Density of States

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Outline

1) Counting states
2) DOS in k-space vs. DOS in E-space
3) Examples
4) Realistic DOS in semiconductors
5) DOS for phonons
Energy levels in Si

Si atom (At. no. 14)

- 1S^2
- 2S^2
- 2P^6
- 3S^2
- 3P^2
- 4S^0

4 valence electrons

8 valence states

“core levels”
States in a Si crystal

- Only the valence states are of interest to us.
- 3s and 3p orbitals hybridize and produce bonding and anti-bonding states.
- The interaction of the electron wavefunctions in the crystal broadens the discrete energy levels of the isolated Si atoms into energy bands.
Energy levels $\rightarrow$ energy bands

Si atom (At. no. 14) Si crystal

$3P^2$ $3S^2$

$E_C^{\text{top}}$ $E_C^{\text{bot}}$

$E_V^{\text{top}}$ $E_V^{\text{bot}}$

$D_C(E)$ conduction “band”

“forbidden gap”

$s$-like

$p$-like

$D_V(E)$ valence “band”

$D(E)$ tells us how the states are distributed with a band.
States in a finite volume of semiconductor

\[
\begin{pmatrix} 0, L_y, -L_z \\ 0, L_y, 0 \end{pmatrix}
\]

Finite volume, \( \Omega \)  
(*part of an infinite volume*)

Finite number of states

Periodic boundary conditions:

\[
\psi(0,0,0) = \psi(L_x,0,0)
\]
\[ \psi(x) = u_k(x)e^{ik_x x} \]

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

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

\[ k_x = \frac{2\pi}{L_x} j \]

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

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

\[ L_x = Na \quad k_x = \frac{2\pi}{a} j \quad j_{\text{max}} = N \]

"Brillouin zone" \[ 0 < k < \frac{2\pi}{a} \]

\[ k_{\text{max}} = \frac{2\pi}{a} \]
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Density-of-states in k-space

1D:
\[ N_k = 2 \times \left( \frac{L}{2\pi} \right) = \frac{L}{\pi} \quad dk \]

2D:
\[ N_k = 2 \times \left( \frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \quad dk_x \, dk_y \]

3D:
\[ N_k = 2 \times \left( \frac{\Omega}{8\pi^2} \right) = \frac{\Omega}{4\pi^3} \quad dk_x \, dk_y \, dk_z \]
DOS: k-space vs. energy space

States are uniformly distributed in k-space, but non-uniformly distributed in energy space.

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

$D(E)dE = N(k)dk$
**Effect of E(k) on the DOS**

How does non-parabolicity affect DOS(E)?

**“Kane bands”**

\[
E'(1 + \alpha E') = \frac{\hbar^2 k^2}{2m^*(0)}
\]

\[
E' = E - \varepsilon_1
\]
Effect on DOS

Nonparabolicity increases the DOS ($E$).
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DOS(E) for 1D nanowire

Find DOS(E) per unit energy, per unit length, a **single subband** assuming parabolic energy bands.

\[ E = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m^*} \]
Example: 1D (single subband)

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

\[ D_{1D}(E) \frac{\#}{J-m} \]

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

\[ N_k \, dk = \frac{L}{\pi} \, dk \]
1D DOS

\[ D_{1D}(E) dE = \frac{N_k dk}{L} \]

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

\[ dE = \frac{\hbar^2 k dk}{m^*} \quad dk = \frac{m^* dE}{\hbar^2 k} \]

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

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

\[ N_k dk = \frac{L}{\pi} dk \]

\[ E = \varepsilon_n + \frac{\hbar^2 k^2}{2m^*} \]
Don’t forget to multiply by 2

Multiply by 2 to account for the negative k-states.

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

(parabolic energy bands)
Multiple subbands

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

\[ D_{1D}^n (E) = \frac{1}{\pi \hbar} \sqrt{\frac{2m_i^*}{(E - \varepsilon_n)}} \]

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In terms of velocity

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

\[ \nu = \frac{\hbar k}{m^*} = \sqrt{2(E - \varepsilon_n)/m^*} \]

**Exercise:** Show that the final expression is independent of bandstructure.
Example 2: DOS(E) for 2D electrons

Find DOS(E) per unit energy, per unit area, for a single subband assuming parabolic energy bands.

\[ E = \varepsilon_n + \frac{\hbar^2 k_\parallel^2}{2m^*} \]
Example 2: DOS(E) for 2D electrons

\[
D(E)dE = \frac{N(k)}{A} dk^2
\]

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

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

Exercise: Show that:

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

Area of each state in k-space:

\[
\frac{4\pi^2}{A}
\]
Valley degeneracy

Conduction band of Si:
6 equivalent valleys: \( g_V = 6 \) (bulk)

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

\[
\Rightarrow g_v m^*_D \sqrt{2m^*_D (E-E_C)} \Theta(E-E_C)
\]

\[
m^*_D \equiv \left( m_\ell m_t \right)^{1/3}
\]
Parabolic bands: 1D, 2D, and 3D

\[ D_{1D}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{E - \epsilon_1}} \Theta(E - \epsilon_1) \]

\[ D_{2D}(E) = g_V \frac{m^*}{\pi \hbar^2} \Theta(E - \epsilon_1) \]

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

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

Exercise: Show that for graphene, the 2D DOS is:

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

\[ E(k) = \pm \hbar v_F k = \pm \hbar v_F \sqrt{k_x^2 + k_y^2} \]
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4) **Realistic DOS in semiconductors**
5) DOS for phonons
DOS for bulk Si

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

\[ E = \varepsilon_j + \frac{\hbar^2 k_{\parallel}^2}{2m_n^*} \]

\[ D_{2D}^j(E) = g_{Vj} \frac{m_n^*}{\pi\hbar^2} \]

\[ E(k_{\parallel}) \]

\[ \varepsilon_1 \]

\[ \varepsilon_2 \]

\[ \frac{\hbar^2 k_{\parallel}^2}{2m_i^*} \]

unprimed

primed

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

\[ g_V = 4 \]

\[ g_V = 2 \]

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DOS for a Si quantum well

\[ D_{2D}^j (E) = g v_j \frac{m_j^*}{\pi \hbar^2} \]

\[ E \]

\[ \varepsilon_1 \quad \varepsilon_2 \]

sp\textsuperscript{3}s\textsuperscript{*}d\textsuperscript{5} TB calculation by Yang Liu, Purdue University, 2007
DOS for a Si quantum well

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

**Exercise:** Show that the DOS for 3D phonons assuming a linear dispersion is

\[
D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2(\hbar\nu_s)^3} \left( J\cdot m^3 \right)^{-1}
\]
Realistic phonon DOS (Si)

\[ D_{ph}(\hbar \omega) \propto E^2 \]

Near room temperature and above, all states are occupied.

(Figure provided by J. Maassen, Dalhousie Univ., CA, 2017)
Summary

1) DOS in energy depends on dimension \textbf{and} on the dispersion.

2) The DOS becomes complicated at high energies.

3) The phonon DOS is generally complicated over the relevant energy range.