Lecture 4: Density of States/
Density of Modes

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA
Datta-Landauer Approach

\[ I = \frac{2q}{\hbar} \int \gamma \pi \frac{D(E)}{2} \left( f_1 - f_2 \right) dE \]

\[ I = \frac{2q}{\hbar} \int T(E) M(E) \left( f_1 - f_2 \right) dE \]

**Key parameters:**

1) Density-of-states (for carrier density)
2) Density of modes (for current)
3) Transmission (to describe scattering)
k-space vs. energy-space

\[ N(k) \, d^3k = \frac{\Omega}{4\pi^3} \, d^3k = D(E) \, dE \]

\( N(k) \): independent of bandstructure

\( D(E) \): depends on \( E(k) \)

\( N(k) \) and \( D(E) \) are proportional to the volume, \( \Omega \), but it is common to express \( D(E) \) per unit energy \textcolor{red}{\textbf{and}} per unit volume. We will use the \textbf{same symbol} in both cases, but the units will be clear from the context.
1) **Density of states**

2) Example: graphene

3) Density of modes

4) Example: graphene

5) Summary
example: 1D DOS

\[ N_{1D}(k)dk = \left( \frac{L}{2\pi} \times 2 \right) dk \]

\[ D_{1D}^+(E)dE = N_{1D}(k)dk / L \]

\[ D_{1D}^+(E)dE = \frac{1}{\pi} dk \]

\[ D_{1D}^+(E) = \frac{1}{\pi} \frac{dk}{dE} = \frac{1}{\pi h \nu} \]

\[ \nu(k) = \frac{1}{h} \frac{dE}{dk} \]

\[ D_{1D}(E) = \frac{2}{\pi h \nu} \]
example: 1D DOS for parabolic bands

\[ E(k) = \frac{\hbar^2 k^2}{2m^*} \]

\[ D_{1D}(E) = \frac{2}{\pi \hbar \upsilon} \]

independent of \( E(k) \)

\[ E(k) = \frac{\hbar^2 k^2}{2m^*} \]

\[ \frac{1}{\hbar} \frac{dE}{dk} = \upsilon = \sqrt{\frac{2E}{m^*}} \]

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density of states in a nanowire

\[ E = \varepsilon_i + \frac{\hbar^2 k^2}{2m^*_i} \]

\[ D_{1D}^{1}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*_i}{(E - \varepsilon_i)}} \]
2D density of states

\[ E = \frac{\hbar^2 k^2}{2m^*} \]

\[ dE = \frac{\hbar^2 kdk}{m^*} \]

\[ N_{2D}(k)dk = \left( \frac{A}{(2\pi)^2} \times 2 \right) dk_x dk_y \]

\[ D_{2D}(E)dE = N_{2D}(k)2\pi kdk/A \]

\[ D_{2D}(E)dE = \frac{1}{2\pi^2} 2\pi kdk \]

\[ D_{2D}(E)dE = \frac{m^*}{\pi\hbar^2} dE \]

\[ D_{2D}(E) = \frac{m^*}{\pi\hbar^2} \]
density of states in a film

\[ E = \varepsilon_i + \frac{\hbar^2 k^2}{2m_i^*} \]

\[ D_{2D}^i(E) = g_V \frac{m_i^*}{\pi \hbar^2} \]

\[ D_{2D}(E) \]
effective mass vs. tight binding

\[ D_{2D}(E) \]

sp\(^3\)s*\(d^5\) tight binding calculation by Yang Liu, Purdue University, 2007

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effective mass vs. tight binding

near subband edge

well above subband edge

sp\textsuperscript{3}s*d\textsuperscript{5} tight binding calculation by Yang Liu, Purdue University, 2007
exercise

\[ E = \varepsilon_1 + E(k_{||}) \]

\[ E_k (1 + \alpha E_k) + \frac{\hbar^2 k_{||}^2}{2 m^*(0)} \]

\[ D_{2D} = ? \]
alternative approach

\[ D_{1D}(E) = \frac{1}{L} \sum_k \delta(E - E_k) \]

\[ D_{2D}(E) = \frac{1}{A} \sum_k \delta(E - E_k) \]

\[ D_{3D}(E) = \frac{1}{\Omega} \sum_k \delta(E - E_k) \]
proof

in k-space, we know:

\[ n_L = \frac{1}{L} \sum_k f_0(E_k) \]

and also work in energy-space:

\[ n_L = \int f_0(E) D_{1D}(E) dE \]

\[ n_L = \int f_0(E) \frac{1}{L} \sum_k \delta(E - E_k) dE \]

\[ n_L = \frac{1}{L} \sum_k \int f_0(E) \delta(E - E_k) dE \]

\[ n_L = \frac{1}{L} \sum_k f_0(E_k) \]
interpretation

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

counts the states between \( E \) and \( E + dE \)
1) Density of states

2) Example: graphene

3) Density of modes

4) Example: graphene

5) Summary
example: DOS for graphene

\[ D(E) = \frac{1}{A} \sum_{k_{\parallel}} \delta(E - E_{k_{\parallel}}) = \frac{1}{A(2\pi^2)} \times 2 \int_{0}^{\infty} \delta(E - E_{k_{\parallel}})2\pi k_{\parallel} dk_{\parallel} \]

\[ E_{k_{\parallel}} = \hbar \nu_{F} k_{\parallel} \quad dE_{k_{\parallel}} = \hbar \nu_{F} dk_{\parallel} \quad k_{\parallel} dk_{\parallel} = E_{k_{\parallel}} dE_{k_{\parallel}} / \hbar^2 \nu_{F}^2 \]

\[ D(E) = \frac{g_{V}}{\pi \hbar^2 \nu_{F}^2} \int_{0}^{\infty} \delta(E - E_{k_{\parallel}}) E_{k_{\parallel}} dE_{k_{\parallel}} \]

\[ D(E) = \frac{2E}{\pi \hbar^2 \nu_{F}^2} \quad E > 0 \]
1) Density of states

2) Example: graphene

3) **Density of modes**

4) Example: graphene

5) Summary
definitions

\[ I = \left\{ \frac{2q^2}{\hbar} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E}\right) dE \right\} V \]

(near-equilibrium)

\[ M(E) = \gamma \pi \frac{D(E)}{2} \]
\[ \gamma(E) = \frac{\hbar}{\tau(E)} \]
\[ T(E) = \frac{\lambda(E)}{\lambda(E) + L} \]
DOS vs. DOM

\[ N = \int D(E) f_0(E) dE \]

\[ G = \int M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \quad (T(E) = 1) \]

Density of states determines the carrier density and density of modes determines the conductance.

1D : \( D(E) \propto L \quad M(E) \propto 1 \)

2D : \( D(E) \propto A \quad M(E) \propto W \)

3D : \( D(E) \propto \Omega \quad M(E) \propto A \)
modes (conducting channels) in 2D

We will assume that \( W \) is wide (small \( W \), is a ‘1D’ nanowire).

\[
M_{2D}(E) = \gamma \pi D_{2D}(E)/2 = ?
\]

\[
\psi(x, y) \propto e^{ik_x x} \sin k_y y
\]

\[
k_y = m\pi / W \quad m = 1, 2, ...
\]

\[
\tan \theta = k_y / k_x
\]
modes (conducting channels) in 2D

\[ M_{2D}(E) = \gamma \pi D_{2D}(E)/2 \]
\[ D_{2D}(E) = A \left( m^*/\pi \hbar^2 \right) \]
\[ (E(k) = \hbar^2 k^2 / 2m^*) \]

\[ \gamma = \hbar/\langle \tau \rangle \]
\[ \langle \cos \theta \rangle = \frac{\int_{-\pi/2}^{+\pi/2} \cos \theta d\theta}{\pi} \]
\[ \gamma = \frac{\hbar \nu}{L} \left( \frac{2}{\pi} \right) \]
\[ \nu = \sqrt{\frac{2(E - \varepsilon_1)}{m^*}} \]

\[ \gamma = \frac{\hbar}{L/\langle v_x \rangle} = \frac{\hbar \nu}{L} \langle \cos \theta \rangle \]
\[ \langle \cos \theta \rangle = \frac{2}{\pi} \]

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modes in 2D

\[ M(E) = \gamma(E) \pi D_{2D}(E)/2 \]

\[ \gamma(E) = \frac{\hbar \nu}{L} \left( \frac{2}{\pi} \right) = \frac{\hbar \sqrt{2(E - \epsilon_1)/m^*}}{L} \left( \frac{2}{\pi} \right) \]

\[ D_{2D}(E) = \frac{m^*}{\pi \hbar^2} WL \]

\[ \gamma \pi D_{2D}/2 = \left( \frac{\hbar}{L} \sqrt{\frac{2(E - \epsilon_1)}{m^*}} \right) \left( \frac{2}{\pi} \right) \pi \left( \frac{m^*}{2 \pi \hbar^2} WL \right) \]

But how do we interpret this result physically?

\[ M_{2D}(E) = W \frac{\sqrt{2m^*(E - \epsilon_1)}}{\pi \hbar} \]
physical interpretation

\[ E(k) = \varepsilon_1 + \frac{\hbar^2 k^2}{2m^*} \]

\[ k(E) = \sqrt{2m^* (E - \varepsilon_1)} \]

\[ k(E) = \frac{2\pi}{\lambda_B(E)} \]

\[
\frac{\sqrt{2m^*(E-\varepsilon_1)}}{\pi \hbar} = \frac{1}{(\lambda_B(E)/2)}
\]

But how do we interpret this result physically?

\[ M_{2D}(E) = W \frac{\sqrt{2m^*(E-\varepsilon_1)}}{\pi \hbar} \]

\[ M_{2D}(E) = \frac{W}{\lambda_B(E)/2} \]
waveguide modes

Assume that there is **one** subband associated with confinement in the $z$-direction. **Many** subbands associated with confinement in the $y$-direction

$$\psi(x, y) \propto e^{ik_yx} \sin k_y y$$

$$k_y = m\pi / W \quad m = 1, 2, ...$$

$M = \# \text{ of electron half wavelengths that fit into } W.$
DOS vs. modes in 2D

\[ D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \theta(E - \varepsilon_i) \]

\[ M_{2D}(E) = \frac{W \sqrt{2m^* [E - \varepsilon_i(0)]}}{\pi \hbar} \theta(E - \varepsilon_1) \]
DOS vs. modes

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

\[ M_{2D}(E) = \frac{W \sqrt{2 m^* \left[ E - \varepsilon_i(0) \right]}}{\pi \hbar} \]

\[ \frac{M_{2D}(E)}{D_{2D}(E)} = \hbar W \sqrt{2 \left[ \frac{E - \varepsilon_i(0)}{m^*} \right]} \]

\[ M(E) = \hbar W D_{2D}(E) v(E) \]

\( M(E) \) is proportional to the DOS(\( E \)) times velocity.
1) Density of states

2) Example: graphene

3) Density of modes

4) **Example:** graphene

5) Summary
We have seen that $M(E)$ depends on dimensionality, but we assumed parabolic energy bands in both cases.

$$E(k) = \varepsilon_1 + \frac{\hbar^2 k^2}{2m^*}$$

But what if our 2D resistor is a sheet of graphene - with linear dispersion?

$$E(k) = \pm \hbar \nu_F k$$

$$\vec{k} = k_x \hat{x} + k_y \hat{y}$$
\[ M(E) = \frac{\gamma(E) \pi D_{2D}(E)}{2} \]

\[ \gamma(E) = \frac{\hbar \nu}{L}\left(\frac{2}{\pi}\right) = \frac{\hbar \nu_F}{L}\left(\frac{2}{\pi}\right) \]

\[ D_{2D}(E) = \frac{2E}{\pi \hbar^2 \nu_F^2} \]

\[ \gamma \pi D_{2D}/2 = \left(\frac{\hbar \nu_F}{L}\right)\left(\frac{2}{\pi}\right)\pi \left(\frac{E}{\pi \hbar^2 \nu_F^2}WL\right) \]

\[ M(E) = \frac{2E}{\pi \hbar \nu_F} = 2 \times \frac{W}{\lambda_B/2} \]

- still proportional to \( W \)
- proportional to \( E \), not \( \sqrt{E} \)
- factor of two is for valley degeneracy

\[ M \text{ depends on dimensionality and on the } E(k). \]
outline

1) Density of states
2) Example: graphene
3) Density of modes
4) Example: graphene
5) Summary
density of states

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

\[ D_{2D}(E) = A \frac{m^*}{\pi \hbar^2} \]

\[ D_{3D}(E) = \Omega \frac{m^* \sqrt{2m^* (E - E_C)}}{2\pi^2 \hbar^3} \]

\[ (E(k) = E_C + \hbar^2 k^2 / 2m^*) \]
modes

\[ M_{1D}(E) = \Theta(E - \varepsilon_1) \]

\[ M_{2D}(E) = W \frac{\sqrt{2m^*(E - \varepsilon_1)}}{\pi \hbar} \]

\[ M_{3D}(E) = A \frac{m^*}{2\pi\hbar^2} (E - E_C) \]

\[ (E(k) = E_C + \hbar^2 k^2 / 2m^*) \]
summary

1) When computing the number of electrons, the important quantity is the density of states, $D(E)$.

2) When computing the current, the important quantity is the number of modes $M(E)$.

3) The number of modes is also the number of subbands at energy, $E$.

4) The number of modes is the number of half wavelengths that fit into the resistor width (2D) or cross section (3D).

5) The number of modes is proportional to $D(E)$ times velocity.