CLASE 21 - Martes 15/06/2021

**La clase pasada vimos:**

Introducción a excitones

Polarización interbanda

Modelo de dos bandas

**En esta clase veremos:**

Elemento de matriz del dipolo eléctrico

Ecuación de movimiento de la polarización interbanda

Polarización interbanda de partícula libre

REPASO

Polarización eléctrica:

$$\mathbf{P(t)} = \sum_s \int d^3r \, \langle \hat{\psi}_s^\dagger(\mathbf{r},t) \, e\mathbf{r} \, \hat{\psi}_s(\mathbf{r},t) \rangle$$

Matriz densidad reducida de una partícula:

$$\rho_{ss'}(\mathbf{r},\mathbf{r}',t) = \langle \hat{\psi}_s^\dagger(\mathbf{r},t)\hat{\psi}_{s'}(\mathbf{r}',t) \rangle$$

Base de **estados de Bloch** del sólido: $\mathcal{H}_0|\lambda\mathbf{k}\rangle = E_\lambda(\mathbf{k})|\lambda\mathbf{k}\rangle = \hbar\epsilon_{\lambda,\mathbf{k}}|\lambda\mathbf{k}\rangle$

$$\psi_\lambda(\mathbf{k},\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} u_\lambda(\mathbf{k},\mathbf{r})$$

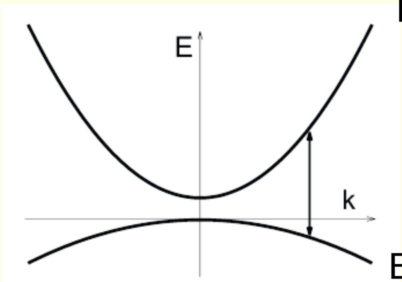
$$\Rightarrow \quad \hat{\psi}_s(\mathbf{r},t) = \sum_{\lambda,\mathbf{k}} a_{\lambda,\mathbf{k},s}(t)\psi_\lambda(\mathbf{k},\mathbf{r})$$

REPASO

$$\mathbf{P}(t) = \sum_{\mathbf{k},s,\lambda,\lambda'} \langle a^{\dagger}_{\lambda,\mathbf{k},s} a_{\lambda',\mathbf{k},s}(t)\rangle \mathbf{d}_{\lambda\lambda'} = \sum_{\mathbf{k},s,\lambda,\lambda'} P_{\lambda\lambda',\mathbf{k},s}(t)\mathbf{d}_{\lambda\lambda'}$$

Donde definimos:

$$P_{\lambda\lambda',\mathbf{k},s}(t) = \langle a^{\dagger}_{\lambda,\mathbf{k},s} a_{\lambda',\mathbf{k},s}(t)\rangle$$




Banda de conducción

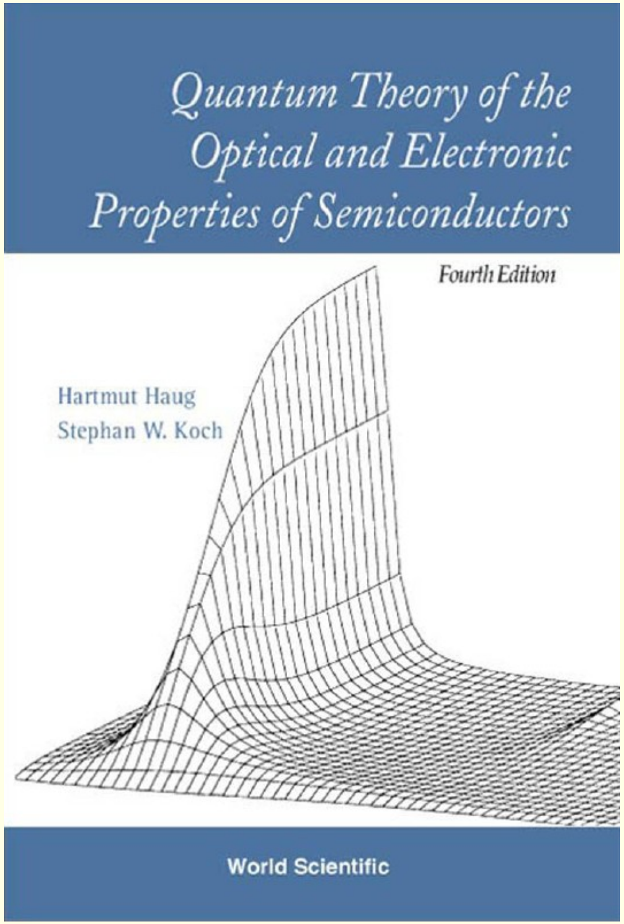
Banda de valencia

$$P_{vc,\mathbf{k}}(t) = \langle a^{\dagger}_{v,\mathbf{k}} a_{c,\mathbf{k}}(t)\rangle$$

Término no diagonal de la matriz densidad

$$\mathcal{H}_I \simeq -\sum_{\mathbf{k}} \mathcal{E}(t)(a^{\dagger}_{c,\mathbf{k}} a_{v,\mathbf{k}} d_{cv} + h.c.)$$

$$\mathcal{H}_{el} = \sum_{\lambda,\mathbf{k}} E_{\lambda,k} a^{\dagger}_{\lambda,\mathbf{k}} a_{\lambda,\mathbf{k}} + \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \mathbf{q}\neq 0 \\ \lambda,\lambda'}} V_q a^{\dagger}_{\lambda,\mathbf{k}+\mathbf{q}} a^{\dagger}_{\lambda',\mathbf{k}'-\mathbf{q}} a_{\lambda',\mathbf{k}'} a_{\lambda,\mathbf{k}}$$


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

# Elemento de matriz del momento dipolar eléctrico

# Elemento de matriz del momento dipolar eléctrico

$$\mathbf{P}(\mathbf{t}) = \sum_s \int d^3r \, \langle \hat{\psi}_s^\dagger(\mathbf{r},t) \, e\mathbf{r} \, \hat{\psi}_s(\mathbf{r},t) \rangle$$

$$\hat{\psi}_s(\mathbf{r},t) = \sum_{\lambda,\mathbf{k}} a_{\lambda,\mathbf{k},s}(t) \psi_\lambda(\mathbf{k},\mathbf{r})$$

$$\mathbf{P}(t) = \sum_{s,\lambda,\lambda',\mathbf{k},\mathbf{k}'} \langle a^\dagger_{\lambda,\mathbf{k},s} a_{\lambda',\mathbf{k}',s} \rangle \int d^3r \, \psi^*_{\lambda,\mathbf{k}}(\mathbf{r}) \, e\mathbf{r} \, \psi_{\lambda',\mathbf{k}'}(\mathbf{r})$$

The integral has been evaluated in Chap. 5, Eqs. (5.11) – (5.20).

$$\int d^3r \, \psi^*_{\lambda,\mathbf{k}}(\mathbf{r}) \, e\mathbf{r} \, \psi_{\lambda',\mathbf{k}'}(\mathbf{r}) \simeq \delta_{\mathbf{k},\mathbf{k}'} \mathbf{d}_{\lambda\lambda'}$$

$\lambda \neq \lambda'$

# Elemento de matriz del momento dipolar eléctrico

$$r_{\lambda'\lambda}(\mathbf{k}', \mathbf{k}) = \langle \lambda'\mathbf{k}' | r | \lambda\mathbf{k} \rangle$$

$$\langle l|x|n\rangle(\epsilon_n - \epsilon_l) = \frac{1}{\hbar}\langle l|[x, \mathcal{H}_0]|n\rangle = -\frac{1}{\hbar}\langle l|[\mathcal{H}_0, x]|n\rangle \quad , \tag{2.26}$$

$$[x, \mathcal{H}_0] = -\frac{\hbar^2}{2m_0}\left(x\frac{d^2}{dx^2} - \frac{d^2}{dx^2}x\right) = \frac{\hbar^2}{m_0}\frac{d}{dx} = \frac{i\hbar}{m_0}p_x \tag{2.31}$$

use the same trick as in Eqs. (2.26) and (2.31) to get

$$\begin{aligned}
\mathbf{r}_{\lambda'\lambda}(\mathbf{k}', \mathbf{k}) &= \frac{1}{E_\lambda(\mathbf{k}) - E_{\lambda'}(\mathbf{k}')}\langle \lambda'\mathbf{k}'|[\mathbf{r}, \mathcal{H}_0]|\lambda\mathbf{k}\rangle \\
&= \frac{i}{m_0(\epsilon_{\lambda,\mathbf{k}} - \epsilon_{\lambda',\mathbf{k}'})}\langle \lambda'\mathbf{k}'|\mathbf{p}|\lambda\mathbf{k}\rangle \quad .
\end{aligned}$$

# Elemento de matriz del momento dipolar eléctrico

$$r_{\lambda'\lambda}(\mathbf{k}',\mathbf{k}) = \langle \lambda'\mathbf{k}'|r|\lambda\mathbf{k}\rangle$$

$$\begin{aligned}\mathbf{r}_{\lambda'\lambda}(\mathbf{k}',\mathbf{k}) &= \frac{1}{E_\lambda(\mathbf{k}) - E_{\lambda'}(\mathbf{k}')}\langle \lambda'\mathbf{k}'|[\mathbf{r},\mathcal{H}_0]|\lambda\mathbf{k}\rangle \\ &= \frac{i}{m_0(\epsilon_{\lambda,\mathbf{k}} - \epsilon_{\lambda',\mathbf{k}'})}\langle \lambda'\mathbf{k}'|\mathbf{p}|\lambda\mathbf{k}\rangle \ .\end{aligned}$$

$$\langle \lambda'\mathbf{k}'|\mathbf{p}|\lambda\mathbf{k}\rangle = \int_{L^3} d^3r\, \psi^*_{\lambda'}(\mathbf{k}',\mathbf{r})\mathbf{p}\psi_\lambda(\mathbf{k},\mathbf{r})$$

$$\psi_\lambda(\mathbf{k},\mathbf{r}) \simeq e^{i\mathbf{k}\cdot\mathbf{r}}\frac{u_\lambda(0,\mathbf{r})}{L^{3/2}}$$

$$\langle \lambda'\mathbf{k}'|\mathbf{p}|\lambda\mathbf{k}\rangle \simeq \frac{1}{L^3}\int_{L^3} d^3r\, e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}u^*_{\lambda'}(0,\mathbf{r})(\hbar\mathbf{k}+\mathbf{p})u_\lambda(0,\mathbf{r})$$

# Elemento de matriz del momento dipolar eléctrico

$$\langle \lambda' \mathbf{k}' | \mathbf{p} | \lambda \mathbf{k} \rangle \simeq \sum_{n=1}^{N} \frac{e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_n}}{N} \int_{l^3} d^3r \frac{e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}}{l^3} u^*_{\lambda'}(0,\mathbf{r})(\hbar\mathbf{k}+\mathbf{p})u_\lambda(0,\mathbf{r})$$

$$\langle \lambda' \mathbf{k}' | \mathbf{p} | \lambda \mathbf{k} \rangle = \frac{\delta_{\mathbf{k},\mathbf{k}'}}{l^3} \int_{l^3} d^3r \, u^*_{\lambda'}(0,\mathbf{r}) \mathbf{p} \, u_\lambda(0,\mathbf{r}) \equiv \delta_{\mathbf{k},\mathbf{k}'} \mathbf{p}_{\lambda'\lambda}(0) \; , \qquad (5.15)$$

The $\delta$-function in Eq. (5.15) shows that the optical dipole matrix element couples identical $\mathbf{k}$-states in different bands, so that optical transitions are "perpendicular" if plotted in an energy–wave–number diagram, as in Fig. 5.1. The *dipole approximation* is equivalent to ignoring the photon momentum in comparison to a typical electron momentum in the Brillouin zone.

# Elemento de matriz del momento dipolar eléctrico

$$e\mathbf{r}_{\lambda'\lambda}(\mathbf{k}',\mathbf{k}) = \frac{ie}{m_0(\epsilon_{\lambda',\mathbf{k}} - \epsilon_{\lambda,\mathbf{k}})}\delta_{\mathbf{k},\mathbf{k}'}\mathbf{p}_{\lambda'\lambda}(0)$$

$$\boldsymbol{e}\mathbf{r}_{\boldsymbol{\lambda}'\boldsymbol{\lambda}}(\mathbf{k}',\mathbf{k}) = \mathbf{d}_{\boldsymbol{\lambda}'\boldsymbol{\lambda}}(\mathbf{k}',\mathbf{k}) = \boldsymbol{\delta}_{\mathbf{k},\mathbf{k}'}\mathbf{d}_{\boldsymbol{\lambda}'\boldsymbol{\lambda}}(\mathbf{0})\frac{\boldsymbol{\epsilon}_{\boldsymbol{\lambda}',\mathbf{0}} - \boldsymbol{\epsilon}_{\boldsymbol{\lambda},\mathbf{0}}}{\boldsymbol{\epsilon}_{\boldsymbol{\lambda}',\mathbf{k}} - \boldsymbol{\epsilon}_{\boldsymbol{\lambda},\mathbf{k}}}$$

**optical dipole matrix element**

$$\mathbf{d}_{\lambda'\lambda}(0) = \frac{ie\mathbf{p}_{\lambda'\lambda}(0)}{m_0(\epsilon_{\lambda',0} - \epsilon_{\lambda,0})}$$

$$\hbar\epsilon_{\lambda',\mathbf{k}} = E_g + \frac{\hbar^2k^2}{2m_{\lambda'}} \quad \text{and} \quad \hbar\epsilon_{\lambda,\mathbf{k}} = \frac{\hbar^2k^2}{2m_\lambda}$$

$$\mathbf{d}_{\lambda'\lambda}(\mathbf{k}',\mathbf{k}) = \delta_{\mathbf{k},\mathbf{k}'}\mathbf{d}_{\lambda'\lambda}(0)\frac{E_g}{E_g + \frac{\hbar^2k^2}{2}\left(\frac{1}{m_\lambda} + \frac{1}{m_{\lambda'}}\right)}$$

# Modelo de dos bandas

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$$\mathcal{H}_{el} = \sum_{\lambda,\mathbf{k}} E_{\lambda,k} a^{\dagger}_{\lambda,\mathbf{k}} a_{\lambda,\mathbf{k}} + \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \mathbf{q}\neq\mathbf{0} \\ \lambda,\lambda'}} V_q a^{\dagger}_{\lambda,\mathbf{k}+\mathbf{q}} a^{\dagger}_{\lambda',\mathbf{k}'-\mathbf{q}} a_{\lambda',\mathbf{k}'} a_{\lambda,\mathbf{k}}$$

$$\lambda, \lambda' = c, v$$

$$\begin{aligned} \mathcal{H}_{el} &= \sum_{\mathbf{k}} \left( E_{c,k} a^{\dagger}_{c,\mathbf{k}} a_{c,\mathbf{k}} + E_{v,k} a^{\dagger}_{v,\mathbf{k}} a_{v,\mathbf{k}} \right) \\ &+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\neq\mathbf{0}} V_q \Big( a^{\dagger}_{c,\mathbf{k}+\mathbf{q}} a^{\dagger}_{c,\mathbf{k}'-\mathbf{q}} a_{c,\mathbf{k}'} a_{c,\mathbf{k}} + a^{\dagger}_{v,\mathbf{k}+\mathbf{q}} a^{\dagger}_{v,\mathbf{k}'-\mathbf{q}} a_{v,\mathbf{k}'} a_{v,\mathbf{k}} \\ &+ 2 a^{\dagger}_{c,\mathbf{k}+\mathbf{q}} a^{\dagger}_{v,\mathbf{k}'-\mathbf{q}} a_{v,\mathbf{k}'} a_{c,\mathbf{k}} \Big) \; . \end{aligned} \tag{10.14}$$

$$E_{c,k} = \hbar\epsilon_{c,k} = E_g + \hbar^2 k^2 / 2m_c$$

$$E_{v,k} = \hbar\epsilon_{v,k} = \hbar^2 k^2 / 2m_v$$

# Modelo de dos bandas

To derive the equation of motion of the polarization, we use the Heisenberg equation for the individual operators. An elementary but lengthy calculation for the isotropic, homogeneous case yields

$$\hbar\left[i\frac{d}{dt}-(\epsilon_{c,k}-\epsilon_{v,k})\right]P_{vc,\mathbf{k}}(t)=\left[n_{c,\mathbf{k}}(t)-n_{v,\mathbf{k}}(t)\right]d_{cv}\mathcal{E}(t)$$
$$+\sum_{\mathbf{k}',\mathbf{q}\neq\mathbf{0}}V_q\Big(\langle a^\dagger_{c,\mathbf{k}'+\mathbf{q}}a^\dagger_{v,\mathbf{k}-\mathbf{q}}a_{c,\mathbf{k}'}a_{c,\mathbf{k}}\rangle+\langle a^\dagger_{v,\mathbf{k}'+\mathbf{q}}a^\dagger_{v,\mathbf{k}-\mathbf{q}}a_{v,\mathbf{k}'}a_{c,\mathbf{k}}\rangle$$
$$+\langle a^\dagger_{v,\mathbf{k}}a^\dagger_{c,\mathbf{k}'-\mathbf{q}}a_{c,\mathbf{k}'}a_{c,\mathbf{k}-\mathbf{q}}\rangle+\langle a^\dagger_{v,\mathbf{k}}a^\dagger_{v,\mathbf{k}'-\mathbf{q}}a_{v,\mathbf{k}'}a_{c,\mathbf{k}-\mathbf{q}}\rangle\Big)\;,$$

$$n_{\lambda,\mathbf{k}}=\langle a^\dagger_{\lambda,\mathbf{k}}a_{\lambda,\mathbf{k}}\rangle$$

# RPA en el Modelo de dos bandas

# RPA en el Modelo de dos bandas

$$\langle a^\dagger_{c,\mathbf{k}'+\mathbf{q}} a^\dagger_{v,\mathbf{k}-\mathbf{q}} a_{c\mathbf{k}'} a_{c,\mathbf{k}} \rangle \simeq P_{vc,\mathbf{k}'} n_{c,\mathbf{k}} \delta_{\mathbf{k}-\mathbf{q},\mathbf{k}'}$$

$$\hbar \left[ i\frac{d}{dt} - (e_{c,k} - e_{v,k}) \right] P_{vc,\mathbf{k}}(t)$$
$$= \left[ n_{c,\mathbf{k}}(t) - n_{v,\mathbf{k}}(t) \right] \left[ d_{cv}\mathcal{E}(t) + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|} P_{vc,\mathbf{q}} \right] . \qquad (10.21)$$

**dynamics of interband polarization (pair) function**

$$e_{\lambda,k} = e_{\lambda,k} + \Sigma_{exc,\lambda}(k)$$

$$\hbar\Sigma_{exc,\lambda}(k) = -\sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|} n_{\lambda,\mathbf{q}}$$

# RPA en el Modelo de dos bandas

$$\boldsymbol{\hbar\left[i\frac{d}{dt}-(e_{c,k}-e_{v,k})\right]P_{vc,\mathbf{k}}(t)}$$
$$\boldsymbol{=\left[n_{c,\mathbf{k}}(t)-n_{v,\mathbf{k}}(t)\right]\left[d_{cv}\mathcal{E}(t)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}\right]}$$

$$n_{c,\mathbf{k}}(t)\rightarrow f_{c,k}\quad\text{and}\quad n_{v,\mathbf{k}}(t)\rightarrow f_{v,k}$$

$$\hbar\left[i\frac{d}{dt}-(e_{c,k}-e_{v,k})\right]P_{vc,\mathbf{k}}(t)$$
$$=\left(f_{c,\mathbf{k}}-f_{v,\mathbf{k}}\right)\left[d_{cv}\mathcal{E}(t)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}\right]$$

Caso sin interacción electrón-electrón

# Caso sin interacción electrón-electrón

$$V_q = 0$$

$$\hbar \left[ i\frac{d}{dt} - (e_{c,k} - \epsilon_{v,k}) \right] P^0_{vc,k}(t) = (f_{c,k} - f_{v,k}) d_{cv} \mathcal{E}(t)$$

$$P^0_{vc,k}(\omega) = (f_{c,k} - f_{v,k}) \frac{d_{cv}}{\hbar[\omega + i\delta - (\epsilon_{c,k} - \epsilon_{v,k})]} \mathcal{E}(\omega)$$

$$P^0_{vc,k}(\omega) = (f_{c,k} - f_{v,k}) \frac{d_{cv}}{\hbar[\omega + i\delta - (\epsilon_{c,k} - \epsilon_{v,k})]} \mathcal{E}(\omega)$$

# Caso sin interacción electrón-electrón

$$P^0_{vc,k}(t) = \int \frac{d\omega}{2\pi}(f_{c,k} - f_{v,k})\frac{d_{cv}}{\hbar[\omega + i\delta - (\epsilon_{c,k} - \epsilon_{v,k})]}\mathcal{E}(\omega)e^{-i\omega t}$$

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

$$P^0(t) = \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi}|d_{cv}|^2 \frac{f_{c,k} - f_{v,k}}{\hbar[\omega + i\delta - (\epsilon_{c,k} - \epsilon_{v,k})]}\mathcal{E}(\omega)e^{-i\omega t} + \text{c.c.}$$

i.e., the free-particle result of Chap. 5.

# Resumen de la clase 21

Elemento de matriz del dipolo eléctrico

Ecuación de movimiento de la polarización interbanda

Polarización interbanda de partícula libre