Quasiparticles in Solids: Electrons, Phonons, Plasmons, …

**Ground state** properties of a solid (can be measured by elastic scattering, \( \delta E = 0 \))

<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>force constant</td>
<td>( f = \partial^2 U/\partial r^2 )</td>
</tr>
</tbody>
</table>

**Excited state** properties of a solid (require excitation by inelastic scattering, \( \delta E \neq 0 \))

<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>vibration amplitude ( \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</td>
<td>electric polarization ( P )</td>
</tr>
<tr>
<td>polaron</td>
<td>( \psi_e ) and ( \delta r )</td>
</tr>
<tr>
<td>exciton</td>
<td>( \psi_e ) and ( \psi_h )</td>
</tr>
</tbody>
</table>

All quasiparticles (= excitations in a solid) are fully characterized by **quantum numbers**:

\[
\text{Energy } E = \hbar \omega, \quad \text{momentum } p = \hbar k
\]

and angular symmetry (given by the point group).

These can be displayed by the **band dispersion** \( E(k) \) with labels for spin and symmetry.
Band Dispersion $E(k)$:

Electrons in Silicon

Band Gap $E_G$

Conduction Band

Valence Band

For the $k$-axis labels see the fcc Brillouin zone in Lecture 10, Slide 3.
**Phonon Bands in the Diamond Structure:**

The diamond structure has two atoms per unit cell, which have $2 \cdot 3 = 6$ degrees of freedom. Therefore, there are **6 branches**: $2\text{TA}$, $2\text{TO}$, $1\text{LA}$, $1\text{LO}$.

The general properties of various phonon modes are:

- For transverse phonons the atoms move perpendicular to the $\mathbf{k}$-vector (= propagation direction)
- For acoustic phonons two atoms in the same unit cell have the same phase, for optical phonons the two are out of phase.
- Atoms in adjacent unit cells have the same phase at the Brillouin zone center $\mathbf{k}=0$. They are out of phase at the zone boundary $\frac{1}{2}\mathbf{G}_{hkl}$ and back in phase at $\mathbf{G}_{hkl}$.

At the zone center:

**TA phonons:**

```
\[ \delta \mathbf{r} \rightarrow \mathbf{k} \]
```

**TO phonons:**

```
\[ \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \]
```

At the zone boundary:

**TA phonons (heavy atom moves):**

```
\[ \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \rightarrow \delta \mathbf{r} \]
```

**TO phonons (light atom moves):**

```
\[ \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \]
```
**Calculation of \( \omega(k) \) for Phonons:**

Consider the simplest case, a linear chain of equal atoms with only nearest neighbors interacting with each other. Start with one unit cell and then connect the unit cells using a plane wave ansatz. Each atom is displaced from the lattice, plus the atoms are displaced relative to each other.

\[
\begin{align*}
\text{u}_n &= \text{u} \cdot e^{i(kn\text{a} - \omega t)} \\
\text{e}^{i(kr - \omega t)}, r &= n \text{a}
\end{align*}
\]

(1) **Hooke’s law:**
\[
F_n = f \cdot (u_{n+1} - u_n) + f \cdot (u_{n-1} - u_n)
\]

(2) **Newton:**
\[
F_n = M \cdot \frac{d^2 u_n}{dt^2}
\]

(3) **Plane wave ansatz:**
\[
F_n = \frac{2f}{M} \cdot \left(2 - \cos(k\text{a})\right) \cdot u_n
\]

\[
\omega = (2f/M)^{\frac{1}{2}} \cdot \left(1 - \cos(k\text{a})\right)^{\frac{1}{2}} = 2(f/M)^{\frac{1}{2}} \cdot |\sin(k\text{a})|
\]

This describes an acoustic phonon:

Classical physics gets the shape of the phonon bands right, but to calculate the force constant \( f \) and the lattice constant \( a \) one needs quantum physics. With density functional theory (DFT) one can obtain both \( f \) and \( a \) by calculating the total energy \( U \) as a function of the bond length.
General Properties of Waves:

Particle-wave duality in quantum physics connects each particle with energy \( E = \hbar \omega \) and momentum \( p = \hbar k \) to a plane wave \( \psi(r,t) = A \cdot \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)] \).

Velocity and Effective Mass

\[ v_{ph} = \frac{E}{|p|} = \frac{\omega}{|k|} \]

**Phase velocity**, for the propagation of an infinite plane wave.

\[ \mathbf{v}_g = \frac{\partial E}{\partial p} = \frac{\partial \omega}{\partial k} \]

**Group velocity**, for the propagation of a wave packet.\[ = \text{slope of } E(p) \]

It determines the speed of signals and of energy transport \( (v_g \leq c) \).

\[ m^* = \frac{1}{\partial^2 E/\partial p^2} \]

**Effective mass**, modeled after the kinetic energy \( E = p^2/2m \).\[ = \text{inverse curvature of } E(p) \]

A wave packet spreads over time, if the phase velocity depends on the frequency \( \omega \) ("dispersion"). Waves with higher frequency tend to move faster due to their higher energy \( E = \hbar \omega \). The center of a wave packet moves with the group velocity \( v_g \). That determines how fast a signal pulse propagates.

Solitons

In a non-linear medium, the phase velocity depends on the amplitude. The spread of a wave packet due to dispersion can be compensated by an opposite spread due to non-linearity. In the figure above the low frequency components with high amplitude are able to catch up with the weaker high frequency components if the phase velocity increases with amplitude. The result is a wave packet that does not change over time. Solitons are used in long distance communications via fiber optics. A tsunami is a soliton.