CLASE 23 - Martes 22/06/2021

La clase pasada vimos:

Ecuación de Wannier.

Excitones de Wannier

En esta clase veremos:

- Cálculo de la polarización interbanda en el problema de excitación óptica de pares electrón-hueco.
- Susceptibilidad óptica electrón-hueco.
- Coeficiente de absorción.
- Espectros de absorción en el borde la banda (band-edge absorption spectrum).

REPASO

Polarización interbanda

$$\left[\hbar(\omega + i\delta) - E_g + \frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] P_{vc}(\mathbf{r}, \omega) = -d_{cv}\mathcal{E}(\omega)\,\delta(\mathbf{r}) L^3$$

$$-\left[\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] \psi_\nu(\mathbf{r}) = E_\nu \psi_\nu(\mathbf{r})$$

Ecuación de Wannier

REPASO

Solución de la ecuación de Wannier

Radio de Bohr renormalizado:

$$a_0 = \frac{\hbar^2 \epsilon_0}{e^2 m_r}$$

Rydberg renormalizado:

$$E_0 = \frac{\hbar^2}{2 m_r a_0^2} = \frac{e^2}{2\epsilon_0 a_0} = \frac{e^4 m_r}{2\epsilon_0^2 \hbar^2}$$

Las soluciones **ligadas** son los **excitones de Wannier**

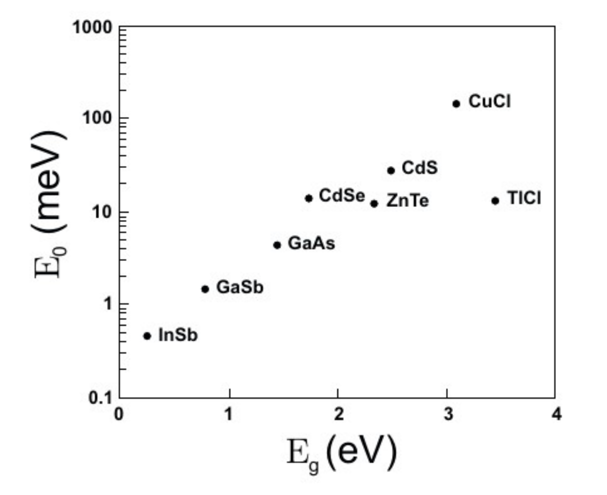
$$E_n = -E_0 \frac{1}{n^2} \quad \text{with } n = 1, 2, \ldots$$

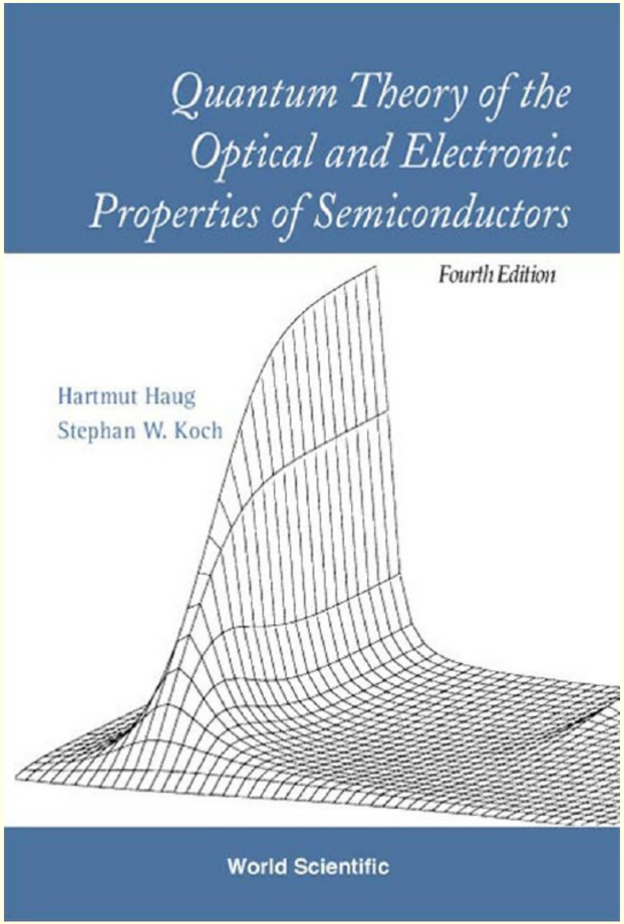
3*D* exciton bound-state energies

$$E_n = -E_0 \frac{1}{(n+1/2)^2} \quad \text{with } n = 0, 1, \ldots ,$$

2*D* exciton bound-state energies

Binding energy experimental

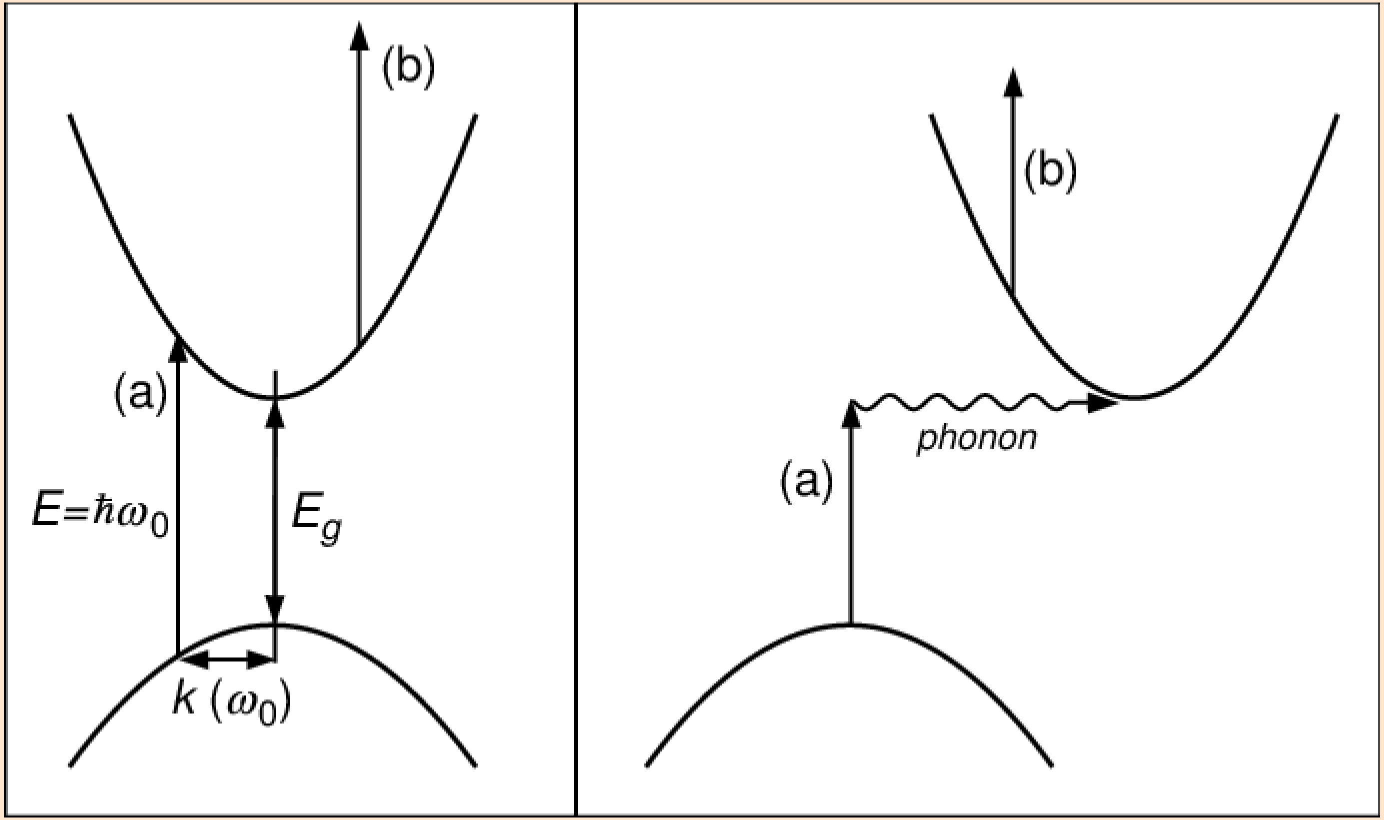



Quantum Theory of the
Optical and Electronic
Properties of Semiconductors
Fourth Edition
Hartmut Haug
Stephan W. Koch
World Scientific

Espectros ópticos de semiconductores

Transiciones ópticas en semiconductores

Band gap directo: Band gap indirecto:



Polarización interbanda

Retomamos la ecuación inhomogénea de la polarización:

$$\left[\hbar(\omega + i\delta) - E_g + \frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] P_{vc}(\mathbf{r},\omega) = -d_{cv}\mathcal{E}(\omega)\,\delta(\mathbf{r})L^3$$

Tratamos de expresar sus soluciones en términos de los autoestados y autofunciones de la ecuación de Wannier:

$$-\left[\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right]\psi_\nu(\mathbf{r}) = E_\nu \psi_\nu(\mathbf{r})$$

$$\Rightarrow \quad P_{vc}(\mathbf{r},\omega) = \sum_\nu b_\nu\, \psi_\nu(\mathbf{r})$$

Polarización interbanda

$$\left[\hbar(\omega + i\delta) - E_g + \frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] P_{vc}(\mathbf{r},\omega) = -d_{cv}\mathcal{E}(\omega)\,\delta(\mathbf{r})L^3$$

$$P_{vc}(\mathbf{r},\omega) = \sum_{\nu} b_\nu\,\psi_\nu(\mathbf{r})$$

Reemplazando y haciendo $\int d^3r\,\psi_\mu^*(\mathbf{r})\cdots$

$$\Rightarrow \sum_\nu b_\nu\left[\hbar(\omega + i\delta) - E_g - E_\nu\right]\int d^3r\,\psi_\mu^*(\mathbf{r})\psi_\nu(\mathbf{r}) = -d_{cv}\,\mathcal{E}(\omega)\,L^3\psi_\mu^*(\mathbf{r}=0)$$

Polarización interbanda

$$\sum_\nu b_\nu \left[\hbar(\omega+i\delta) - E_g - E_\nu\right] \underbrace{\int d^3r\, \psi_\mu^*(\mathbf{r})\psi_\nu(\mathbf{r})}_{\delta_{\mu,\nu}} = -d_{cv}\,\mathcal{E}(\omega)\, L^3 \psi_\mu^*(\mathbf{r}=0)$$

$$\Rightarrow \quad \left.\begin{aligned} b_\mu &= -\frac{d_{cv} L^3 \psi_\mu^*(\mathbf{r}=0)}{\hbar(\omega+i\delta) - E_g - E_\mu}\mathcal{E}(\omega) \\ P_{vc}(\mathbf{r},\omega) &= \sum_\nu b_\nu\, \psi_\nu(\mathbf{r}) \end{aligned}\right\}$$

$$\Rightarrow \quad P_{vc}(\mathbf{r},\omega) = -\sum_\nu \mathcal{E}(\omega) \frac{d_{cv}\, L^3\, \psi_\nu^*(\mathbf{r}=0)}{\hbar(\omega+i\delta) - E_g - E_\nu}\psi_\nu(\mathbf{r})$$

Polarización interbanda

$$\sum_{\nu} b_{\nu} \left[\hbar(\omega + i\delta) - E_g - E_{\nu}\right] \underbrace{\int d^3r \, \psi^*_{\mu}(\mathbf{r})\psi_{\nu}(\mathbf{r})}_{\delta_{\mu,\nu}} = -d_{cv} \, \mathcal{E}(\omega) \, L^3 \psi^*_{\mu}(\mathbf{r} = 0)$$

$$\Rightarrow \quad b_{\mu} = -\frac{d_{cv} L^3 \psi^*_{\mu}(\mathbf{r} = 0)}{\hbar(\omega + i\delta) - E_g - E_{\mu}} \mathcal{E}(\omega)$$

$$P_{vc}(\mathbf{r}, \omega) = \sum_{\nu} b_{\nu} \, \psi_{\nu}(\mathbf{r})$$

$$\Rightarrow \quad P_{vc}(\mathbf{r}, \omega) = -\sum_{\nu} \mathcal{E}(\omega) \frac{d_{cv} \, L^3 \, \psi^*_{\nu}(\mathbf{r} = 0)}{\hbar(\omega + i\delta) - E_g - E_{\nu}} \psi_{\nu}(\mathbf{r})$$

Polarización interbanda

$$P_{vc}(\mathbf{r},\omega) = -\sum_{\nu} \mathcal{E}(\omega) \frac{d_{cv}\, L^3\, \psi_\nu^*(\mathbf{r}=0)}{\hbar(\omega + i\delta) - E_g - E_\nu} \psi_\nu(\mathbf{r})$$

Transformada de Fourier para volver al dominio ***k***

$$\Rightarrow \quad P_{vc,\mathbf{k}}(\omega) = -\sum_{\nu} \mathcal{E}(\omega) \frac{d_{cv}\psi_\nu^*(\mathbf{r}=0)}{\hbar(\omega + i\delta) - E_g - E_\nu} \int d^3r\, \psi_\nu(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Polarización interbanda

$$P_{vc,\mathbf{k}}(\omega) = -\sum_{\nu} \mathcal{E}(\omega) \frac{d_{cv}\psi_{\nu}^{*}(\mathbf{r}=0)}{\hbar(\omega+i\delta) - E_g - E_{\nu}} \int d^3r\, \psi_{\nu}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Ya podemos calcular la polarización total:

$$P(t) = \sum_{\mathbf{k}} P_{cv,\mathbf{k}}(t) d_{vc} + \text{c.c.} \qquad (10.28)$$

Su transformada de Fourier temporal tiene la forma:

$$\begin{aligned} P(\omega) &= \sum_{\mathbf{k}} \int dt\, (P_{cv,\mathbf{k}}(t) d_{vc} + P^{*}_{cv,\mathbf{k}}(t) d_{vc}) e^{i\omega t} \\ &= \sum_{\mathbf{k}} (P_{cv,\mathbf{k}}(\omega) d_{vc} + P^{*}_{cv,\mathbf{k}}(-\omega) d_{vc}) \ . \end{aligned}$$

Polarización interbanda

$$P(\omega) = \sum_{\mathbf{k}} (P_{cv,\mathbf{k}}(\omega) d_{vc} + P^*_{cv,\mathbf{k}}(-\omega) d_{vc})$$

$$\mathcal{E}^*(-\omega) = \mathcal{E}(\omega)$$

$$\sum_{\mathbf{k}} \int d^3r\, \psi_\nu(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} = 2L^3\, \psi_\nu(\mathbf{r}=0)$$

espín

$$P(\omega) = -2L^3 \sum_\nu |d_{cv}|^2 |\psi_\nu(\mathbf{r}=0)|^2 \mathcal{E}(\omega) \qquad (10.101)$$

$$\times \left[\frac{1}{\hbar(\omega + i\delta) - E_g - E_\nu} - \frac{1}{\hbar(\omega + i\delta) + E_g + E_\nu} \right] ,$$

Susceptibilidad de pares electrón-hueco

Susceptibilidad de pares electrón-hueco

Recordamos la definición de la susceptibilidad óptica:

$$\boxed{\chi(\omega) = \frac{\mathcal{P}(\omega)}{\mathcal{E}(\omega)} = \frac{P(\omega)}{L^3\mathcal{E}(\omega)}}$$

$$P(\omega) = -2L^3 \sum_{\nu} |d_{cv}|^2 |\psi_\nu(\mathbf{r}=0)|^2 \mathcal{E}(\omega) \times \left[\frac{1}{\hbar(\omega + i\delta) - E_g - E_\nu} - \frac{1}{\hbar(\omega + i\delta) + E_g + E_\nu} \right] , \tag{10.101}$$

Susceptibilidad de pares electrón-hueco

Suma sobre estados de excitón

Amplitud de que el electrón y el hueco estén en la misma posición

$$\chi(\omega) = -2|d_{cv}|^2 \sum_{\mu} |\psi_{\mu}(\mathbf{r}=0)|^2$$

$$\times \left[\underbrace{\frac{1}{\hbar(\omega + i\delta) - E_g - E_{\mu}}}_{\text{Término resonante}} - \underbrace{\frac{1}{\hbar(\omega + i\delta) + E_g + E_{\mu}}}_{\text{No resonante no contribuye a la absorción}} \right]$$

Susceptibilidad de pares electrón-hueco

Ahora hay que especializar:

$$\chi(\omega) = -2|d_{cv}|^2 \sum_{\mu} |\psi_\mu(\mathbf{r}=0)|^2$$

$$\times \left[\frac{1}{\hbar(\omega + i\delta) - E_g - E_\mu} - \frac{1}{\hbar(\omega + i\delta) + E_g + E_\mu} \right]$$

a los casos 3D, 2D, y 1D

Susceptibilidad de pares electrón-hueco

Coeficiente de absorción:

$$\alpha(\omega) = \alpha_0^{3D} \frac{\hbar\omega}{E_0} \left[\sum_{n=1}^{\infty} \frac{4\pi}{n^3} \delta(\Delta + \frac{1}{n^2}) + \Theta(\Delta) \frac{\pi e^{\frac{\pi}{\sqrt{\Delta}}}}{\sinh(\frac{\pi}{\sqrt{\Delta}})} \right]$$

Fórmula de Elliot 3D

$$\Delta = (\hbar\omega - E_g)/E_0$$

$$\alpha_0^D = \frac{4\pi^2 |d_{cv}|^2}{\hbar n_b c} \frac{1}{(2\pi a_0)^D} \Omega_D \frac{1}{L_c^{3-D}} \tag{5.81}$$

$$\alpha(\omega) = \alpha_0^D \frac{\hbar\omega}{E_0} \left(\frac{\hbar\omega - E_g - E_0^{(D)}}{E_0} \right)^{\frac{D-2}{2}} \Theta(\hbar\omega - E_g - E_0^{(D)}) A(\omega) \;, \tag{5.80}$$

absorption coefficient for free carriers

Espectro de absorción de partícula libre

Espectro de absorción en el borde de banda (band edge) sin interacción e-e

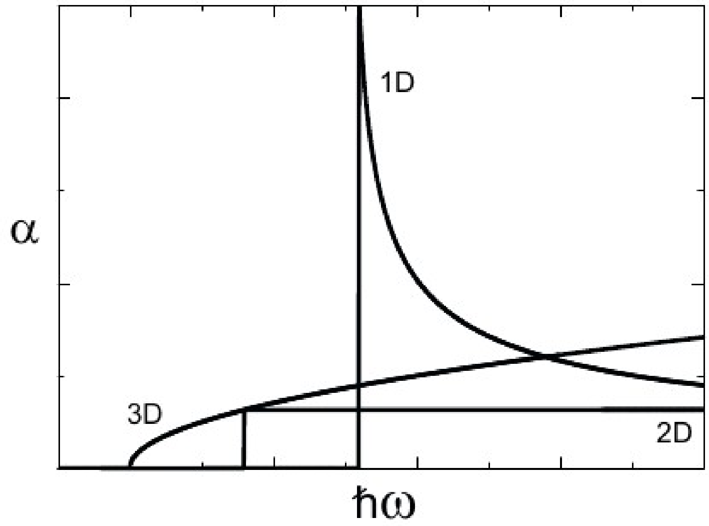


Fig. 5.3 Free electron absorption spectra for semiconductors, where the electrons can move freely in one, two, or three space dimensions.

Espectro de absorción de pares partícula-hueco

Espectro de absorción en el borde de banda (band edge) con interacción e-e

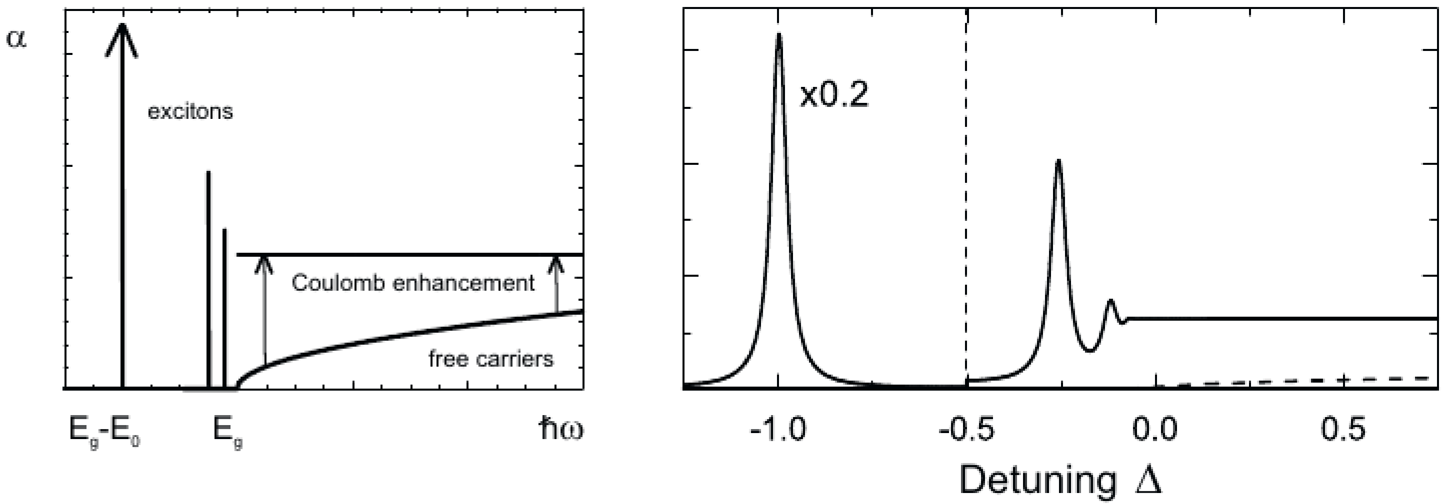


Fig. 10.2 Schematic (left figure) and calculated (right figure) band edge absorption spectrum for a $3D$ semiconductor. Shown are the results obtained with and without including the Coulomb interaction. The $1s$-exciton part of the computed absorption spectra has been scaled by a factor of 0.2 .

Espectro de absorción de pares partícula-hueco

Espectro de absorción en el borde de banda (band edge) con interacción e-e

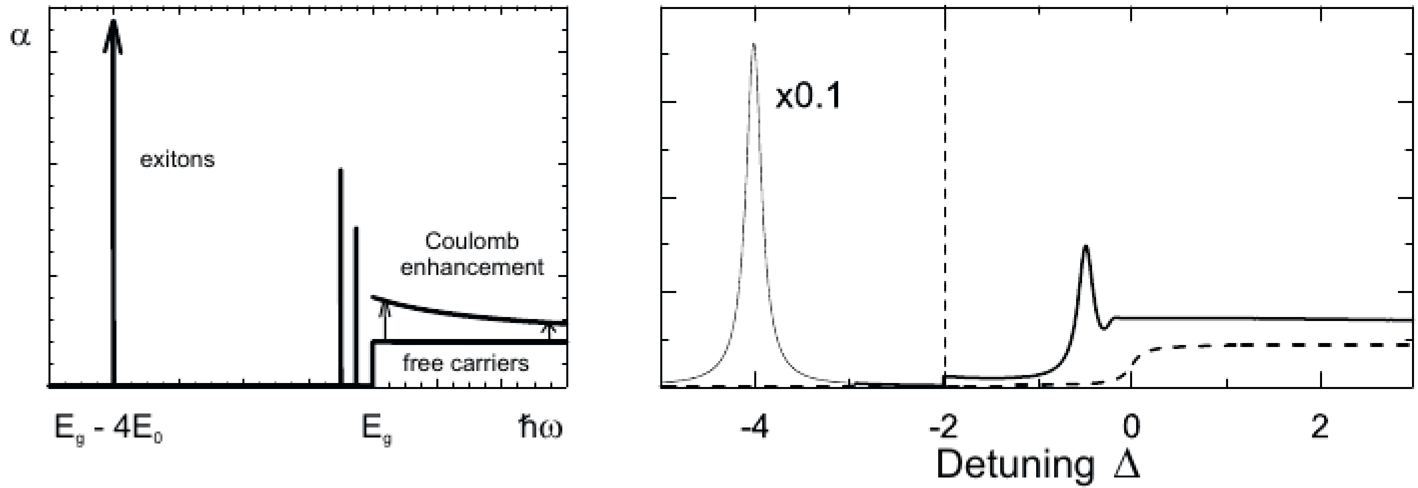


Fig. 10.3 Schematic (left figure) and calculated (right figure) band edge absorption spectrum for a $2D$ semiconductor. Shown are the results obtained with and without including the Coulomb interaction. The $1s$-exciton part of the computed absorption spectra has been scaled by a factor of 0.1 .

Resumen de la clase 23

- Cálculo de la polarización interbanda en el problema de excitación óptica de pares electrón-hueco.
- Susceptibilidad óptica electrón-hueco.
- Coeficiente de absorción.
- Espectros de absorción en el borde la banda (bandedge absorption spectrum).