion
- 5) Summary

bulk semiconductor



finite volume, Ω
(part of an infinite volume)

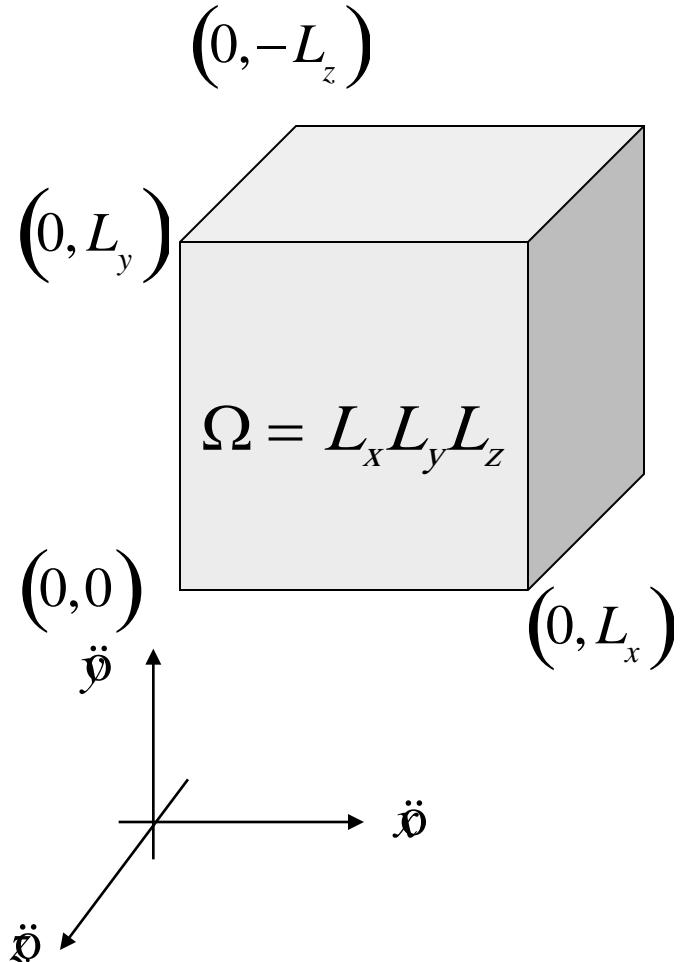
$N_a \Omega$ atoms and $2N_a \Omega$ states in Ω

Periodic boundary conditions:

$$\psi(\mathbf{r}) = u_k(\mathbf{r}) e^{ik\mathbf{g}\cdot\mathbf{r}}$$

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

bulk semiconductor

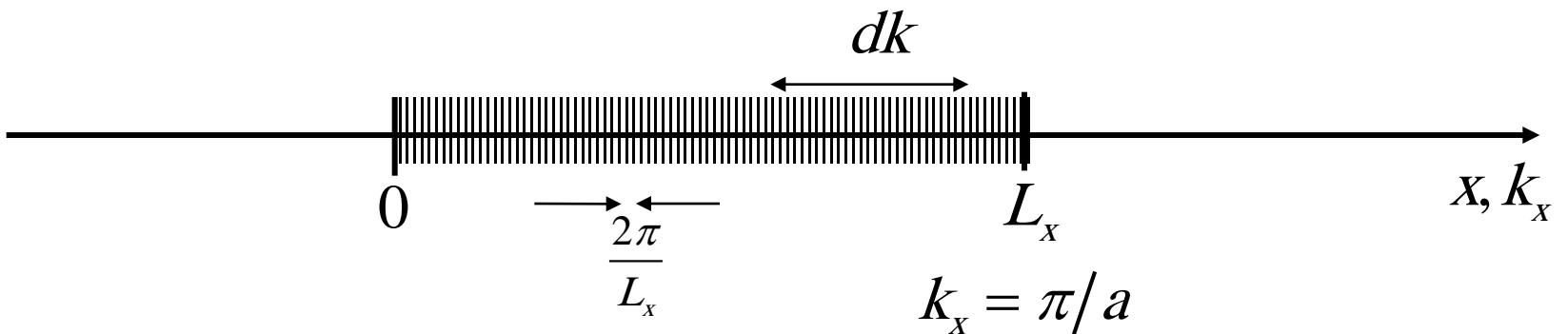


$$N = \sum_k f_0(E(k))$$

$$n = \frac{1}{\Omega} \sum_k f_0(E_k)$$

$$n = \frac{1}{\Omega} \int_k f_0(E_k) N_k d^3 k$$

bulk semiconductor: x -direction



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

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

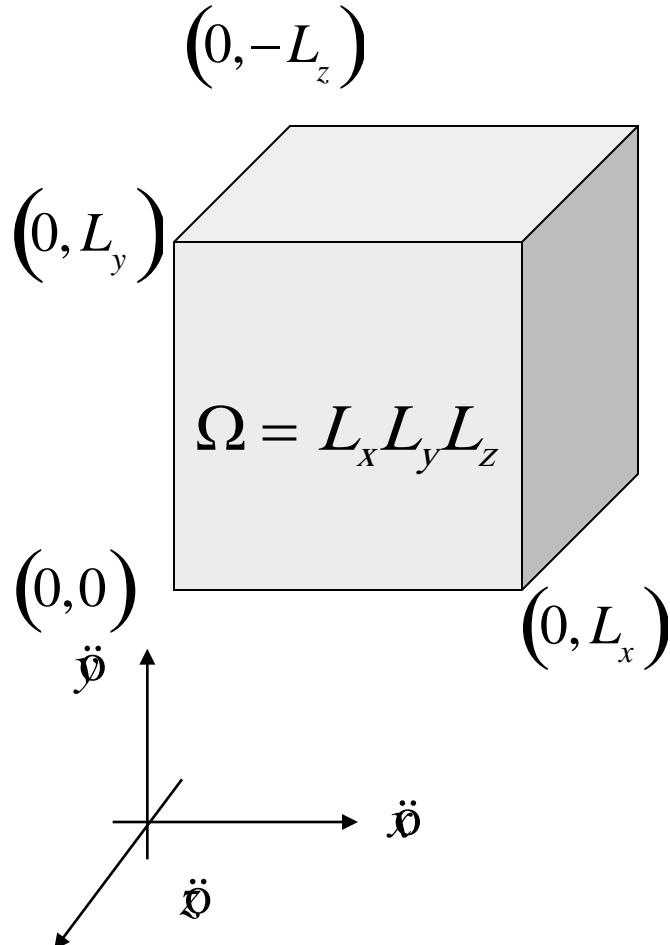
$$k_x L_x = 2\pi j \quad j = 1, 2, 3, \dots$$

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

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

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

density of states in 3D

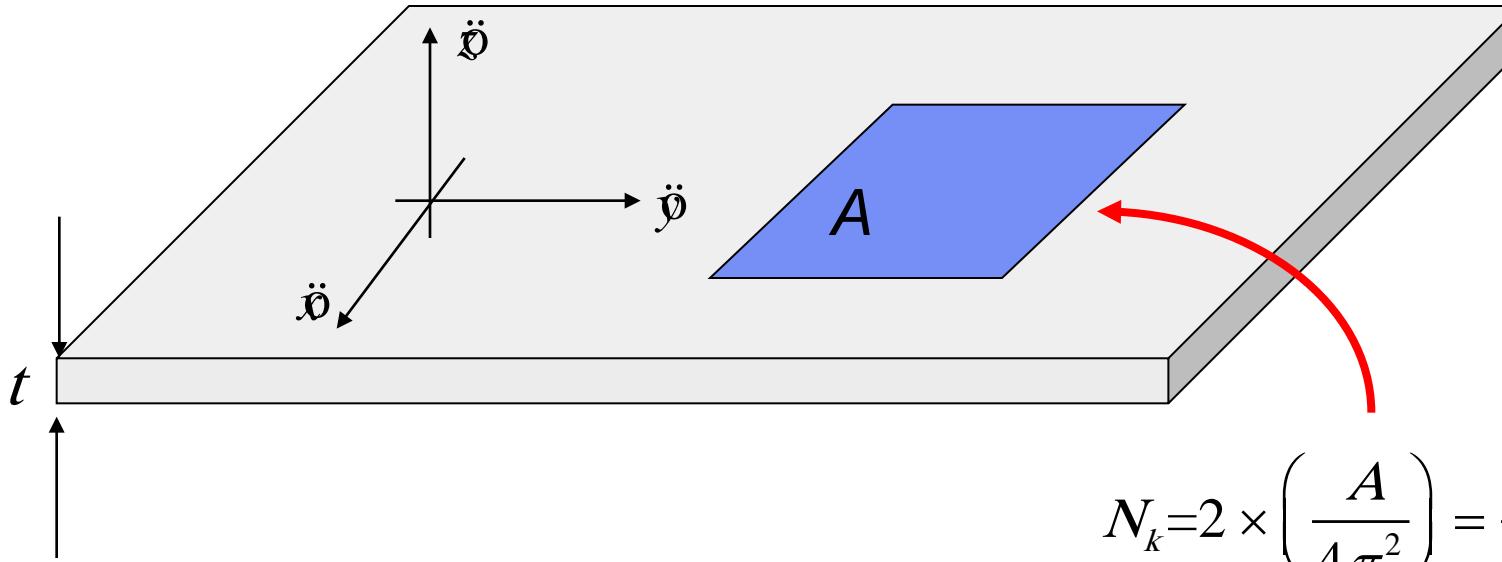


$$N_k = 2 \times \left(\frac{L_x}{2\pi} \right) \times \left(\frac{L_y}{2\pi} \right) \times \left(\frac{L_z}{2\pi} \right)$$

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

$$\sum_{\vec{k}} \bullet \rightarrow \frac{\Omega}{4\pi^3} \int_{BZ} \bullet d^3 k$$

density of states in 2D



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

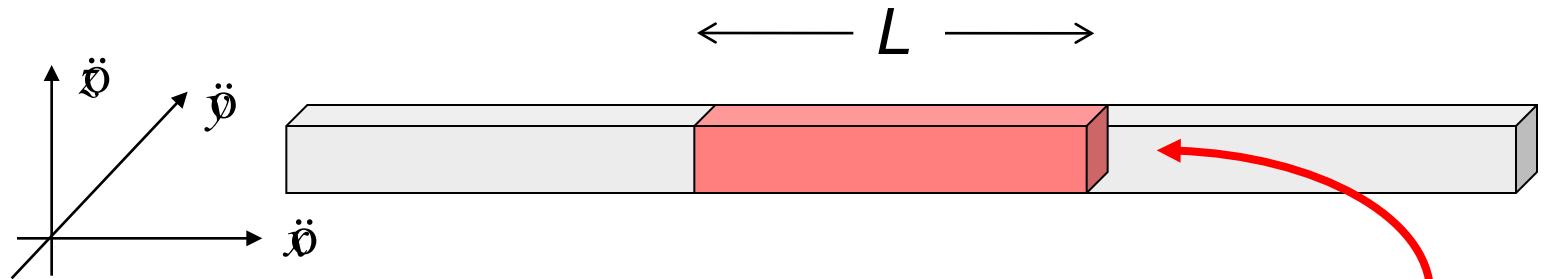
$$N = \sum_k f_0(E_k)$$

$$n_s = \frac{1}{A} \sum_k f_0(E_k) \text{ cm}^{-2}$$

$$n_s = \sum_j \frac{1}{2\pi^2} \int_{BZ}^{\infty} f_0(E_k) dk_x dk_y$$

sum over subbands

density of states in 1D



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

$$N = \sum_k f_0(E_k)$$

$$n_L = \frac{1}{L_x} \sum_{k_x} f_0(E_k) \text{ cm}^{-1}$$

$$n_L = \sum_j \frac{1}{\pi} \int_{BZ} f_0(E_k) dk_x$$

sum over subbands

density of states in k-space

1D:

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

2D:

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

independent of $E(k)$

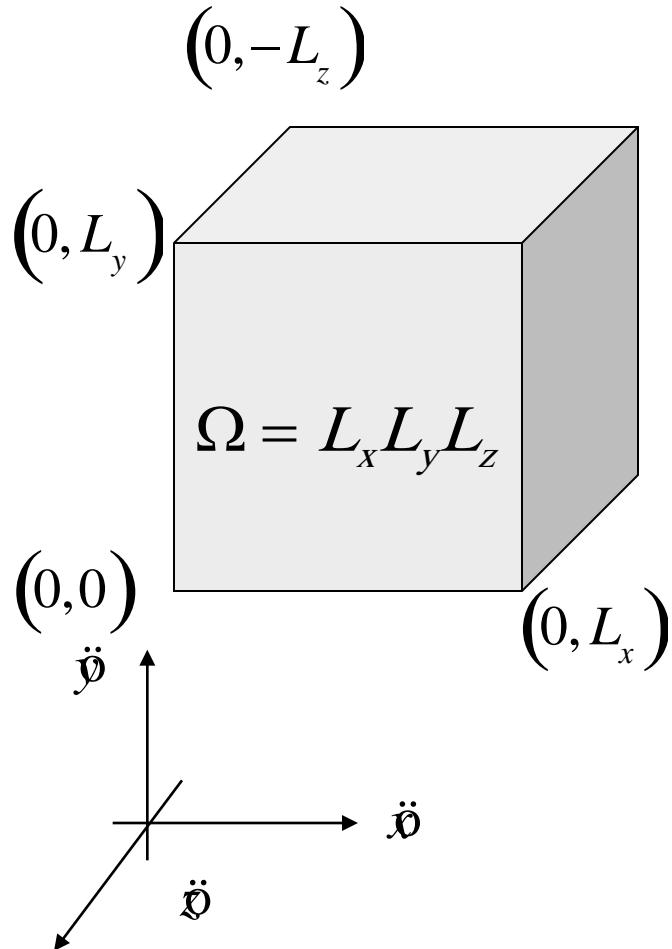
3D:

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

outline

- 1) Density of states in k-space
- 2) Example
- 3) Working in energy space
- 4) Discussion
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example: electron density in 3D



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

$$n = \frac{1}{\Omega} \sum_k f_0(E_k) \text{ cm}^{-3}$$

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

example: cont.

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

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

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

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

$$n = \frac{1}{\pi^2} \int_0^\infty \frac{k^2 dk}{1 + e^{(E_C + \hbar^2 k^2 / 2m^* - E_F) / k_B T}}$$

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

$$n = \frac{1}{\pi^2} \int_0^\infty \frac{k^2 dk}{1 + e^{-\eta_F} e^{\hbar^2 k^2 / 2m^* k_B T}}$$

example: cont.

$$n = \frac{1}{\pi^2} \int_0^\infty \frac{k^2 dk}{1 + e^{-\eta_F} e^{\hbar^2 k^2 / 2 m^* k_B T}}$$

$$n = \frac{(2m^*k_B T)^{3/2}}{2\pi^2 \hbar^3} \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

$$n = \frac{(2m^*k_B T)^{3/2}}{2\pi^{3/2} \hbar^3} \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

$$n = N_C \mathcal{F}_{1/2}(\eta_F)$$

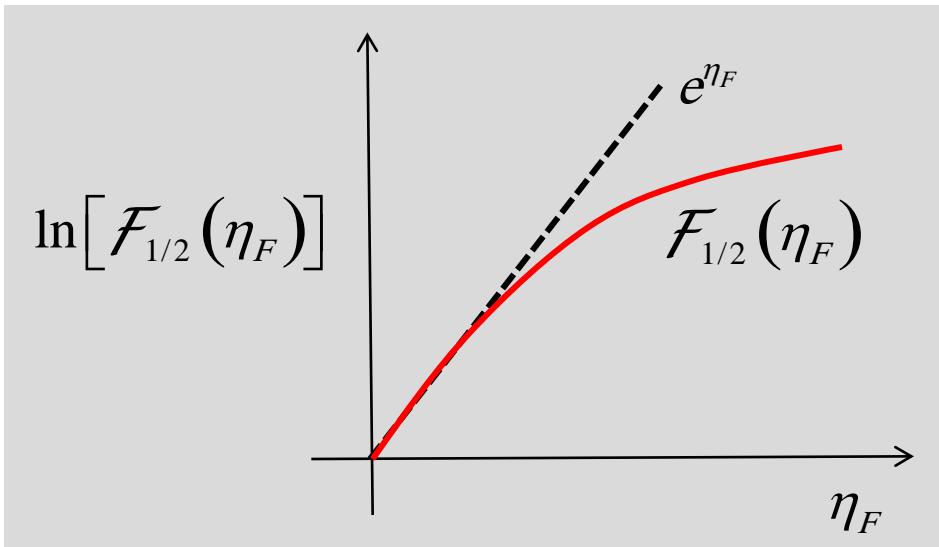
$$\eta_F = (E_F - E_C) / k_B T$$

$$\eta = \hbar^2 k^2 / 2 m^* k_B T$$

$$k^2 dk = \frac{(2m^*k_B T)^{3/2}}{2\hbar^3} \eta^{1/2} d\eta$$

example: cont.

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



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

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

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

$$\eta_F \ll 0 \quad E_F \ll E_C \quad \mathcal{F}_{1/2}(\eta_F) \rightarrow e^{\eta_F} \quad n = N_C e^{\eta_F} \text{ cm}^3$$

(non-degenerate semiconductor)

Fermi-Dirac integrals

$$\mathcal{F}_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{\eta^j d\eta}{1 + e^{\eta - \eta_F}}$$

$$\Gamma(n) = (n-1)! \quad (n \text{ integer})$$

$$\Gamma(1/2) = \sqrt{\pi}$$

$$\Gamma(p+1) = p\Gamma(p)$$

$$\mathcal{F}_j(\eta) \rightarrow e^\eta \quad \eta \ll 1$$

$$(E_F - E_C)/k_B T \ll 1$$

$$\frac{d\mathcal{F}_j}{d\eta} \rightarrow \mathcal{F}_{j-1}$$

don't confuse with.... $F_j(\eta) = \int_0^{+\infty} \frac{x^j dx}{1 + e^{x-\eta}}$

For an introduction to Fermi-Dirac integrals, see: "Notes on Fermi-Dirac Integrals," 3rd Ed., by R. Kim and M. Lundstrom) <https://www.nanohub.org/resources/5475>

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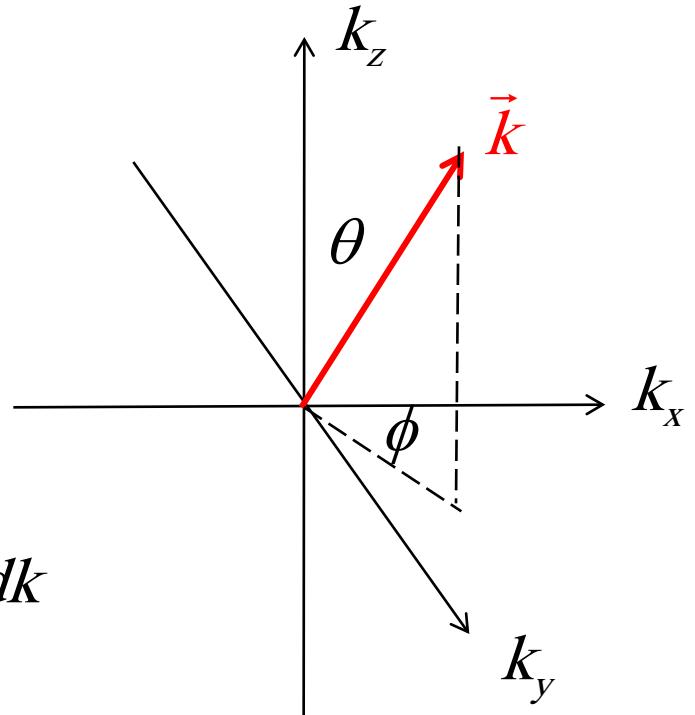
working in energy space

$$n = \frac{1}{\Omega} \sum f_0(E_k) \text{ cm}^3$$

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

$$n = \frac{1}{4\pi^3} \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_0^\infty f_0(E_k) k^2 dk$$

$$n = \frac{1}{4\pi^3} \times 2\pi \times 2 \times \int_0^\infty f_0(E_k) k^2 dk$$



$$n = \frac{1}{4\pi^3} \int_0^\infty f_0(E_k) 4\pi k^2 dk$$

working in energy space

$$n = \frac{1}{\pi^2} \int_0^\infty f_0(E_k) k^2 dk \quad \text{cm}^3$$

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

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

$$dk = \frac{\sqrt{2m^*}}{2\hbar} (E - E_C)^{-1/2} dE$$

$$k^2 dk = \frac{(2m^*)^{3/2}}{2\hbar^3} (E - E_C)^{1/2} dE$$

$$n = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} \int_{E_C}^\infty f_0(E_k) (E - E_C)^{1/2} dE$$

energy space

$$n = \frac{(2m^*)^{3/2}}{2\pi^2 h^3} \int_{E_C}^{\infty} f_0(E_k) (E - E_C)^{1/2} dE$$

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

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

energy space: cont.

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

$$n = \frac{(2m^*)^{3/2}}{2\pi^2 h^3} \int_{E_C}^{\infty} \frac{(E - E_C)^{1/2}}{1 + e^{(E - E_F)/k_B T}} dE$$

$$n = \frac{(2m^* k_B T)^{3/2}}{2\pi^2 h^3} \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

$$n = N_C \mathcal{F}_{1/2}(\eta_F) \text{cm}^{-3}$$

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

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

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

$$\eta = (E - E_C)/k_B T$$

k-space vs. energy-space

k-space:

$$n = \frac{1}{\Omega} \sum_k f_0(E_k) = \frac{1}{\Omega} \int_{BZ} f_0(E_k) N_k d^3k \text{ cm}^{-3}$$

$$N_k d^3k = \frac{\Omega}{4\pi^3}$$

$$n = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3}$$

energy-space:

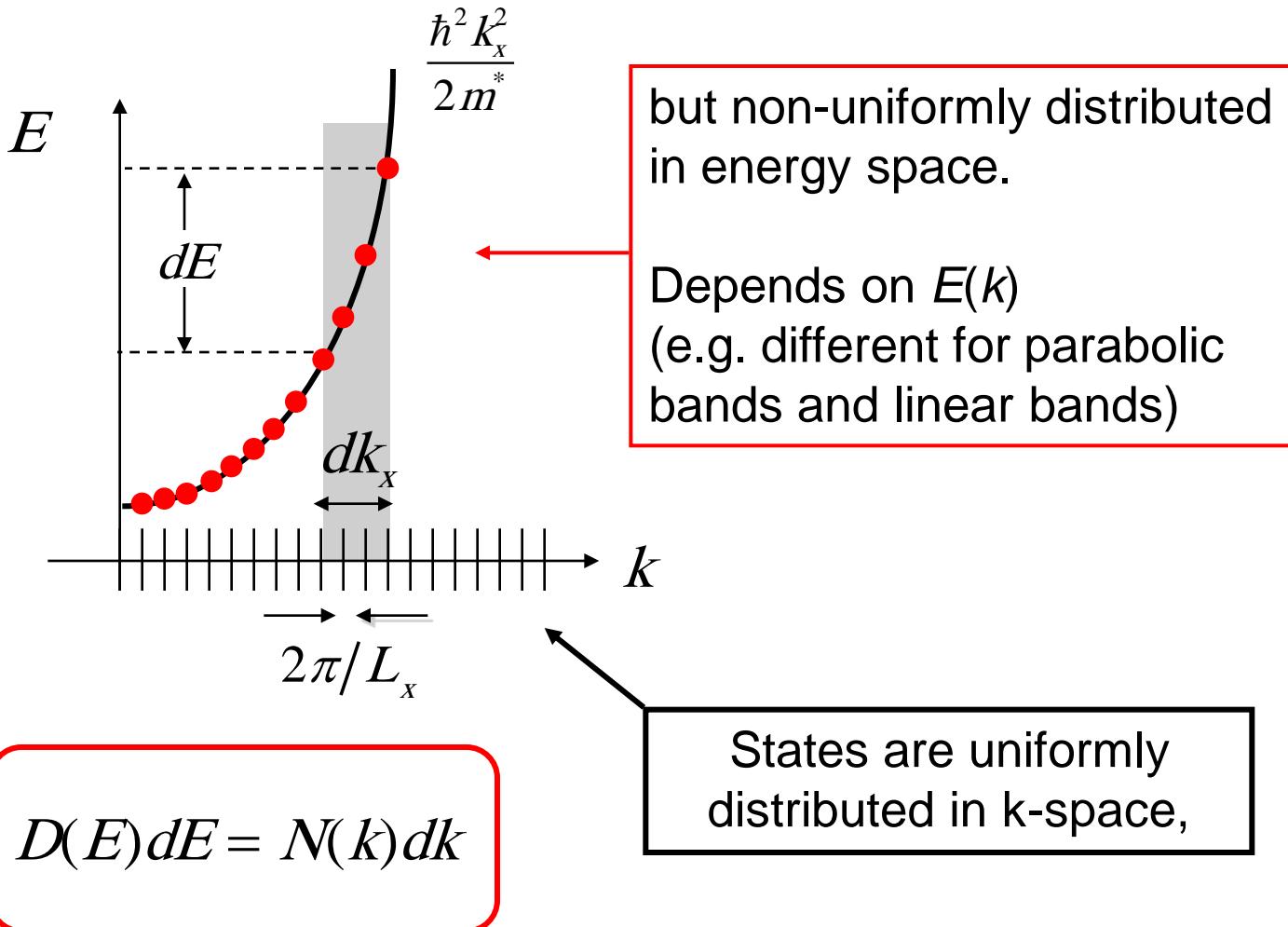
$$n = \int_{E_C}^{\infty} f_0(E) D(E) dE$$

$$D(E) dE = \frac{(2m^*)^{3/2}}{2\pi^2 h^3} (E - E_C)^{1/2} dE$$

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DOS: k-space vs. energy-space



DOS

parabolic bands

$$D_{3D}(E) = g_V \frac{(2m^*)^{3/2}}{2\pi^2 h^3} (E - E_C)^{1/2}$$
$$D_{2D}(E) = g_V \frac{m^*}{\pi h^2}$$
$$D_{1D}(E) = g_V \frac{1}{\pi h} \sqrt{\frac{m^*}{2(E - E_C)}}$$

$E > E_C$

graphene

$$D(E) = \frac{2|E|}{\pi h^2 v_F^2}$$

$$D(E) = 2 \frac{(|E|/v_F^2)}{\pi h^2}$$

$$|E| = m^*(E)v_F^2$$

other moments of the Fermi function

$$n = \frac{1}{\Omega} \sum_k f_0(E_k) \text{ cm}^{-3}$$

$$\langle E - E_C \rangle = u = \frac{\frac{1}{\Omega} \sum_k (E_k - E_C) f_0(E_k)}{\frac{1}{\Omega} \sum_k f_0(E_k)} \text{ J} \quad \begin{aligned} \langle E - E_C \rangle &= \frac{3}{2} k_B T \\ (\eta_F \ll 0) \end{aligned}$$

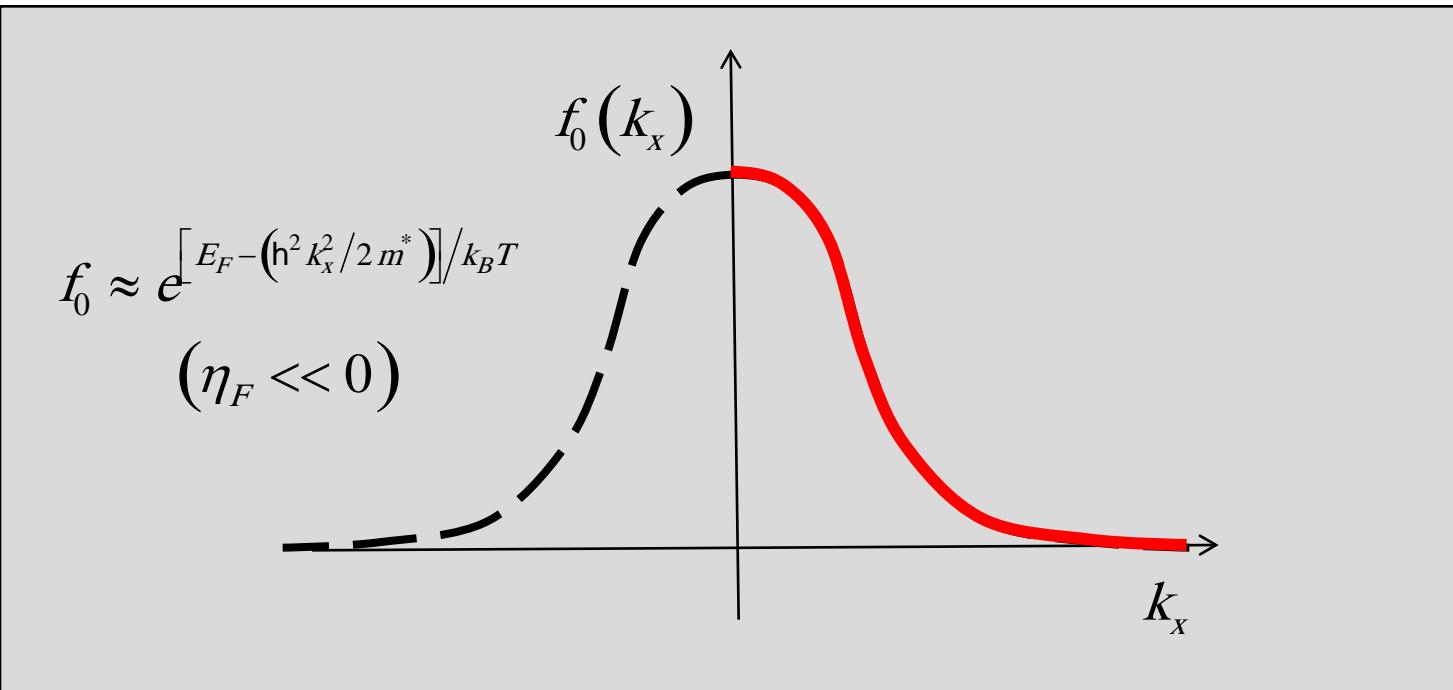
$$\langle v \rangle = 0$$

$$\langle v^+ \rangle = \frac{\frac{1}{\Omega} \sum_{k_x > 0, k_y, k_z} v_k f_0(E_k)}{\frac{1}{\Omega} \sum_{k_x > 0, k_y, k_z} f_0(E_k)} \text{ cm/s} = \mathcal{V}_T \quad v_T = \sqrt{\frac{2 k_B T}{\pi m^*}} \quad (\eta_F \ll 0)$$

thermal velocity

$$\langle v^+ \rangle = \frac{\frac{1}{\Omega} \sum_{k_x > 0, k_y, k_z} v_k f_0(E_k)}{\frac{1}{\Omega} \sum_{k_x > 0, k_y, k_z} f_0(E_k)} \text{ cm/s}$$

$$v_T = \sqrt{\frac{2k_B T}{\pi m^*}} \quad (\eta_F \ll 0)$$



rms thermal velocity

$$\langle E - E_C \rangle = \frac{3}{2} k_B T \quad E - E_C = \frac{1}{2} m^* v^2(E)$$

$$\frac{1}{2} m^* \langle v^2 \rangle = \frac{3}{2} k_B T \quad \langle E - E_C \rangle = \frac{1}{2} m^* \langle v^2 \rangle$$

$$\langle v^2 \rangle^{1/2} = v_{rms} = \sqrt{\frac{3k_B T}{m^*}} \neq v_T = \sqrt{\frac{2k_B T}{\pi m^*}}$$

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suggested practice

- 1) Work out the moments on slide 25 for $T = 0\text{K}$.
- 2) Work out the moments on slide 25 for $T > 0\text{K}$.
- 3) Work out the moments on page 25 for 1D and 2D carriers.
- 4) Finally, work them out for the conduction band of graphene to see how they depend on bandstructure.

questions

- 1) Density of states in k-space
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