CLASE 6 - martes 13/04/2021

La clase pasada vimos:

Heteroestructuras de semiconductores

- Técnicas de crecimiento de cristales capa por capa
- Ley de Vegard
- Ingeniería de bandas:
  - Regla de Anderson
  - Tipos de alineación de bandas
- Ejemplos de estructuras cuánticas
  - Barrera, pozo, doble barrera, superlattice

En esta clase veremos:

- Pozos cuánticos dobles y parabólicos
- Aproximación de masa efectiva : una impureza

REPASO

Hetero-estructuras

Regla de Anderson

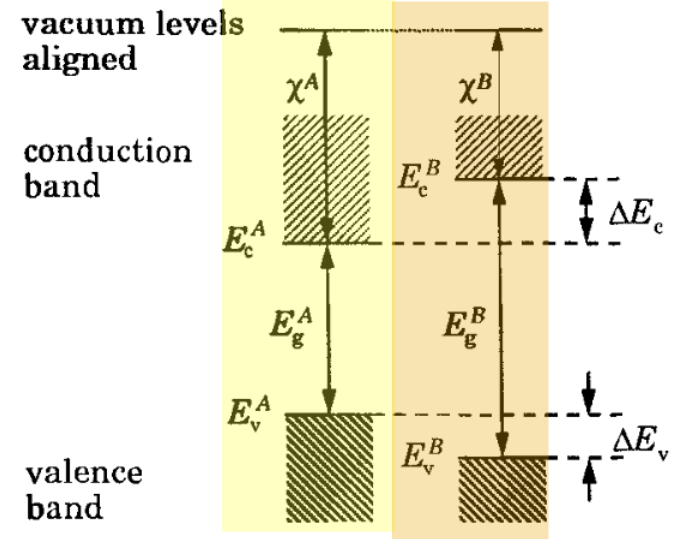
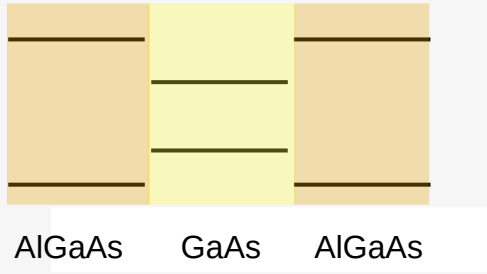


FIGURE 3.4. Anderson's rule for the alignment of the bands at a heterojunction between materials *A* and *B*, based on aligning the vacuum levels.

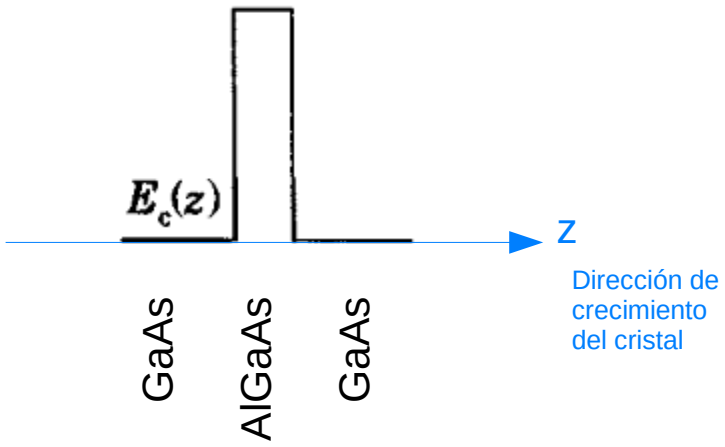
En un sandwich BAB se confinan en A tanto electrones como huecos



REPASO

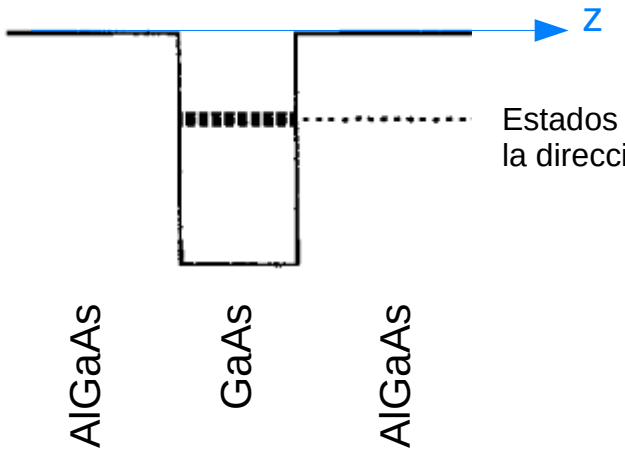
Ejemplos de estructuras cuánticas en capas

Barrera túnel



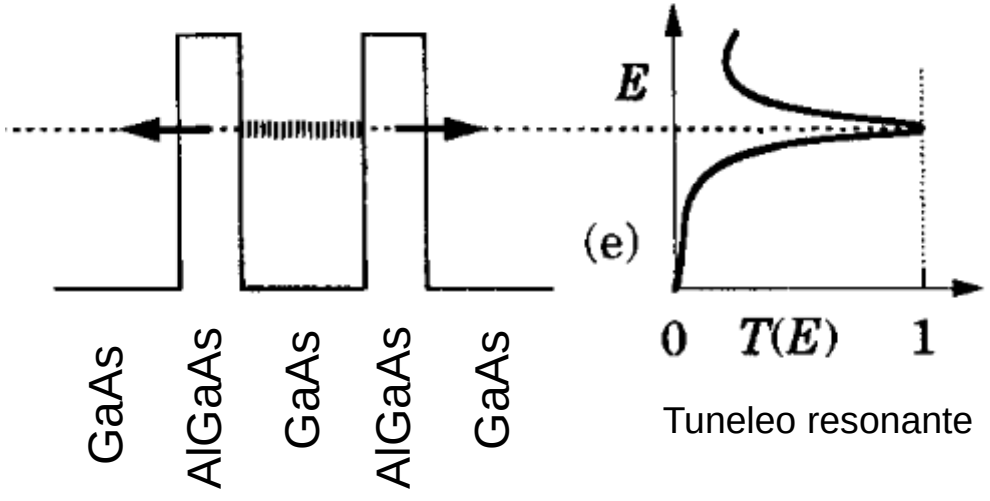
Dirección de crecimiento del cristal

Pozo cuántico



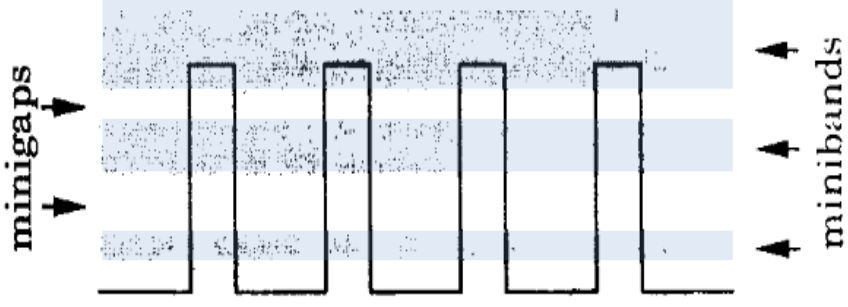
Estados ligados en la dirección z

Barrera doble



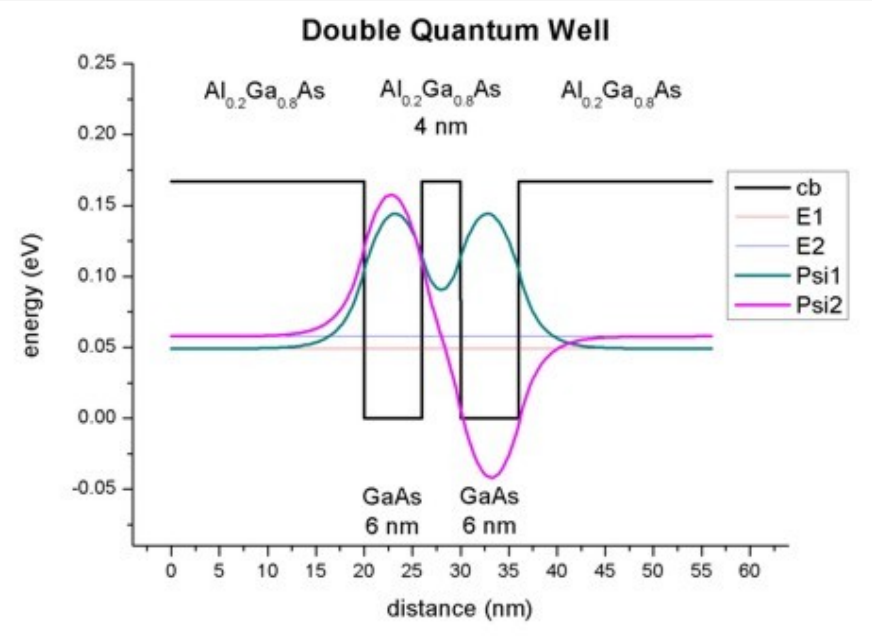
Tuneleo resonante

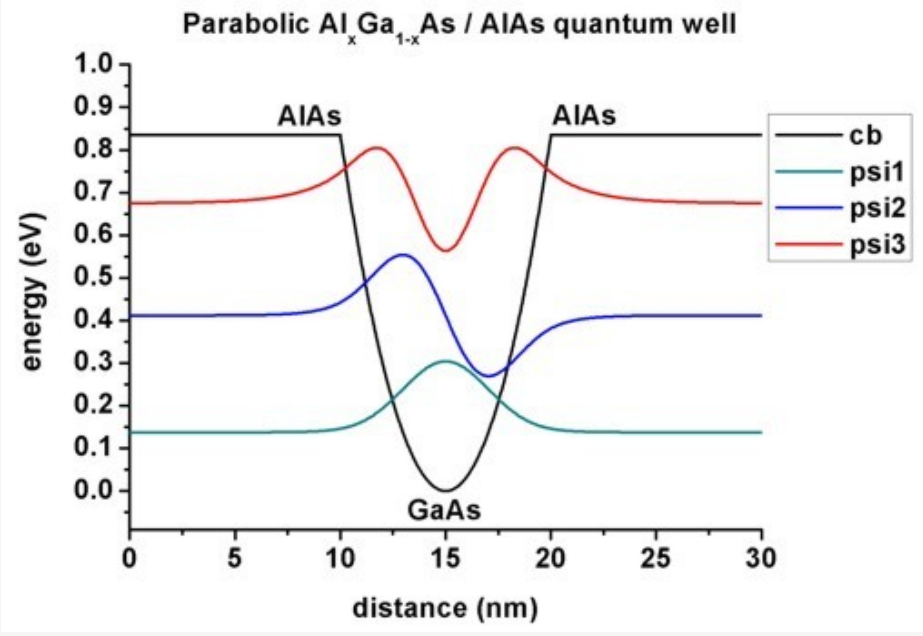
Superlattice



Algunos ejemplos más de pozos cuánticos

Pozos cuánticos dobles y parabólicos





Pozos dobles

VOLUME 73, NUMBER 14 PHYSICAL REVIEW LETTERS 3 OCTOBER 1994

Vertex-Correction-Driven Intersubband Spin-Density Excitonic Instability in Double Quantum Well Structures

S. Das Sarma and P. I. Tamborenea
Department of Physics, University of Maryland, College Park, Maryland 20742-4111
(Received 15 March 1994)

We show that exchange-correlation induced many-body excitonic vertex correction may lead to an instability in the normal ground state of a semiconductor double quantum well structure by suppressing the symmetric-antisymmetric intersubband gap at low but accessible ($\sim 0.7 \times 10^{11}$ cm^{-2}) electron densities. We predict as a consequence a novel electronic phase transition where the lowest intersubband spin-density-excitation gap vanishes giving rise to a new many-body triplet excitonic liquid ground state which is more stable at low densities than the usual two dimensional Fermi liquid phase.

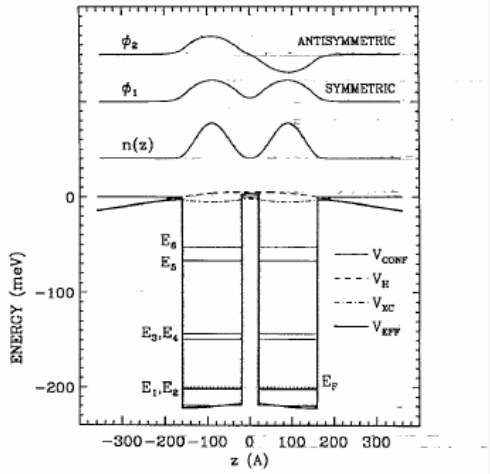


FIG. 1. The typical double quantum well structure ($N_S = 10^{11}$ cm^{-2}) with the self-consistent local-density-approximation calculated energy levels and wave functions for the symmetric-antisymmetric levels. The bare (V_{conf}), Hartree (V_H), and exchange-correlation (V_{xc}) contributions to the effective potential (V_{EFF}) are shown. (The SAS gap $\Delta_{SAS} = | E_2 - E_1 |$.)

Pozos parabólicos con imperfecciones

PHYSICAL REVIEW B VOLUME 49, NUMBER 23 15 JUNE 1994-I

Collective excitations in imperfect parabolic quantum wells with in-plane magnetic fields

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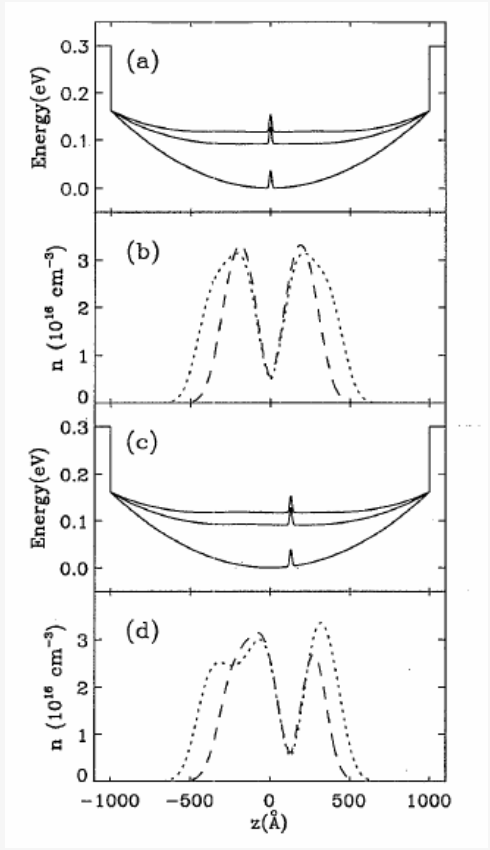
(Received 7 July 1993; revised manuscript received 25 January 1994)



Pozos parabólicos asimétricos, con dos curvaturas diferentes

Pergamon

Solid State Communications, Vol. 89, No. 12, pp. 1009-1012, 1994
Elsevier Science Ltd

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COLLECTIVE EXCITATIONS IN ASYMMETRIC PARABOLIC QUANTUM WELLS

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(*Received 12 January 1994 by A. Pinczuk*)

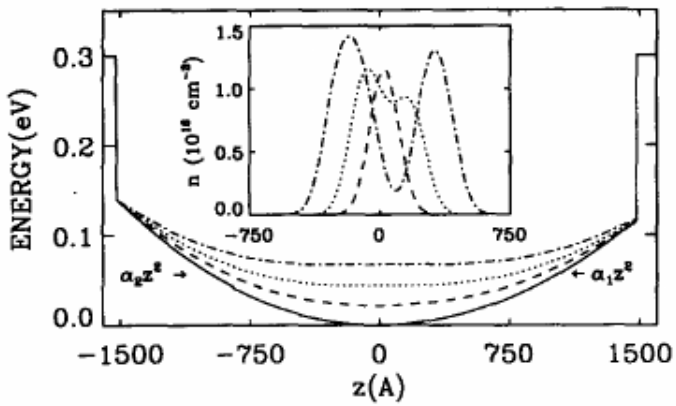
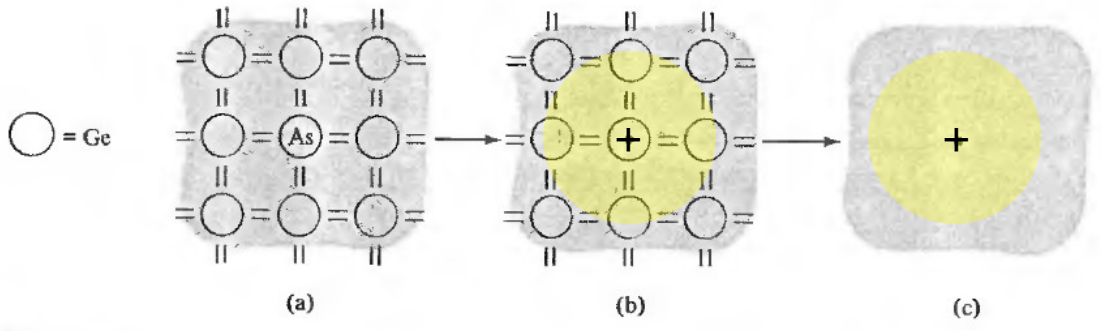


Fig. 1. Model bare potential of the asymmetric parabolic well (solid line), and calculated self-consistent potentials with an in-plane magnetic field of $B = 5.8\ T$, for $N_s = 2.4$ (dash line), 4.7 (dotted line), and $7.5 \times 10^{10}\ cm^{-2}$ (dash-dot line); inset: corresponding calculated self-consistent densities.

Aproximación de masa efectiva

Aproximación de masa efectiva

Supongamos que se agrega al material algo nanométrico que perturba su periodicidad, por ejemplo, una impureza:



Impureza sustitucional

Figure 28.11
(a) Schematic representation of a substitutional arsenic (valence 5) donor impurity in a germanium (valence 4) crystal. (b) The arsenic (As) can be represented as a germanium atom *plus* an additional unit of positive charge fixed at the site of the atom (circled dot). (c) In the semiclassical approximation, in which the pure semiconductor is treated as a homogeneous medium, the arsenic impurity is represented as a fixed point charge $+e$ (dot).

Ashcroft y Mermin

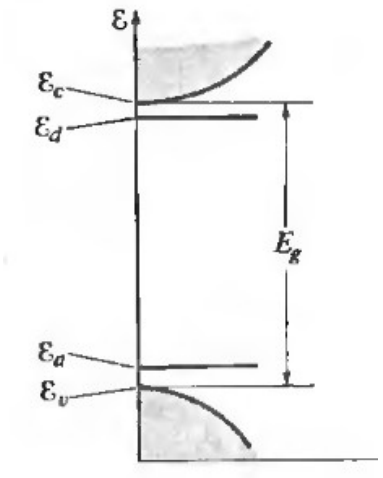
Aproximación de masa efectiva

Ecuación de Schrödinger para el electrón donado al material:

$$[\hat{H}_{\text{per}} + V_{\text{imp}}(\mathbf{R})]\psi(\mathbf{R}) = E\psi(\mathbf{R})$$

Queremos ver como se llega a un modelo simplificado sin H_{per}

En el problema de la impureza sustitucional se llega a un problema equivalente al átomo de hidrógeno con *constante dieléctrica* y *masa efectiva*:



$$\left[-\frac{\hbar^2\nabla^2}{2m^*} - \frac{e^2}{\epsilon r}\right]\psi(\mathbf{r}) = E^*\psi(\mathbf{r})$$

Ecuación de Schrödinger efectiva

$$r_0 = \frac{m}{m^*}\epsilon a_0$$

radio de Bohr efectivo (decenas de angstroms)

$$\varepsilon = \frac{m^*}{m}\frac{1}{\epsilon^2} \times 13.6\ \text{eV}$$

Rydberg efectivo (meV) (5 meV en GaAs)

Aproximación de masa efectiva

Estados de Bloch y energías del cristal puro: $\hat{H}_{\text{per}}\phi_{nk}(x) = \varepsilon_n(k)\phi_{nk}(x)$

Expandimos el estado del electrón con la impureza presente :

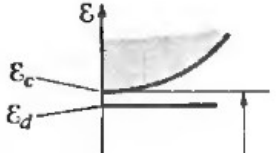
$$\psi(x) = \sum_n \int_{-\pi/a}^{\pi/a} \tilde{\chi}_n(k)\phi_{nk}(x)\frac{dk}{2\pi}$$

Coeficientes de la expansión

Aproximaciones :

(1) Una sola banda, por ejemplo banda de conducción
(un solo n en la suma)

(2) Integrar *k* cerca del mínimo



Aproximación de masa efectiva

$$\psi(x) = \sum_n \int_{-\pi/a}^{\pi/a} \tilde{\chi}_n(k)\phi_{nk}(x)\frac{dk}{2\pi}$$

(2) Integrar *k* cerca del mínimo :

Aproximamos la función de Bloch cerca de *k* = 0 :

$$\phi_{nk}(x) = u_{nk}(x)\, e^{ikx} \approx u_{n0}(x)\, e^{ikx} = \phi_{n0}(x)\, e^{ikx}$$

$$\longrightarrow \quad \psi(x) \approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k) \exp(ikx)\frac{dk}{2\pi} = \phi_{n0}(x)\, \chi(x)$$

Aproximación de masa efectiva

$$\psi(x) \approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k) \exp(ikx) \frac{dk}{2\pi} = \phi_{n0}(x)\, \chi(x)$$

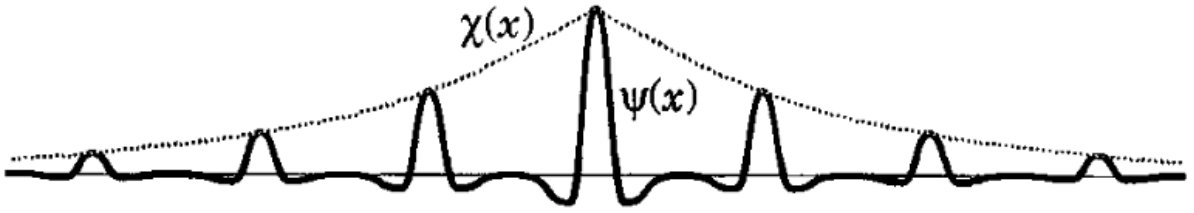


FIGURE 3.21. Wave function around an impurity, showing the envelope function $\chi(x)$ that modulates the Bloch function to give the full wave function $\psi(x)$.

La función envolvente contiene valores chicos de k en su expansión de Fourier, por lo tanto es **suave** comparada con el parámetro de red

Vamos a ver que en este caso es el ground state hidrogenoide: $\chi(r) \sim e^{-r/a_0^*}$

Aproximación de masa efectiva

Falta obtener la ecuación para la función envolvente. Teníamos el problema exacto:

$$\begin{cases} [\hat{H}_{\text{per}} + V_{\text{imp}}(\mathbf{R})]\psi(\mathbf{R}) = E\psi(\mathbf{R}) \\ \psi(x) = \sum_n \int_{-\pi/a}^{\pi/a} \tilde{\chi}_n(k)\phi_{nk}(x)\frac{dk}{2\pi} \end{cases}$$

Nos quedamos con una sola banda en la expansión:

$$\hat{H}_{\text{per}}\psi(x) = \hat{H}_{\text{per}} \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\,\phi_{nk}(x)\frac{dk}{2\pi} = \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\,\varepsilon_n(k)\,\phi_{nk}(x)\frac{dk}{2\pi}$$

$$\approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\,\varepsilon_n(k)\,e^{ikx}\frac{dk}{2\pi}.$$

Aproximación de masa efectiva

Supongamos que: $\varepsilon_n(k) = \sum_m a_m k^m$

Reemplazando:

$$\hat{H}_{\text{per}}\psi(x) \approx \phi_{n0}(x) \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, \varepsilon_n(k)\, e^{ikx} \frac{dk}{2\pi}$$

$$\approx \phi_{n0}(x) \sum_m a_m \int_{-\pi/a}^{\pi/a} \tilde{\chi}(k)\, k^m\, e^{ikx} \frac{dk}{2\pi}$$

Integración por partes y transf. de Fourier

$$\approx \phi_{n0}(x) \sum_m a_m \left(-i\frac{d}{dx}\right)^m \chi(x)$$

$$\equiv \phi_{n0}(x)\, \varepsilon_n\left(-i\frac{d}{dx}\right) \chi(x)$$

Aproximación de masa efectiva

Entonces obtuvimos: $$\left[\varepsilon_n\left(-i\frac{d}{dx}\right) + V_{\text{imp}}(x)\right]\chi(x) = E\chi(x).$$

Ecuación de Schrödinger efectiva para la función envolvente

In 3D: $\varepsilon_n(-i\,d/dx) \longrightarrow \varepsilon_n(-i\nabla)$

Cerca del mínimo de la banda de conducción:

$$\varepsilon_n(\mathbf{K}) \approx E_c + \frac{\hbar^2 K^2}{2m_0 m_e} \longrightarrow \varepsilon_n(-i\nabla) \approx E_c - \frac{\hbar^2}{2m_0 m_e}\nabla^2$$

$$\longrightarrow \boxed{\left[-\frac{\hbar^2}{2m_0 m_e}\nabla^2 + V_{\text{imp}}(\mathbf{R})\right]\chi(\mathbf{R}) = (E - E_c)\chi(\mathbf{R})}$$

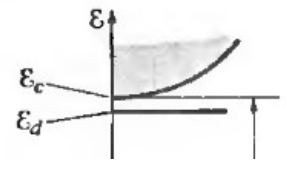
Aproximación de masa efectiva

Incluyendo el potencial de la impureza ionizada:

$$\left(-\frac{\hbar^2}{2m_0 m_e}\nabla^2 - \frac{e^2}{4\pi\epsilon_0\epsilon_b R}\right)\chi(\mathbf{R}) = (E - E_c)\chi(\mathbf{R})$$

$\chi(R) = (\pi a_B^3)^{-1/2}\exp(-R/a_B)$, where a_B is the *Bohr radius*

$$\mathcal{R} = \left(\frac{e^2}{4\pi\epsilon}\right)^2 \frac{m}{2\hbar^2} = \frac{\hbar^2}{2ma_B^2} = \frac{1}{2}\frac{e^2}{4\pi\epsilon a_B}$$



$$a_B = \frac{4\pi\epsilon\hbar^2}{me^2}.$$

$\mathcal{R} \approx 5\,\text{meV}$ and $a_B \approx 10\,\text{nm}$ for electrons in GaAs

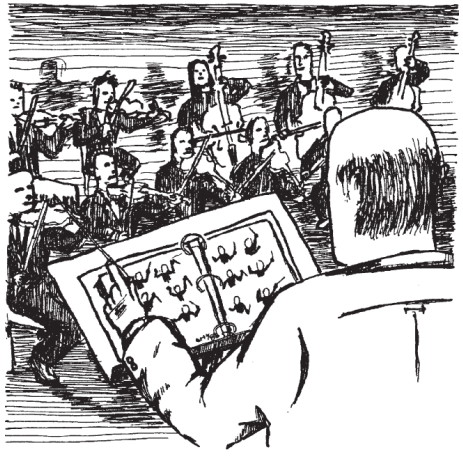
The lowest state has a binding energy of $4\mathcal{R}$, four times larger than the corresponding three-dimensional result. This is particularly important for an *exciton*. an

Peter Y. Yu
Manuel Cardona

Aproximación de masa efectiva

Fundamentals of Semiconductors

Physics and Materials Properties



A SEMI-CONDUCTOR

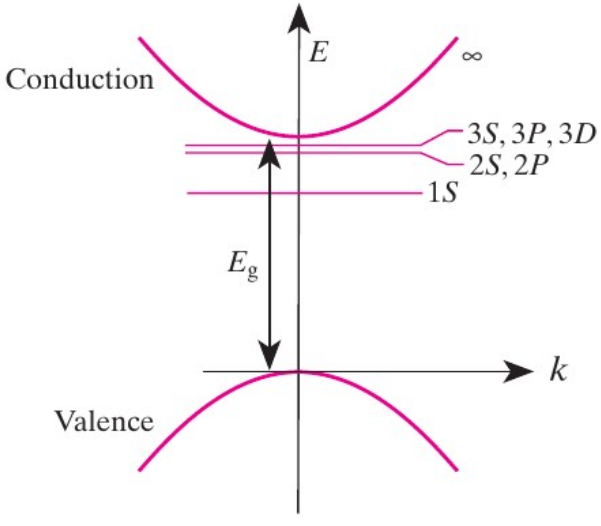


Fig. 4.1. Schematic diagram of the n=1, 2, and 3 bound states of a shallow donor electron near a nondegenerate and parabolic conduction band (corresponding to $n = \infty$). E_g is the bandgap

Aproximación de masa efectiva

Table 4.1. Experimental binding energies of the 1*s* state of shallow donors in some zinc-blende-type semiconductors (from [Ref. 4.4, p. 224]) compared with the predictions of (4.24)

Semiconductor	Binding energy from (4.24) [meV]	Experimental binding energy of common donors [meV]
GaAs	5.72	Si_{Ga}(5.84); Ge_{Ga}(5.88) S_{As}(5.87); Se_{As}(5.79)
InP	7.14	7.14
InSb	0.6	Te_{Sb}(0.6)
CdTe	11.6	In_{Cd}(14); Al_{Cd}(14)
ZnSe	25.7	Al_{Zn}(26.3); Ga_{Zn}(27.9) F_{Se}(29.3); Cl_{Se}(26.9)

$$R = \left(\frac{m^*}{m_0}\right)\left(\frac{1}{\varepsilon_0^2}\right)\left(\frac{e^4 m_0}{2\hbar^2}\right)\frac{1}{(4\pi\varepsilon_0)^2}, \qquad (4.24)$$

Resumen de la clase 6

Pozos cuánticos dobles y parabólicos

Aproximación de masa efectiva : una impureza