# Density of States Derivation

The density of states gives the number of allowed electron (or hole) states per volume at a given energy. It can be derived from basic quantum mechanics.
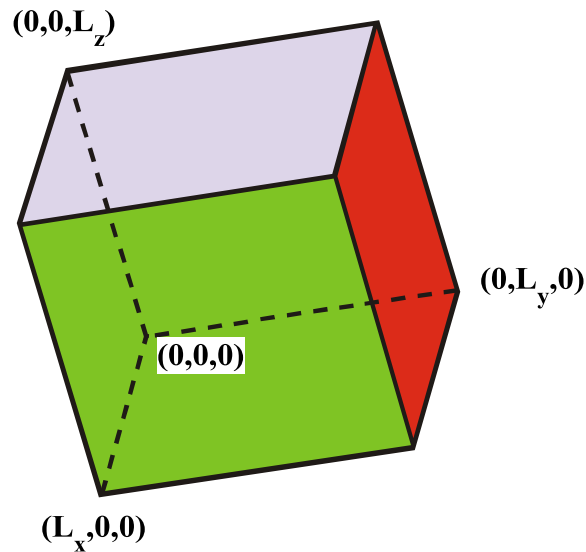
**Electron Wavefunction**

The position of an electron is described by a wavefunction $\psi(x, y, z)$. The probability of finding the electron at a specific point (x,y,z) is given by $|\psi(x, y, z)|^2$, where total probability $\int_{\substack{all \\ space}} |\psi(x, y, z)|^2 dxdydz$ is normalized to one.

**Particle in a Box**

The electrons at the bottom of a conduction band (and holes at the top of the valence band) behave approximately like free particles (with an effective mass) trapped in a box. We will consider here conduction band electrons, but the result for holes is similar. For our parabolic conduction band:

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



For electrons in a rectangular volume $L_x$ by $L_y$ by $L_z$ with an infinite confining potential ((U(x,y,z)=0 inside the box and $\infty$ outside), the electron wavefunction $\psi$ must go to zero on the boundaries, and takes the form of a harmonic function within the region. The wavefunction solution is:

$$\psi(x, y, z) = \sin(k_x x)\sin(k_y y)\sin(k_z z) \tag{1}$$

and $k_x$, $k_y$, and $k_z$ are the wavevectors for an electron in the x, y, and z directions. The real wavefunction in a solid is more complex and periodic (with the crystal lattice), but this is a good approximation for the parabolic regions near the band edges.
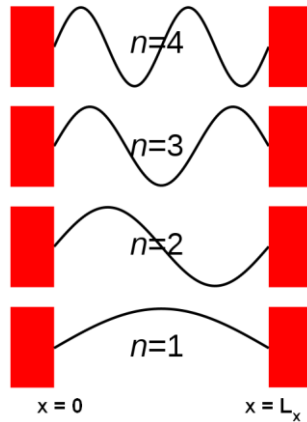


First 4 particle in a box wavefunctions across the x direction.
Orthogonal directions are analogous.

Enforcing the boundary conditions: At x, y, or z = 0, the sine functions go to zero. At the opposite boundaries of the rectangular region, $\sin(k_x L_x) = 0$, $\sin(k_y L_y) = 0$, and $\sin(k_z L_z) = 0$ for the x, y, and z directions. The allowed wavevectors satisfy:

$$k_x L_x = \pi n_x, k_y L_y = \pi n_y, k_z L_z = \pi n_z, \text{ for } n_x, n_y, n_z \text{ integers} \qquad (2)$$

**K Space**

The allowed states can be plotted as a grid of points in k space, a 3-D visualization of the directions of electron wavevectors. Allowed states are separated by $\pi / L_{x,y,z}$ in the 3 directions in k space.

The k space volume taken up by each allowed state is $\pi^3 / L_x L_y L_z$. The reciprocal is the state density in k space (# of states per volume in k space), $V / \pi^3$ where $V$ is the volume of the semiconductor (in real space).

The number of states available for a given magnitude of wavevector |k| is found by constructing a spherical shell of radius |k| and thickness $dk$. The volume of this spherical shell in k space is $4\pi k^2 dk$.
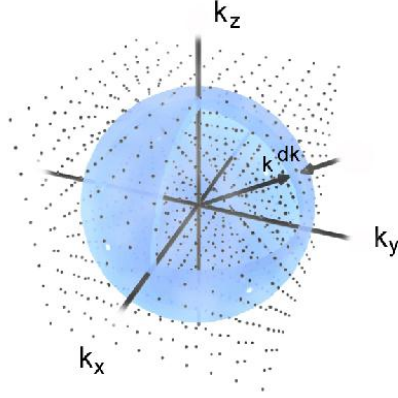
Allowed wavevector states in k space form a lattice.
A spherical shell gives the number of allowed states at a specific radius |k|.

The number of k states within the spherical shell, $g(k)dk$, is (approximately) the k space volume times the k space state density:

$$g(k)dk = 4\pi k^2 \left[\frac{V}{\pi^3}\right] dk \qquad (3)$$

Each k state can hold 2 electrons (of opposite spins), so the number of electron states is:

$$g(k)dk = 8\pi k^2 \left[\frac{V}{\pi^3}\right] dk \qquad (4a)$$

Finally, there is a relatively subtle issue. Wavefunctions that differ only in sign are indistinguishable. Hence we should count only the positive $n_x$, $n_y$, $n_z$ states to avoid multiply counting the same quantum state. Thus, we divide (4a) by 1/8 to get the result:

$$g(k)dk = \pi k^2 \left[\frac{V}{\pi^3}\right] dk = \left[\frac{Vk^2}{\pi^2}\right] dk \qquad (4b)$$

This is an expression for the number of unique electron states available at a given $|k|$ over a range $dk$. We need an expression in terms of energy rather than wavevector k. We proceed from the relationships between wavevector, momentum $p$, and energy $E$:

$$p = \hbar k , E = p^2 / 2m^* \quad E = \frac{\hbar^2 k^2}{2m^*} \qquad (5)$$

with $m^*$ as the effective mass. Rewriting, and noting that the energy of carriers in the conduction band is given with respect to the conduction band edge energy $E_c$:

$$k^2 = \frac{(E - E_c)2m^*}{\hbar^2} \qquad (6)$$

Differentiating:

$$2kdk = \frac{2m^* dE}{\hbar^2} \qquad (7a)$$

Combining (6) and (7a):

$$dk = \frac{2m^* dE}{2k\hbar^2} = \frac{m^* dE}{k\hbar^2} = \frac{m^* dE}{\hbar^2 \sqrt{2m^*(E - E_c)/\hbar^2}}$$
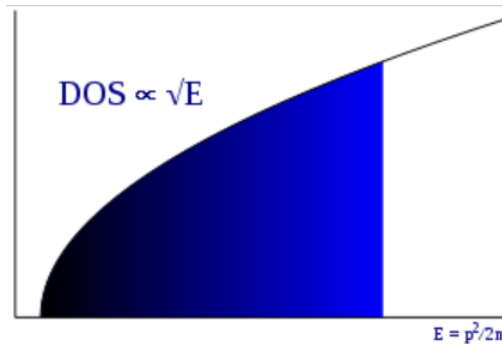
$$= \frac{m^* dE}{\hbar\sqrt{2m^*(E - E_c)}} \tag{7b}$$

Plugging (6) and (7) into (4b):

$$g(k)dk = \frac{Vk^2}{\pi^2} \frac{m^* dE}{\hbar\sqrt{2m^*(E - E_c)}}$$

$$= \frac{V\left[2m^*(E - E_c)/\hbar^2\right]\left(m^* dE\right)}{\pi^2\hbar\left[2m^*(E - E_c)\right]^{1/2}} \tag{8}$$

$$= \frac{Vm^*\left[2m^*(E - E_c)\right]^{1/2}}{\pi^2\hbar^3} dE$$

Dividing through by $V$, the number of electron states in the conduction band per unit volume over an energy range $dE$ is:

$$g(E)dE = \frac{m^*\left[2m^*(E - E_c)\right]^{1/2}}{\pi^2\hbar^3} dE \tag{9}$$

This is equivalent to the density of the states given without derivation in the textbook.



DOS ∝ √E

E = p²/2m

3-D density of states, which are filled in order of increasing energy.

## Dimensionality

The derivation above is for a 3 dimensional semiconductor volume. What happens if the semiconductor region is very thin and effectively 2 dimensional?

Confining the electron in the $x$-$y$ plane, the wavevector $z$ component $k_z = 0$. The allowed states in k space becomes a 2 dimensional lattice of $k_x$ and $k_y$ values, spaced $\pi/L_{x,y}$ apart. The 2-D k space area taken up by each state is $\pi^2/L_x L_y$. The number of states per area in k space is $A/\pi^2$ with $A$ as the real-space area of the thin semiconductor.

The number of states available at a given |k| is found using an annular region of radius |k| and thickness *dk* rather than the spherical shell from the 3-D case. There is a factor of ¼ due to the equivalent nature of the +/- states (just as there was 1/8 in the 3D case). The area is $\pi k dk$. The number of k space states is:

$$g(k)dk = \left[\frac{A}{\pi^2}\right] 2\pi k dk \times 2 \text{ spin states} \div 4 \text{ equivalent states} = k\left[\frac{A}{\pi}\right]dk \qquad (10)$$

Converting to energy using (7b):

$$g(k)dk = k\left[\frac{A}{\pi}\right]dk = \frac{A\left[2m^*\left(E-E_c\right)/\hbar^2\right]^{1/2}}{\pi}\left(\frac{m^*}{\hbar\left[2m^*\left(E-E_c\right)\right]^{1/2}}\right)dE \qquad (11)$$

Cleaning up and dividing through by area, the density of states per area at an energy *E* over a range *dE* is:

$$g(E)dE = \frac{m^* dE}{\pi\hbar^2} \qquad (12)$$

Unlike the 3-D case, this expression is independent of energy *E*!

In a real structure (which is not perfectly 2-D), there are finite energy ranges over which the energy independence holds (the derivation holds for each single, well separated possible value of $k_z$). The resulting density of states for a quantum well is a staircase, as below in red.

Further restriction of the semiconductor dimensionality to 1-D (quantum wire) and 0-D (quantum dot) results in more and more confined density of states functions.
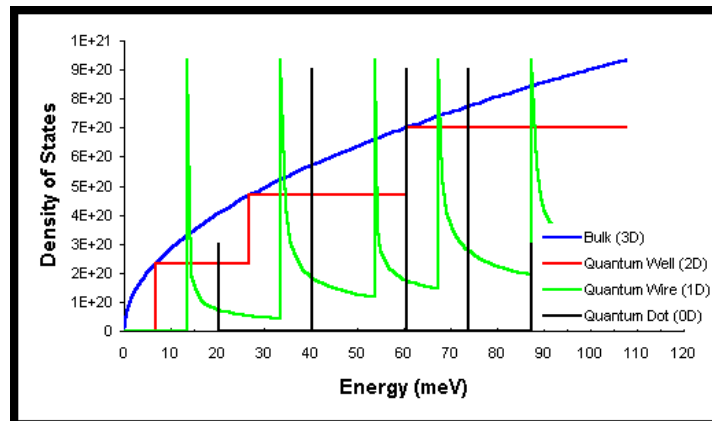


Density of states for 0-D through 3-D regions.

Low dimensional and confining nanostructures have lots of applications controlling carriers in semiconductor devices.