

Energy Bands of Electrons and Phonons

**Ground State** of a Solid

<table>
<thead>
<tr>
<th>property</th>
<th>measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>charge density</td>
<td>( \rho )</td>
</tr>
<tr>
<td>spin density</td>
<td>( \rho^\uparrow - \rho^\downarrow )</td>
</tr>
<tr>
<td>total energy</td>
<td>( U )</td>
</tr>
<tr>
<td>magnetic moment</td>
<td>( -\partial U/\partial B )</td>
</tr>
<tr>
<td>bulk modulus</td>
<td>( \partial^2 U/\partial V^2 )</td>
</tr>
</tbody>
</table>

**Excited State** of a Solid

<table>
<thead>
<tr>
<th>quasiparticle</th>
<th>wave, oscillating quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>electron, hole</td>
<td>wave function ( \psi_e, \psi_h )</td>
</tr>
<tr>
<td>photon</td>
<td>electromagnetic field ( A )</td>
</tr>
<tr>
<td>phonon</td>
<td>atomic displacement ( \delta r )</td>
</tr>
<tr>
<td>plasmon</td>
<td>charge density ( \rho )</td>
</tr>
<tr>
<td>magnon</td>
<td>magnetization ( M )</td>
</tr>
<tr>
<td>polariton = photon / phonon</td>
<td>polarization ( P )</td>
</tr>
<tr>
<td>polaron = electron + phonon</td>
<td>( \psi_e + \delta r )</td>
</tr>
<tr>
<td>exciton = electron + hole</td>
<td>( \psi_e + \psi_h )</td>
</tr>
</tbody>
</table>

Fundamental excitations in a solid are fully characterized by **quantum numbers**, such as **energy** \( E \), **momentum** \( p \), spin \( \sigma \), and angular symmetries ( = point group symmetry). These are usually displayed as the **band dispersion** \( E(k) \) which contains labels for spin and symmetry.

Particle-wave duality in quantum mechanics says that each **wave** \( \psi = A \cdot \exp[i(kr - \omega t)] \) corresponds to a **quasiparticle** with energy \( E = \hbar \omega \) and momentum \( p = \hbar k \).

In a periodic crystal a plane wave becomes a **Bloch function** \( \psi_{\text{Bloch}} = u_k(r) \exp[i(kr - \omega t)] \) where \( u_k(r) \) is a **periodic** function. It can be expanded into a Fourier series that is summed over reciprocal lattice vectors \( G \): \( u_k(r) = \Sigma_G u_G \exp[i(Gr)] \)
Energy Bands $E(k)$

Electrons in Silicon:

![Electron Band Structure Diagram]

Phonons in Silicon:

![Phonon Frequency Diagram]
Density of States \( D(E) \)

\( D(E) = \) number of states (\( = \) modes) per energy interval. The density of states in \( k \)-space is constant, with a spacing \( \delta k = 2\pi/L \) between states. Electrons have two spin states (\( \uparrow, \downarrow \)).

**General Case (3D):** \( D(E) \sim \int \frac{1}{|v_{\text{group}}(k)|} \, dS \)

Integrate over the surface \( S \) in \( k \)-space where \( E(k) = \) constant = \( E \).

\( v_{\text{group}} = 0 \) leads to van Hove singularities in \( D(E) \).

**Spherical Symmetry (3D):** \( D(E) = \frac{dn}{dE} = \frac{(dn/dp)/(dp/dE)}{p(E)/v_{\text{group}}(E)} \approx \frac{p^2(E)}{v_{\text{group}}(E)} \)

\( S = \) sphere with area \( 4\pi p^2 \). Convert the variable \( p \) to \( E \) by inverting \( E(p) \) to \( p(E) \).

Examples:

**Acoustic phonons:**

\( E = v_{\text{sound}} \cdot p \rightarrow p^2(E) = (v_{\text{sound}})^2 \cdot E^2 \), \( v_{\text{group}} = v_{\text{sound}} \), \( D(E) \sim (v_{\text{sound}})^{-3} \cdot E^2 \)

**Free electrons** in various dimensions:

\[
\begin{align*}
\text{3D:} & & \quad \sqrt{E} \\ 
\text{2D:} & & \quad 1 \\ 
\text{1D:} & & \quad 1/\sqrt{E}
\end{align*}
\]

Density of states for phonons in silicon (top), obtained from the band dispersion (bottom).

Bands with low \( v_{\text{group}} \) produce high density of states.

The Debye approximation emphasizes acoustic phonons, the Einstein approximation optical phonons.
Phonon Modes

Phonon frequency: $\omega \approx \sqrt{\kappa/m}$ $\kappa$ = force constant, $m$ = mass (harmonic oscillator).

Measure $E(k)$ from the $E,k$ transfer in inelastic neutron scattering.

Phonon modes:
1. Transverse: $\delta r \perp k$
   Longitudinal: $\delta r \parallel k$
2. Acoustic: In Phase
   Optical: Out of Phase

N atoms per unit cell $\rightarrow$ 3N phonon bands $\quad$ (Each atom can move in x, y, z.)