Sums and Integrals

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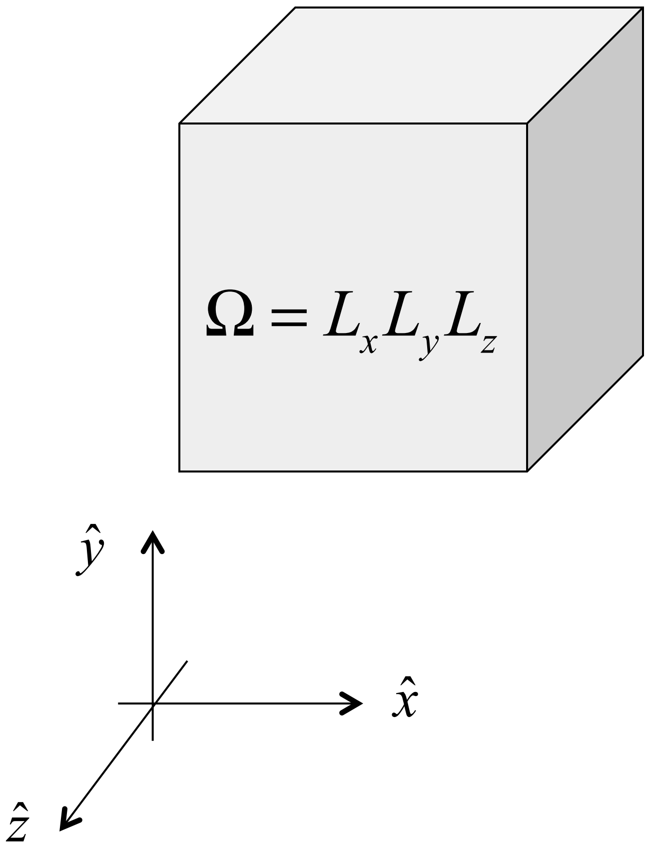
Outline

1) **Carrier densities in 3D, 2D, and 1D**
2) Working in k-space
3) Working in energy space
4) Other important moments
5) Alternative definition of DOS
5) Summary

3D bulk semiconductor



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

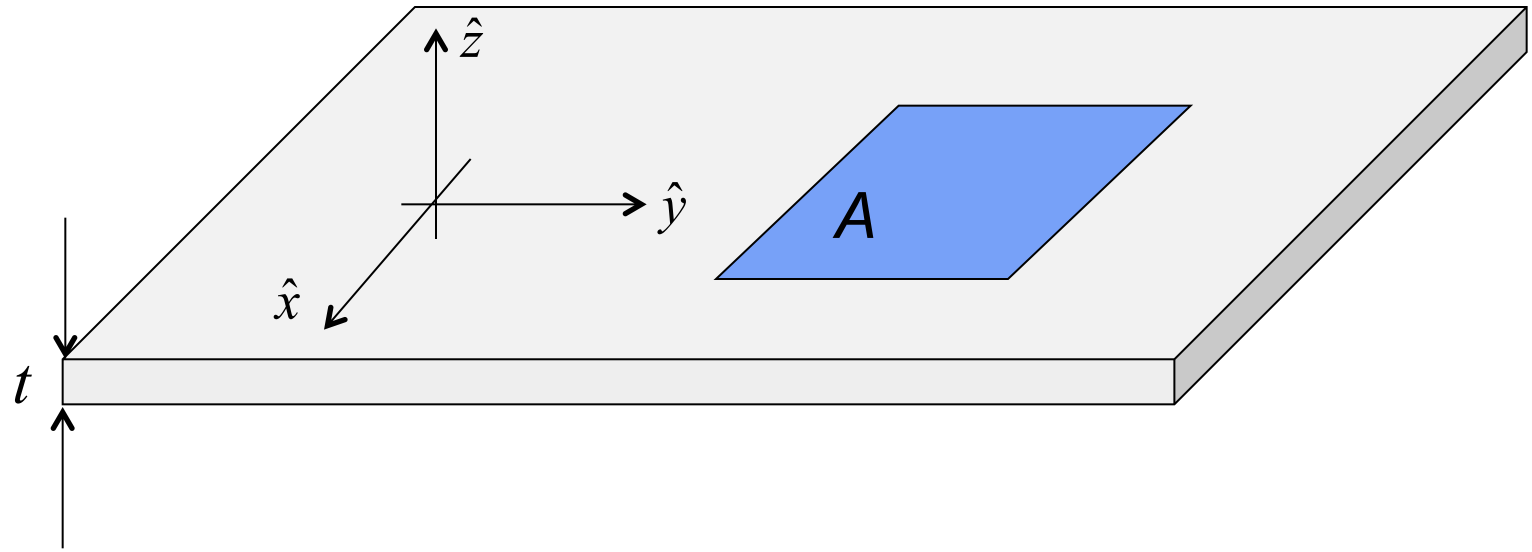
$$n = \frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)$$

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

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

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

2D “bulk” semiconductor



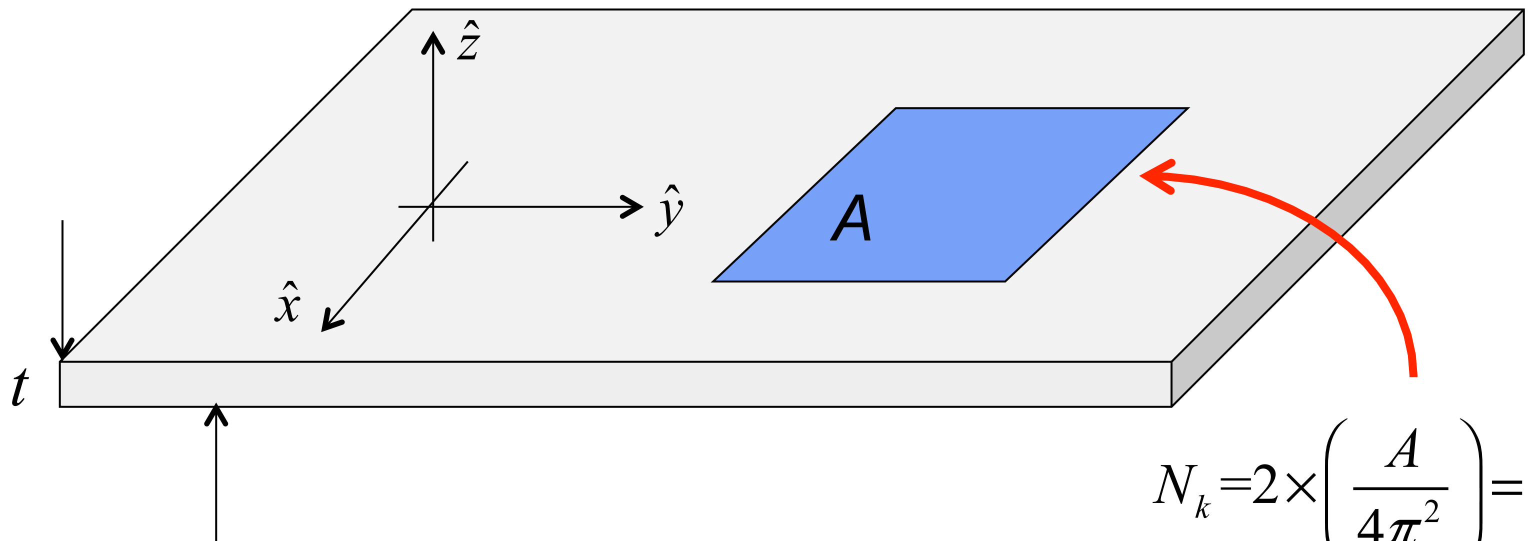
$$N = \sum_{\vec{k}} f_0(E_k)$$

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

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

sum over subbands

2D bulk semiconductor: single subband



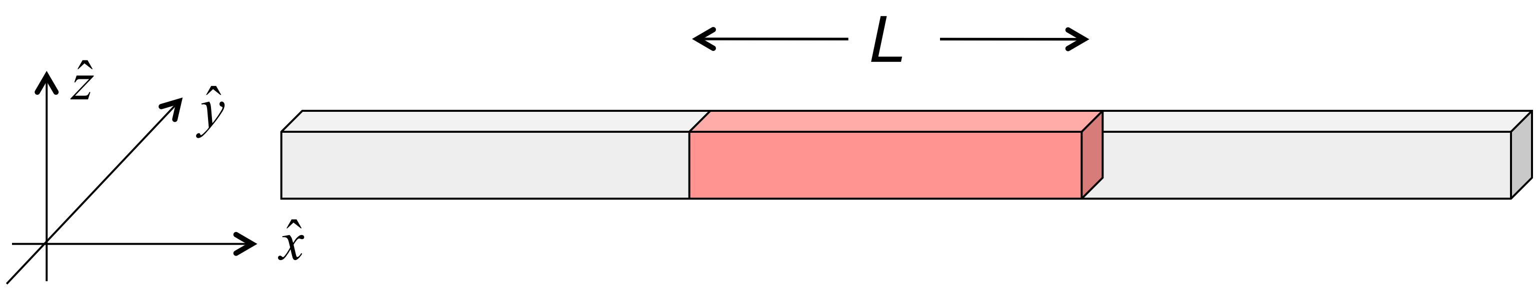
$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2}$$

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

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

$$\sum_{\vec{k}} \bullet \rightarrow \frac{A}{2\pi^2} \int_{BZ} \bullet \, d^2k$$

1D "bulk" semiconductor



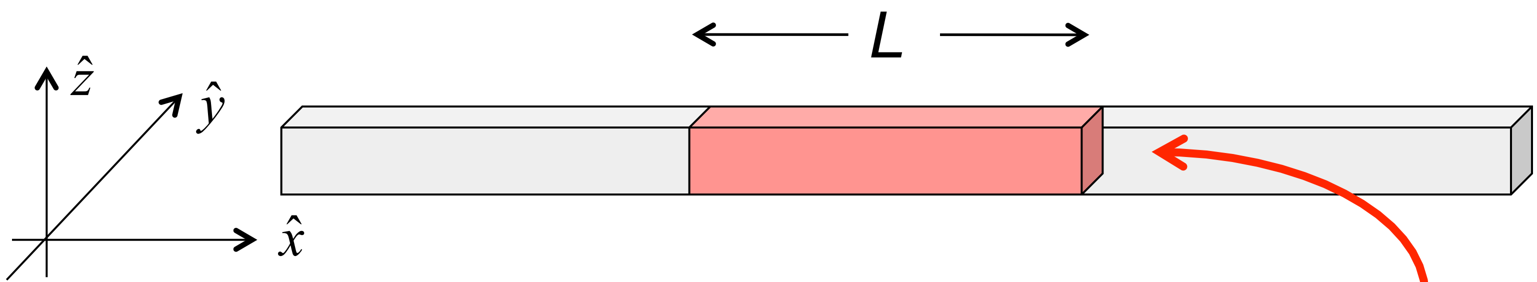
$$N = \sum_{k_x} f_0\left(E_k\right)$$

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

$$n_L = \sum_j \frac{1}{L} \sum_{k_x} f_0\left(E_k\right) \text{ cm}^{-1}$$

sum over subbands

1D bulk semiconductor: single subband



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

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

$$n_L = \frac{1}{L}\int_{BZ} f_0\left(E_k\right) N_k\ dk_x$$

$$\sum_{k_x} \bullet \rightarrow \frac{L}{\pi}\int_{BZ} \bullet\ dk$$

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Density-of-states in k-space

1D:

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

2D:

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

3D:

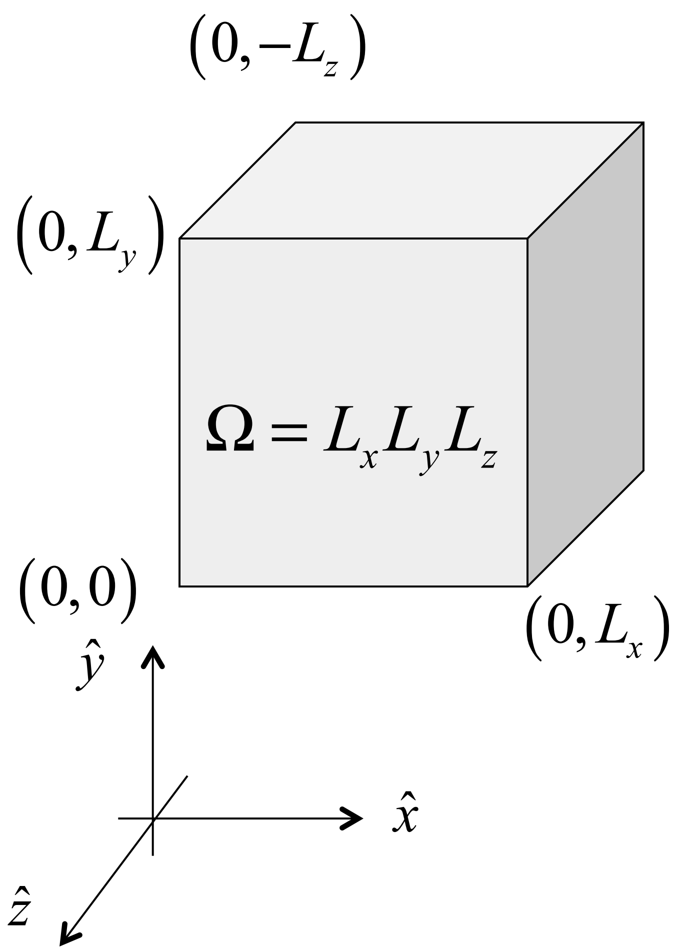
$$N_k = 2 \times \left(\frac{\Omega}{8\pi^2} \right) = \frac{\Omega}{4\pi^3} \qquad dk_x dk_y dk_z$$

N_k independent of *E*(*k*)

$$\sum_{\vec{k}} \bullet \rightarrow N_k \int_{BZ} \bullet \, dk$$

(Should include valley degeneracy factor, g_V.)

Example 1: Electron density in 3D



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

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

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

Example: cont.

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

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

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

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

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

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

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

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

Example: cont.

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

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

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

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

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

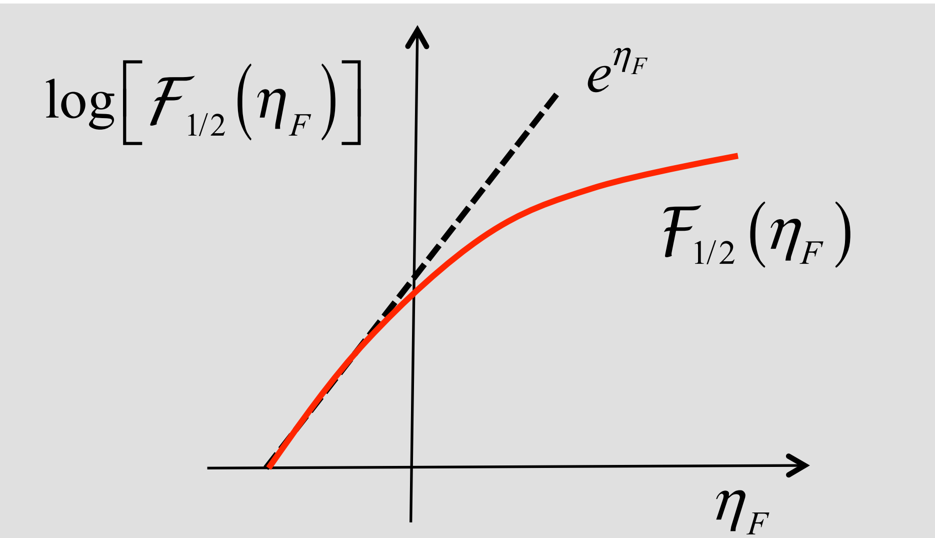
$$\eta \equiv \left(E - E_C\right)/k_BT$$

$$\eta = \hbar^2k^2/2m^*k_BT$$

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

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

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

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

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

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

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

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

$$\frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}$$

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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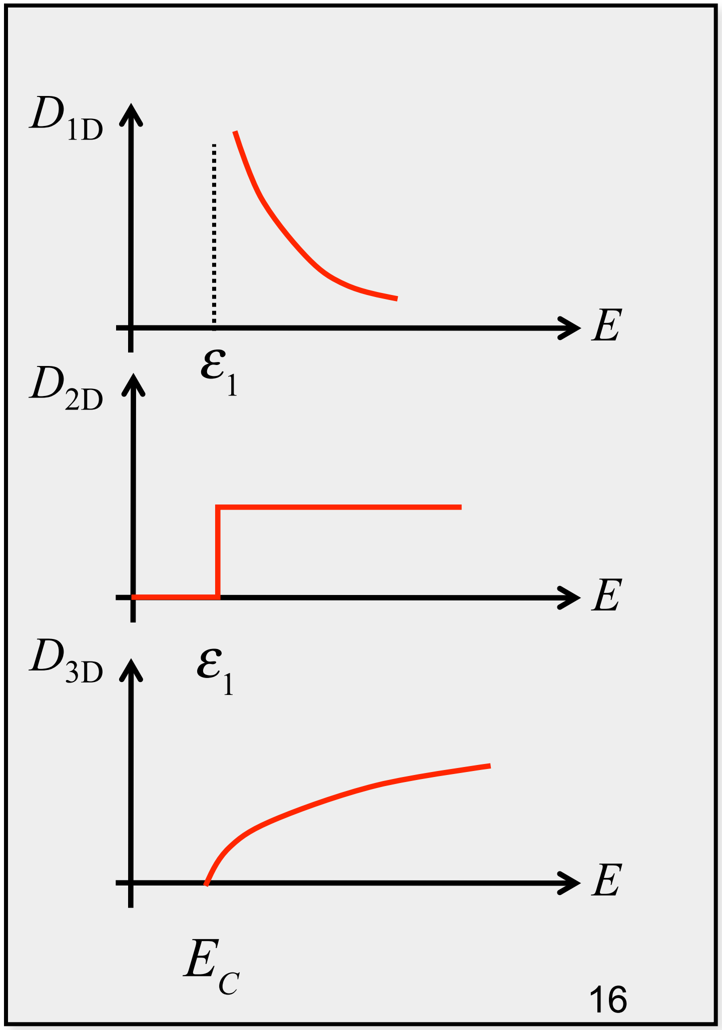
Parabolic bands: 1D, 2D, and 3D

$$D_{1D}(E) = g_V \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{(E-\varepsilon_1)}}\,\Theta(E-\varepsilon_1)$$

$$D_{2D}(E) = g_V \frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

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

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



Energy space (3D)

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

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

$$n = \frac{\left(2m^* k_B T\right)^{3/2}}{2\pi^2\hbar^3} \int_{0}^{\infty} \frac{\eta^{1/2} d\eta}{1 + e^{\eta-\eta_F}}$$

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

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

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

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

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

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

k-space vs. energy-space

k-space:

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

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

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

energy-space:

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

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

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Moments of the Fermi function

In equilibrium, physical quantities are various moments of the Fermi function.

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

$$\phi\left(\vec{k}\right) = 1$$

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

$$\phi\left(\vec{k}\right) = \upsilon_x\left(\vec{k}\right)$$

$$\left\langle \upsilon_x \right\rangle = \frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x\left(\vec{k}\right) f_0\left(E_k\right) = 0$$

$$\frac{\left\langle \upsilon_x \right\rangle}{n} = \frac{\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x\left(\vec{k}\right) f_0\left(E_k\right)}{\frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)} = 0$$

Other moments

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

$$\phi\left(\vec{k}\right) = 1 \qquad n \quad \text{cm}^{-3}$$

$$\phi\left(\vec{k}\right) = \upsilon_x\left(\vec{k}\right) \qquad \left\langle \upsilon_x \right\rangle = 0$$

$$\phi\left(\vec{k}\right) = E\left(\vec{k}\right) \qquad \left\langle E_k \right\rangle$$

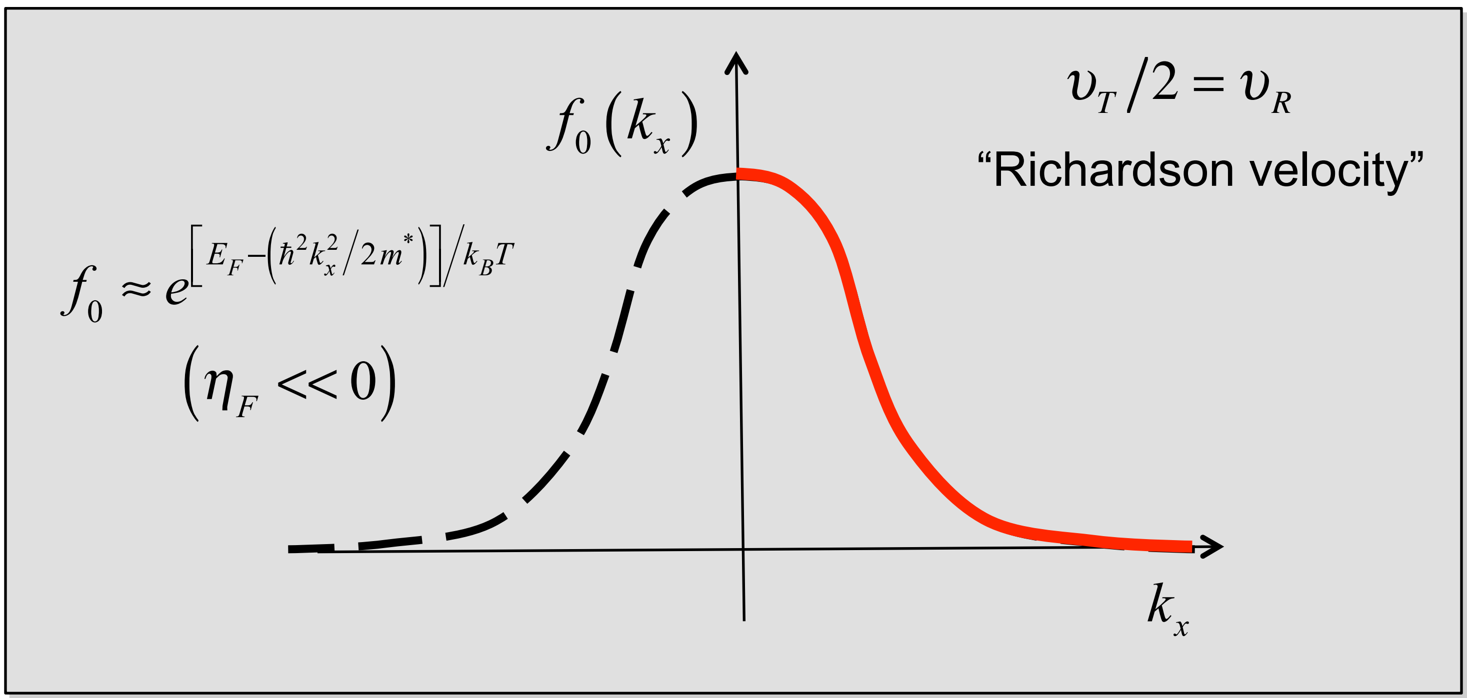
$$\frac{\left\langle E_k \right\rangle}{n} = u = \frac{\frac{1}{\Omega}\sum_{\vec{k}} E_k f_0\left(E_k\right)}{\frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)} \quad \text{J}$$

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

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

Uni-directional thermal velocity

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



About thermal velocities

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

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

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

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

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An alternative way to define the DOS

$$D_{1D}(E) = \frac{1}{L}\sum_{k}\delta\left(E - E_k\right) \quad \frac{\#}{\text{J-m}}$$

$$D_{2D}(E) = \frac{1}{A}\sum_{\vec{k}}\delta\left(E - E_{\vec{k}}\right) \quad \frac{\#}{\text{J-m}^2}$$

$$D_{3D}(E) = \frac{1}{\Omega}\sum_{\vec{k}}\delta\left(E - E_{\vec{k}}\right) \quad \frac{\#}{\text{J-m}^3}$$

Proof (1D)

in k-space, we know:

$$n_L = \frac{1}{L}\sum_k f_0\left(E_k\right)$$

can also work in energy-space:

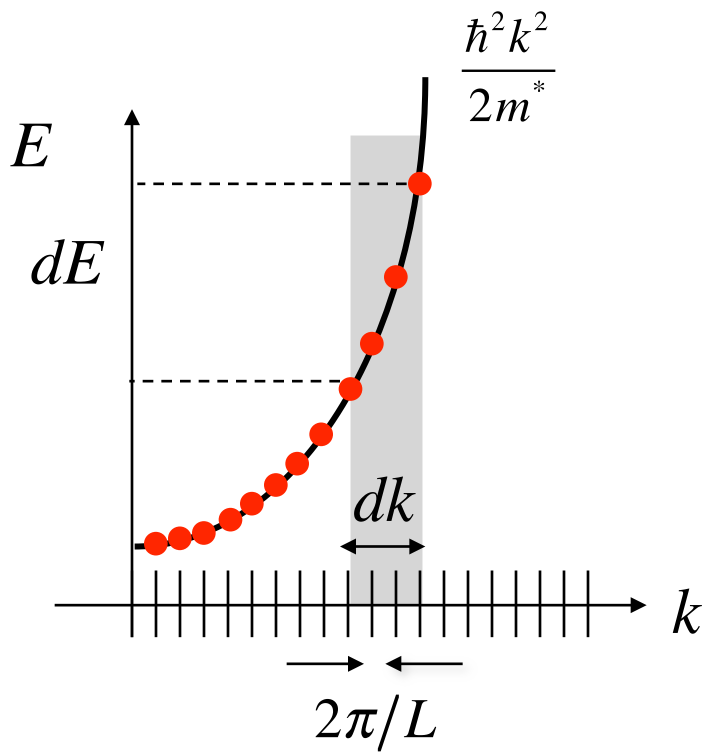
$$n_L = \int f_0\left(E\right) D_{1D}(E) dE$$

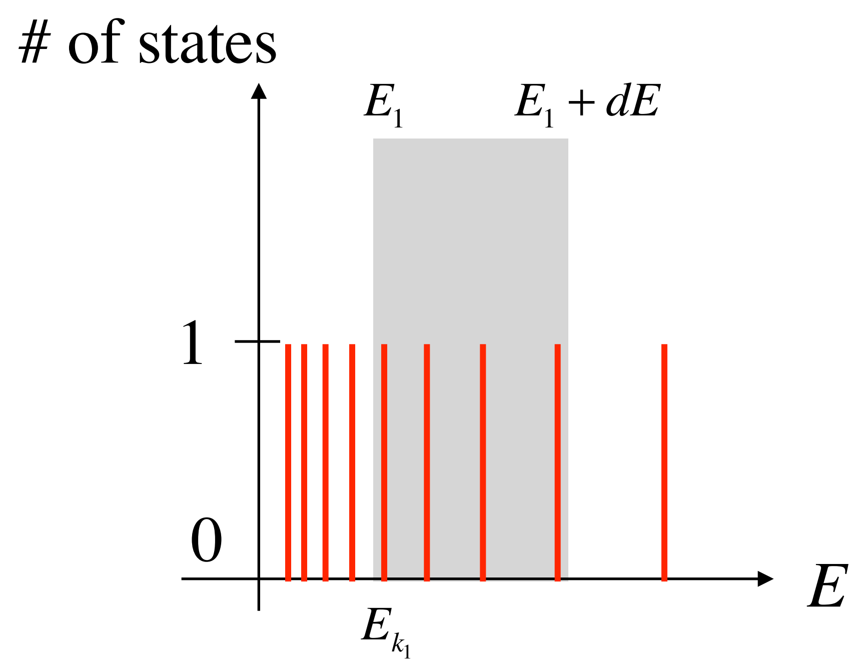
$$n_L = \int f_0\left(E\right) \frac{1}{L}\sum_k \delta\left(E - E_k\right) dE$$

$$n_L = \frac{1}{L}\sum_k \int f_0\left(E\right) \delta\left(E - E_k\right) dE$$

$$n_L = \frac{1}{L}\sum_k f_0\left(E_k\right)$$

Interpretation





$$\int_{E_1}^{E_1+dE} D_{1D}(E)\,dE = \int_{E_1}^{E_1+dE} \frac{1}{L}\sum_k \delta\left(E - E_k\right)dE = \frac{1}{L}\sum_k \int_{E_1}^{E_1+dE} \delta\left(E - E_k\right)dE$$

counts the states between E and E +dE

Example: 2D DOS for parabolic energy bands

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \delta\left(E_1 - E_{\mathbf{k}}\right) \quad \frac{\#}{\text{J-m}^2}$$

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \delta\left(E_1 - E_{\mathbf{k}}\right) \rightarrow \frac{1}{A} g_V \frac{A}{(2\pi)^2} \times 2\int_0^\infty \delta\left(E_1 - E_{\mathbf{k}}\right) 2\pi k\, dk$$

$$D_{2D}(E_1) = g_V \frac{1}{\pi} \times \int_0^\infty \delta\left(E_1 - E(k)\right) k dk$$

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \qquad dE = \frac{\hbar^2 2kdk}{2m^*} \qquad kdk = \frac{m^*}{\hbar^2} dE$$

$$D_{2D}(E_1) = g_V \frac{m^*}{\pi\hbar^2} \times \int_0^\infty \delta\left(E_1 - E(k)\right) dE \qquad D_{2D}(E_1) = g_V \frac{m^*}{\pi\hbar^2} \checkmark$$

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Summary

1) Be familiar with how to work out sums in k-space and integrals in energy space.

2) Become familiar with Fermi-Dirac integrals.

3) Understand the uni-directional thermal velocity.

4) Understand the delta-function definition of the DOS.