ECE-656: Fall 2011

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

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outline

1) Density of states in k-space

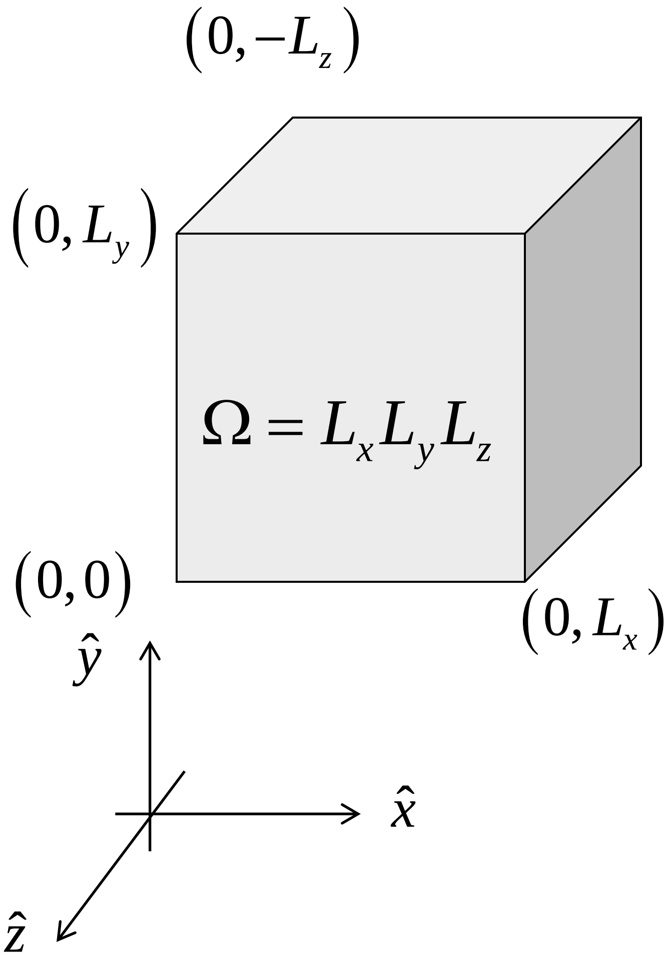
2) Example

3) Working in energy space

4) Discussion

5) Summary

bulk semiconductor



finite volume, Ω
(***part of an infinite volume***)

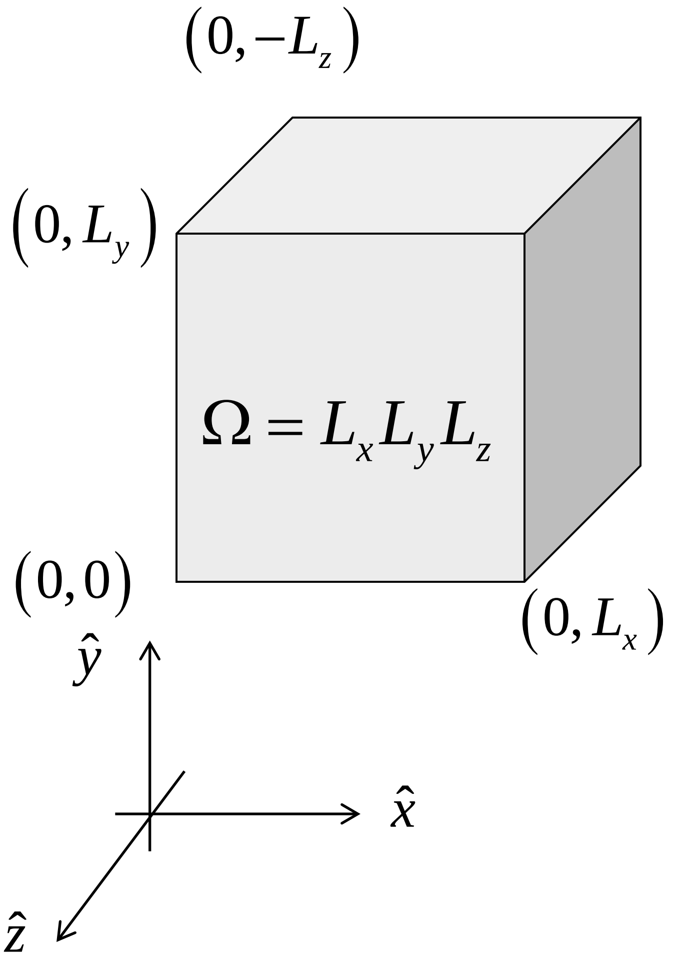
N_a atoms and $2N_a$ states in Ω

Periodic boundary conditions:

$$\psi\left(\vec{r}\right) = u_k(\vec{r})e^{i\vec{k}\bullet\vec{r}} \qquad k = 2\pi/\lambda$$

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

bulk semiconductor

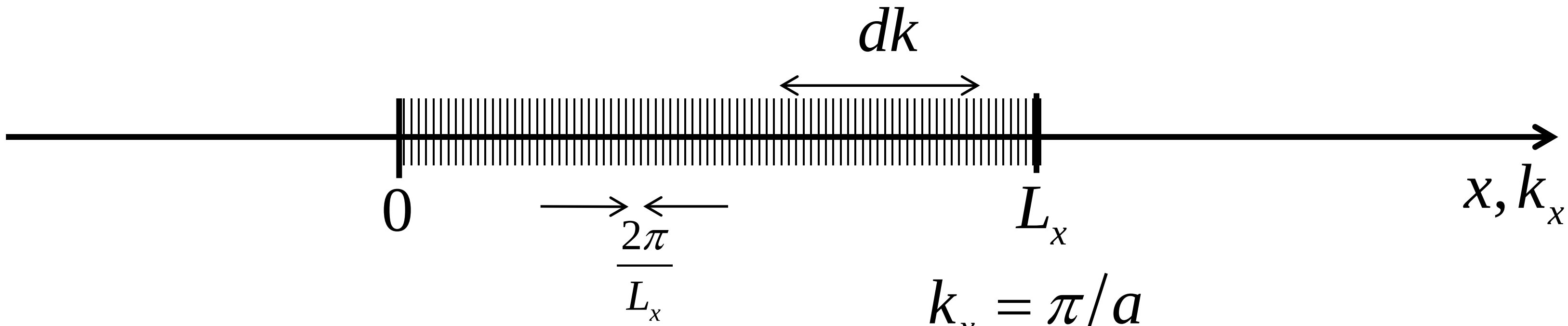


$$N = \sum_{\vec{k}} f_0\left[E\left(\vec{k}\right)\right]$$

$$n = \frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)$$

$$n = \frac{1}{\Omega}\int_{\vec{k}} f_0\left(E_k\right) N_k d^3k$$

bulk semiconductor: *x*-direction



$$k_x = \pi / a$$

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

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

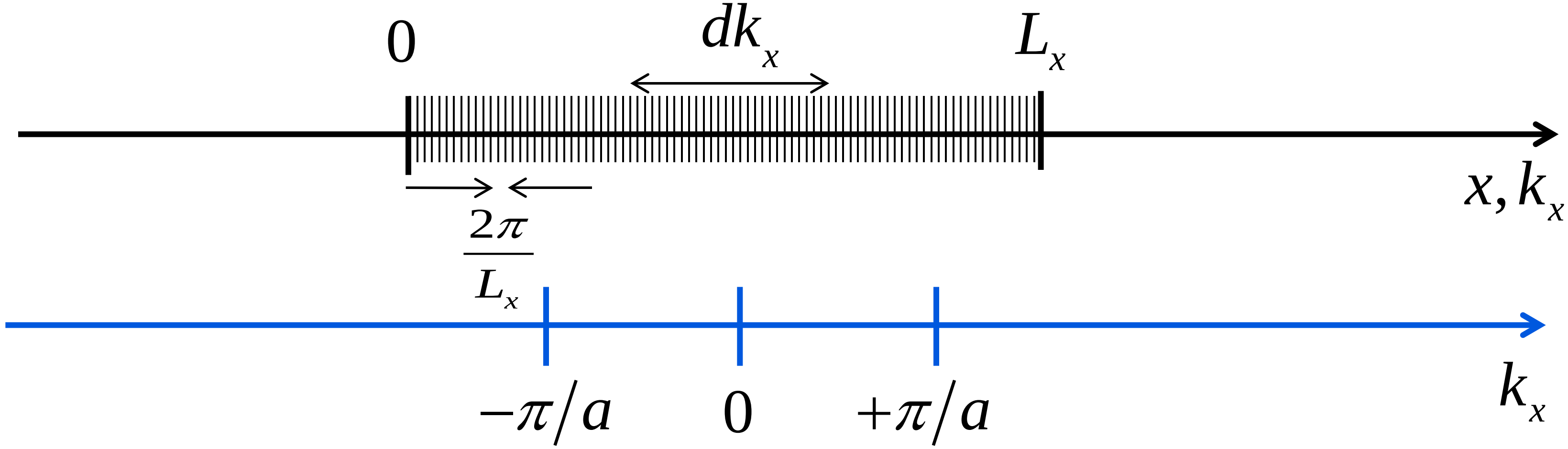
$$k_x L_x = 2\pi j \quad j = 1, 2, 3, \ldots$$

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

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

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

counting states



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

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

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

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

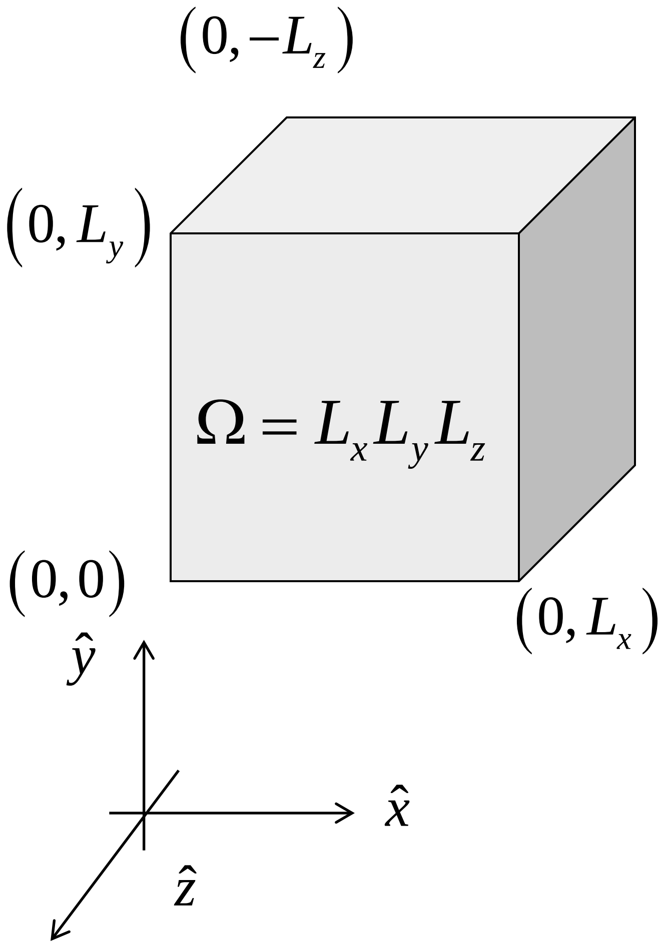
$$L_x = N_A a$$

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

$$\theta = i k_x x = i\left(2\pi \frac{j}{N_A}\right)\frac{x}{a}$$

$$j_{max} = N_A \qquad k_{max} = \frac{2\pi}{a}$$

density of states in 3D

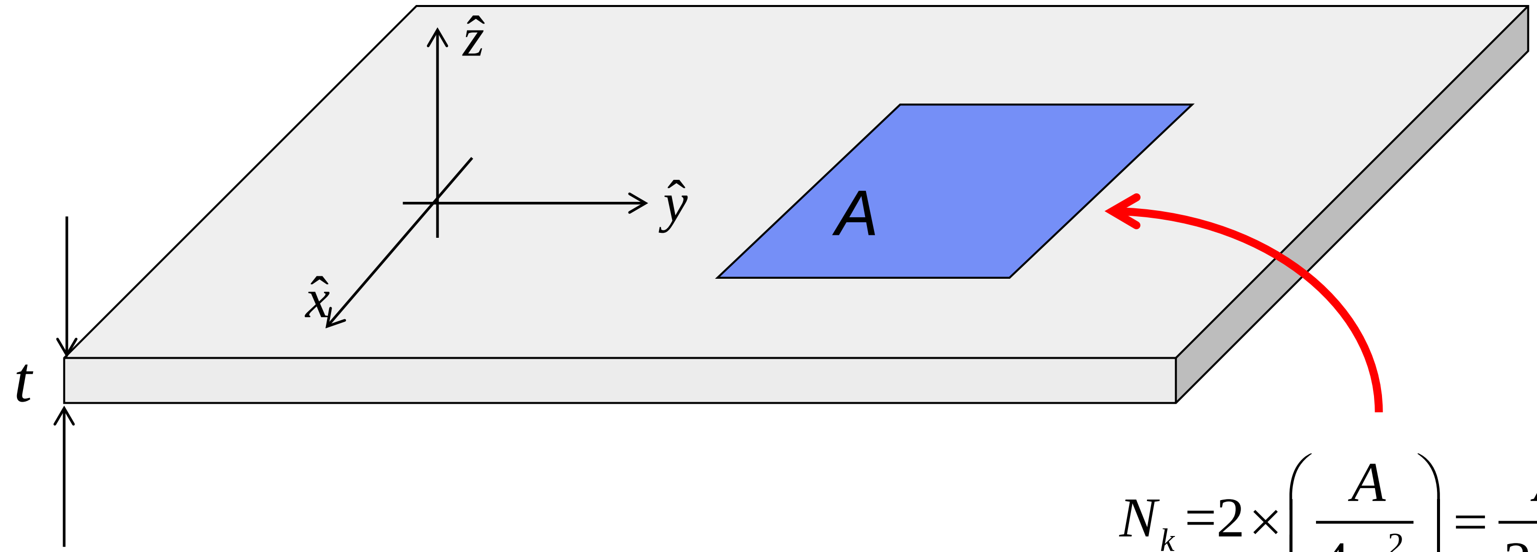


$$N_k d^3k = 2 \times \left(\frac{L_x}{2\pi}\right) \times \left(\frac{L_y}{2\pi}\right) \times \left(\frac{L_z}{2\pi}\right) d^3k$$

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

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

density of states in 2D



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

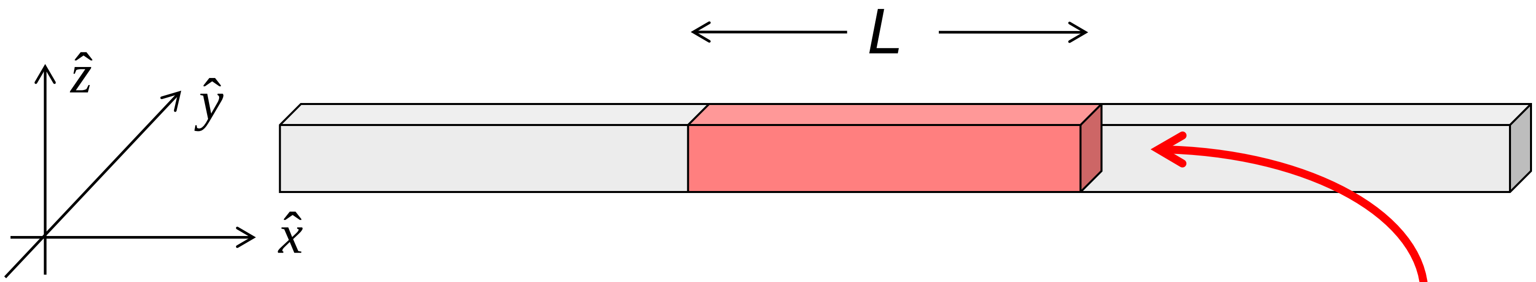
$$N = \sum_{\vec{k}} f_0\left(E_k\right)$$

$$n_S = \frac{1}{A} \sum_{\vec{k}} f_0\left(E_k\right) \text{ cm}^{-2}$$

$$n_S = \sum_j \frac{1}{2\pi^2} \int_{BZ} f_0\left(E_k\right) dk_x \, dk_y$$

sum over subbands

density of states in 1D



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

$$N = \sum_{\vec{k}} f_0(E_k)$$

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

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

sum over subbands

density of states in k-space

1D:

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

2D:

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

independent of *E*(*k*)

3D:

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

outline

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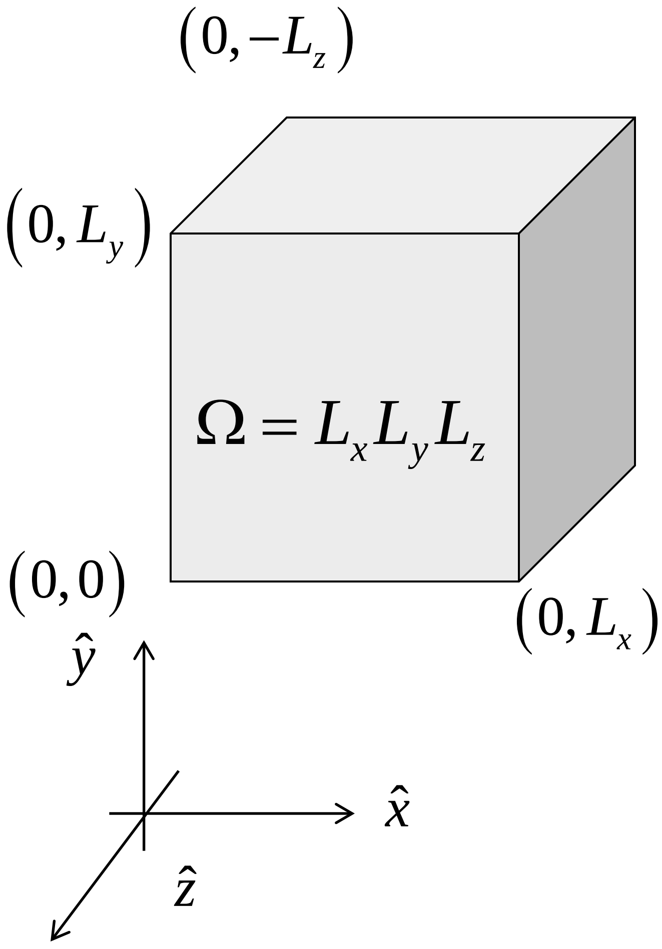
example: electron density in 3D



$$N = \sum_{\vec{k}} f_0(E_k) \qquad f_0 = \frac{1}{1+e^{(E-E_F)/k_BT}}$$

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

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

example: cont.

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

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

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

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

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

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

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

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

example: cont.

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

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

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

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

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

$$n = \frac{\left(2m^* k_B T\right)^{3/2}}{4\pi^{3/2} \hbar^3} \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

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

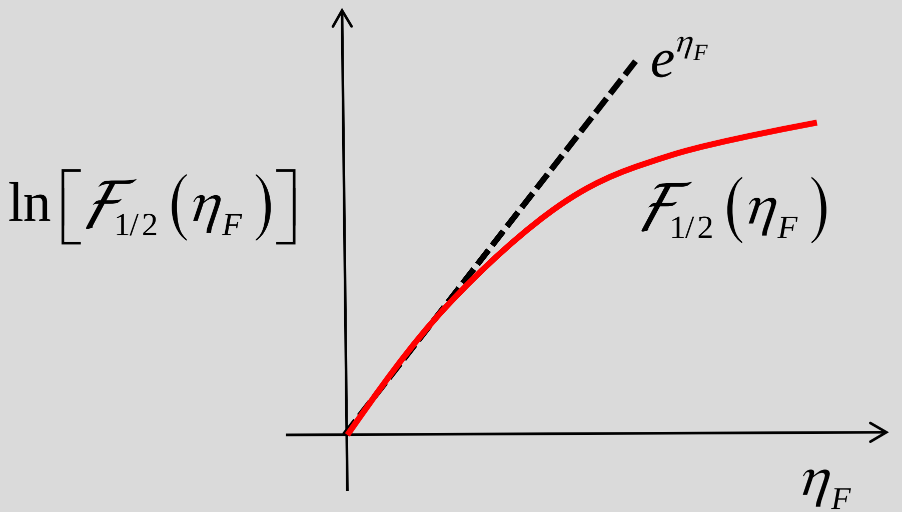
example: cont.

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

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

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

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



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

(non-degenerate semiconductor)

Fermi-Dirac integrals

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

$$\Gamma(n) = (n-1)!$$ (n integer)

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

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

$$\mathcal{F}_j(\eta) \to e^{\eta} \quad \eta << 1$$

$$(E_F - E_C)/k_B T << 1$$

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

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

exercises

1) Work out the corresponding expression for n_L in 1D

2) Work out the corresponding expression for n_S in 2D

3) Work out the average energy per electron in 1D, 2D, 3D

$$U = nu = \frac{1}{\Omega}\sum_{\vec{k}} E_k f_0\left(E_k\right) \text{ cm}^{-3}$$

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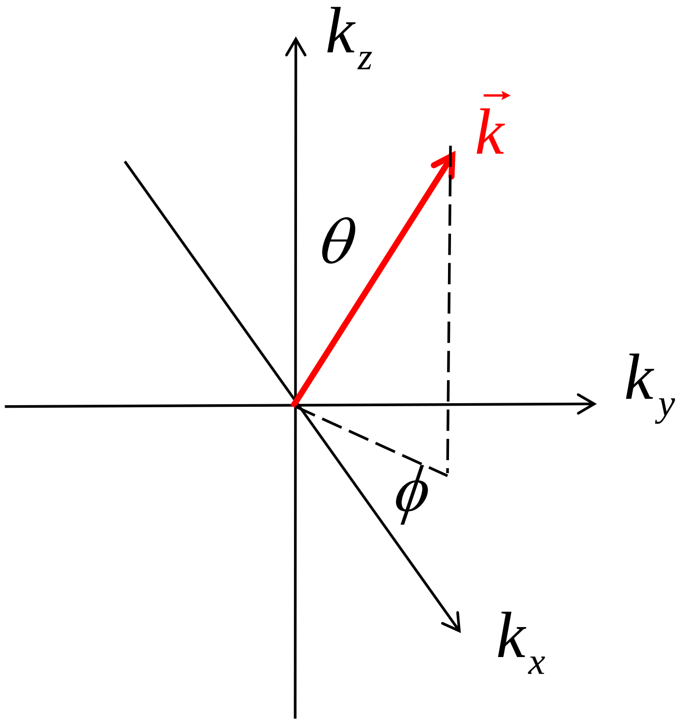
working in energy space

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

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

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



(no bandstructure yet)

working in energy space

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

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

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

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

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

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

energy space

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

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

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

energy space: cont.

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

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

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

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

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

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

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

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

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

k-space vs. energy-space

k-space:

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

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

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

energy-space:

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

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

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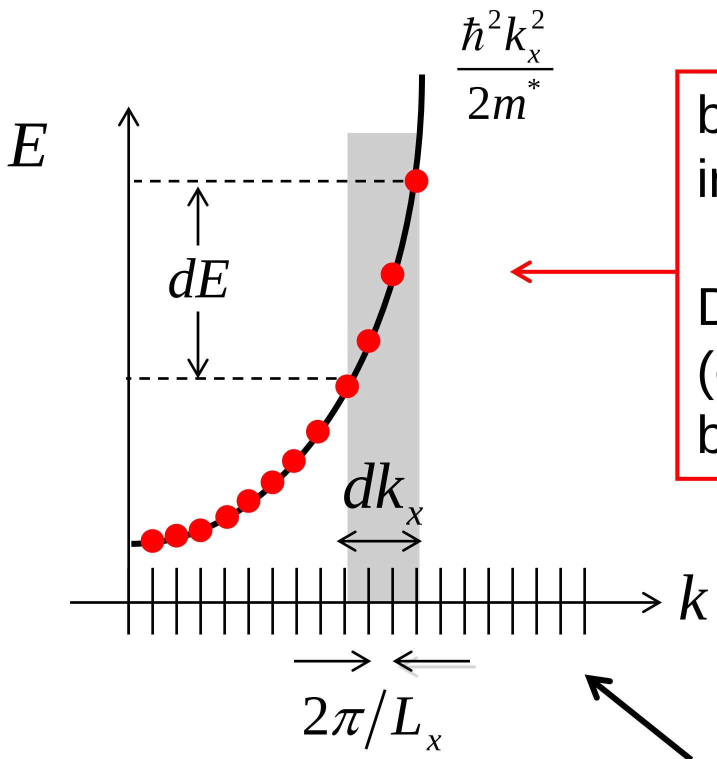
DOS: k-space vs. energy-space



but non-uniformly distributed in energy space.

Depends on *E*(*k*)
(e.g. different for parabolic bands and linear bands)

States are uniformly distributed in k-space,

$$D(E)dE = N(k)dk$$

DOS

parabolic bands

$$E = \hbar^2 k^2 / 2m^*$$

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

$$D_{2D}(E) = g_V \frac{m^*}{\pi\hbar^2}$$

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

$E > E_C$

graphene

$$E = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2}$$

$$D_{2D}(E) = \frac{2|E|}{\pi\hbar^2\upsilon_F^2}$$

other moments of the Fermi function

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

$$\frac{\left\langle E_k \right\rangle}{n} = u = \frac{\frac{1}{\Omega}\sum_{\vec{k}} E_k f_0\left(E_k\right)}{\frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)} \quad \text{J}$$

$$u = \frac{3}{2} k_B T$$

$$\left(\eta_F << 0\right)$$

$$\left\langle \upsilon \right\rangle = 0$$

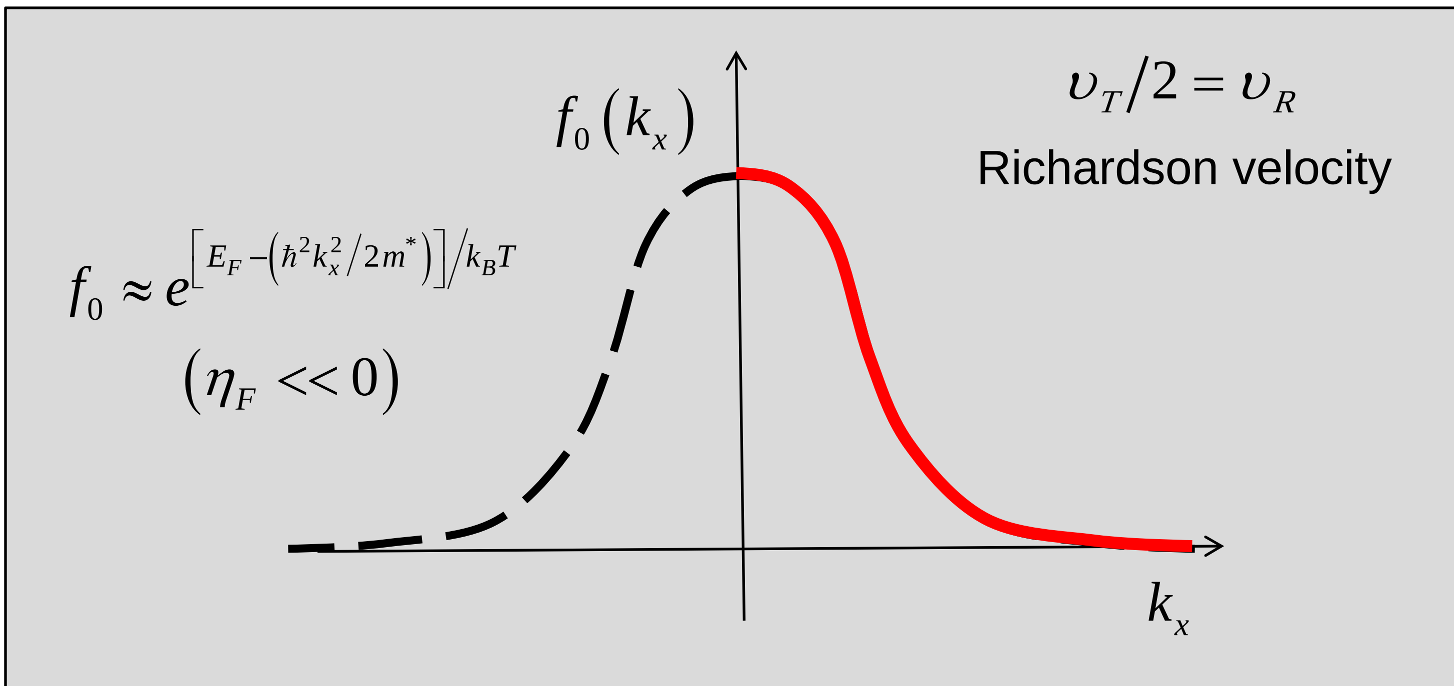
$$\left\langle \upsilon^+ \right\rangle = \frac{\frac{1}{\Omega}\sum_{k_x>0,k_y,k_z} \upsilon_k f_0\left(E_k\right)}{\frac{1}{\Omega}\sum_{k_x>0,k_y,k_z} f_0\left(E_k\right)} \quad \text{cm/s} = \tilde{\upsilon}_T \qquad \upsilon_T = \sqrt{\frac{2k_B T}{\pi m^*}} \qquad \left(\eta_F << 0\right)$$

uni-directional thermal velocity

$$\left\langle \upsilon^{+} \right\rangle = \frac{\dfrac{1}{\Omega}\displaystyle\sum_{k_x>0,k_y,k_z} \upsilon_k f_0\left(E_k\right)}{\dfrac{1}{\Omega}\displaystyle\sum_{k_x>0,k_y,k_z} f_0\left(E_k\right)} \quad \text{cm/s} = \tilde{\upsilon}_T$$

$$\upsilon_T = \sqrt{\frac{2k_BT}{\pi m^*}}$$

$$\left(\eta_F << 0\right)$$



rms thermal velocity

$$u = \frac{3}{2} k_B T \qquad u = \frac{1}{2} m^* \left\langle \upsilon^2 (E) \right\rangle$$

$$\frac{1}{2} m^* \left\langle \upsilon^2 \right\rangle = \frac{3}{2} k_B T$$

$$\left\langle \upsilon^2 \right\rangle^{1/2} = \upsilon_{rms} = \sqrt{\frac{3k_B T}{m^*}} \neq \upsilon_T = \sqrt{\frac{2k_B T}{\pi m^*}}$$

i) unidirectional thermal velocity
ii) Richardson thermal velocity
iii) rms thermal velocity

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suggested practice (slide 28)

1) Work out the moments for $T = 0\text{K}$.

2) Work out the moments for $T > 0\text{K}$.

3) Work out the moments for 1D and 2D carriers.

4) Finally, work them out for the conduction band of graphene to see how they depend on bandstructure.

questions

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