

VII. SEMICONDUCTOR PHOTONICS

A. PRELIMINARIES: SEMICONDUCTOR BACKGROUND²⁹

THE CRYSTAL HAMILTONIAN

For an assembly of atoms the classical energy is the sum of the following:

- the kinetic energy of the nuclei;
 - the potential energy of the nuclei in one another's electrostatic field;
- the kinetic energy of the electrons;
- the potential energy of the electrons in the field of the nuclei;
- the potential energy of the electrons in one another's electrostatic field;
- the magnetic energy associated with spin and orbital variables.

Dividing the electrons into core and valence electrons and leaving out magnetic effects leads to the following expression for the crystal Hamiltonian:

$$\mathcal{H} = \sum_l \frac{\vec{p}_l^2}{2M} + U(\vec{\mathbf{R}}) + \sum_{l,m} \frac{\vec{p}_l^2}{2m_l} + \sum_{l,m} V(\vec{\mathbf{r}}_l - \vec{\mathbf{R}}_m) + \sum_{l,m} \frac{e^2/4}{|\vec{\mathbf{r}}_l - \vec{\mathbf{r}}_m|} \quad [\text{VII-0}]$$

where l and m label the ions, l and m label the electrons, \vec{p} is the momentum, M is an ionic mass, m is the mass of an electron, $U(\vec{\mathbf{R}})$ is the interionic potential, and $V(\vec{\mathbf{r}}_l - \vec{\mathbf{R}}_m)$ is the valence-electron-ion potential.

The quantum mechanics of the assembly is treated to a good approximation by taking the total wavefunction of the system as the product

$$\Psi(\vec{\mathbf{r}}; \vec{\mathbf{R}}) = \Psi(\vec{\mathbf{r}}) \Psi(\vec{\mathbf{R}}) \quad [\text{VII-1}]$$

²⁹ This discussion draws heavily on B. K. Ridley, *Quantum Processes in Semiconductors* (3rd edition), Clarendon Press (1993).

where $\left(\vec{\mathbf{R}}\right) = \left(\vec{\mathbf{R}}_1, \vec{\mathbf{R}}_2, \vec{\mathbf{R}}_3, \vec{\mathbf{R}}_4, \dots\right)$ is the wavefunction of all the ions and $\left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) = \left(\vec{\mathbf{r}}_k, \vec{\mathbf{r}}_l, \vec{\mathbf{r}}_m, \vec{\mathbf{r}}_n, \dots; \vec{\mathbf{R}}_1, \vec{\mathbf{R}}_2, \vec{\mathbf{R}}_3, \vec{\mathbf{R}}_4, \dots\right)$ is the wavefunction of all the electrons at the instantaneous ionic positions. The Schrödinger equation is then written

$$\begin{aligned} &\left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \mathcal{H}_{lattice} \left(\vec{\mathbf{R}}\right) + \left(\vec{\mathbf{R}}\right) \mathcal{H}_{elec} \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \\ &+ \left[\mathcal{H}_{lattice} \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \left(\vec{\mathbf{R}}\right) - \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \mathcal{H}_{lattice} \left(\vec{\mathbf{R}}\right) \right] = E \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \left(\vec{\mathbf{R}}\right) \quad [\text{VII-2}] \end{aligned}$$

where the total Hamiltonian is parsed into two independent components -- viz.

$$\mathcal{H}_{lattice} = \frac{\vec{\mathbf{p}}^2}{2M} + U \left(\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2 \right) . \quad [\text{VII-3a}]$$

$$\mathcal{H}_{elec} = \sum_l \frac{\vec{\mathbf{p}}_l^2}{2m_l} + \sum_{l, m} V \left(\vec{\mathbf{r}}_l - \vec{\mathbf{r}}_m \right) + \sum_{l, m} \frac{e^2/4}{|\vec{\mathbf{r}}_l - \vec{\mathbf{r}}_m|} . \quad [\text{VII-3b}]$$

The essential assumption of the *adiabatic approximation* is that the bracketed term is negligible and that the global problem may be treated as two independent problems -- viz.

$$\mathcal{H}_{lattice} \left(\vec{\mathbf{R}}\right) = E_{lattice} \left(\vec{\mathbf{R}}\right) \quad [\text{VII-4a}]$$

$$\mathcal{H}_{elec} \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) = E_{elec} \left(\vec{\mathbf{r}}; \vec{\mathbf{R}}\right) \quad [\text{VII-4b}]$$

As a further refinement, the electron problem must be parsed once more as

$$\mathcal{H}_{elec} = \left\{ \mathcal{H}_{elec} \right\}_{static} + \left\{ \mathcal{H}_{elec} \right\}_{dynamic}$$

where $\{\mathcal{H}_{elec}\}_{static}$ defines the problem of the many electron system interacting with the static ionic lattice and $\{\mathcal{H}_{elec}\}_{dynamic}$ incorporates the effects of the electron-phonon interaction.

LATTICE VIBRATIONS

For a brief overview of lattice vibrations see the webpage entitled *Self Study Materials on Solid State Electronics 2* at

http://deas.harvard.edu/courses/ap216/lectures/ls_2/ls2_u7/sse_tut_2/solid2.html

BLOCH ELECTRONS - Solutions of the Schrödinger equation for a **single electron** or **quasi-particle** moving in a periodic lattice

If the electron-electron is averaged out, deviations from the average may be treated perturbations -- *i.e.*, we make the replacement

$$\frac{e^2/4}{|\vec{\mathbf{r}}_l - \vec{\mathbf{r}}_m|} \quad (\mathcal{H}_{elec})_0 + (\mathcal{H}_{elec})_1 \quad [VII-5]$$

where $(\mathcal{H}_{elec})_0$ leads to a constant repulsive electronic energy component and $(\mathcal{H}_{elec})_1$ is a small fluctuating electron-electron interaction. If we neglect these fluctuations, each electron interacts independently with a screened lattice potential. In this approximation, the electronic wavefunction can be expressed as

$$\psi(\vec{\mathbf{r}}; \vec{\mathbf{R}}_0) = \prod_n \psi_n(\vec{\mathbf{r}}_n; \vec{\mathbf{R}}_0) \quad [VII-6]$$

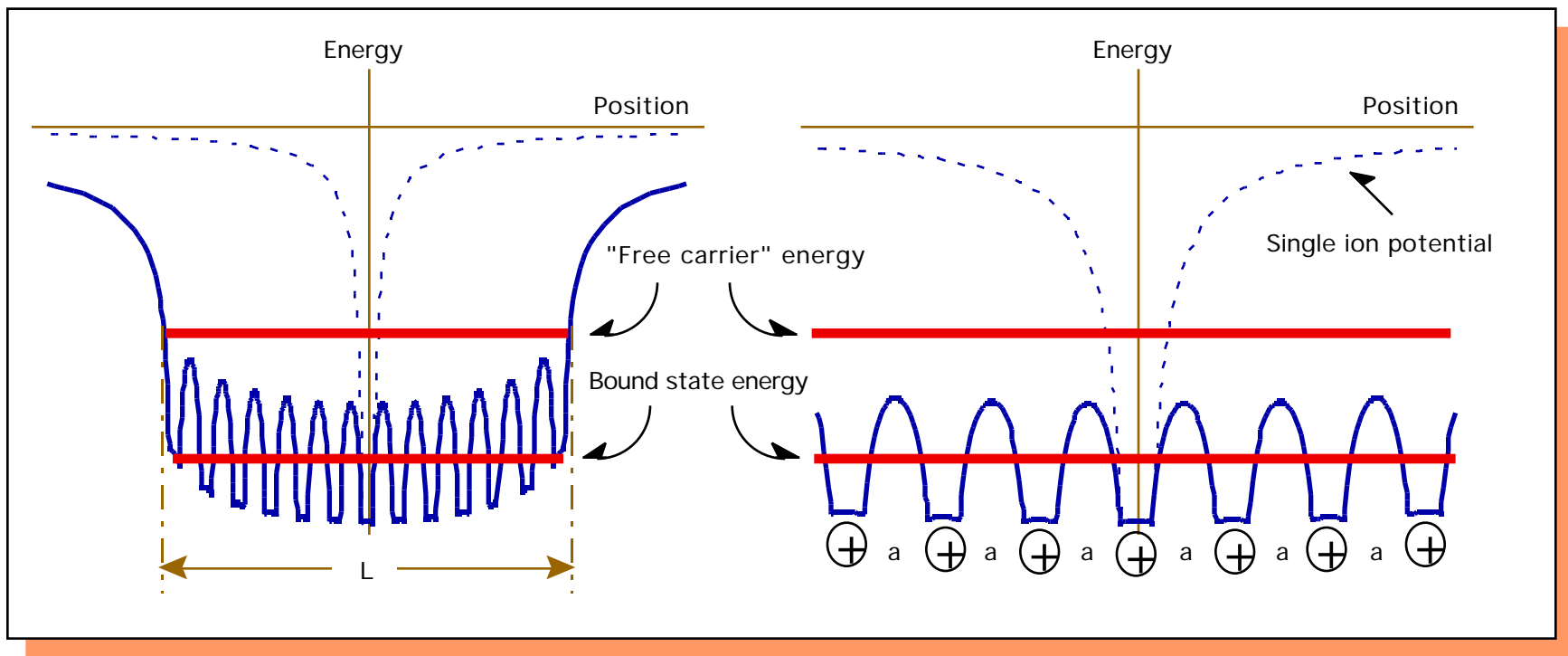
with the requirement that the occupation of one-electron states is in accordance with Pauli exclusion principle. Thus, each the wavefunction for each electrons satisfies a Schrödinger equation in the form

$$\left(\mathcal{H}_{elec}^{(n)} \right)_{static} \psi_n(\vec{r}_n; \vec{R}_0) = -\frac{\hbar^2}{2m} \nabla_n^2 \psi_n(\vec{r}_n; \vec{R}_0) + V(\vec{r}_n) \psi_n(\vec{r}_n; \vec{R}_0) = E_n \psi_n(\vec{r}_n; \vec{R}_0) \quad [VII-7a]$$

or simplifying the notation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) \quad [VII-7b]$$

SCHEMATIC PERIODIC LATTICE POTENTIAL



The lattice potential far from the surface of the crystal has the property that, for all lattice vectors $\bar{\mathbf{R}}_{[\ell]} = \ell_1 \bar{\mathbf{a}}_1 + \ell_2 \bar{\mathbf{a}}_2 + \ell_3 \bar{\mathbf{a}}_3$

$$V(\bar{\mathbf{r}}) = V(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) \quad [\text{VII-8}]$$

Bloch's (Floquet's) theorem: The function

$$\bar{\psi}_{\mathbf{k}}(\bar{\mathbf{r}}) = (\mathcal{V})^{-1/2} u_{\mathbf{k}}(\bar{\mathbf{r}}) \exp(i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}) \quad [\text{VII-9}]$$

where $u_{\mathbf{k}}(\bar{\mathbf{r}})$ is a function with the same spatial periodicity as $V(\bar{\mathbf{r}})$ that is an eigenfunction of Equation [VII-7].

Proof of theorem:

First rewrite Equation [VII-7b] as

$$\mathcal{H}(\bar{\mathbf{r}}) \bar{\psi}(\bar{\mathbf{r}}) = E \bar{\psi}(\bar{\mathbf{r}}) \quad [\text{VII-7b}']$$

Shifting the origin by a lattice vector, we again rewrite Equation [VII-7b] as

$$\mathcal{H}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) \bar{\psi}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) = E \bar{\psi}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) \quad [\text{VII-7b}'']$$

In light of periodicity expressed in Equation [VII-8], it follows that

$$\mathcal{H}(\bar{\mathbf{r}}) \bar{\psi}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) = E \bar{\psi}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]}) \quad [\text{VII-10}]$$

Thus, any linear combination of the possible eigenfunctions $\bar{\psi}(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]})$ is a valid eigenstate of the energy ! In particular, let us choose the combination

$$\begin{aligned} \bar{u}_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) &= \sum_{[\ell]} \left(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]} \right) \exp \left(-i \bar{\mathbf{k}} \cdot \bar{\mathbf{R}}_{[\ell]} \right) \\ &= \exp \left(i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}} \right) \sum_{[\ell]} \left(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]} \right) \exp \left[-i \bar{\mathbf{k}} \cdot \left(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]} \right) \right] \end{aligned} \quad [\text{VII-11}]$$

where $\bar{\mathbf{k}}$ is, for the moment, taken to be an arbitrary **complex** vector. Since the summation includes all possible lattice vectors it must be a periodic function of $\bar{\mathbf{r}}$ with the period of the lattice and may be identified with $u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})$ of Equation [VII-9].³⁰ If we impose cyclical boundary conditions on $\bar{u}_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})$, we see that, of necessity, $\bar{\mathbf{k}}$ is a real vector! **QED**

In light of Bloch's theorem, Equation [VII-7b] may be rewrite in the form

$$\mathcal{H}_{\bar{\mathbf{k}}} \bar{u}_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) = -\frac{\hbar^2}{2m} \left(\nabla^2 + i \bar{\mathbf{k}} \cdot \nabla \right) u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) = \epsilon_{\bar{\mathbf{k}}} u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) . \quad [\text{VII-12}]$$

Since the reciprocal lattice vectors of crystal are defined³¹ so that $\exp \left(i \bar{\mathbf{R}}_{[\ell]} \cdot \bar{\mathbf{G}}_{[m]} \right) = 1$, any function written in the form

$$\sum_{[m]} C_{[m]} \exp \left(i \bar{\mathbf{G}}_{[m]} \cdot \bar{\mathbf{r}} \right)$$

³⁰ We keep for the record $\bar{u}_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) = \sum_{[\ell]} \left(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]} \right) \exp \left[-i \bar{\mathbf{k}} \cdot \left(\bar{\mathbf{r}} + \bar{\mathbf{R}}_{[\ell]} \right) \right]$

³¹ The reciprocal lattice vectors: $\bar{\mathbf{G}}_{[m]} = m_1 \bar{\mathbf{b}}_1 + m_2 \bar{\mathbf{b}}_2 + m_3 \bar{\mathbf{b}}_3$
where

$$\bar{\mathbf{b}}_1 = 2 \frac{\bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3}{\bar{\mathbf{a}}_1 \cdot \bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3}; \quad \bar{\mathbf{b}}_2 = 2 \frac{\bar{\mathbf{a}}_3 \times \bar{\mathbf{a}}_1}{\bar{\mathbf{a}}_1 \cdot \bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3}; \quad \bar{\mathbf{b}}_3 = 2 \frac{\bar{\mathbf{a}}_1 \times \bar{\mathbf{a}}_2}{\bar{\mathbf{a}}_1 \cdot \bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3}$$

has the spatial periodicity of the lattice. Conversely, we are allowed to expand $V(\vec{r})$ and $u_{\vec{k}}(\vec{r})$ in Fourier series -- viz.

$$V(\vec{r}) = \sum_{[m]} V_{[m]} \exp\left(i \vec{G}_{[m]} \cdot \vec{r} \right) \quad [\text{VII-13a}]$$

$$u_{\vec{k}}(\vec{r}) = \sum_{[m]} u_{[m]}(\vec{k}) \exp\left(i \vec{G}_{[m]} \cdot \vec{r} \right) \quad [\text{VII-14a}]$$

where
$$V_{[m]} = \mathcal{V}^{-1} \int d\vec{r} V(\vec{r}) \exp\left(-i \vec{G}_{[m]} \cdot \vec{r}\right) \quad [\text{VII-13b}]$$

and
$$u_{[m]}(\vec{k}) = \mathcal{V}^{-1} \int d\vec{r} u_{\vec{k}}(\vec{r}) \exp\left(-i \vec{G}_{[m]} \cdot \vec{r}\right) \quad [\text{VII-14b}]$$

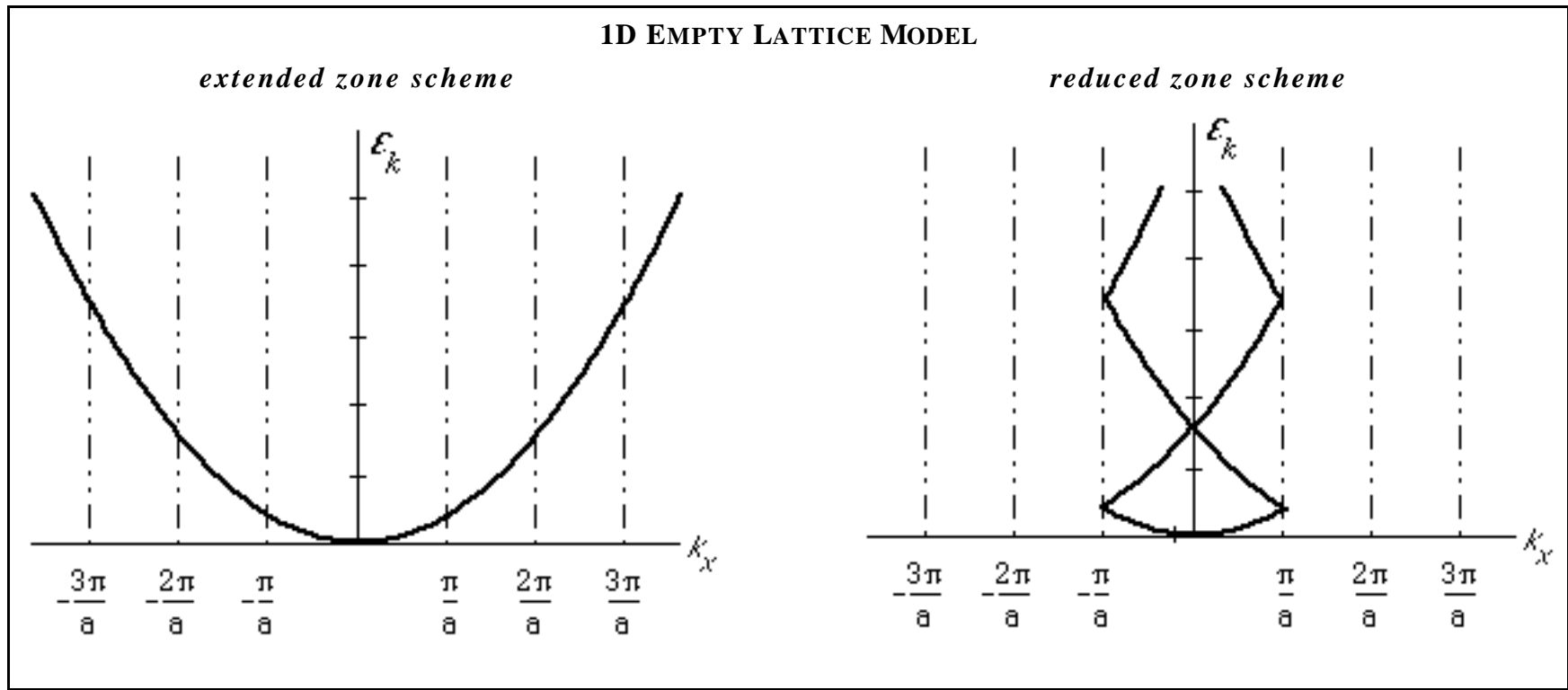
Substituting these expressions into Equation [VII-12] and equating various Fourier components, we obtain the following infinite set of algebraic equations:

$$\frac{\hbar^2}{2m} \left(\vec{G}_{[m]} + \vec{k} \right)^2 u_{[m]}(\vec{k}) + \sum_{[m']} V_{[m']} u_{[m]-[m']}(\vec{k}) = \epsilon_{\vec{k}} u_{[m]}(\vec{k}) \quad [\text{VII-15}]$$

which can, in principle, be solved for $\epsilon_{\vec{k}}$ and $u_{[m]}(\vec{k})$. If we were to turn off the lattice potential off to effectuate the *empty lattice approximation*, the eigenfunctions and eigenvalues should, obviously, be those of a **free electron** and given by

$$u_{\vec{k}}(\vec{r}) = \epsilon_{\vec{k}}(\vec{r}) = \mathcal{V}^{-1/2} \exp\left(i \vec{k} \cdot \vec{r} \right) \quad [\text{VII-16}]$$

and
$$\epsilon_{\vec{k}} = \frac{\hbar^2 |\vec{k}|^2}{2m} \quad [\text{VII-17}]$$



With gradual restoration of the lattice potential, the wave function is gradually transformed from a plane wave, Equation [VII-16], to a Bloch function, Equation [VII-9]. In general, the value of $\bar{\mathbf{k}}$ is well defined since it does not change from its original value and the plane wave merely becomes modulated by the function $u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})$. Clearly, it is also possible to write the Bloch wave function in the form

$$u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) = (\mathcal{V})^{-1/2} \left\{ u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}}) \exp \left(i \bar{\mathbf{G}}_{[m]} \cdot \bar{\mathbf{r}} \right) \right\} \exp \left[i \left(\bar{\mathbf{k}} - \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \quad [\text{VII-18}]$$

and since both $u_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})$ and $\exp \left(i \bar{\mathbf{G}}_{[m]} \cdot \bar{\mathbf{r}} \right)$ are spatially periodic, so is their product. Thus, the wave function can be considered as obeying the Bloch theorem with any empty lattice wave vector $\bar{\mathbf{k}} - \bar{\mathbf{G}}_{[m]}$. Accordingly, the theorem allows for two

alternative modes of classifying solutions -- *i.e.* a solution may be specified with the original value of $\bar{\mathbf{k}}$ (extended zone scheme) or with that value "reduced" by a reciprocal lattice vector plus a *band index* (reduced zone scheme).

In the *nearly free electron* approximation we use the $\psi_{\bar{\mathbf{k}}}^0(\bar{\mathbf{r}})$ functions as a basis set and take the periodic potential $V(\bar{\mathbf{r}})$ as a small static perturbation. Using Equations [A-6c] and [A-7b] of this set of lecture notes (at the end of the Section II, *Review of Basic Quantum Mechanics: Dynamic Behavior of Quantum Systems*) we obtain

$$\left| \frac{1}{\bar{\mathbf{k}}} \right\rangle = \left| \frac{0}{\bar{\mathbf{k}}} \right\rangle + \left| \frac{0}{\bar{\mathbf{k}}} \right\rangle \frac{\left\langle \frac{0}{\bar{\mathbf{k}}} \left| V \right| \frac{0}{\bar{\mathbf{k}}} \right\rangle}{\frac{0}{\bar{\mathbf{k}}} - \frac{0}{\bar{\mathbf{k}}}} \quad \text{[VII-19]}$$

$$\frac{0}{\bar{\mathbf{k}}} + \frac{\left| \left\langle \frac{0}{\bar{\mathbf{k}}} \left| V \right| \frac{0}{\bar{\mathbf{k}}} \right\rangle \right|^2}{\frac{0}{\bar{\mathbf{k}}} - \frac{0}{\bar{\mathbf{k}}}} \quad \text{[VII-20]}$$

In light of Equation [VII-13a] we may write

$$\begin{aligned} \left\langle \frac{0}{\bar{\mathbf{k}}} \left| V \right| \frac{0}{\bar{\mathbf{k}}} \right\rangle &= (\mathcal{V})^{-1} \int d\bar{\mathbf{r}} \exp(-i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}) V(\bar{\mathbf{r}}) \exp(i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}) \\ &= (\mathcal{V})^{-1} \int d\bar{\mathbf{r}} \exp[-i(\bar{\mathbf{k}} - \bar{\mathbf{k}}) \cdot \bar{\mathbf{r}}] V_{[m]} \exp(i \bar{\mathbf{G}}_{[m]} \cdot \bar{\mathbf{r}}) \quad \text{[VII-21]} \\ &= V_{[m]} (\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]} - \bar{\mathbf{k}}) \end{aligned}$$

so that Equations [VII-19] and [VII-20] become

$$\left| \frac{1}{\bar{\mathbf{k}}} \right\rangle = \left| \frac{0}{\bar{\mathbf{k}}} \right\rangle + \left| \frac{0}{\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]}} \right\rangle \frac{V_{[m]}}{\frac{0}{\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]}} - \frac{0}{\bar{\mathbf{k}}}} \quad \text{[VII-22]}$$

$$\bar{\mathbf{k}} = \frac{\bar{\mathbf{k}}}{[m]} + \frac{|V_{[m]}|^2}{\frac{\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]}}{[m]} - \frac{\bar{\mathbf{k}}}{[m]}} \quad [\text{VII-23}]$$

Clearly, the strongest departure from free electron behavior occurs when the denominator vanishes -- *i.e.* when

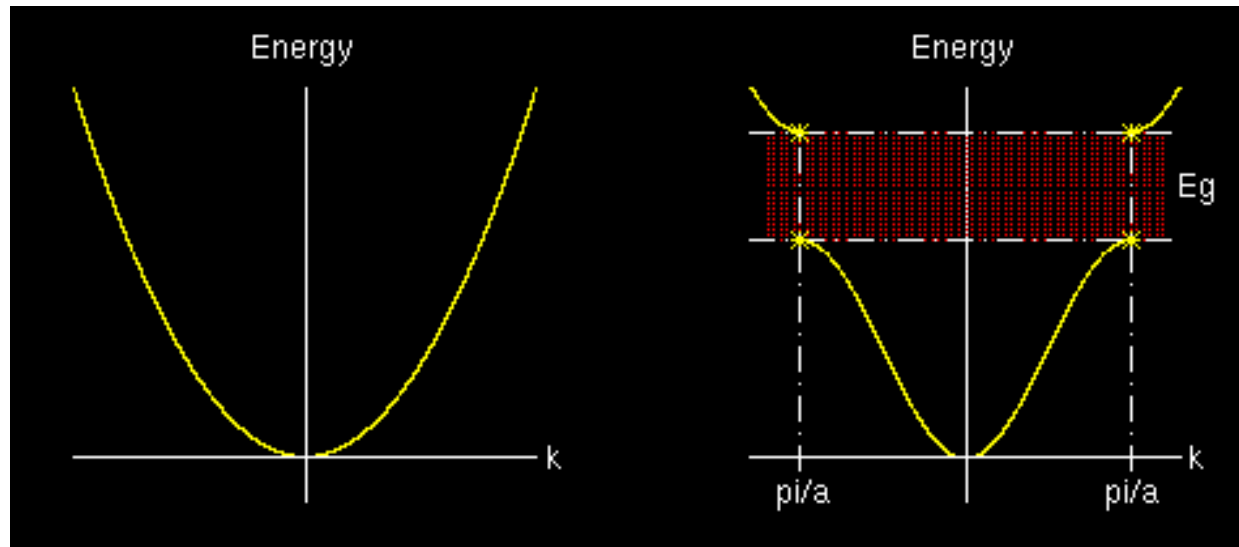
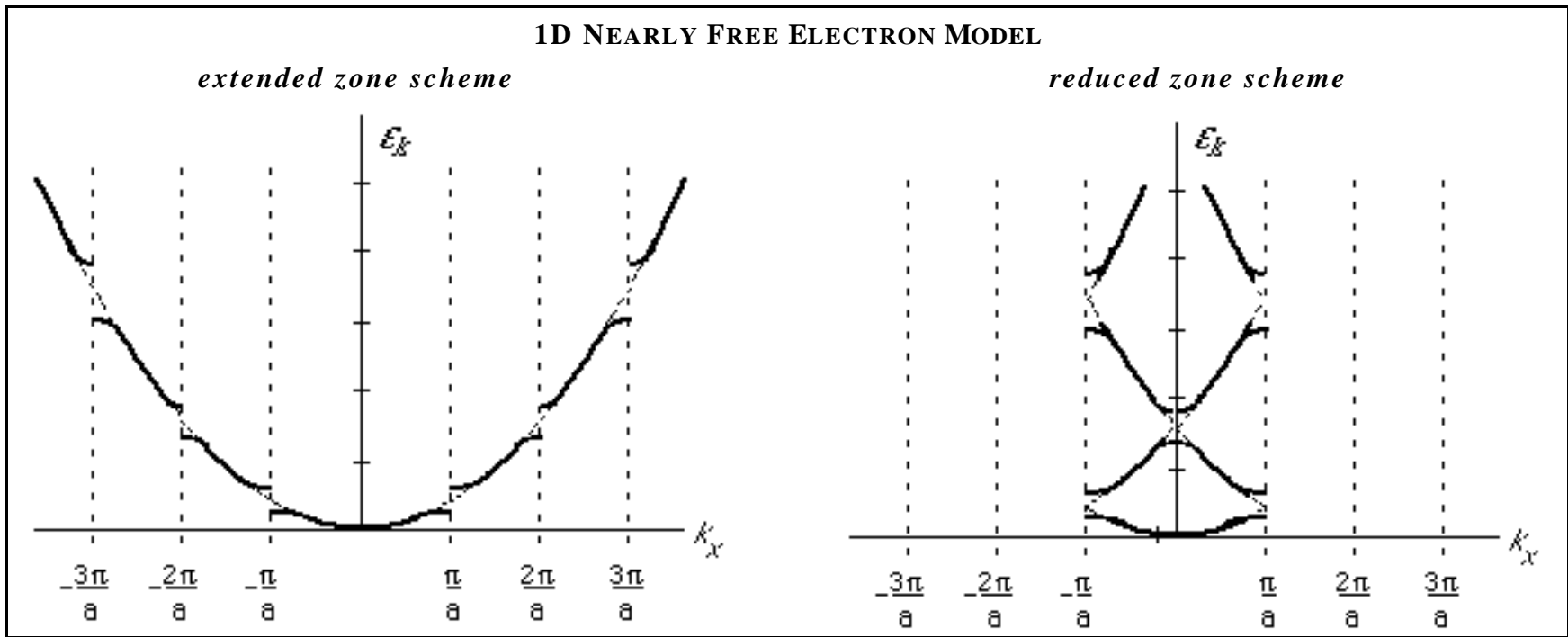
$$\begin{aligned} \frac{\bar{\mathbf{k}}}{[m]} - \frac{\bar{\mathbf{k}}}{[m]} &= \frac{\hbar^2}{2m} \left| \bar{\mathbf{G}}_{[m]} + \bar{\mathbf{k}} \right|^2 - \left| \bar{\mathbf{k}} \right|^2 \\ &= \frac{\hbar^2}{2m} \left| \bar{\mathbf{G}}_{[m]} \right|^2 + 2\bar{\mathbf{G}}_{[m]} \cdot \bar{\mathbf{k}} = 0 \end{aligned} \quad [\text{VII-24}]$$

Equation [VII-24] is the famous **Bragg scattering condition** or the condition which defines the boundaries of the Brillouin zones. At the zone edge for a particular pair of degenerate free electron states the appropriate pair of equation from the set in Equation [VII-19] may be approximated

$$\begin{aligned} \left[\frac{\bar{\mathbf{k}}}{[m]} - \frac{\bar{\mathbf{k}}}{[m]} \right] u_{[0]}(\bar{\mathbf{k}}) + V_{[m]} u_{[m]}(\bar{\mathbf{k}}) &= 0 \\ \left[\frac{\bar{\mathbf{k}}}{[m]} - \frac{\bar{\mathbf{k}}}{[m]} \right] u_{[m]}(\bar{\mathbf{k}}) + V_{[m]} u_{[0]}(\bar{\mathbf{k}}) &= 0 \end{aligned} \quad [\text{VII-25a}]$$

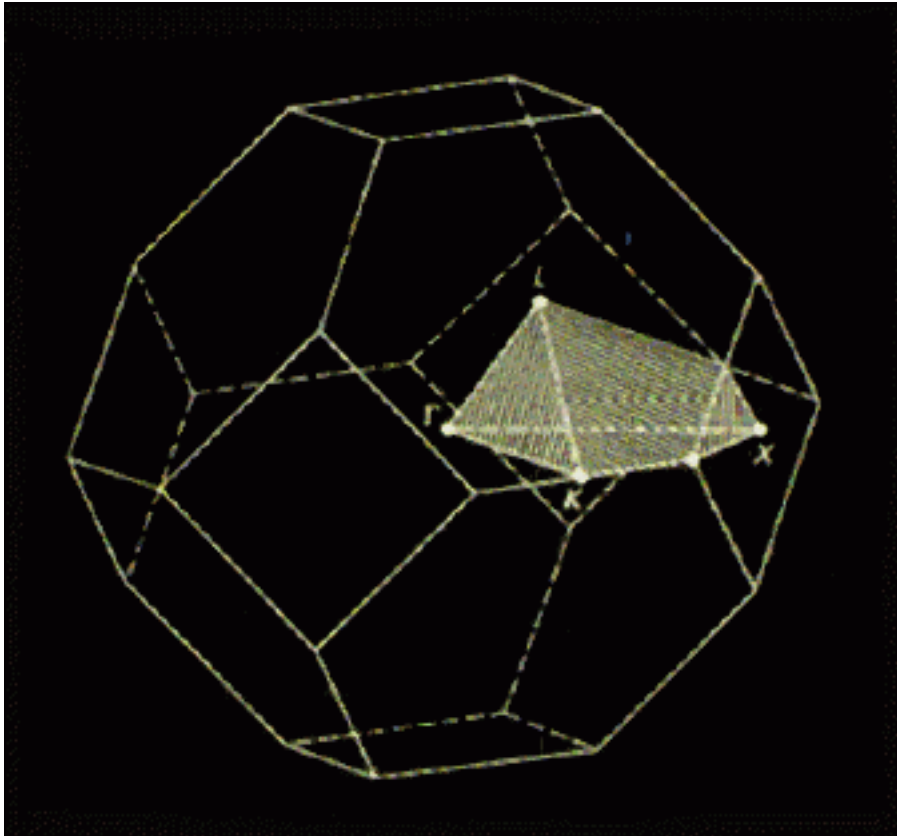
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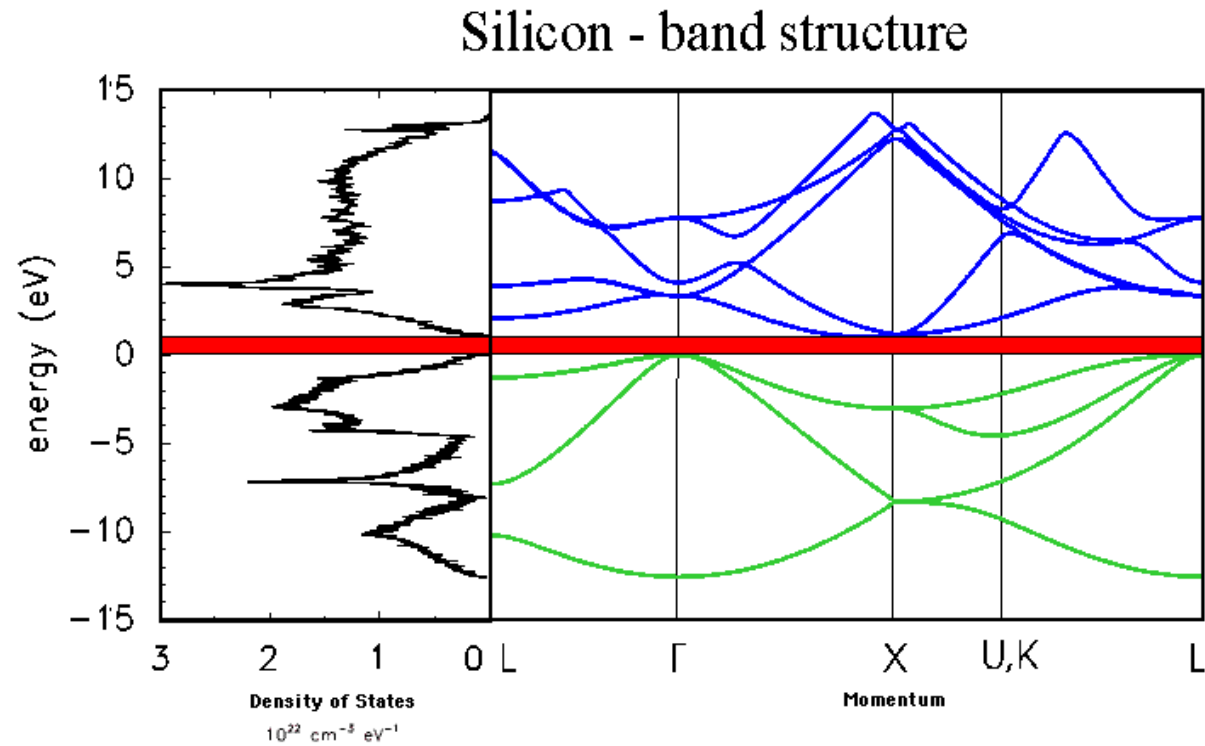
$$\bar{\mathbf{k}} = \frac{1}{2} \left(\frac{\bar{\mathbf{k}}}{[m]} + \frac{\bar{\mathbf{k}}}{[m]} \right) \pm \sqrt{\left(\frac{\bar{\mathbf{k}}}{[m]} - \frac{\bar{\mathbf{k}}}{[m]} \right)^2 + 4 |V_{[m]}|^2} \quad [\text{VII-25b}]$$



These considerations then provide the context for the examination of *real* band structures.

Diamond Structure Brillouin Zone and Nomenclature





For more on band structures go to:

http://www.deas.harvard.edu/courses/ap216/images/bandgap_engineering/bandgap_engineering.html

For more on pn junction physics go to:

http://www.deas.harvard.edu/courses/ap216/images/pn_junction/pn_junction.html

B. OPTICAL PROPERTIES OF BULK (3-D) SEMICONDUCTOR³²**FREE-CARRIER THEORY**

For most of our considerations a **parabolic-band model** provides a reasonable picture of optical properties. In this model we assume that near a band edge the single particle energy of the electron **measured with respect to the edge** is given by

$$\bar{\epsilon}_{\mathbf{k}} = \frac{\hbar^2 |\bar{\mathbf{k}}|^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad [\text{VII-26a}]$$

where the *effective mass* m is a measure of the inverse curvature of the band.³³ Introducing the notion of a deficiency of electrons in the valence band -- *i.e.* **holes** -- as positive charge carriers, the parabolic-band model is re-interpreted as, respectively, the quasiparticle energies of an electron in the conduction band and a hole in the valence band

$${}_{e,\mathbf{k}} \bar{\epsilon}_{\mathbf{k}} = \frac{\hbar^2 |\bar{\mathbf{k}}|^2}{2m_e} = \frac{\hbar^2 k^2}{2m_e} \quad [\text{VII-26b}]$$

$${}_{h,\mathbf{k}} \bar{\epsilon}_{\mathbf{k}} = \frac{\hbar^2 |\bar{\mathbf{k}}|^2}{2m_h} = \frac{\hbar^2 k^2}{2m_h} \quad [\text{VII-26c}]$$

³² This section draws heavily on Weng W. Chow, Stephan W. Koch and Murray. Sargent III, *Semiconductor-Laser Physics*, Springer-Verlag (1994)

³³ That is, the effective mass is given by

$$\frac{1}{m} = \frac{1}{\hbar^2} \frac{\partial^2 \bar{\epsilon}_{\mathbf{k}}}{\partial k^2} \Bigg|_{\text{Band edge}}$$

and, thus, in the **conduction band the effective mass of electrons is positive and in the valence band it is negative** -- *i.e.* $m_c > 0$ and $m_v < 0$.

where $m_e = m_c > 0$ and $m_h > 0$ accounts for aggregate dynamics of all the electron in the valence minus the single empty state.³⁴ Of course, the single particle picture discussed thus far, does not include the critically important effects of the inter-electronic Coulomb interactions and, in particular, *carrier-carrier scattering*. In what is usually called *free-carrier theory*, it is assumed that carrier-carrier scattering causes a rapid "thermalization" (relaxation times less than 0.1 picoseconds) of excited conduction band electrons (and valence band holes) and, consequently, it is assumed that carriers **within a band** are in *quasiequilibrium* with energies distributed according to a Fermi-Dirac distribution (see illustration on the next page).^{35,, 36} Accordingly, the carrier density for a given band (*i.e.* = e for the conduction band and = h for the valence band) is determined by the condition

$$N = \frac{1}{V} \sum_{\text{states}} f_{\vec{k}} = \frac{1}{V} \sum_{\text{states}} \exp \left(\frac{E_{\vec{k}} - \mu}{k_B T} \right) + 1^{-1} \quad [\text{VII-27}]$$

where V is the volume of the sample and μ is the carrier *quasichemical potential* (or *imref quasi-Fermi energy*).³⁷ In the discussion of Equation

³⁴ The hole energy is the energy of the filled valence minus the energy of the filled with a vacant electronic state so that an increase in hole momentum leads to an increase in hole energy. Since m_h must of necessity include the many-body Coulomb interactions among the valence electrons.

³⁵ See a Derivation of the Fermi-Dirac distribution function at http://ece-www.colorado.edu/~bart/book/fermi-dirac_derivation.htm

³⁶ See the applets Fermi Level vs. Carrier Concentration and Doping of Donor and Acceptor Impurities (at <http://www.acsu.buffalo.edu/~wie/applet/fermi/fermi.html>) and Fermi Level, Fermi Function and Electron Occupancy of Localized Energy States (at <http://www.acsu.buffalo.edu/~wie/applet/fermi/functionAndStates/functionAndStates.html>).

³⁷ As are the electron and hole energies $E_{\vec{k}}$, the imrefs μ are measured with respect to the appropriate band edge -- *viz.*

$$\mu_e = (E_F)_C - E_C \quad \text{and} \quad \mu_h = E_V - (E_F)_V$$

Thus, if $\mu < 0$ the band does contain enough carriers to populate any state with a probability greater than one-half.

[IV-5] of this set of lectures, it was argued that the 3-D density of states in \vec{k} space is given by

$$g(k) dk = \frac{V}{2\pi^2} k^2 dk \quad [VII-28]$$

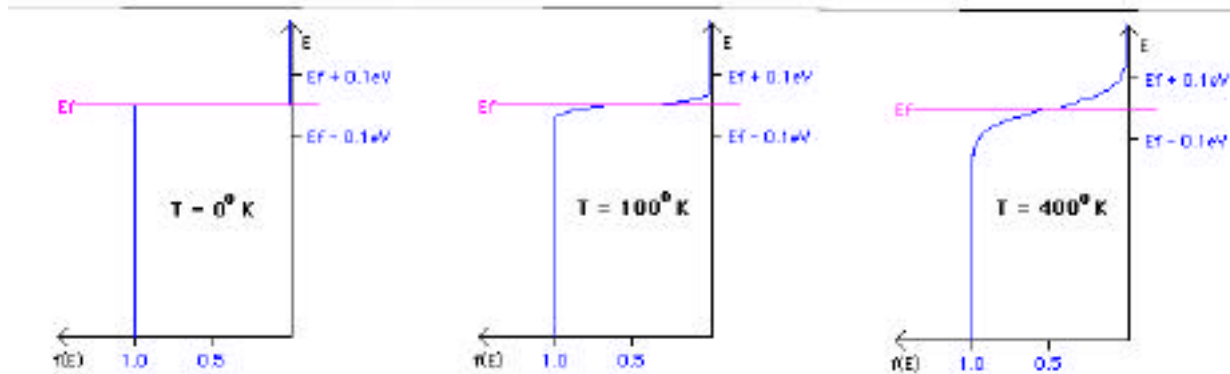
which translates (within a given band) into a density of states per unit energy per unit volume of

$$g(\vec{k}) = \frac{1}{V} g(k) \frac{dk}{d\epsilon_{\vec{k}}} = \frac{1}{2\pi^2} \frac{2m}{\hbar^2} \sqrt{\epsilon_{\vec{k}}} \quad [VII-29]$$

Hence, for a 3D semiconductor, Equation [VII-27] becomes

$$N = \int_0^\infty g(\epsilon) f(\epsilon) d\epsilon = \frac{1}{2\pi^2} \frac{2m}{\hbar^2} \int_0^\infty \sqrt{\epsilon} \left\{ \exp\left[\frac{\epsilon - \mu}{k_B T} \right] + 1 \right\}^{-1} d\epsilon \quad [VII-30]$$

Fermi Function



OPTICAL MATRIX ELEMENTS

Since optical interactions in a semiconductor are essential **distributed**, it is probably more precise and appropriate in this case to write the interaction Hamiltonian as ³⁸

$$\mathcal{H}_I = -\frac{q}{m} \bar{\mathbf{A}} \cdot \bar{\mathcal{P}} = \frac{e}{m} \bar{\mathbf{A}} \cdot \bar{\mathcal{P}} = \frac{eA_0}{2m} [\hat{\epsilon} \cdot \bar{\mathcal{P}}] \exp \left[i \left(\omega_{\text{rad}} t - \bar{\mathbf{k}}_{\text{rad}} \cdot \bar{\mathbf{r}} \right) \right] + \dots \quad \text{[VII-31]}$$

Thus, the critical optical matrix element ³⁹ between a state in the valence band and one in the conduction band is

$$\left\langle v_{\bar{\mathbf{k}}} \left| \mathcal{H}_I \right| c_{\bar{\mathbf{k}}} \right\rangle = \frac{eA_0}{2m} \exp \left[i \omega_{\text{rad}} t \right] \bar{\mathbf{M}}_{v_{\bar{\mathbf{k}}} c_{\bar{\mathbf{k}}}} \quad \text{[VII-32a]}$$

where the so called **transition matrix element** is given by

$$\bar{\mathbf{M}}_{v_{\bar{\mathbf{k}}} c_{\bar{\mathbf{k}}}} = \int d\bar{\mathbf{r}} u_{v_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})} \exp \left[-i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}} \right] \left\{ \hat{\epsilon} \cdot \bar{\mathcal{P}} \exp \left[-i \bar{\mathbf{k}}_{\text{rad}} \cdot \bar{\mathbf{r}} \right] \right\} u_{c_{\bar{\mathbf{k}}}(\bar{\mathbf{r}})} \exp \left[i \bar{\mathbf{k}} \cdot \bar{\mathbf{r}} \right] \quad \text{[VII-32b]}$$

Using the expansion for $u_{n\bar{\mathbf{k}}}$ in Equation [VII-12a] the matrix element becomes

$$\begin{aligned} \bar{\mathbf{M}}_{v_{\bar{\mathbf{k}}} c_{\bar{\mathbf{k}}}} &= \sum_{[m][m']} u_{v_{[m]}(\bar{\mathbf{k}})} u_{c_{[m]}(\bar{\mathbf{k}})} \\ &\times \int d\bar{\mathbf{r}} \exp \left[-i \left(\bar{\mathbf{k}} + \bar{\mathbf{k}}_{\text{rad}} + \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \left\{ \hat{\epsilon} \cdot \bar{\mathcal{P}} \right\} \exp \left[i \left(\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \end{aligned} \quad \text{[VII-33]}$$

³⁸ In the next set of lectures, *The Interaction of Radiation and Matter: Quantum Theory*, we develop the following expression for the **nonrelativistic Hamiltonian of a single charged particle**:

$$\mathcal{H} = q \phi + \frac{1}{2m} \left[\bar{\mathcal{P}} - q \bar{\mathbf{A}} \right]^2$$

where $\bar{\mathcal{P}}$ is the canonical conjugate momentum of the charged particle.

³⁹ The Fermi Golden Rule and first-order perturbation theory tells us that the **radiation-induced transition rate** is given by

$$\frac{2}{\hbar} \left| \langle f | \mathcal{H}_{\text{int}} | i \rangle \right|^2 \rho_f \left(\omega_f - \omega_i \right).$$

However, $\bar{P} = i \hbar^{-1}$ so that

$$\bar{M}_{\bar{k}c\bar{k}} = \sum_{[m][m]} \left\{ \hbar \hat{e} \left(\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]} \right) \right\} u_{v[m]}(\bar{\mathbf{k}}) u_{c[m]}(\bar{\mathbf{k}}) \times \int d\bar{\mathbf{r}} \exp \left[-i \left(\bar{\mathbf{k}} + \bar{\mathbf{k}}_{\text{rad}} - \bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]} - \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \quad [\text{VII-34}]$$

With the parsing $\bar{\mathbf{r}} = \bar{\mathbf{R}}_{[\ell]} + \bar{\mathbf{r}}_{\text{uc}}$ and using the defining relationship $\exp \left(i \bar{\mathbf{R}}_{[\ell]} \cdot \bar{\mathbf{G}}_{[m]} \right) = 1$, the volume integral may be expressed

$$\int d\bar{\mathbf{r}} \{ \bar{\mathbf{r}} \} \exp \left[i \left(\bar{\mathbf{k}} - \bar{\mathbf{k}} - \bar{\mathbf{k}}_{\text{rad}} + \bar{\mathbf{G}}_{[m]} - \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] = \int_{\text{unit cell}} d\bar{\mathbf{r}} \{ \bar{\mathbf{r}} \} \exp \left[i \left(\bar{\mathbf{k}} - \bar{\mathbf{k}} - \bar{\mathbf{k}}_{\text{rad}} + \bar{\mathbf{G}}_{[m]} - \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \times \exp \left[i \left(\bar{\mathbf{k}} - \bar{\mathbf{k}} - \bar{\mathbf{k}}_{\text{rad}} \right) \cdot \bar{\mathbf{R}}_{[\ell]} \right] \quad [\text{VII-35}]$$

The summation $\sum_{[\ell]} \exp \left[i \left(\bar{\mathbf{k}} - \bar{\mathbf{k}} - \bar{\mathbf{k}}_{\text{rad}} \right) \cdot \bar{\mathbf{R}}_{[\ell]} \right] = 0$ unless

$$\bar{\mathbf{k}} = \bar{\mathbf{k}} + \bar{\mathbf{k}}_{\text{rad}} - \bar{\mathbf{k}}. \quad [\text{VII-36}]$$

-- *i.e.* essentially **only vertical transitions are allowed!** Therefore,

$$\bar{M}_{\bar{k}c\bar{k}} = \sum_{\bar{k}\bar{k}} \frac{V_{\text{sample}}}{V_{\text{unit cell}}} \sum_{[m][m]} \left\{ \hbar \hat{e} \left(\bar{\mathbf{k}} + \bar{\mathbf{G}}_{[m]} \right) \right\} u_{v[m]}(\bar{\mathbf{k}}) u_{c[m]}(\bar{\mathbf{k}}) \times \int_{\text{unit cell}} d\bar{\mathbf{r}} \exp \left[i \left(\bar{\mathbf{G}}_{[m]} - \bar{\mathbf{G}}_{[m]} \right) \cdot \bar{\mathbf{r}} \right] \quad [\text{VII-37a}]$$

For a given polarization of the applied field, the transition matrix can be written

$$\bar{\bar{M}}_{\nu \bar{k} c \bar{k}} = \{ \text{polarization factor} \} \bar{\bar{M}} . \quad [\text{VII-37b}]$$

where the polarization factors are of order one and typical values of $|\mathbf{M}|^2$ are given in the following table:⁴⁰

Material system	$2 \mathbf{M} ^2/m$ (in eV)
Ga As	28.8
$\text{Al}_x \text{Ga}_{1-x} \text{As}$ ($x < 0.3$)	$29.83 + 2.85 x$
$\text{In}_x \text{Ga}_{1-x} \text{As}$	$28.8 - 6.6 x$
In P	19.7
$\text{In}_{1-x} \text{Ga}_x \text{As}_y \text{P}_{1-y}$ ($x = 0.47 y$)	$19.7 + 5.6 y$

Of course, the radiation must also satisfy the energy conservation condition

$$\bar{k} = \hbar \bar{k} = \hbar \left(\frac{k^2}{2m_e} + \frac{k^2}{2m_h} \right) = \hbar \frac{k^2}{2m_r} \quad [\text{VII-38a}]$$

where

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h} . \quad [\text{VII-38b}]$$

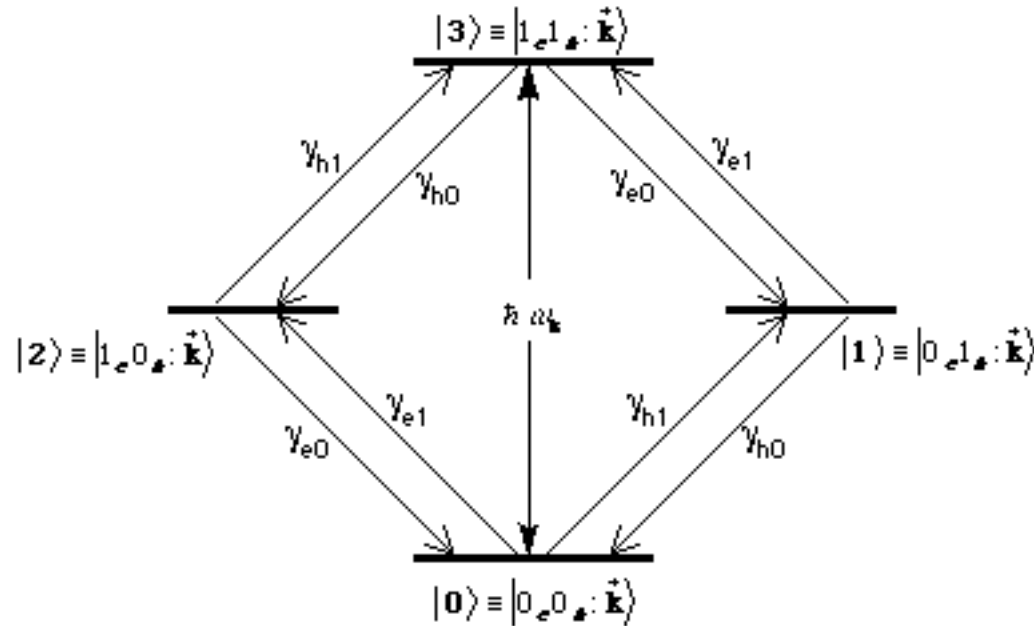
"FREE-CARRIER THEORY" OF OPTICAL PROCESSES

The *bottom line* is that in the *free-carrier theory* of optical interactions, the effective Hamiltonian for the carriers -- *i.e.* "free" particle kinetic energy plus electromagnetic interaction -- is separable into a series of \bar{k} -dependent terms.⁴¹ Thus,

⁴⁰ From *Diode Lasers and Photonic Integrated Circuits* by Larry A. Coldren and Scott W. Corzine, Wiley (1995)

⁴¹ In particular, it can be shown -- see Weng W. Chow, Stephan W. Koch and Murray Sargent III, *Semiconductor-Laser Physics*, Springer-Verlag (1994) -- that

if we neglect $\bar{\mathbf{k}}\bar{\mathbf{k}}$ correlations in the treatment of optical properties, we need only consider the following manifold of states:

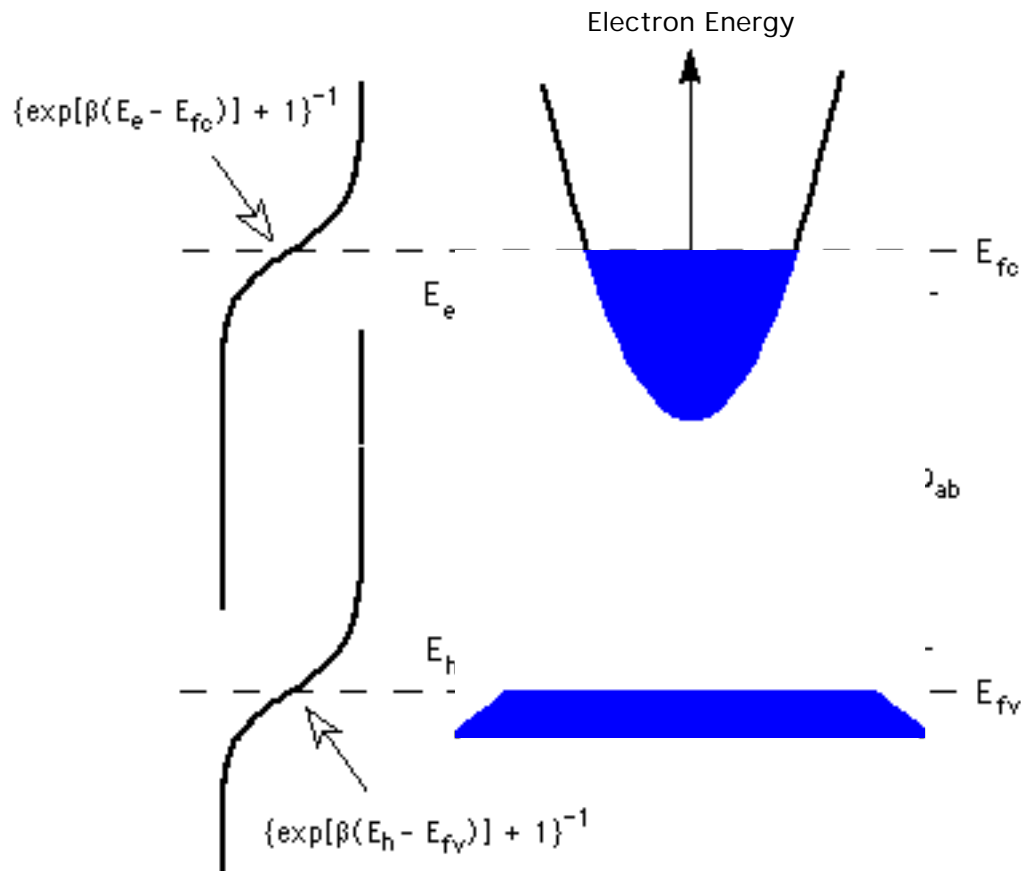


Equation [VII-37a] tells us that the absorption or emission of a single photon connect only the two states in the manifold which can be identified as $|0_e 0_h : \vec{k}\rangle$ and $|1_e 1_h : \vec{k}\rangle$ where the first number in the ket specifies **electron occupancy** of a state with momentum $\hbar \vec{k}$ and the second **hole occupancy** of a state with momentum $-\hbar \vec{k}$.

$$\mathcal{H}_{\text{eff}} = \frac{\hbar^2 k^2}{2m_{ec}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{\hbar^2 k^2}{2m_{hv}} b_{-\vec{k}}^\dagger b_{-\vec{k}} - [\mu_{\vec{k}} a_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger + \mu_{\vec{k}} a_{\vec{k}} b_{-\vec{k}}] E(z, t)$$

where $\{a_{\vec{k}}^\dagger, a_{\vec{k}}\}$ and $\{b_{\vec{k}}^\dagger, b_{\vec{k}}\}$ are, respectively, electron and hole {**creation, destruction**} operators. $\mu_{\vec{k}}$ is the dipole matrix element between vertical states in the valence and conduction bands.

ENERGY DIAGRAM FOR BULK LASERS



Since no $\bar{\mathbf{k}}\bar{\mathbf{k}}$ correlations are involved in the free carrier theory, the density operator of the complete system may be expressed as a product of component density operators

$$= \prod_{\mathbf{k}} \rho(\bar{\mathbf{k}}) \quad [\text{VII-39}]$$

so that the Schrödinger equation of motion for the density operator is also separable -- viz.

$$\dot{\psi}(\bar{\mathbf{k}}) = -\frac{i}{\hbar} \left[\mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}), \psi(\bar{\mathbf{k}}) \right]. \quad [\text{VII-39}]$$

C. INJECTION LASER THEORY

(For pictorials on laser configurations go to:

http://www.deas.harvard.edu/courses/ap216/images/injection_lasers/laser_structures/laser_structures.html)

A fairly satisfactory model of lasing (and other optical processes) in semiconductors may be obtained by adaptation of the two-level, semiclassical discussed earlier. In light of the discussion in the previous section, we adapt the two-level theory by making the identifications

$$\begin{aligned} {}_{aa}(\bar{\mathbf{k}}) \quad {}_{1111}(\bar{\mathbf{k}}) &= \langle 1_e 1_h : \bar{\mathbf{k}} \mid \mid 1_e 1_h : \bar{\mathbf{k}} \rangle = \langle 3 : \bar{\mathbf{k}} \mid \mid 3 : \bar{\mathbf{k}} \rangle = {}_{33}(\bar{\mathbf{k}}) \\ {}_{bb}(\bar{\mathbf{k}}) \quad {}_{0000}(\bar{\mathbf{k}}) &= \langle 0_e 0_h : \bar{\mathbf{k}} \mid \mid 0_e 0_h : \bar{\mathbf{k}} \rangle = \langle 0 : \bar{\mathbf{k}} \mid \mid 0 : \bar{\mathbf{k}} \rangle = {}_{00}(\bar{\mathbf{k}}) \\ {}_{ab}(\bar{\mathbf{k}}) \quad {}_{1100}(\bar{\mathbf{k}}) &= \langle 1_e 1_h : \bar{\mathbf{k}} \mid \mid 0_e 0_h : \bar{\mathbf{k}} \rangle = \langle 3 : \bar{\mathbf{k}} \mid \mid 0 : \bar{\mathbf{k}} \rangle = {}_{30}(\bar{\mathbf{k}}) \end{aligned} \quad [\text{VII--40}]$$

Given the **free carrier effective Hamiltonian** discussed above and the equation of motion expressed in Equation [VII-31], we can write

$$\begin{aligned} \dot{{}_{30}}(\bar{\mathbf{k}}) &= \langle 3 : \bar{\mathbf{k}} \mid \dot{\psi}(\bar{\mathbf{k}}) \mid 0 : \bar{\mathbf{k}} \rangle \\ &= -\frac{i}{\hbar} \left[\langle 3 : \bar{\mathbf{k}} \mid \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) \mid 3 : \bar{\mathbf{k}} \rangle - \langle 0 : \bar{\mathbf{k}} \mid \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) \mid 0 : \bar{\mathbf{k}} \rangle \right] {}_{30}(\bar{\mathbf{k}}) \\ &\quad + \frac{i}{\hbar} \langle 3 : \bar{\mathbf{k}} \mid \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) \mid 0 : \bar{\mathbf{k}} \rangle \left[{}_{33}(\bar{\mathbf{k}}) - {}_{00}(\bar{\mathbf{k}}) \right] \end{aligned} \quad [\text{VII--41a}]$$

$$\begin{aligned} \dot{{}_{33}}(\bar{\mathbf{k}}) &= \langle 3 : \bar{\mathbf{k}} \mid \dot{\psi}(\bar{\mathbf{k}}) \mid 3 : \bar{\mathbf{k}} \rangle = \frac{i}{\hbar} \left[{}_{30}(\bar{\mathbf{k}}) \langle 0 : \bar{\mathbf{k}} \mid \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) \mid 3 : \bar{\mathbf{k}} \rangle \right] \\ &\quad - \frac{i}{\hbar} \left[{}_{03}(\bar{\mathbf{k}}) \langle 3 : \bar{\mathbf{k}} \mid \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) \mid 0 : \bar{\mathbf{k}} \rangle \right] \end{aligned} \quad [\text{VII--41b}]$$

$$\begin{aligned} \dot{\rho}_{00}(\bar{\mathbf{k}}) = \langle 0:\bar{\mathbf{k}} | \dot{\rho}(\bar{\mathbf{k}}) | 0:\bar{\mathbf{k}} \rangle = & -\frac{i}{\hbar} \left[\rho_{30}(\bar{\mathbf{k}}) \langle 0:\bar{\mathbf{k}} | \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) | 3:\bar{\mathbf{k}} \rangle \right] \\ & + \frac{i}{\hbar} \left[\rho_{03}(\bar{\mathbf{k}}) \langle 3:\bar{\mathbf{k}} | \mathcal{H}_{\text{eff}}(\bar{\mathbf{k}}) | 0:\bar{\mathbf{k}} \rangle \right] \end{aligned} \quad [\text{VII--41c}]$$

which tells us, once again, that ρ_{ab} is driven by $\rho_{aa} - \rho_{bb}$ and *vice versa*. There is, however, an important new element to be considered in this problem to wit, as we have illustrated above, we are, in fact, actually dealing with a **four-level system** which includes of the states $|1_e 0_h; \bar{\mathbf{k}}\rangle$ and $|0_e 1_h; \bar{\mathbf{k}}\rangle$ as well as the pseudo "a" and "b" states. Fortunately, inclusion of these states does not unduly complicate the analysis since, as discussed above, electron-electron scattering induces a rapid relaxation or "thermalization" of the probability of finding a given state occupied. After thermalization, the probability of finding a state with a particular momentum value in a given band is provided by a Fermi-Dirac distribution referenced to a quasi-Fermi energy or **imref** appropriate to that band. To obtain an expression for $\rho_{aa} - \rho_{bb}$ we note that⁴²

$$\text{tr} \left[\rho(\bar{\mathbf{k}}) \right] = \rho_{00}(\bar{\mathbf{k}}) + \rho_{11}(\bar{\mathbf{k}}) + \rho_{22}(\bar{\mathbf{k}}) + \rho_{33}(\bar{\mathbf{k}}) = 1 \quad [\text{VII--42}]$$

so that

$$\begin{aligned} \rho_{aa} - \rho_{bb} = \rho_{33}(\bar{\mathbf{k}}) - \rho_{00}(\bar{\mathbf{k}}) = & \left\{ \rho_{33}(\bar{\mathbf{k}}) + \rho_{22}(\bar{\mathbf{k}}) \right\} + \left\{ \rho_{33}(\bar{\mathbf{k}}) + \rho_{11}(\bar{\mathbf{k}}) \right\} - 1 \\ = & n_e(\bar{\mathbf{k}}) + n_h(\bar{\mathbf{k}}) - 1 \end{aligned} \quad [\text{VII--43}]$$

where $n_e(\bar{\mathbf{k}})$ is the probability⁴³ of finding a electron with momentum $\hbar \bar{\mathbf{k}}$ independent of whether or not there is a hole with momentum $-\hbar \bar{\mathbf{k}}$ and $n_h(\bar{\mathbf{k}})$ is the corresponding

⁴² That is, there must be either 0 or 1 electrons and 0 or 1 holes in the given $\bar{\mathbf{k}}$ state.

⁴³ In the second quantization representation of the problem, the n 's are expectation values of the appropriate number operators.

probability for a hole. Adapting Equations [VI-13a-c] from earlier in this set of lecture notes,⁴⁴ we may write

$$\dot{n}_e(\bar{\mathbf{k}}) = \dot{n}_{e\bar{\mathbf{k}}} - n_{nr} n_e(\bar{\mathbf{k}}) - \dot{n}_{\bar{\mathbf{k}}} n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}}) - \dot{n}_e(\bar{\mathbf{k}}) \Big|_{c-c} - \left[i \hbar^{-1} \mathcal{V}'_{ab}(z, t; \bar{\mathbf{k}}) n_{ab}(\bar{\mathbf{k}}) + c.c \right] \quad [\text{VII--44a}]$$

$$\dot{n}_h(\bar{\mathbf{k}}) = \dot{n}_{h\bar{\mathbf{k}}} - n_{nr} n_h(\bar{\mathbf{k}}) - \dot{n}_{\bar{\mathbf{k}}} n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}}) - \dot{n}_h(\bar{\mathbf{k}}) \Big|_{c-c} - \left[i \hbar^{-1} \mathcal{V}'_{ab}(z, t; \bar{\mathbf{k}}) n_{ab}(\bar{\mathbf{k}}) + c.c \right] \quad [\text{VII--44b}]$$

$$\dot{n}_{ab}(\bar{\mathbf{k}}) = -\left(i \dot{n}_{ab} + \dot{n}_{ab} \right) n_{ab}(\bar{\mathbf{k}}) + i \hbar^{-1} \mathcal{V}'_{ab}(z, t; \bar{\mathbf{k}}) \left[n_e(\bar{\mathbf{k}}) + n_h(\bar{\mathbf{k}}) - 1 \right] \quad [\text{VII--44c}]$$

where $\dot{n}_{\bar{\mathbf{k}}}$ (= e or h) represents the pumping rate due to carrier injection and $\dot{n}_e(\bar{\mathbf{k}}) \Big|_{c-c}$ the effect of carrier-carrier scattering. $n_{nr} n_e(\bar{\mathbf{k}})$ and $\dot{n}_{\bar{\mathbf{k}}} n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}})$ are, respectively, phenomenological representations of nonradiative decay and radiative “bimolecular” recombination (**spontaneous emission**), respectively. The probability difference (**gain factor**)

$$n_{ab}(\bar{\mathbf{k}}) = n_e(\bar{\mathbf{k}}) + n_h(\bar{\mathbf{k}}) - 1 = n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}}) \left[\frac{1}{n_e(\bar{\mathbf{k}})} - 1 - \frac{1}{n_h(\bar{\mathbf{k}})} - 1 \right] \quad [\text{VII--45}]$$

is the **critical factor** in the analysis of **stimulated** processes -- *i.e.* for inversion $n_{ab}(\bar{\mathbf{k}}) > 0$. This gain factor may be written as $n_{ab}(\bar{\mathbf{k}}) = n_e(\bar{\mathbf{k}}) - [1 - n_h(\bar{\mathbf{k}})]$ -- *i.e.* the population inversion is proportional to the probability difference of an electron in corresponding $\bar{\mathbf{k}}$ -states in the conduction and valence bands. Alternatively and more usefully, we see that it varies directly with the product of

⁴⁴ That is

$$\begin{aligned} \dot{n}_{aa} &= \dot{n}_a - \dot{n}_a - \dot{n}_{aa} - \left[i \hbar^{-1} \mathcal{V}'_{ab} \dot{n}_{ab} + c.c. \right] \\ \dot{n}_{bb} &= \dot{n}_b - \dot{n}_b - \dot{n}_{bb} + \left[i \hbar^{-1} \mathcal{V}'_{ab} \dot{n}_{ab} + c.c. \right] \\ \dot{n}_{ab} &= -\left(i \dot{n}_{ab} + \dot{n}_{ab} \right) \dot{n}_{ab} + i \hbar^{-1} \mathcal{V}'_{ab} \left[\dot{n}_{aa} - \dot{n}_{bb} \right] \end{aligned}$$

the **spontaneous emission factor**

$$n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}})$$

and the so called **absorption factor**

$$1 - \frac{1}{n_e(\bar{\mathbf{k}})} - 1 - \frac{1}{n_h(\bar{\mathbf{k}})} - 1 .$$

In the spirit of the **free carrier model** and in the unsaturated limit the $n_\ell(\bar{\mathbf{k}})$'s are given by the *quasi equilibrium* Fermi-Dirac distributions -- viz.

$$n(\bar{\mathbf{k}}) = f_{\bar{\mathbf{k}}} = \exp \left(\frac{\epsilon_{\bar{\mathbf{k}}} - \mu}{k_B T} \right) + 1^{-1} \quad [\text{VII--46}]$$

Thus, the **absorption factor** is given by

$$\begin{aligned} 1 - \frac{1}{n_e(\bar{\mathbf{k}})} - 1 - \frac{1}{n_h(\bar{\mathbf{k}})} - 1 &= 1 - \exp \left(\frac{\epsilon_{e\bar{\mathbf{k}}} + \epsilon_{h\bar{\mathbf{k}}} - \mu_e - \mu_h}{k_B T} \right) \\ &= 1 - \exp \left[\frac{\epsilon_{\bar{\mathbf{k}}} - \mu}{k_B T} \right] \end{aligned} \quad [\text{VII--47}]$$

and the **spontaneous emission factor** is given by

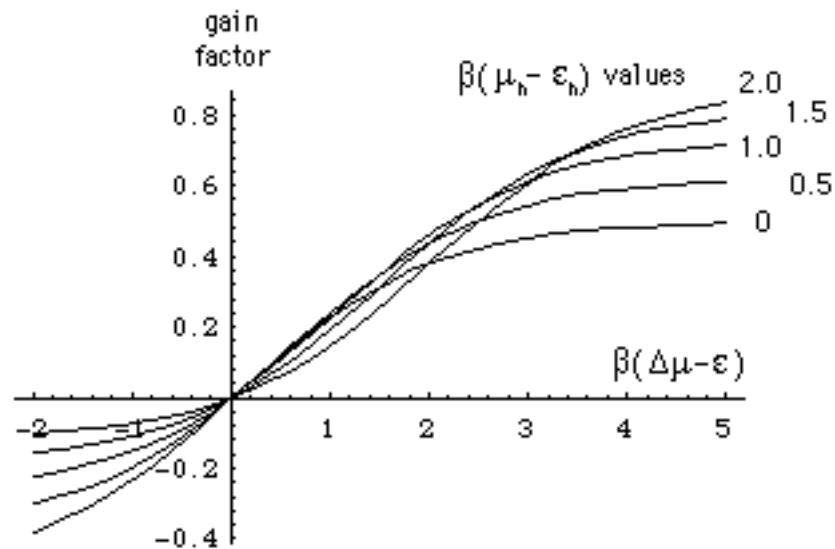
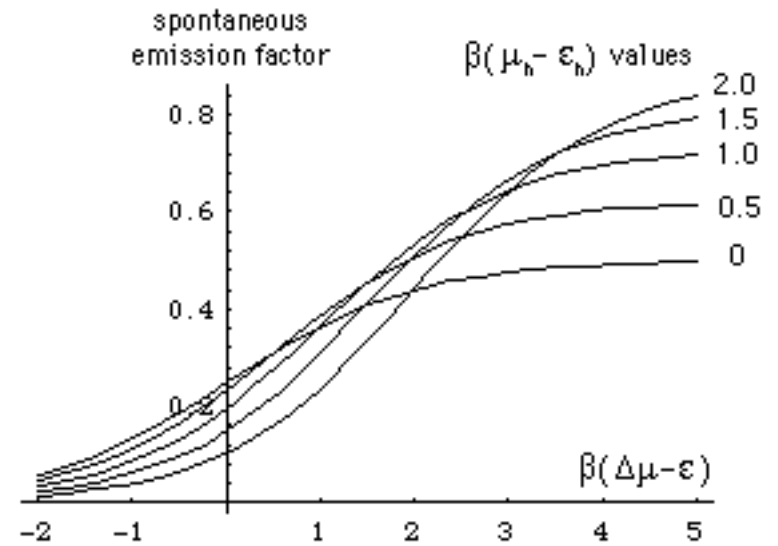
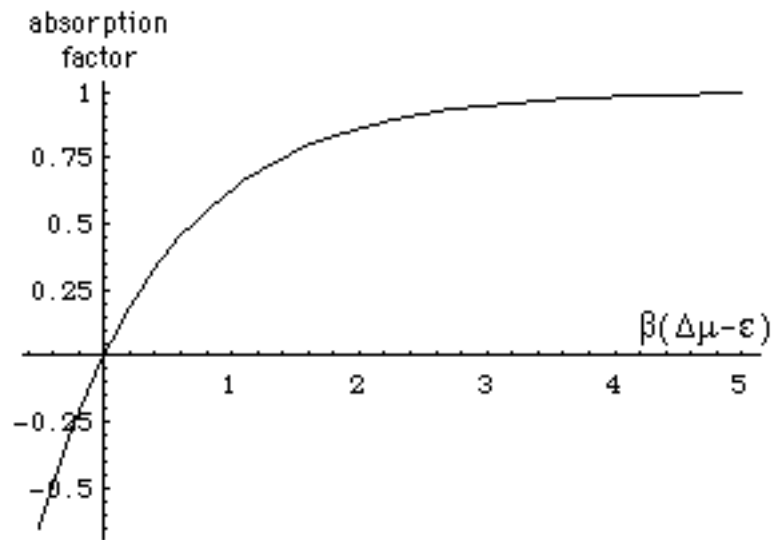
$$n_e(\bar{\mathbf{k}}) n_h(\bar{\mathbf{k}}) = \exp \left(\frac{\epsilon_{h\bar{\mathbf{k}}} - \mu_h}{k_B T} \right) \exp \left[\frac{\epsilon_{\bar{\mathbf{k}}} - \mu}{k_B T} \right] + 1^{-1} \exp \left(\frac{\epsilon_{e\bar{\mathbf{k}}} - \mu_e}{k_B T} \right) + 1^{-1} \quad [\text{VII--48}]$$

where $\epsilon_{\bar{\mathbf{k}}} = \frac{\hbar^2 k^2}{2m_r}$ and $\mu = \mu_e + \mu_h = (E_F)_C - (E_F)_V - \epsilon_g$.⁴⁵

⁴⁵ For plotting purposes it is useful to write the complete **gain factor** as

$$G(\bar{\mathbf{k}}) = \exp \left[g \left(\frac{x}{1+r} + \frac{r}{1+r} - x_F + x_h \right) \right] + 1^{-1} - \exp \left[g \left(-\frac{r}{1+r} x + \frac{r}{1+r} + x_h \right) \right] + 1^{-1}$$

where $r = m_e/m_h$, $x = \hbar k / m_g v_g$, $x_F = E_F / \epsilon_g$, and $x_h = \mu_h / \epsilon_g$.



Therefore, **for population inversion** $\mu - = (E_F)_C - (E_F)_V - (k_B T \ln 2) > 0$ **which is a very stringent condition!**

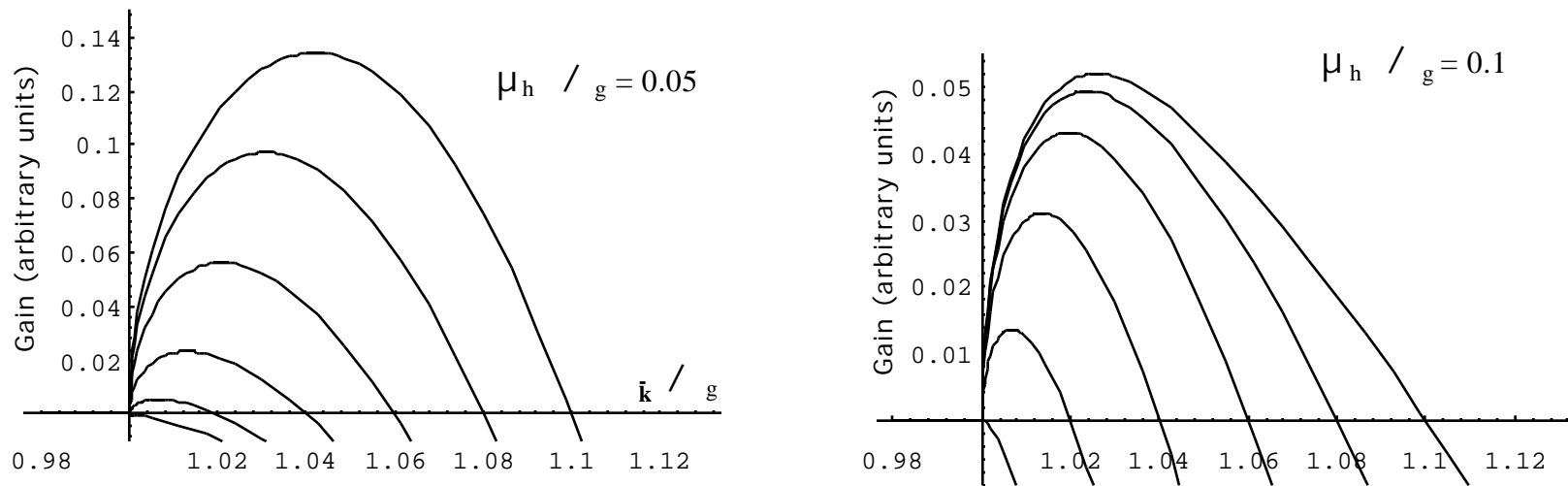
Adapting Equation [VI-26a] from earlier in this set of lecture notes,⁴⁶ we may see that

the **small signal gain** in a semiconductor, may be expressed in the form

$$Gain(\bar{k}) = \left| \bar{M}_{v\bar{k}c\bar{k}} \right|^{-1} (\bar{k}) \left\{ \text{the density of paired states at } \bar{k} \right\} \mathcal{L}(\bar{k} - \epsilon_n; ab) \quad [VII-49]$$

in bulk material the density of paired states varies as the square root of the energy.

Therefore, we may draw the following gain curves:

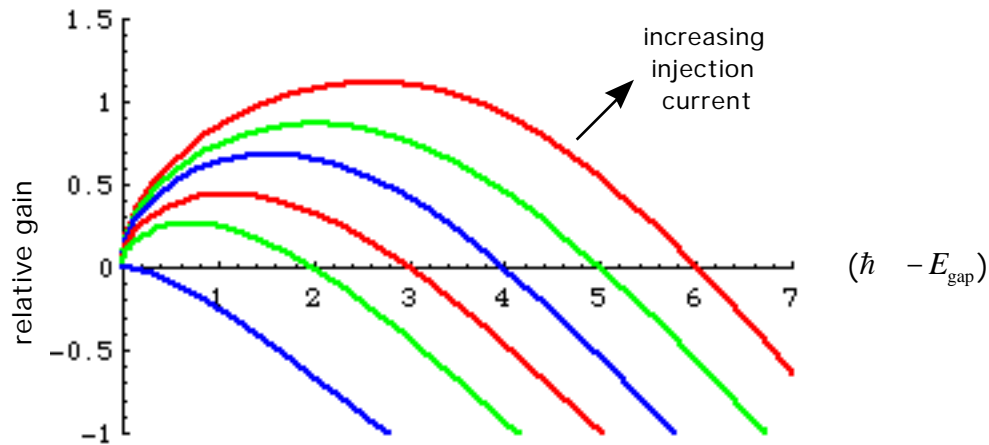


Gain in a bulk semiconductor with $E_F / \epsilon_g = 1.00, 1.02, 1.04, 1.06, 1.08, \text{ and } 1.10$

⁴⁶ That is

$$n = \frac{1}{2} n \frac{2}{\hbar \omega} \frac{1}{ab} \mathcal{L}(ab - \epsilon_n; ab) \bar{N} - \frac{n}{2Q_n}$$

GAIN VARIATION WITH CARRIER CONCENTRATION



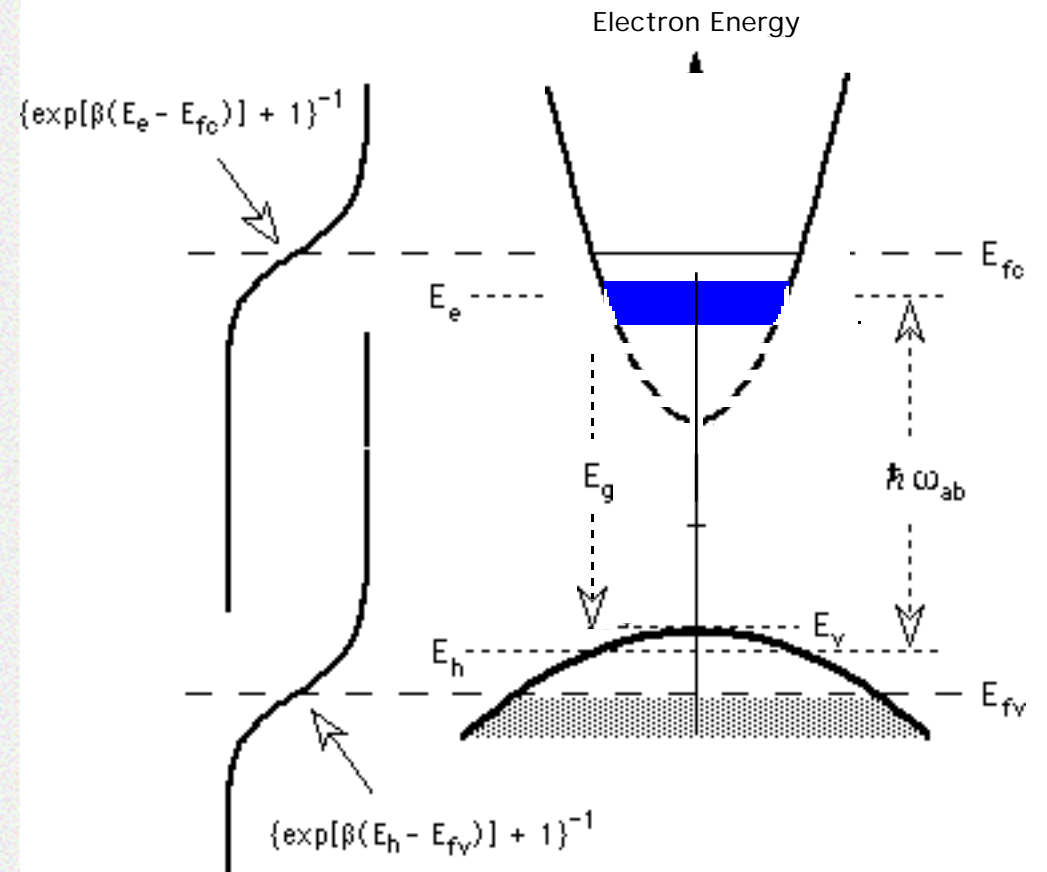
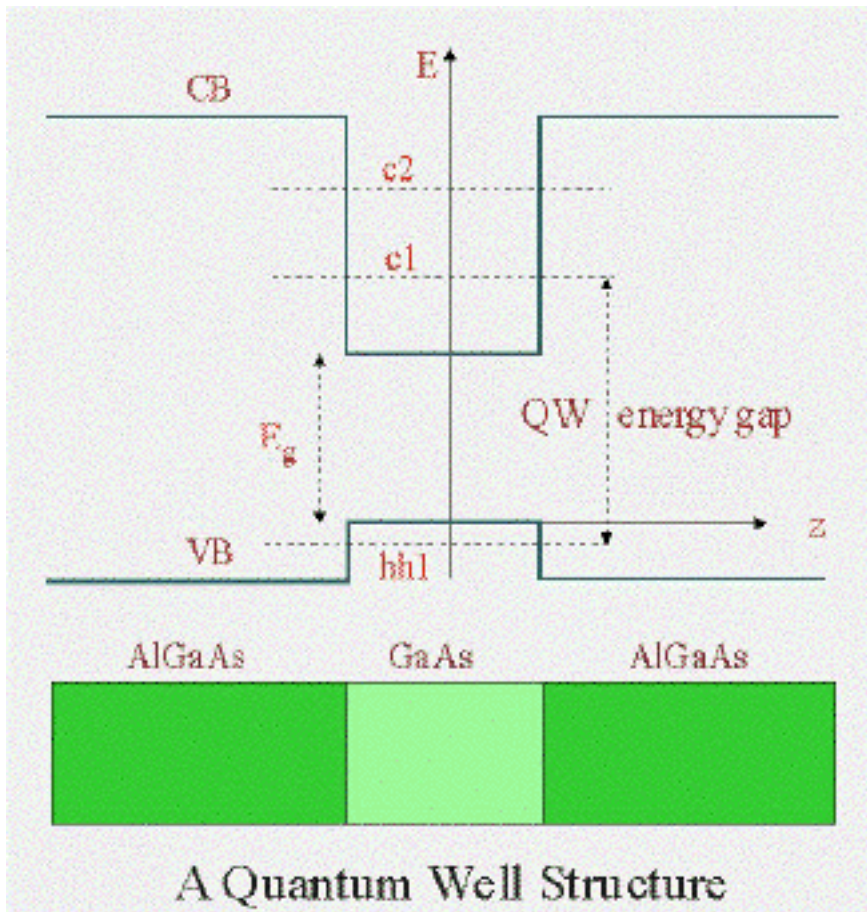
QUANTUM CONFINEMENT

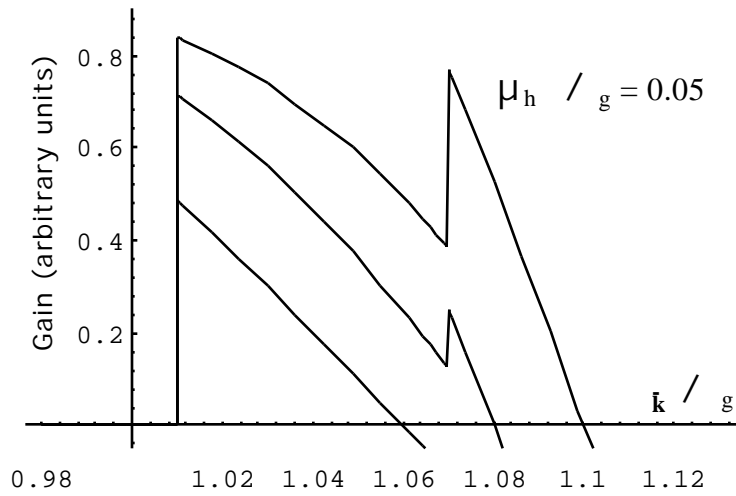
In an idealized quantum well
$$V(z) = \begin{cases} 0 & |z| < L_c/2 \\ \infty & |z| > L_c/2 \end{cases}$$

which yields a single electron energy

$$E_n(\vec{k}) = \frac{\hbar^2 n^2 \pi^2}{2 m_z L_c^2} + \frac{\hbar^2 |\vec{k}|^2}{2 m}$$

and density of paired states which is a constant or a staircase.





Gain in a 2D semiconductor with $E_F / \epsilon_g = 1.06, 1.08, \text{ and } 1.10$

