**Density of States $D(E)$**

$D(E) =$ Number of electron states (or phonon modes) per energy interval

$D(E)$ is derived via **box quantization**, which produces a square grid of states in $k$-space, spaced by $\delta k = 2\pi/L$ (L= size of the box).

The density of $k$-points is: $n = 1/\delta k^3 = (L/2\pi)^3$

Two ways to calculate $D(E)$:

A) $D(E) = dN/dE$, $N(E) = n \int d^3k$

(Integration over the $k$-volume with $E(k) \leq E$)

B) $D(E) \propto n \int |v_g|^{-1} d^2k$

(Integration over the $k$-surface with $E(k) = E$)

This form of $D(E)$ shows that flat bands have high density of states, and steep bands low $D(E)$.

**$D(E)$ for free electrons** in various dimensions:

As the dimensionality is reduced, $D(E)$ becomes more singular at the bottom of the band. Zero-dimensional electrons have sharp energy levels like atoms and molecules. They can be represented by $\delta$-functions, something even more singular than the $1/\sqrt{E}$ singularity.

**Acoustic phonons** as example, using method B) in spherical symmetry ($|p| = p$):

1) $E(k) = v_s \cdot p = v_s \cdot \hbar k$ \hspace{1cm} $v_s =$ sound velocity

2) $|v_g| \propto \frac{dE/dk} \propto v_s$

3) Convert $k$ to $E$ by inverting $E(k)$ to $k(E)$:

$E(k) = v_s \cdot \hbar k \Rightarrow k(E) = E / \hbar v_s$

The $k$-integration takes place over a sphere with area $4\pi k^2$ (where the integrand is constant). After integrating one must convert the variable $k$ to the variable $E$:

$D(E) \propto n \cdot |v_g|^{-1} \cdot 4\pi k^2 \propto n \cdot v_s^{-1} \cdot (E/v_s)^2 \propto L^3 v_s^{-3} \cdot E^2$
Density of states for phonons in silicon (top), obtained from the band dispersion (bottom).

Bands with low $v_g$ have high $D(E)$. $k$-points with $v_g=0$ produce van Hove singularities in $D(E)$.

The Debye approximation is matched to acoustic phonons, using the dashed quadratic density of states calculated on the previous page. The upper cutoff is placed such that the area under the dashed curve is the same as for the real acoustic phonon spectrum (full line). The energy of this cutoff $E_{cut} = k_B \Theta_D$ corresponds to the average phonon energy. It defines the Debye temperature $\Theta_D$.

Typical Debye temperatures are listed below. Strong covalent bonding corresponds to a large force constant $f$ and high $\Theta_D$:

<table>
<thead>
<tr>
<th>Material</th>
<th>$\Theta_D$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diamond</td>
<td>2230</td>
</tr>
<tr>
<td>Si</td>
<td>640</td>
</tr>
<tr>
<td>Al</td>
<td>428</td>
</tr>
<tr>
<td>Au</td>
<td>170</td>
</tr>
<tr>
<td>Pb</td>
<td>105</td>
</tr>
</tbody>
</table>

\[ E_{cut} = k_B \Theta_D \]