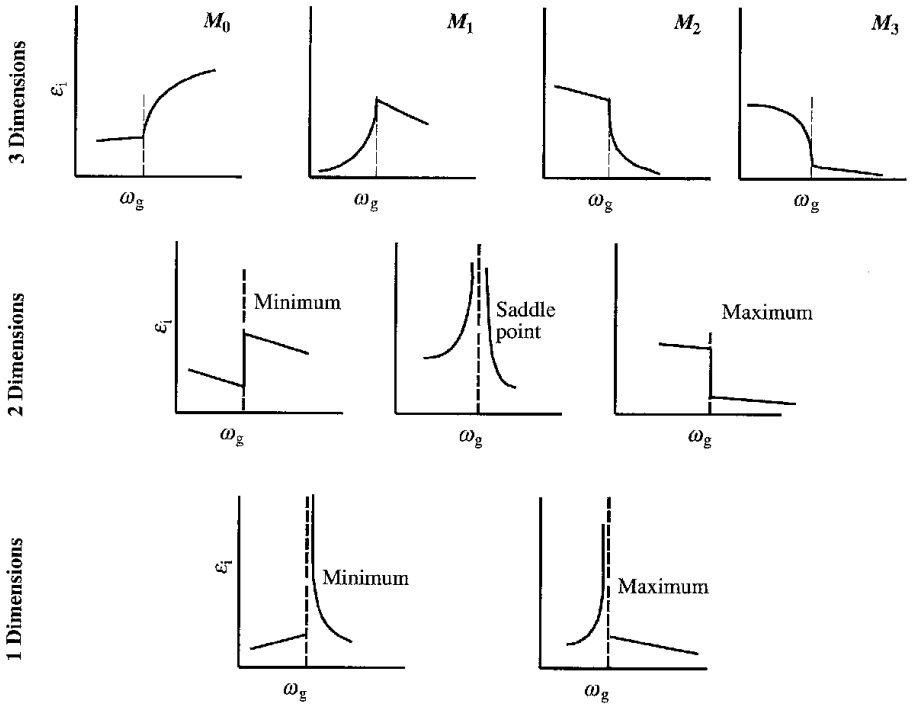
6.2.4. Van Hove Singularities

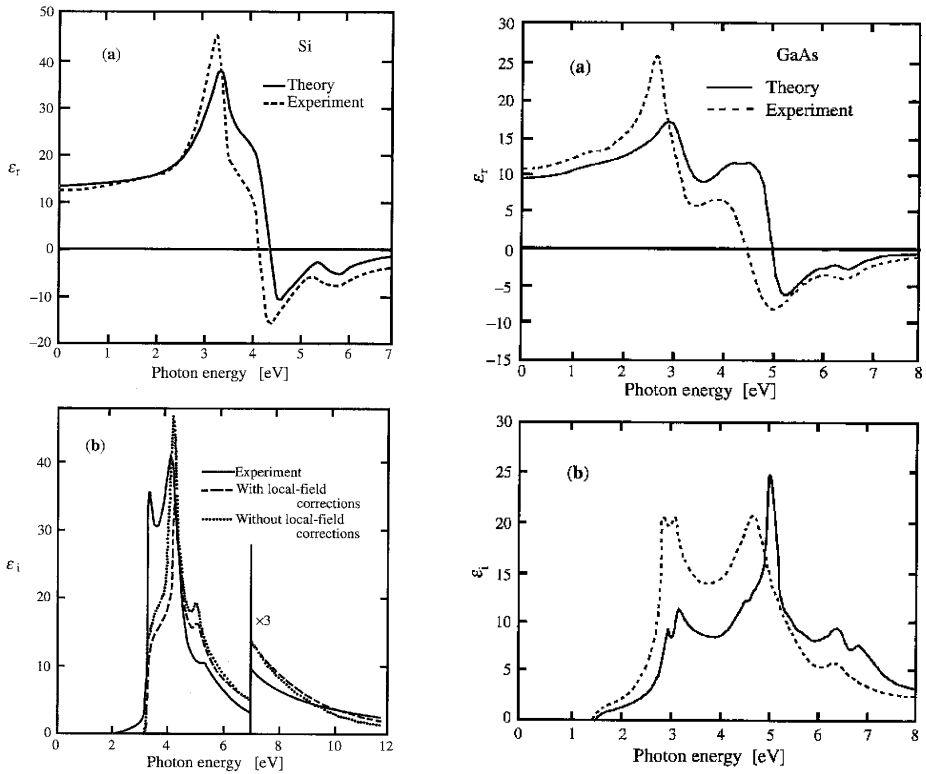
Van Hove singularities in DOS arise from $|\nabla_{\mathbf{k}}| \rightarrow 0$ and are called critical points. Assume $\mathbf{k} = 0$ is a critical point and expand

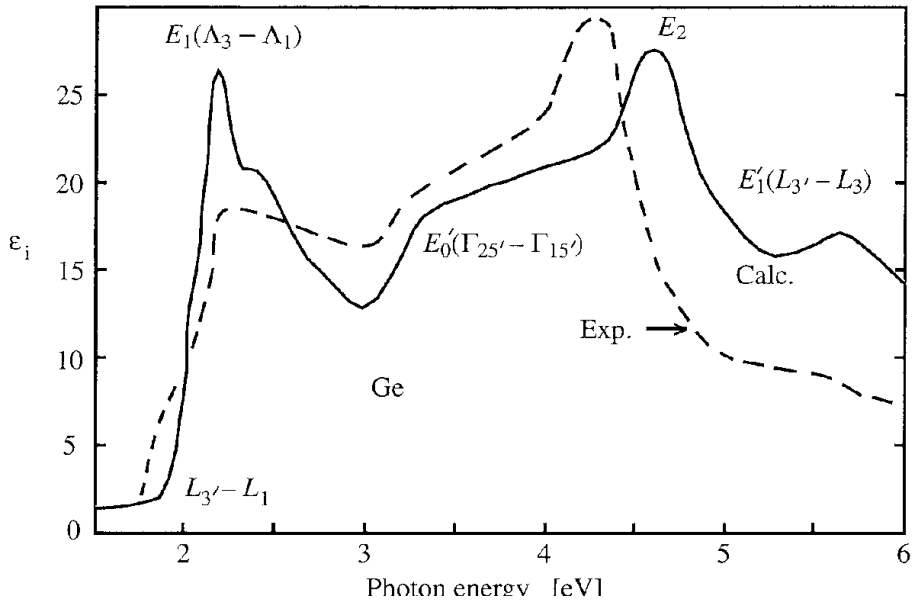
Note! $D_j(E) \propto \varepsilon_i(E) \propto$ absorption.

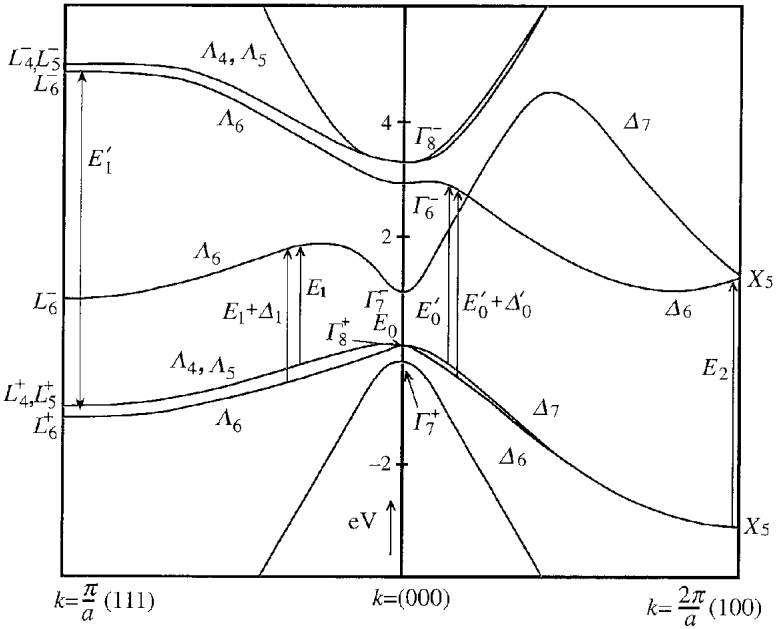


Concepts and common features in absorption, ε_i :

- *fundamental absorption edge:* the lowest energy transitions over the *fundamental band gap* E_g,
  - direct E_0 strong $\Gamma_{4v} \leftrightarrow \Gamma_{1c}$ in zinc-blende & dia
  - indirect weaker
  - may involve split-off $E_0 + \Delta_0$
- E_1 transition involving M_1 type critical point, $\langle 111 \rangle$-direction $E_1 + \Delta_1$ ($\Delta_1 \approx 2/3\ \Delta_0$)
- E_2 transition, usually absolute maximum, may involve M_2 type critical point, $\langle 100 \rangle$- and $\langle 110 \rangle$-directions
- E_0' and E_1' transitions from valence to higher conduction b







Naming system by Cardona:

6.2.5. Direct Absorption Edges

For the direct band gap semiconductor let us expand the conduction band and valence band at Γ-point assuming spherical symmetry as

$$E_c(k) = E_{CBM} + (\hbar^2/2m_c)\, k^2$$

and

$$E_v(k) = E_{VBM} - (\hbar^2/2m_v)\, k^2,$$

where m_v and m_v are the respective effective masses. These lead, in the vicinity of the band gap, to the transition energy

6.2.6. Indirect Absorption Edges

Transitions over the indirect fundamental band gap can be mediated by phonons to obey the conservation laws. If E_p and $\mathbf{Q}$ are the phonon energy and wavevector, then

$$\hbar\omega = E_{cv} \pm E_p$$

and (6.60)

$$\mathbf{k}_c - \mathbf{k}_v = \pm(-\mathbf{Q})$$

are the conservation conditions for phonon-assisted indirect transitions, where the upper and lower signs correspond to absorption and emission of a photon, respectively.

Consider Si and indirect transition $|0\rangle$ to $|f\rangle$ via an intermediate virtual state $|i\rangle = |\Gamma_{15}\rangle$ or $|\Delta_5\rangle$, i.e., $|0\rangle \rightarrow |i\rangle \rightarrow |f\rangle$.

The second order perturbation theory gives the next higher order term to Fermi's Golden Rule

6.2. Excitons

So far, we have described the created electron–hole pairs with the delocalized one-electron Bloch wavefunctions. However, the created e–h pair may lower the total energy by a hydrogen atom or positronium like localized quantum state. This bound or correlated electron–hole pair is called exciton.

In case of strong Coulomb attraction the exciton may localize in a unit cell or nearest neighbor unit cells. Such a particle is called *Frenkel exciton.* In most semiconductors the Coulomb interaction is screened and weak resulting in larger size excitons, called as *Wannier–Mott excitons* or simply as *Wannier excitons.*

Properties of Wannier excitons can be calculated using the effective mass approximation and separating the center-of-mass (CM) motion and relative motion with the respective masses

$$M = m_e + m_h$$

and μ from

$$\mu^{-1} = m_e^{-1} + m_h^{-1},$$

respectively.

The CM motion is translationally invariant with the wavevector

$$\mathbf{K} = \mathbf{k}_e + \mathbf{k}_h ,$$

where $\mathbf{k}_e$ and $\mathbf{k}_h$ are the wavevectors of the electron and the hole.

Note! For a direct transition $\mathbf{k}_e \approx -\mathbf{k}_h$.