This is the *electric dipole approximation*

$$e/m\ \mathbf{A}\cdot\mathbf{p} \quad \rightarrow \quad -e\ \mathbf{r}\cdot\mathbf{E}$$

for the *electron–radiation interaction Hamiltonian.* We see that it means approximation of the transitions to be direct (suora).

Thus, the corresponding integral, *electric dipole transition matrix element* is

In the following assume that $\mathbf{k}_c \approx \mathbf{k}_v$ and simplify

The *Fermi Golden Rule* from the time-dependent perturbation theory for transition probabilities (or transition rate) per unit volume is

Now, the absorbed energy (in form of quanta $\hbar\omega$) per unit of time is

$$\text{power loss} = R\,\hbar\omega. \tag{6.44}$$

On the other hand, for absorbed intensity

$$-\,dI/dt = -\,dI/dx\ \ dx/dt = c/n\ \ \alpha\, I, \tag{6.45}$$

where α is the absorption coefficient, earlier met in Eq. (6.9). As $\alpha = \varepsilon_i\,\omega\,/\,(nc)$,

Thus,

$$\varepsilon_i(\omega) = \frac{1}{4\pi\varepsilon_0}\left(\frac{2\pi e}{m\omega}\right)^2 \frac{1}{\hbar} \sum_{\mathbf{k}} |P_{cv}|^2\, \delta(\omega_{cv} - \omega)\ , \tag{6.48}$$

where $E_c(\mathbf{k}) - E_v(\mathbf{k}) = E_{cv} = \hbar\omega_{cv}$.

By using KKR (6.14)

$$\varepsilon_r(\omega) = 1 + \frac{2}{\pi} \mathcal{P} \int_0^\infty \frac{\omega' \varepsilon_i(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$\varepsilon_r(\omega) = 1 + \frac{e^2}{\varepsilon_0 m} \sum_{\mathbf{k}} \frac{2}{m\, \hbar\omega_{cv}} \frac{|P_{cv}|^2}{\omega_{cv}^2 - \omega^2} . \qquad (6.49)$$

Compare this with the dielectric function of N_i classical harmonic oscillator dipoles with resonance frequencies ω_i

6.2.3. Joint Density-of-States

The density-of-states (DOS) of the 3-dimensional band structure $E_c(\mathbf{k})$ or $E_v(\mathbf{k})$ is defined by

Similarly, for the transition energy $E_{cv}(\mathbf{k}) = E_c(\mathbf{k}) - E_v(\mathbf{k})$ define the joint density-of-states (jDOS) by

The DOS may become singular at the limit $|\nabla_{\mathbf{k}}| \to 0$. Off from the Γ-point the singularity may become stronger.

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