ECE 656: Fundamentals of Carrier Transport Fall 2013

Week 2 Summary

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(revised 8/31/13)

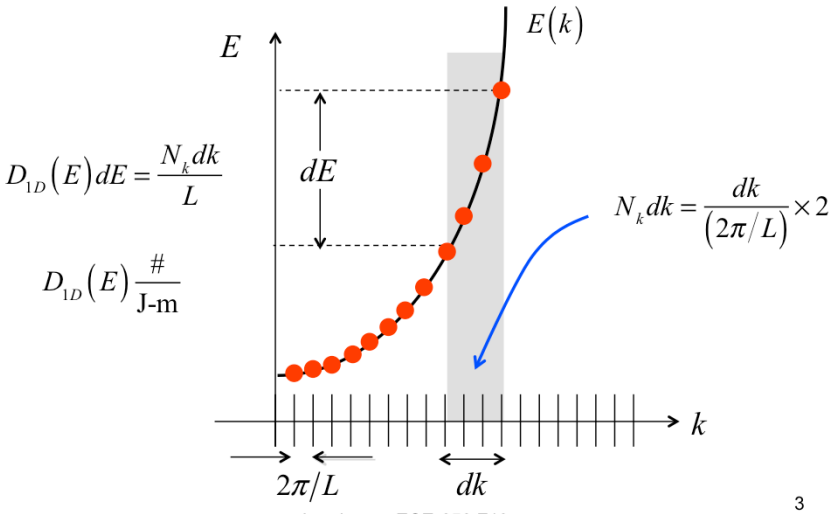
topics

1) Density of states (in energy)

2) DOS examples

3) (Intro to scattering)

mapping from k-space to energy-space

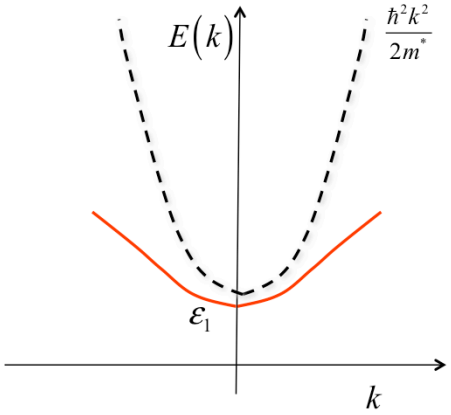


$$D_{1D}(E)\,dE = \frac{N_k\,dk}{L}$$

$$D_{1D}(E)\ \frac{\#}{\text{J-m}}$$

$$N_k\,dk = \frac{dk}{(2\pi/L)} \times 2$$

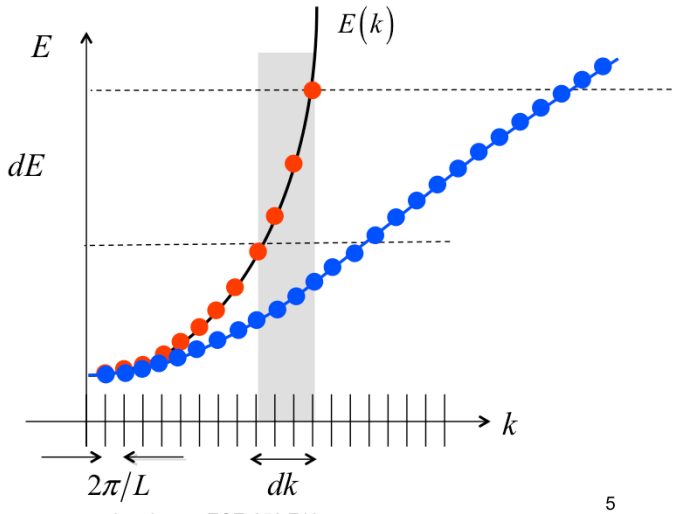
conduction band non-parabolicity



$$E'\left(1+\alpha E'\right)=\frac{\hbar^2 k^2}{2m^*(0)}$$

$$E'=E-\varepsilon_1$$

mapping from k-space to energy-space



alternative expression for DOS

$$D_{1D}(E)dE = \frac{1}{L}\sum_{k}\Delta_{E,E_k}$$

$$D_{2D}(E)dE = \frac{1}{A}\sum_{\vec{k}}\Delta_{E,E_k}$$

$$D_{3D}(E) = \frac{1}{\Omega}\sum_{\vec{k}}\Delta_{E,E_k}$$

like a "Kronecker delta"

one if: $E - dE/2 < E_k < E + dE/2$

otherwise zero

example: 2D DOS for parabolic energy bands

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \Delta_{E',E_k}$$

$$D_{2D}\left(E_1\right)dE = \frac{1}{A}\sum_{\vec{k}} \Delta_{E',E_k} \rightarrow D_{2D}\left(E_1\right) = \frac{1}{A}\frac{A}{\left(2\pi\right)^2} \times 2\int_0^\infty 2\pi k\, dk\delta\left(E_1 - E\left(k\right)\right)$$

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

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

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

example: 2D DOS for parabolic energy bands

$$D_{2D}(E_1)dE = \frac{1}{A}\sum_{\vec{k}} \Delta_{E_1,E_k} \rightarrow D_{2D}(E_1) = g_V \frac{m^*}{\pi\hbar^2}$$ ✓

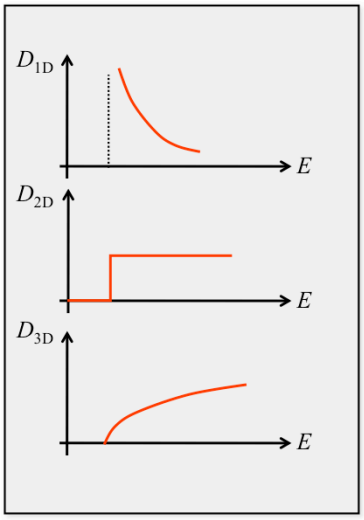
parabolic bands: 1D, 2D, and 3D

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

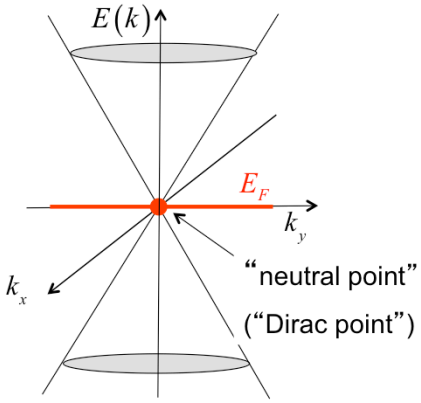
$$D_{2D}(E) = g_V \frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

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

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

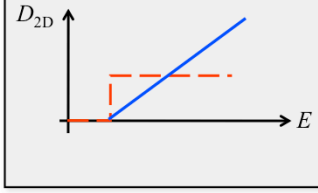


graphene (2D)

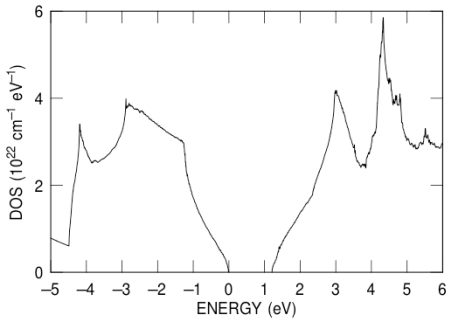


$$E(k) = \pm\hbar\upsilon_F k = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2}$$

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



DOS for bulk Si



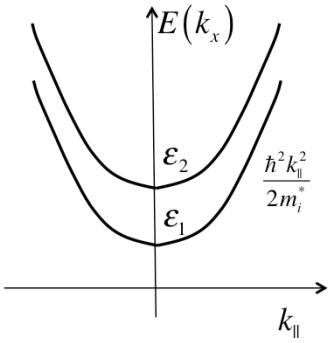
$$D_{3D}(E_1) = \frac{1}{\Omega}\sum_{\vec{k}} \delta_{E_1, E_{\vec{k}}}$$

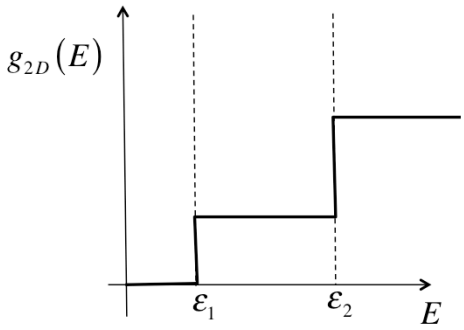
The DOS is calculated with nonlocal empirical pseudopotentials including the spin-orbit interaction.
(Courtesy Massimo Fischetti, August, 2011.)

DOS for a Si quantum well

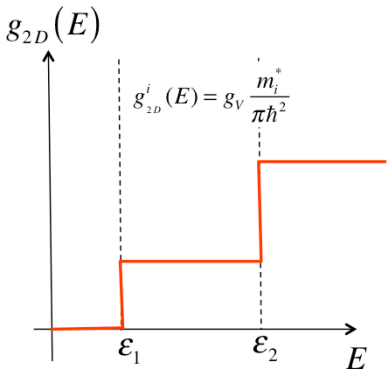
$$E = \varepsilon_i + \frac{\hbar^2 k_{\|}^2}{2m_i^*}$$

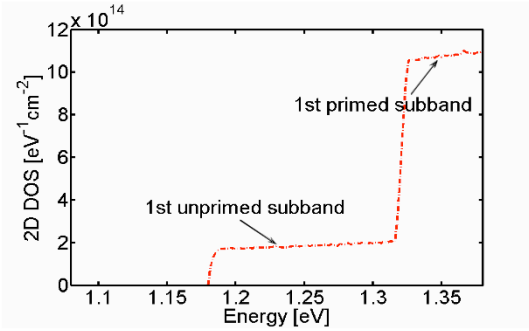
$$g_{2D}^{i}(E) = g_V \frac{m_i^*}{\pi\hbar^2}$$





DOS for a Si quantum well





$sp^3s^*d^5$ TB calculation by Yang Liu, Purdue University, 2007

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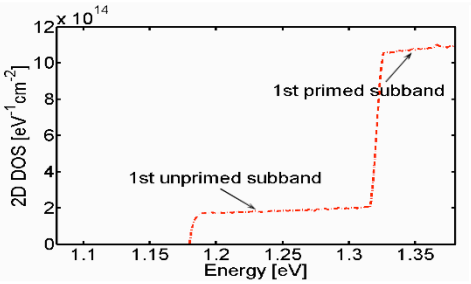

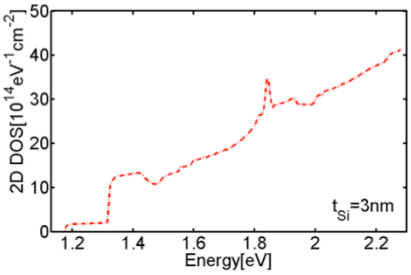

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