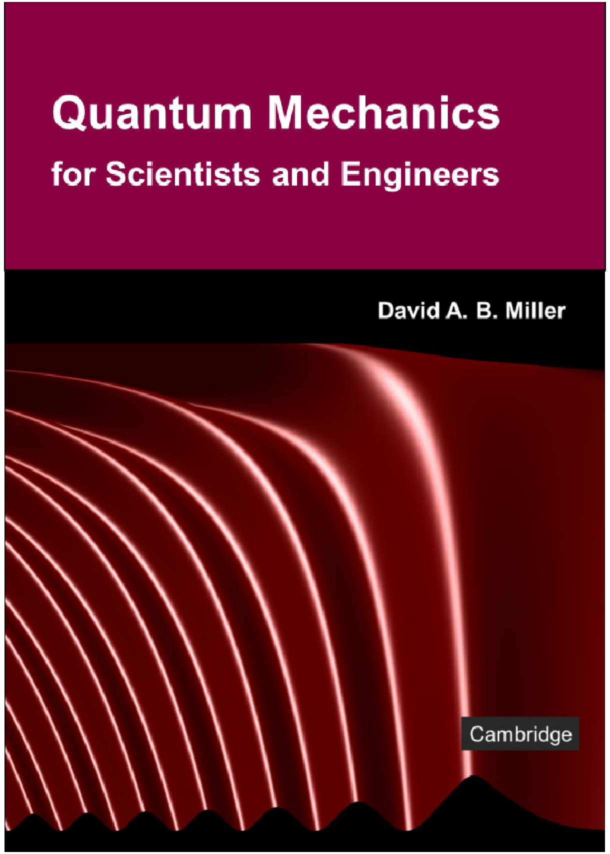
32 Optical absorption in semiconductors

Slides: Lecture 32a Introduction to optical absorption in semiconductors

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.10 (beginning)



Optical absorption in semiconductors

Quantum mechanics for scientists and engineers

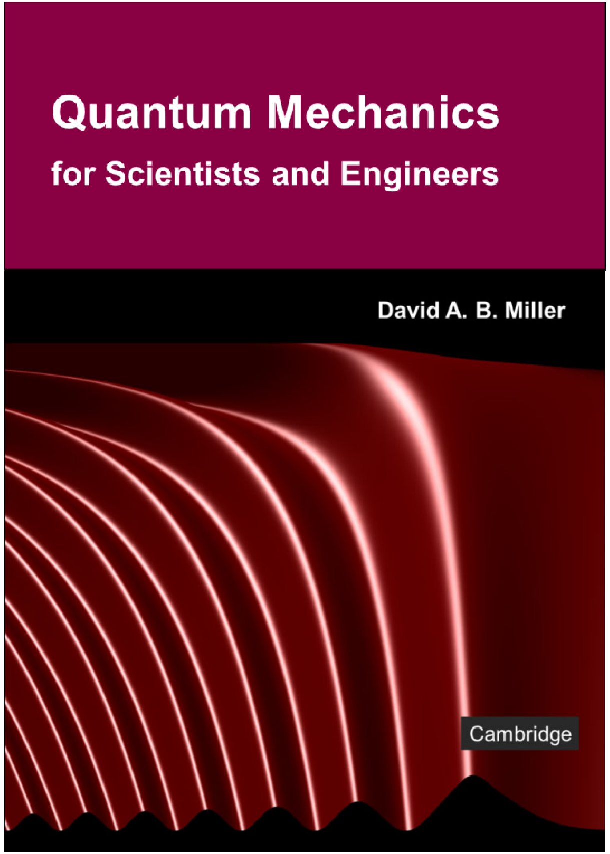
David Miller

32 Optical absorption in semiconductors

Slides: Lecture 32b Perturbing Hamiltonian

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.10 through "Form of the perturbing …" (with Appendix E for optional background)



Optical absorption in semiconductors

Perturbing Hamiltonian

Quantum mechanics for scientists and engineers

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Direct optical absorption

The transition rate for absorption

from an initial electron state $|\psi_i\rangle$

with energy E_i

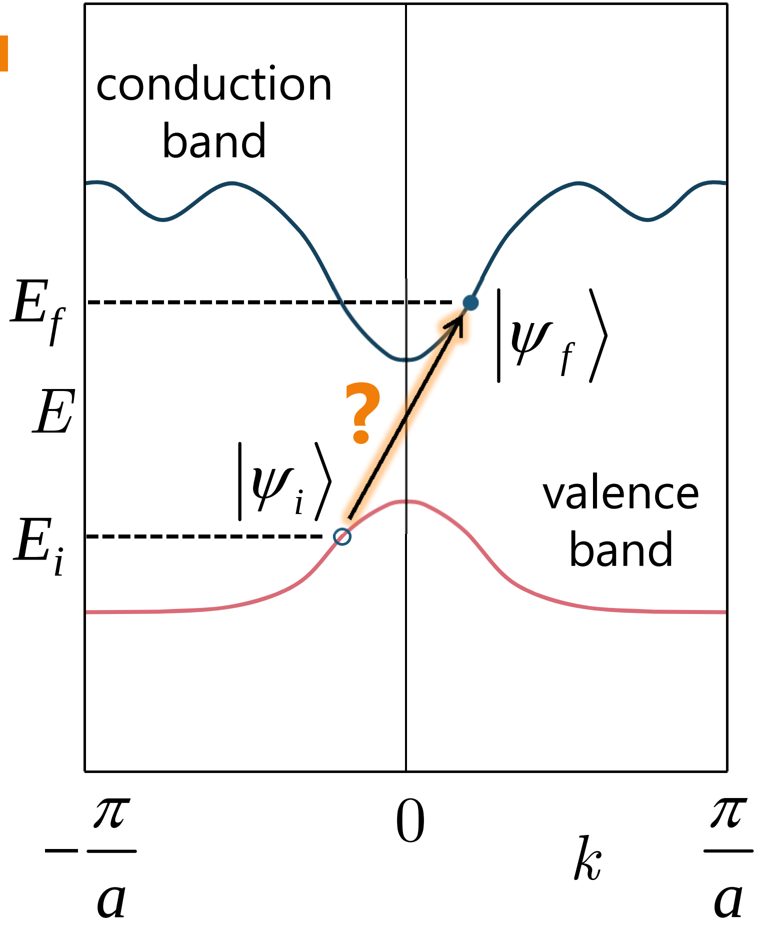
to a final state $|\psi_f\rangle$ with energy E_f

with an oscillating perturbation of

angular frequency ω

is, from Fermi's Golden Rule

$$w_{abs} = \frac{2\pi}{\hbar}\left|\left\langle \psi_f \middle| \hat{H}_{po} \middle| \psi_i \right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$



Direct optical absorption

In Fermi's Golden Rule $w_{abs} = \frac{2\pi}{\hbar}\left|\left\langle \psi_f \middle| \hat{H}_{po} \middle| \psi_i \right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$

$\hat{H}_{po}$ is the amplitude of a perturbation oscillating in time at (angular) frequency ω, such as is defined in

$$\hat{H}_p(t) = e\mathrm{E}(t)z = \hat{H}_{po}\left[\exp(-i\omega t) + \exp(i\omega t)\right]$$

where E is the electric field in the z direction

We are also now interested in the spatial variation of $\hat{H}_{po}$ through the spatial dependence of the electromagnetic wave amplitude, as explicitly in

$$\hat{H}_p(\mathbf{r},t) = \hat{H}_{po}(\mathbf{r})\left[\exp(-i\omega t) + \exp(i\omega t)\right]$$

Direct optical absorption

The matrix element in Fermi's Golden Rule, $\left\langle \psi_f \middle| \hat{H}_{po} \middle| \psi_i \right\rangle$

can now be written explicitly as

$$\left\langle \psi_f \middle| \hat{H}_{po} \middle| \psi_i \right\rangle = \int \psi_f^*(\mathbf{r}) \hat{H}_{po}(\mathbf{r}) \psi_i(\mathbf{r}) d^3\mathbf{r}$$

where $\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$ are, respectively,

the wave functions of the initial and final states

and we explicitly allow $\hat{H}_{po}(\mathbf{r})$ to vary in space

because the electromagnetic field at

(angular) frequency ω will vary in space

Perturbing Hamiltonian for electromagnetic field

Though we could continue with the “electric dipole” version of the perturbing Hamiltonian $\hat{H}_p(\mathbf{r},t) = e\mathrm{E}(\mathbf{r},t)z$

we can connect to other semiconductor phenomena

if we switch to using the magnetic vector potential $\mathbf{A}$ instead of the electric field, and write

$$\hat{H}_p(\mathbf{r},t) \cong -\frac{e}{m_o}\mathbf{A}\cdot\hat{\mathbf{p}}$$

where m_o is the usual free electron mass and

$\hat{\mathbf{p}} = -i\hbar\nabla$ is the momentum operator

(Note: both the electric and magnetic fields can be deduced from the vector potential $\mathbf{A}$)

Perturbing Hamiltonian for electromagnetic field

Now we write the vector potential of a wave at frequency ω

$$\mathbf{A} = \mathbf{e}\left\{\frac{A_0}{2}\exp\left[i\left(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t\right)\right]+\frac{A_0}{2}\exp\left[-i\left(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t\right)\right]\right\}$$

Here $\mathbf{k}_{op}$ is the wave vector of the optical field inside the material, and

we take the field to be linearly polarized

with its electric vector in the direction of the unit vector $\mathbf{e}$

Perturbing Hamiltonian for electromagnetic field

Now in $\mathbf{A} = \mathbf{e}\left\{\frac{A_0}{2}\exp\left[i\left(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t\right)\right]+\frac{A_0}{2}\exp\left[-i\left(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t\right)\right]\right\}$

we are going to keep only the term in $\exp(-i\omega t)$

because we know from our previous discussion of Fermi's Golden Rule that this term

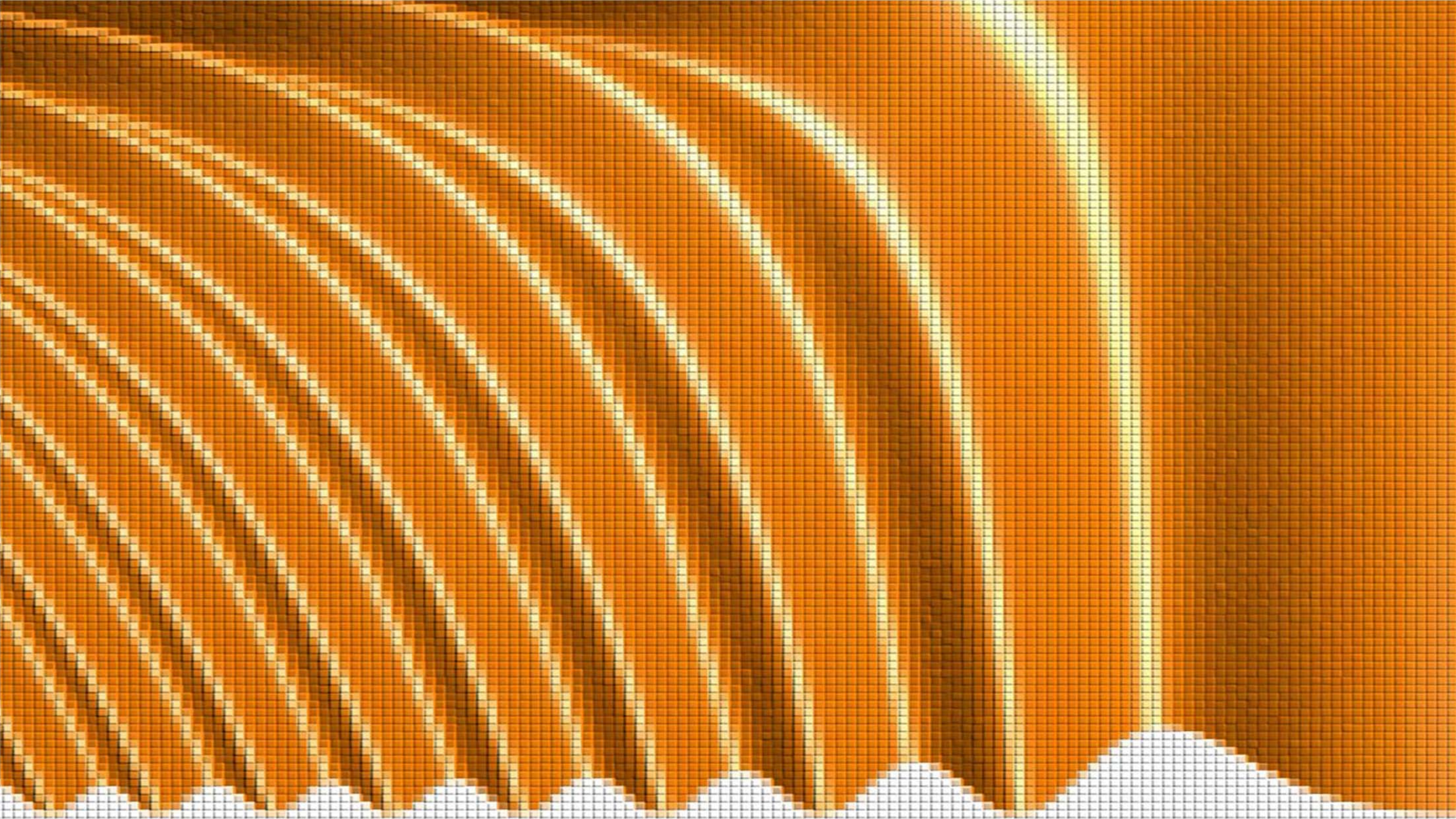
corresponds to absorption rather than emission

So the spatial part of our perturbing Hamiltonian is

$$\hat{H}_{po}(\mathbf{r}) = -(e/2m_o)A_0\exp\left(i\mathbf{k}_{op}\cdot\mathbf{r}\right)\mathbf{e}\cdot\hat{\mathbf{p}}$$

and the total perturbing Hamiltonian is

$$\hat{H}_p(\mathbf{r},t) = \hat{H}_{po}(\mathbf{r})\exp(-i\omega t)$$

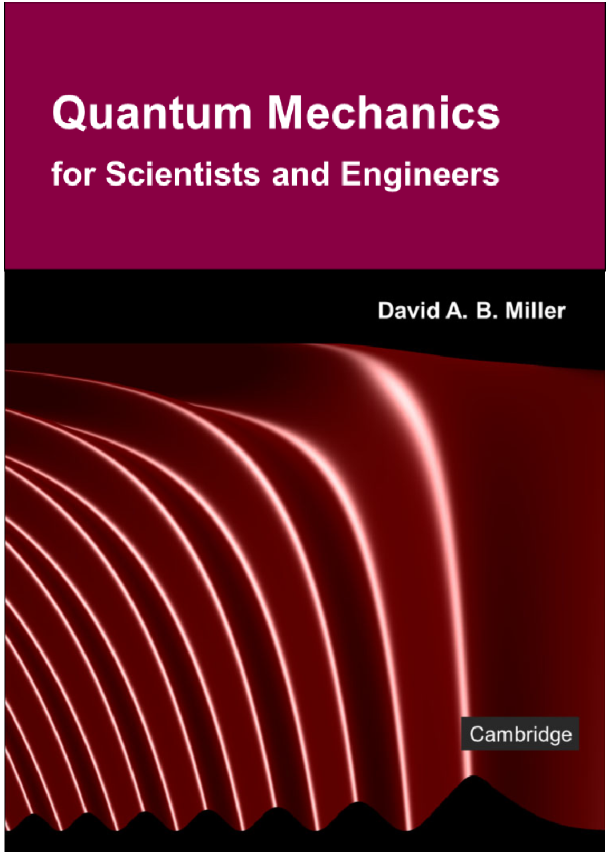


32 Optical absorption in semiconductors

Slides: Lecture 32c Direct transitions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.10 subsection "Direct valence …" through paragraph after Eq. 8.98



Optical absorption in semiconductors

Direct transitions

Quantum mechanics for scientists and engineers

David Miller

Direct optical absorption

To proceed, we need to know

the initial and final wavefunctions

We are most interested in the transitions between

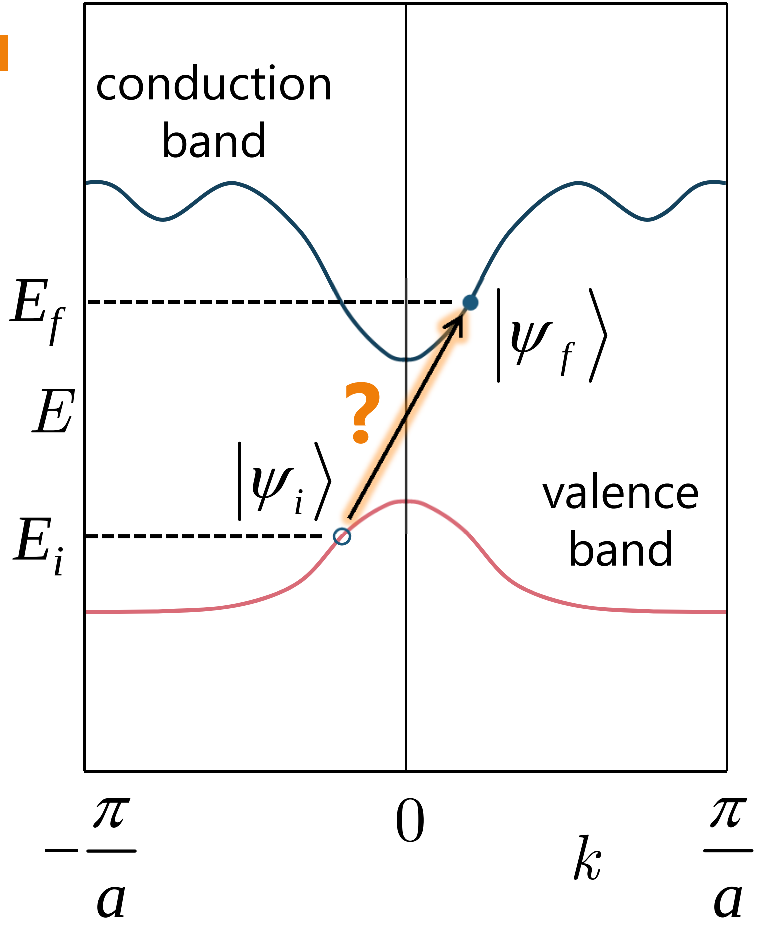
an initial valence band state $|\psi_i\rangle$ and

a final conduction band state $|\psi_f\rangle$

We presume that we can write them as "single-electron" Bloch states

and to calculate matrix elements

we must normalize them



Normalizing Bloch functions

With normalization constants B_i and B_f, we have

$$\psi_i(\mathbf{r}) = B_i u_v(\mathbf{r}) \exp(i\mathbf{k}_v \cdot \mathbf{r})$$

and

$$\psi_f(\mathbf{r}) = B_f u_c(\mathbf{r}) \exp(i\mathbf{k}_c \cdot \mathbf{r})$$

Here, and below, for simplicity

we presume u_v and u_c do not depend on $\mathbf{k}$

a good approximation for an "allowed" process

so we omit the "$\mathbf{k}$" subscripts on u_v and u_c

We do, however, now explicitly allow the conduction (u_v) and valence (u_c) unit cell functions to be different

Normalizing Bloch functions

We choose $u_v(\mathbf{r})$ and $u_c(\mathbf{r})$ to be normalized over a unit cell

$$\int_{unit\ cell} u_v^*(\mathbf{r}) u_v(\mathbf{r}) d^3\mathbf{r} = 1$$ and similarly for $u_c(\mathbf{r})$

Hence, normalizing $\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$, we have, e.g., for $\psi_i(\mathbf{r})$

$$\int_V \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) d^3\mathbf{r} = 1 = B_i^2 \int_V u_v^*(\mathbf{r})\exp(-i\mathbf{k}_v\cdot\mathbf{r}) u_v(\mathbf{r})\exp(i\mathbf{k}_v\cdot\mathbf{r}) d^3\mathbf{r}$$

$$= B_i^2 \int_V u_v^*(\mathbf{r}) u_v(\mathbf{r}) d^3\mathbf{r} = B_i^2 N \int_{unit\,cell} u_v^*(\mathbf{r}) u_v(\mathbf{r}) d^3\mathbf{r} = B_i^2 N$$

where V is the volume of the crystal

where N is the number of unit cells and

Hence we have $B_i = B_f = 1/\sqrt{N}$

Matrix element for Fermi's Golden Rule

With $\hat{H}_{po}(\mathbf{r}) = -(e/2m_o)A_o \exp\left(i\mathbf{k}_{op} \cdot \mathbf{r}\right)\mathbf{e} \cdot \hat{\mathbf{p}}$

$\psi_i(\mathbf{r}) = \frac{1}{\sqrt{N}} u_v(\mathbf{r}) \exp\left(i\mathbf{k}_v \cdot \mathbf{r}\right)$ and $\psi_f(\mathbf{r}) = \frac{1}{\sqrt{N}} u_c(\mathbf{r}) \exp\left(i\mathbf{k}_c \cdot \mathbf{r}\right)$

the matrix element for Fermi's Golden Rule is

$$\left\langle \psi_f \middle| \hat{H}_{po}(\mathbf{r}) \middle| \psi_i \right\rangle =$$

$$-\frac{eA_o}{2m_o N} \int_V \left[u_c^*(\mathbf{r}) \exp\left(-i\mathbf{k}_c \cdot \mathbf{r}\right)\right] \exp\left(i\mathbf{k}_{op} \cdot \mathbf{r}\right)\mathbf{e} \cdot \hat{\mathbf{p}} \left[u_v(\mathbf{r}) \exp\left(i\mathbf{k}_v \cdot \mathbf{r}\right)\right] d^3\mathbf{r}$$

Matrix element for Fermi's Golden Rule

We are interested in transitions involving states near the center of the Brillouin zone, so

$|\mathbf{k}_v|$ and $|\mathbf{k}_c|$ are both $\ll \pi / a$

Though strictly $\hat{\mathbf{p}} = -i\hbar\nabla$ operates on all of $u_v(\mathbf{r})\exp(i\mathbf{k}_v \cdot \mathbf{r})$

with these small values of $\mathbf{k}_v$

$\exp(i\mathbf{k}_v \cdot \mathbf{r})$ changes very slowly compared to the rate of change of $u_v(\mathbf{r})$

so, at least as a first approximation, we take

$$\hat{\mathbf{p}}\left[u_v(\mathbf{r})\exp(i\mathbf{k}_v \cdot \mathbf{r})\right] = \exp(i\mathbf{k}_v \cdot \mathbf{r})\hat{\mathbf{p}}u_v(\mathbf{r}) + u_v(\mathbf{r})\hat{\mathbf{p}}\exp(i\mathbf{k}_v \cdot \mathbf{r})$$

$$\simeq \exp(i\mathbf{k}_v \cdot \mathbf{r})\hat{\mathbf{p}}u_v(\mathbf{r})$$

Matrix element for Fermi's Golden Rule

For definiteness, we choose the polarization direction (i.e., unit vector **e**) in the *x* direction

- *x* will be one of the directions perpendicular to the propagation of the electromagnetic wave

With this choice and our approximations so far

$$\left\langle \psi_f \left| \hat{H}_{po}(\mathbf{r}) \right| \psi_i \right\rangle =$$

$$-\frac{eA_0}{2m_o N}\int_V \left[u_c^*(\mathbf{r})\exp(-i\mathbf{k}_c\cdot\mathbf{r})\right]\exp\left(i\mathbf{k}_{op}\cdot\mathbf{r}\right)\mathbf{e}\cdot\hat{\mathbf{p}}\left[u_v(\mathbf{r})\exp(i\mathbf{k}_v\cdot\mathbf{r})\right]d^3\mathbf{r}$$

$$\simeq -\frac{eA_0}{2m_o N}\int_V \exp\left[i\left(\mathbf{k}_v-\mathbf{k}_c+\mathbf{k}_{op}\right)\cdot\mathbf{r}\right]\left[u_c^*(\mathbf{r})\,\hat{p}_x u_v(\mathbf{r})\right]d^3\mathbf{r}$$

Matrix element for Fermi’s Golden Rule

The optical wave vector $\mathbf{k}_{op}$ corresponds to wavelengths

of 100's of nm or more (even inside the material)

A typical crystal unit cell size is, e.g., $a \sim 0.5\ \text{nm}$

so $\exp\left(i\mathbf{k}_{op}\cdot\mathbf{r}\right)$ is slowly varying over a unit cell

Hence, since we have already restricted $\left|\mathbf{k}_v\right|$ and $\left|\mathbf{k}_c\right|$ to being small by assumption

then the entire factor

$$\exp\left[i\left(\mathbf{k}_v-\mathbf{k}_c+\mathbf{k}_{op}\right)\cdot\mathbf{r}\right]$$

varies slowly over the length scale, a, of a unit cell

Matrix element for Fermi's Golden Rule

As a result, we can approximately separate the integral

$$\left\langle \psi_f \left| \hat{H}_{po}(\mathbf{r}) \right| \psi_i \right\rangle \simeq -\frac{eA_o}{2m_o N} \int_V \exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} \right) \cdot \mathbf{r} \right] \left[u_c^*(\mathbf{r})\, \hat{p}_x u_v(\mathbf{r}) \right] d^3\mathbf{r}$$

into a sum of integrals over a unit cell

treating the value of $\exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} \right) \cdot \mathbf{r} \right]$

as approximately constant within a unit cell, i.e.,

$$\left\langle \psi_f \left| \hat{H}_{po}(\mathbf{r}) \right| \psi_i \right\rangle = -\frac{eA_o}{2m_o N} \left\langle c \left| \hat{p}_x \right| v \right\rangle \sum_{m(i.e.,\, unit\, cells)} \exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} \right) \cdot \mathbf{R}_m \right]$$

where $\mathbf{R}_m$ is the position of (the center of) the *m*th unit cell

and $\left\langle c \left| \hat{p}_x \right| v \right\rangle \equiv \int_{\text{unit cell}} u_c^*(\mathbf{r})\, \hat{p}_x u_v(\mathbf{r})\, d^3\mathbf{r} \equiv p_{cv}$

Matrix element for Fermi's Golden Rule

The summation in

$$\left\langle \psi_f \middle| \hat{H}_{po}(\mathbf{r}) \middle| \psi_i \right\rangle = -\frac{eA_o}{2m_o N}\langle c|\hat{p}_x|v\rangle \sum_{m(i.e.,\, unit\, cells)} \exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op}\right)\cdot\mathbf{R}_m\right]$$

will average approximately to zero unless $\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} = 0$

because otherwise

the function $\exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op}\right)\cdot\mathbf{r}\right]$ is oscillatory

(Note this condition $\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} = 0$ can be seen to correspond to conservation of crystal momentum $\hbar\mathbf{k}$)

In this case, the sum becomes

$$\sum_m \exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op}\right)\cdot\mathbf{R}_m\right] = \sum_m \exp(0) = N$$

Fermi's Golden Rule transition rate

Hence

$$\left\langle \psi_f \left| \hat{H}_{po}(\mathbf{r}) \right| \psi_i \right\rangle = -\frac{eA_o}{2m_o N}\left\langle c \left| \hat{p}_x \right| v \right\rangle \sum_{m(i.e.,\, unit\, cells)} \exp\left[i\left(\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op}\right)\cdot \mathbf{R}_m \right]$$

becomes $\left\langle \psi_f \left| \hat{H}_{po}(\mathbf{r}) \right| \psi_i \right\rangle = -\frac{eA_o}{2m_o} p_{cv}$

and Fermi's Golden Rule gives a transition rate

$$w_{abs} = \frac{2\pi}{\hbar}\left| \left\langle \psi_f \left| \hat{H}_{po} \right| \psi_i \right\rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

$$= \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}\left| p_{cv} \right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

Direct valence to conduction band absorption

Hence, for an incident optical wave of frequency ω, wavevector $\mathbf{k}_{op}$ and magnetic vector potential amplitude A_o

- for an initial state of energy E_i and Bloch wavevector $\mathbf{k}_v$ in the valence band
- and a final state of energy E_f and Bloch wavevector $\mathbf{k}_c$ in the conduction band
  - if and only if $\mathbf{k}_v - \mathbf{k}_c + \mathbf{k}_{op} = 0$, we have a "direct transition rate"

$$w_{abs} = \frac{2\pi}{\hbar} \frac{e^2 A_o^2}{4m_o^2} |p_{cv}|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

Direct valence to conduction band absorption

Note also that the transition rate

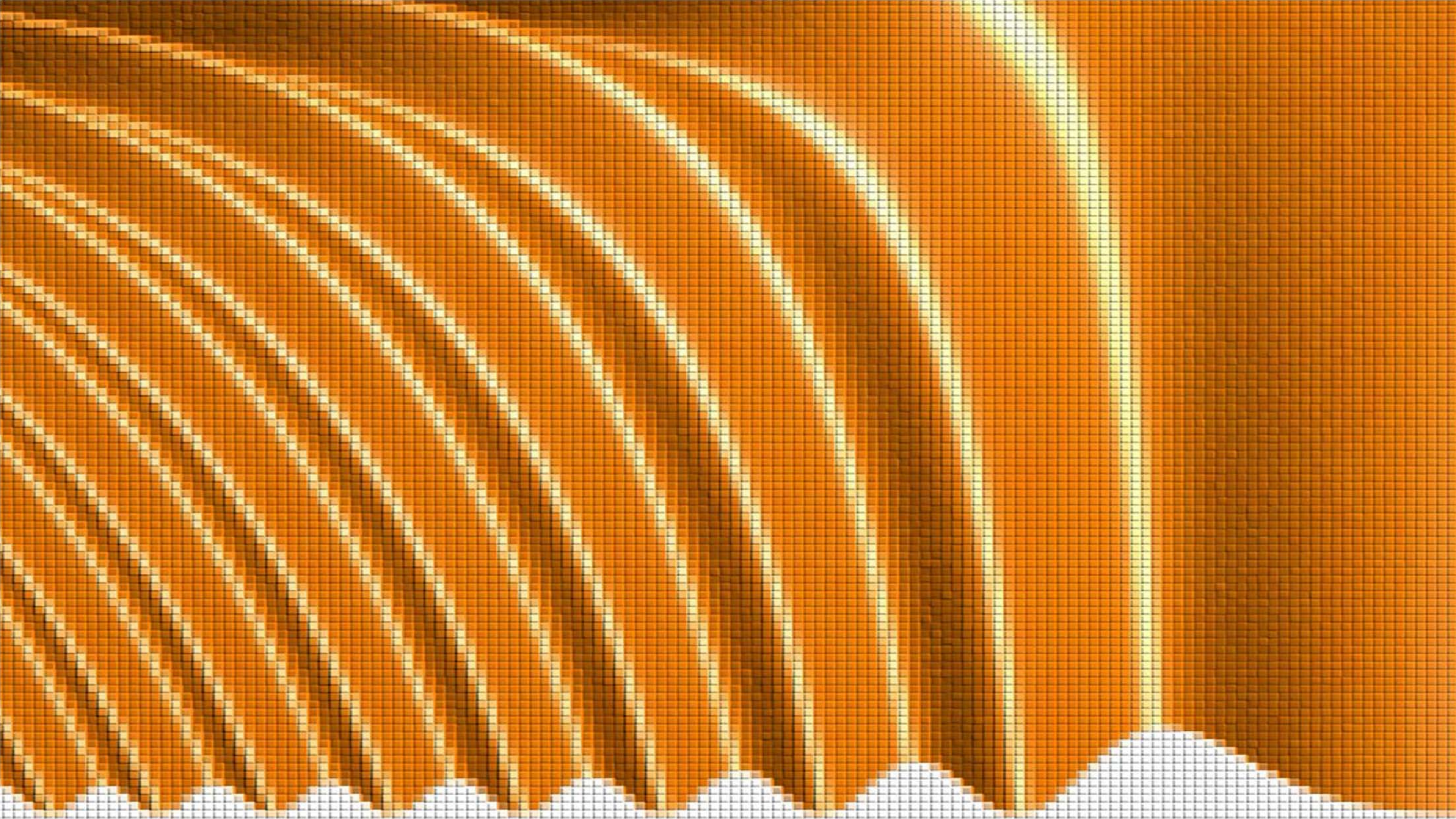
$$w_{abs} = \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}\left|p_{cv}\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

is proportional to

a (squared) matrix element, $\left|p_{cv}\right|^2$

the optical intensity (which is proportional to A_o^2)

and hence to the average arrival rate of photons in the semiconductor (per unit area)

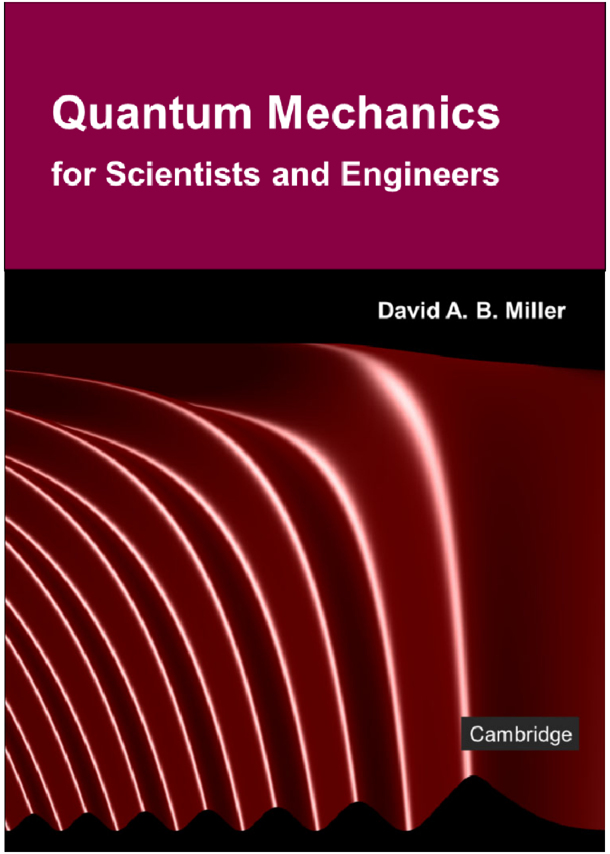


32 Optical absorption in semiconductors

Slides: Lecture 32d Transitioning from sums to integrals

Text reference: Quantum Mechanics for Scientists and Engineers

Section 5.3



Optical absorption in semiconductors

Transitioning from sums to integrals

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Transitioning from sums to integrals

Suppose we have some states

    indexed by an integer q

For each of these states

    some quantity

        such as energy

    has a value f_q

Hence, summing all of these quantities would give a result

$$S = \sum_q f_q$$

Transitioning from sums to integrals

It could be that f_q can also equivalently be written as a function of some parameter u

such as momentum

that takes on some value u_q for each q

i.e., $f_q \equiv f(u_q)$

e.g., f_q might be the energy associated with momentum u_q

and q might be indexing all the allowed values of $\mathbf{k}$

So, we could write $S = \sum_q f(u_q)$

Transitioning from sums to integrals

Suppose now that the u_q and the f_q

are very closely spaced as we change q

and vary relatively smoothly with q

We suppose that this smooth change of u_q with q is such that

we can approximately represent u as some smooth and differentiable function of a continuous variable q

i.e., $u(q)$

that is the same as u_q for all integer values of q

Transitioning from sums to integrals

We can define the difference between two specific adjacent values as $u_{q+1} - u_q \equiv \delta u$

With $\delta q = (q+1) - q$

then, trivially

$$\delta u = \frac{\delta u}{\delta q} \delta q$$

Because of the presumed "smoothness" of $u(q)$

$$u_{q+1} - u_q \equiv \delta u = \frac{\delta u}{\delta q} \delta q \simeq \frac{du}{dq} \delta q = \frac{du}{dq}$$

where in the last step we use the fact

$$\delta q = (q+1) - q = 1$$

Transitioning from sums to integrals

So, considering some small range Δu

within which the separation δu between adjacent values of u

was approximately constant

the number of different terms in the sum that would lie within that range is

$$\Delta u / \delta u \simeq \Delta u / \left(du / dq \right)$$

Transitioning from sums to integrals

Equivalently, defining a density of states $g(u) = \dfrac{1}{(du/dq)}$

we could say, equivalently, that the number of terms

in the sum that lie within Δu is $\dfrac{\Delta u}{\delta u} \simeq \dfrac{\Delta u}{du/dq} = g(u)\Delta u$

Hence, instead of summing over q we could instead

consider a set of values of u each separated by Δu

and spanning the same range

and write the sum over all those values

i.e., $S = \sum_q f_q \equiv \sum_q f(u_q) \simeq \sum_u f(u)\,g(u)\,\Delta u$

Transitioning from sums to integrals

Finally we formally let Δu in $S \simeq \sum_u f(u)g(u)\Delta u$

become very small

so we can approximate the sum by an integral

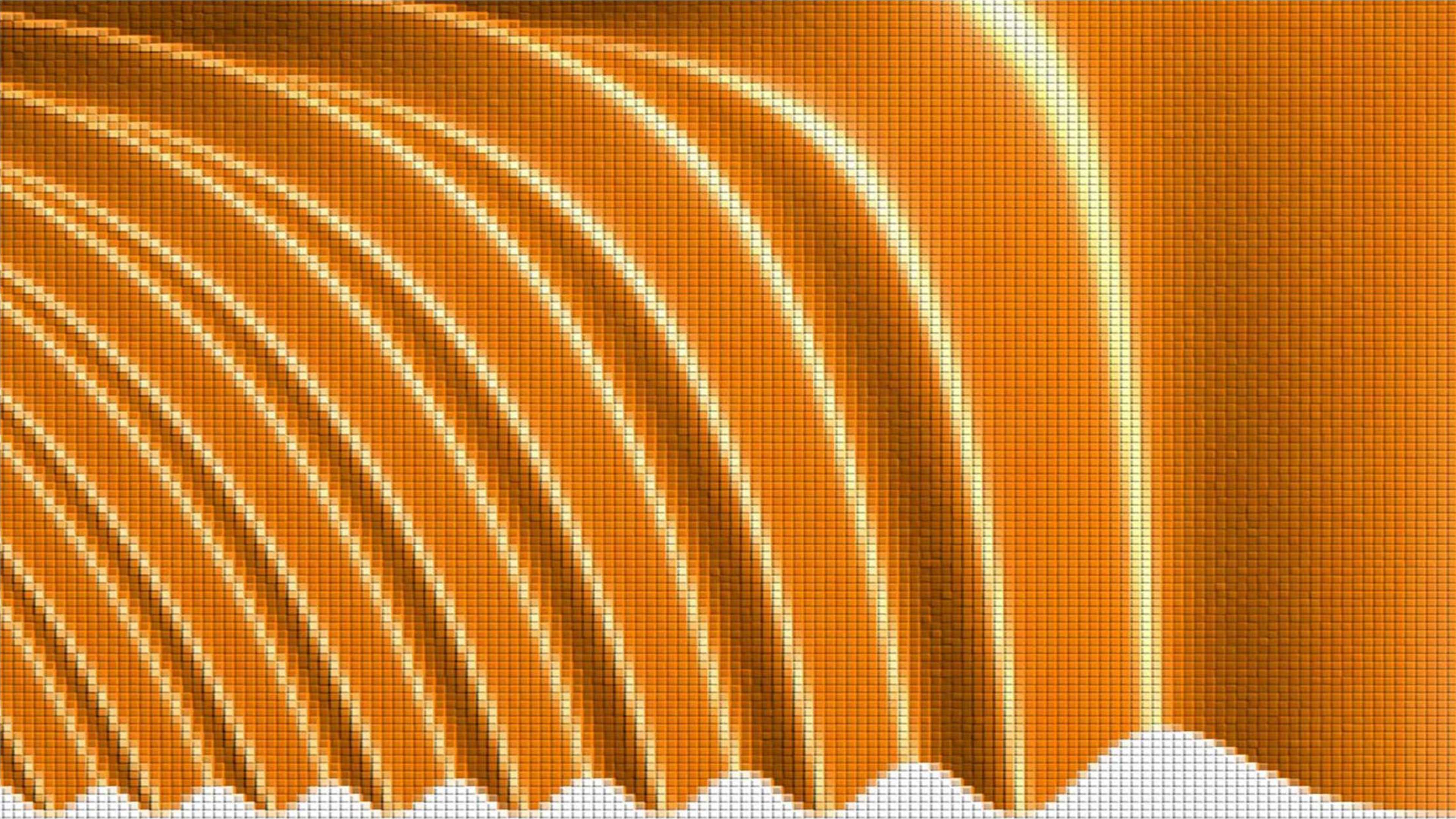
to obtain $S \simeq \int f(u)g(u)du$

So in going from a sum to an integral, we

insert the density of states in the integration variable into the integrand

i.e., $\boxed{\sum_q \ldots \rightarrow \int \ldots g(u)du}$

(The integral limits must correspond to the limits in the sum)

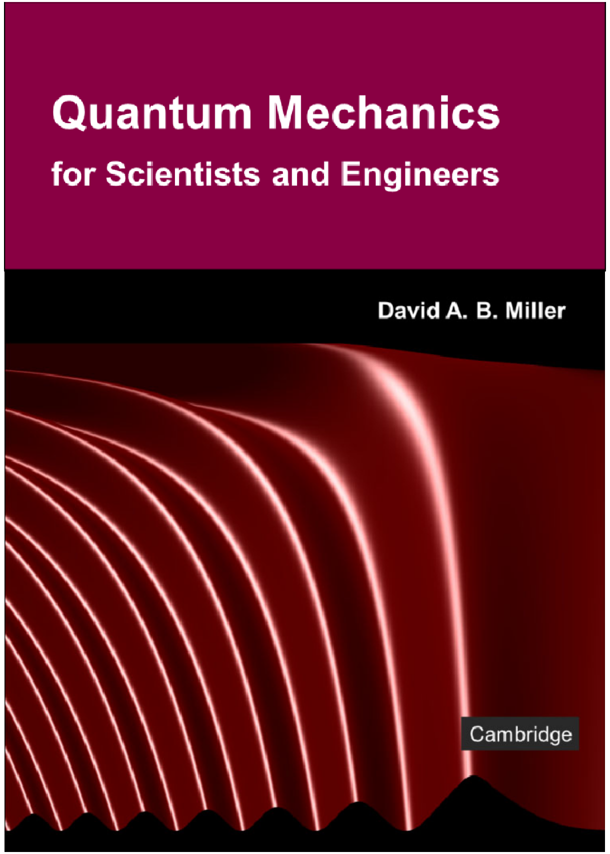


32 Optical absorption in semiconductors

Slides: Lecture 32e Total transition rate

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.10 subsection "Direct valence …" starting above Eq. 8.99 through Eq. 8.107


Quantum Mechanics
for Scientists and Engineers
David A. B. Miller
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Optical absorption in semiconductors

Total transition rate

Quantum mechanics for scientists and engineers

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Total transition rate

$$w_{abs} = \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}\left|p_{cv}\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

is transition rate from

an initial valence band state with Bloch wavevector $\mathbf{k}_v$

to the conduction band state with wave vector

$\mathbf{k}_c = \mathbf{k}_v + \mathbf{k}_{op}$

To get the total transition rate

and hence the optical absorption rate of photons

we need to sum over all the possible initial and final states

Total transition rate

The total transition rate W_{TOT} is formally

$$W_{TOT} = \sum_i \sum_f w_{abs} = \frac{2\pi}{\hbar} \frac{e^2 A_o^2}{4m_o^2} \left|p_{cv}\right|^2 \sum_i \sum_f \delta\left(E_f - E_i - \hbar\omega\right)$$

where we presume $\left|p_{cv}\right|^2$ is ~ independent of $\mathbf{k}$

We have shown above that

for a given initial state with wave vector $\mathbf{k}_v$

the only final state possible is the conduction band state with $\mathbf{k}_c = \mathbf{k}_v + \mathbf{k}_{op}$

With this knowledge

we can drop the separate sum over final states

Total transition rate

Since $\left|\mathbf{k}_{op}\right|$ is generally a very small fraction of the size of the Brillouin zone

- we will now neglect it for simplicity, taking $\mathbf{k}_c = \mathbf{k}_v$

This negligible size of the optical wavevector means that

- the direct optical transitions are essentially "vertical" on the energy-momentum diagram

Hence, for a given initial state $\mathbf{k}_v$

- only one term remains in the sum over the final states
  - namely, the one with $\mathbf{k}_c = \mathbf{k}_v$

From now on, we drop the suffixes "v" and "c", using just $\mathbf{k}$

Total transition rate

Hence the total transition rate becomes

$$W_{TOT} = \frac{2\pi}{\hbar} \frac{e^2 A_o^2}{4m_o^2} |p_{cv}|^2 \sum_{\mathbf{k},\,\text{spin}} \delta\left[E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega\right]$$

now including a sum over the two possible spin states

Now we formally rewrite (considering unit volume)

$$\sum_{\mathbf{k},\,\text{spin}} = 2\sum_{\mathbf{k}} \approx 2\int_{\mathbf{k}} g(\mathbf{k}) d^3\mathbf{k}$$

where $g(\mathbf{k})$ is the density of states in k space

We will next change variables in the integral

to the energy $E_c(\mathbf{k}) - E_v(\mathbf{k})$

Direct optical absorption

Assuming parabolic bands

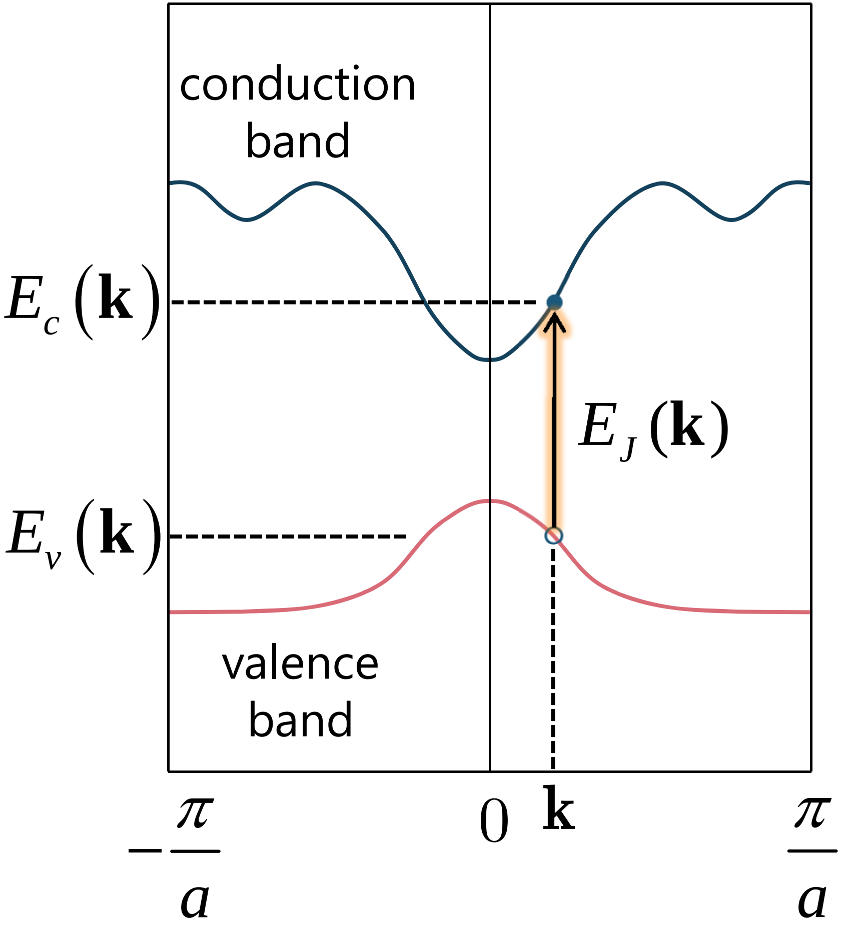
with m_{effe} and m_{effh} as the hole and electron effective masses

both positive by convention

we can define the transition energy

$$E_J(\mathbf{k}) = E_c(\mathbf{k}) - E_v(\mathbf{k})$$

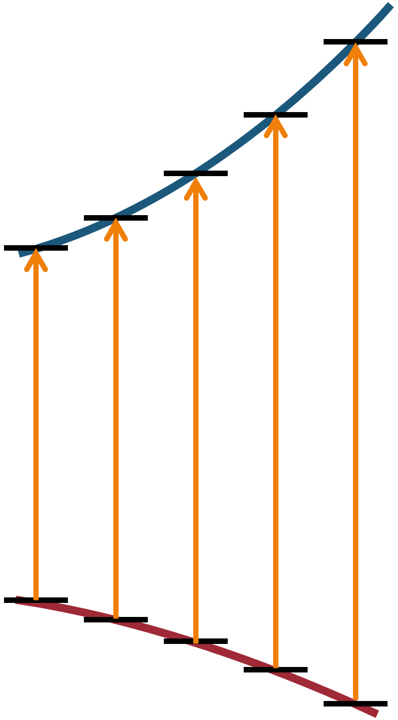
$$= \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_{effe}} + \frac{1}{m_{effh}}\right) + E_g$$



Dense sets of possible transitions

Now we can think of a set of possible transitions

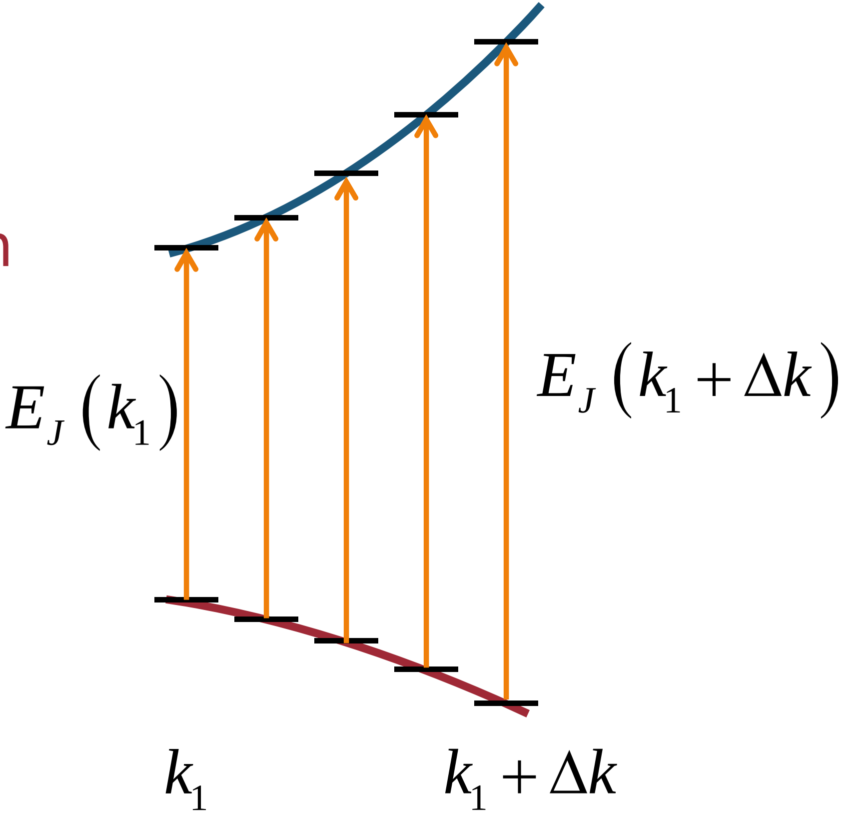
- corresponding to transitions between a specific k-state in the valence band
  - and the corresponding k-state in the conduction band
    - as sketched here for some portion of the Brillouin zone



Dense sets of possible transitions

Here, in a one-dimensional visualization

- the transition energy E_J goes from
  - $E_J(k_1)$ at one end, to
  - $E_J(k_1 + \Delta k)$ at the other



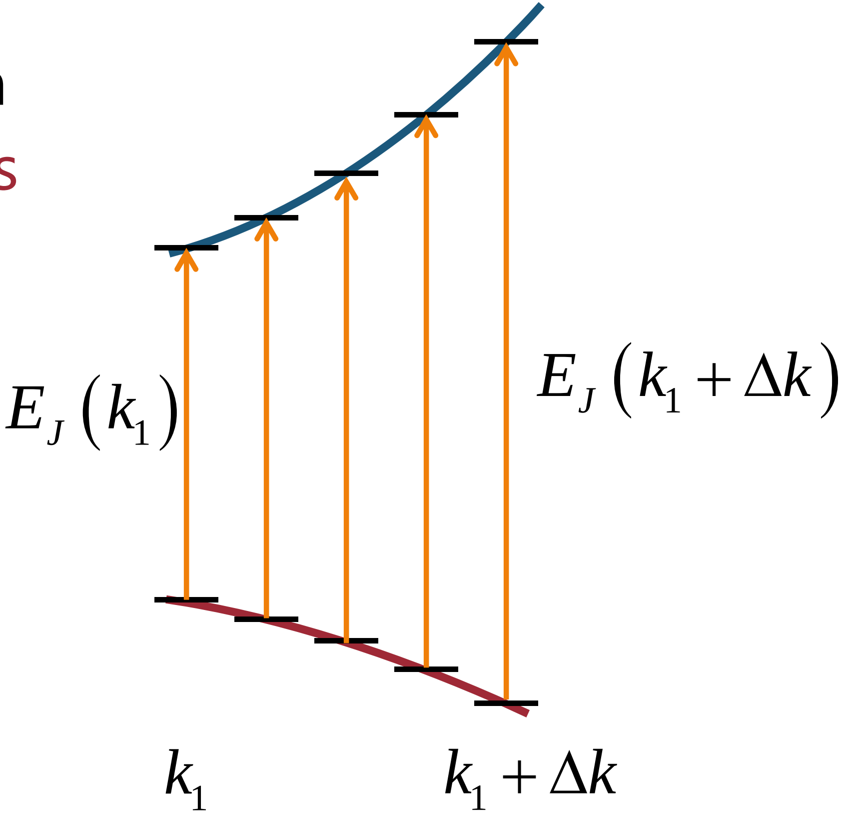
Dense sets of possible transitions

In what follows, we are interested in

- the number of different transitions possible
  - in a range of photon energies
    - from $E_J(k_1)$ to $E_J(k_1 + \Delta k)$
      - that is, within a range

$$\Delta E_J = E_J(k_1 + \Delta k) - E_J(k_1)$$

in the vicinity of $E_J(k_1)$



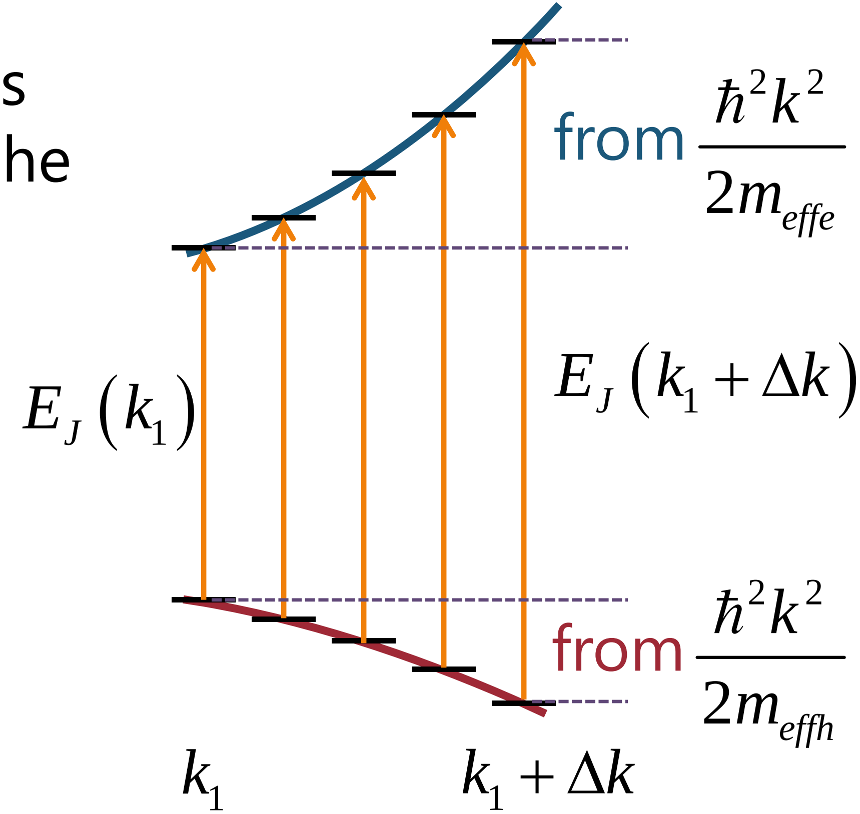
Dense sets of possible transitions

The difference in transition energies from one side of this diagram to the other

is the sum of two parts

one from $\dfrac{\hbar^2 k^2}{2m_{effe}}$

the other from $\dfrac{\hbar^2 k^2}{2m_{effh}}$



Dense sets of possible transitions

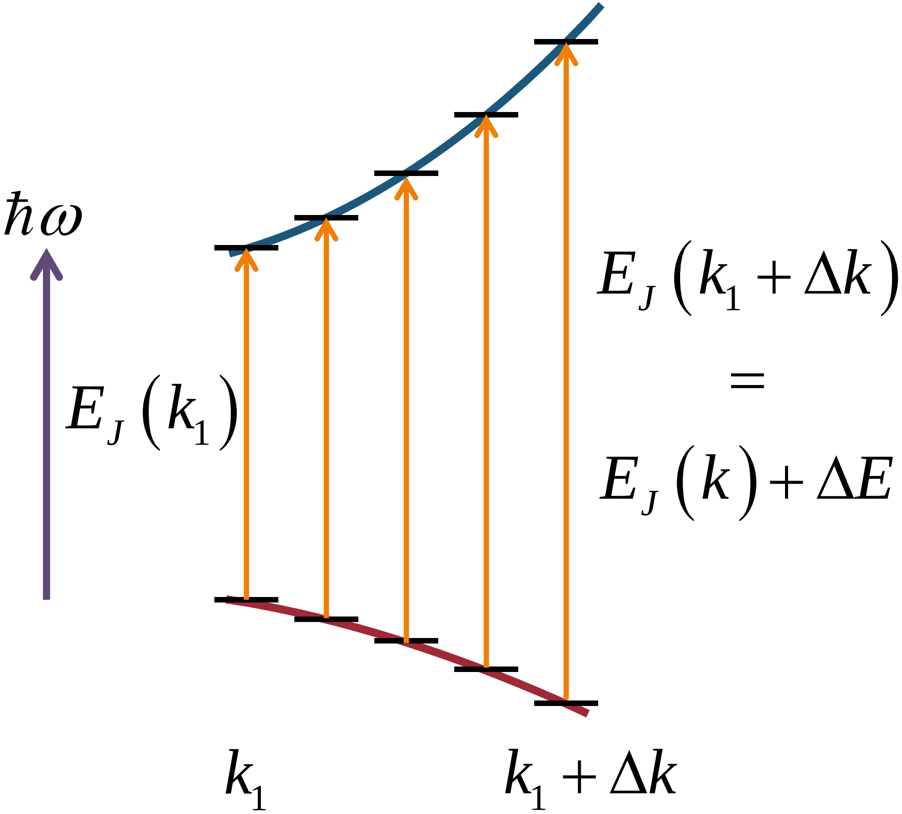
We presume this set of possible transitions is very dense

with density $g_J(\hbar\omega)$ per unit energy near photon energy $\hbar\omega$

giving $g_J(\hbar\omega)\Delta E$ transitions within energy range ΔE

$g_J(\hbar\omega)$ is known as a "joint density of states"

since it refers to transitions between states



Joint density of states

So, we can write the transition energies as

$$E_J(\mathbf{k}) = E_c(\mathbf{k}) - E_v(\mathbf{k}) = \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_{effe}} + \frac{1}{m_{effh}}\right) + E_g = \frac{\hbar^2 k^2}{2\mu_{eff}} + E_g$$

where we have introduced a convenient parameter

a “reduced effective mass”

$$\frac{1}{\mu_{eff}} = \frac{1}{m_{effe}} + \frac{1}{m_{effh}}$$

Joint density of states

We can then define a “joint density of states” $g_J\left(E_J\right)$

the number of transitions per unit (photon) energy

where we view E_J as being a function of $\boldsymbol{k}$

Like the energy density of states in a band, we can write

$$g_J(E_J)dE_J = 2g(\mathbf{k})d^3\mathbf{k}$$

including a factor of 2 for spin

where $g\left(\mathbf{k}\right)$ is the density of states in k-space

just as before

Joint density of states

Because our expression for the transition energy

$$E_J(\mathbf{k}) = \frac{\hbar^2 k^2}{2\mu_{eff}} + E_g$$

has exactly the same form as the energy of k-states in a given parabolic band

we now follow mathematically identical arguments to those used to deduce

the density of states in energy

from the density of states in k-space

Joint density of states

Now we deduce

the density of transitions per unit photon energy

now called the "joint density of states"

obtaining, for photon energy greater than the bandgap energy

i.e., $E_J \geq E_g$

the "joint density of states"

$$g_J(E_J) = \frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(E_J - E_g\right)^{1/2}$$

Total transition rate

So, from $W_{TOT} = \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}|p_{cv}|^2 \sum_{\mathbf{k},\,\mathrm{spin}} \delta\left[E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega\right]$

using $\sum_{\mathbf{k},\,\mathrm{spin}} = 2\sum_{\mathbf{k}} \approx 2\int_{\mathbf{k}} g(\mathbf{k})d^3\mathbf{k} = \int_{E_J \geq E_g} g_J\left(E_J - E_g\right)dE_J$

with $g_J(E_J) = \frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(E_J - E_g\right)^{1/2}$

then

$$W_{TOT} = \frac{2\pi}{\hbar}\frac{e^2 A_0^2}{4m_0^2}|p_{cv}|^2 \int_{E_J \geq E_g} \frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(E_J - E_g\right)^{1/2}\delta\left(E_J - \hbar\omega\right)dE_J$$

Total transition rate

Integrating to eliminate the delta function in

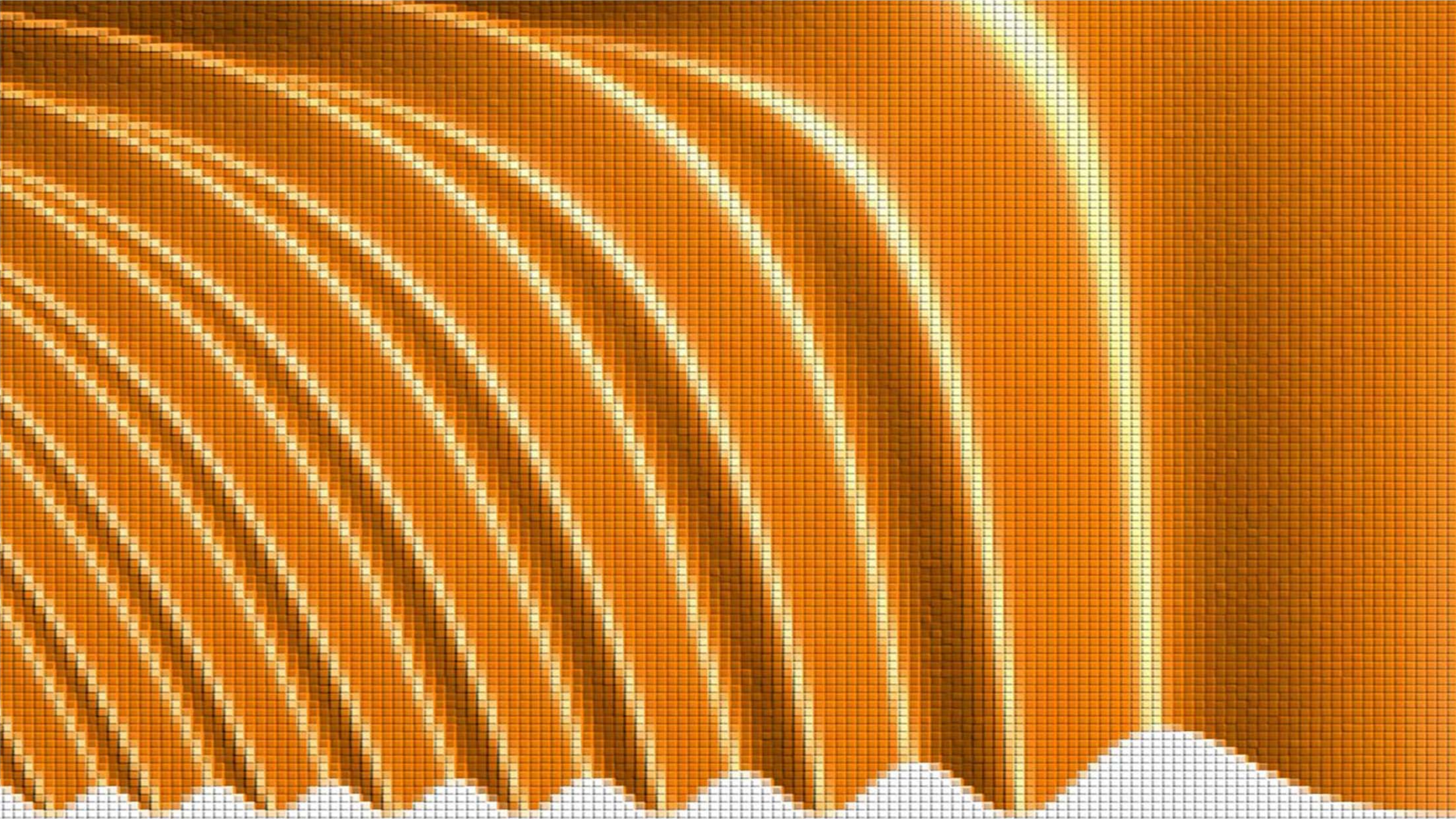
$$W_{TOT} = \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}\left|p_{cv}\right|^2 \int_{E_J \geq E_g} \frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(E_J - E_g\right)^{1/2}\delta\left(E_J - \hbar\omega\right)dE_J$$

we finally obtain, for $\hbar\omega \geq E_g$

$$W_{TOT}(\hbar\omega) = \frac{2\pi}{\hbar}\frac{e^2 A_o^2}{4m_o^2}\left|p_{cv}\right|^2 \frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(\hbar\omega - E_g\right)^{1/2}$$

Hence we finally see how Fermi's Golden Rule can be used with an appropriate density of states

to give a total transition rate

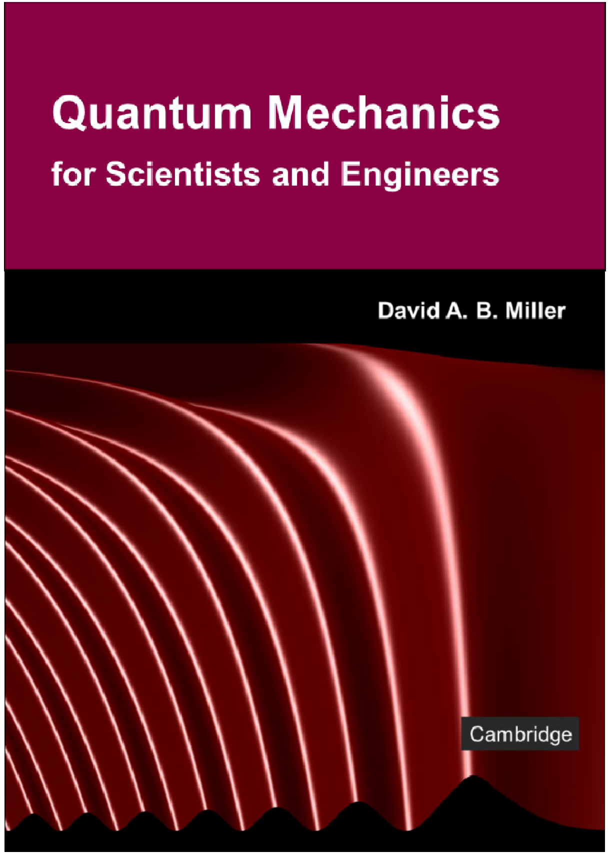


32 Optical absorption in semiconductors

Slides: Lecture 32f Absorption coefficient

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.10 starting just above Eq. 8.108



Optical absorption in semiconductors

Absorption coefficient

Quantum mechanics for scientists and engineers

David Miller

Absorption coefficient

The final step is to relate the absorption coefficient, α

the probability of absorption of a photon per unit length

to the total transition rate per unit volume W_{TOT}

With photon energy $\hbar\omega$

the number of photons incident per unit area per second

is, by definition $n_p = I / \hbar\omega$

where I is the optical intensity (power per unit area)

So the probability a photon is absorbed per unit length is

$$\alpha = \frac{W_{TOT}}{n_p} = \frac{\hbar\omega W_{TOT}}{I}$$

Absorption coefficient

From electromagnetism, we can deduce the intensity from the vector potential amplitude through

$$I = \frac{n_r c \varepsilon_0 \omega^2 A_o^2}{2}$$

where

n_r is the refractive index

c is the velocity of light, and

ε_o is the permittivity of free space (electric constant)

Absorption coefficient

Hence

$$\alpha(\hbar\omega)=\frac{\hbar\omega}{I}W_{TOT}=\frac{2\hbar\omega}{n_r c\varepsilon_0\omega^2 A_o^2}\frac{2\pi}{\hbar}\frac{e^2A_o^2}{4m_o^2}\frac{1}{2\pi^2}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left|p_{cv}\right|^2\left(\hbar\omega-E_g\right)^{1/2}$$

$$=\frac{e^2}{2\pi m_o^2 c\varepsilon_o}\frac{1}{n_r\omega}\left|p_{cv}\right|^2\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(\hbar\omega-E_g\right)^{1/2}$$

The parameter $E_p=\left(2/m_o\right)\left|p_{cv}\right|^2$ (~ 20 eV in many semiconductors) is often used in calculations

in which case we can rewrite

$$\alpha\left(\hbar\omega\right)=\frac{\hbar e^2}{4\pi m_o c\varepsilon_o}\frac{1}{n_r}\frac{E_p}{\hbar\omega}\left(\frac{2\mu_{eff}}{\hbar^2}\right)^{3/2}\left(\hbar\omega-E_g\right)^{1/2}$$

Optical absorption

In direct gap semiconductors

- the optical absorption in this model
  - rises as $\left(\hbar\omega - E_g\right)^{1/2}$ above the bandgap energy E_g

This model is used as the starting point for optical calculations in semiconductors