Polaritons, polarons, excitons

Transverse optical phonons will couple to photons with the same ω and *k*.



Light Bragg reflects off the sound wave; sound Bragg reflects off the light wave.

The dispersion relation for light

$$\varepsilon \varepsilon_0 \mu_0 \omega^2 = \frac{\varepsilon \omega^2}{c^2} = k^2$$

For an insulator

 $\epsilon_r(\omega) = \epsilon(\infty) + rac{\omega_0^2(\epsilon(0)-\epsilon(\infty))}{\omega_0^2-\omega^2+i\gamma\omega}$



Ignore the loss term $i\gamma\omega$

$$\varepsilon(\omega) = \varepsilon(\infty) + \frac{\omega_0^2 \left(\varepsilon(0) - \varepsilon(\infty)\right)}{\omega_0^2 - \omega^2}$$

Multiply through by $\omega_0^2 - \omega^2$
$$\varepsilon(\omega) = \frac{\varepsilon(\infty) \left(\omega_0^2 - \omega^2\right)}{\omega_0^2 - \omega^2} + \frac{\omega_0^2 \left(\varepsilon(0) - \varepsilon(\infty)\right)}{\omega_0^2 - \omega^2}$$

Define $\omega_L \quad \omega_0^2 \varepsilon(0) = \varepsilon(\infty) \omega_L^2$
$$\varepsilon(\omega) = \varepsilon(\infty) \frac{\omega_L^2 - \omega^2}{\omega_0^2 - \omega^2}$$

$$\varepsilon(\infty)\frac{\omega_L^2-\omega^2}{\omega_0^2-\omega^2}\frac{\omega^2}{c^2}=k^2$$



There are two solutions for every *k*, one for the upper branch and one for the lower branch.

A gap exists in frequency.

Polaritons are the normal modes near the avoided crossing.

Polaritons allow us to study the properties of phonons using optical measurements



By looking at the reflectance in different crystal directions, you can determine the frequencies of the transverse optical phonons.

Polarons

A polaron is a quasiparticle consisting of an electron and an ionic polarization field. The electron density is low so the screening by electrons can be neglected.



Electronic charge is partially screened by lattice ions. This is a charge - phonon coupling.

Large polaron (Fröhlich polaron)

The spatial extent of the polaron is much larger than the lattice constant.

Large polarons typically form bands.



Electrons move in bands with a large effective mass (432 m_e for NaCl)

Small polaron (Holstein polaron)

For a small polaron, the polarization is about the size of the lattice contant.



Small polaron - Holstein Hamiltonian - electrons are localized and hop (thermally activated or tunneling). Small polarons often form in organic material. In soft materials the energy for making a distortion is smaller.

Bipolarons

Two polarons can bind together to form a bipolaron (a quasiparticle).

Elastic strain energy is reduced by sharing the polarization field.

Bipolarons have integral spin -> they are bosons.

It is possible that the condensation of bipolarons into the same ground state could lead to superconductivity.

Bipolarons



Figure 10. Evolution of the polypyrrole band structure upon doping: (a) low doping level, polaron formation; (b) moderate doping level, bipolaron formation; (c) high (33 mol %) doping level, formation of bipolaron bands.

J. L. Breda and G. B. Street, Acc. Chem. Res. 1985, 18, 309-315.

Excitons

Bound state of an electron and a hole in a semiconductor or insulator



Mott-Wannier Excitons

Bound state of an electron and a hole in a semiconductor or insulator (like positronium)



Excitons



Gross & Marx

Excitons



See: C. D. Jeffries, Electron-Hole Condensation in Semiconductors, Science 189 p. 955 (1975).

A Frenkel exciton is localized on an atom or molecule in a crystal.

The band gap of solid krypton is 11.7 eV. Lowest atomic transition in the solid is 10.17 eV.

Excitons transport energy but not charge. Frenkel excitons are occur in organic solar cells, organic light emitting diodes, and photosynthesis.