Describing p-Doped Quantum Dots

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2 Quantum Dots
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   - Nondegenerate Case
   - Spin Orbit Coupling

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   - Kohn-Luttinger Hamiltonian
   - Envelope Functions

5 Summary
We want to have magnetic quantum dots.

Doping with Manganese (Mn)
- Mn has an magnetic moment of $\frac{5}{2} \hbar$
- Mn acts as an acceptor in GaAs
  → Holes are main charge carriers.

We can not use the description for quantum dots with electrons.
- The valence bands are degenerate at the bandgap.
- We have to use a more difficile description.
We can confine electrons in all three spatial directions in an heterojunction made of GaAs/GaAlAs.
Quantum Dots Today

- Only QD with electrons are good explored.
- Manufacture of QD with holes is difficult.
- Experiments on them are running.
- First results on Mn-doped QD are uncertain.
The $k \cdot p$ Theory

Basic Approach for the Hamiltonian

$$
\left( \frac{p^2}{2m_e} + V(r) \right) e^{ikr} u_{nk}(r) = E_{nk} e^{ikr} u_{nk}(r)
$$

$V(r)$: Periodic Crystal Potential

This leads to an equation for the Bloch functions $u_{nk}$:

$$
\left( \frac{\hbar^2 k^2}{2m_e} + \frac{\hbar}{m_e} k \cdot p + \frac{p^2}{2m_e} + V(r) \right) u_{nk}(r) = E_{nk} u_{nk}(r)
$$
Centrum Of The Brillouin-Zone: \( k = 0 \)

\[
\left( \frac{p^2}{2m_e} + V \right) u_{n0} = E_{n0} u_{n0}
\]

In the vicinity of \( k = 0 \) we can thread the \( \mathbf{k} \cdot \mathbf{p} \)- and the \( k^2 \) - term as an perturbation to this equitation.

This is called the \( \mathbf{k} \cdot \mathbf{p} \) method.
Perturbation Theory

First Order Eigenstates:

\[ u_{nk} = u_{n0} + \frac{\hbar}{m} \sum_{n' \neq n} \frac{\langle u_{n0} | \mathbf{k} \cdot \mathbf{p} | u_{n'0} \rangle}{E_{n0} - E_{n'0}} u_{n'0} \]

Second Order Energy:

\[ E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n' \neq n} \left| \langle u_{n0} | \mathbf{k} \cdot \mathbf{p} | u_{n'0} \rangle \right|^2 \frac{E_{n0} - E_{n'0}}{E_{n0} - E_{n'0}} \]

We can abbreviate this to:

\[ E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*} \]
**Effective Mass**

With the Definition of an Effective Mass:

\[
\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2} \sum_{n' \neq n} \frac{| \langle u_{n0} | \mathbf{k} \cdot \mathbf{p} | u_{n'0} \rangle |^2}{E_{n0} - E_{n'0}}
\]

The matrix elements \( \langle u_{n0} | \mathbf{k} \cdot \mathbf{p} | u_{n'0} \rangle \) can be calculated from group-theoretical considerations:

- GaAs has a crystal structure of zinc-blende. \( \rightarrow \) cubic symmetry
- \( u_{n0} \) must follow the symmetry at the center of the Brillouin-Zone.
- \( u_{n0} \) are an orthonormal basis set.
- \( \mathbf{p} \) can couple only certain \( u_{n'0} \) to \( u_{n0} \).
We can tread the electron in the crystal almost just like a free particle with a different mass. But...

**Assumptions made:**
- The conduction band is not degenerate.
- Bandgap is at $k = 0$ (direct semiconductor).
- The conduction band is well separated from other bands.
- No Spin-Orbit coupling!!!
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Spin Orbit Coupling

We have to add the Spin-Orbit Potential to our Hamiltonian:

\[ H_{SO} = \frac{\hbar}{4c^2m^2} (\nabla V \times \mathbf{p}) \cdot \sigma \]

\[ \sigma : \text{Pauli-Matrices} \]
\[ V : \text{crystal potential} \]

Since \( V \) has the crystal periodicity we can find some Bloch functions \( \tilde{u}_n \) which are eigenfunctions to our old \( H \) plus \( H_{SO} \).

We restrict our considerations to bands of our interest.
Spin Orbit Coupling

Holes

Motion of holes $\rightarrow$ look at the top of the valence band

Without Spin-Orbit coupling in crystals with diamond or zinc-blende structure we have 6 degenerate functions at the top of the valence band: $|X\pm\rangle$, $|Y\pm\rangle$, $|Z\pm\rangle$

$|X\rangle$, $|Y\rangle$, $|Z\rangle$ have symmetry like atomic p-states.
$\pm$ denotes the possible spin states.

Spin-Orbit States:

We construct the states like in atomic physics!
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**Spin Orbit Coupling**

### "l=1" -like states in zinc-blende crystals

\[
|lm_l\rangle = \begin{cases} 
|1, 1\rangle = -(X + iY)/\sqrt{2} \\
|1, 0\rangle = Z \\
|1, -1\rangle = (X - iY)/\sqrt{2}
\end{cases}
\]

### "j=3/2" and "j=1/2" -like states in zinc-blende crystals

\[
|jm_j\rangle = \begin{cases} 
|3/2, 3/2\rangle = |1, 1, -\rangle \\
|3/2, 1/2\rangle = (1/\sqrt{3})(|1, 1, -\rangle + \sqrt{2}|1, 0, -\rangle) \\
|3/2, -1/2\rangle = (1/\sqrt{3})(|1, -1, -\rangle + \sqrt{2}|1, 0, -\rangle) \\
|3/2, -3/2\rangle = |1, -1, -\rangle \\
|1/2, 1/2\rangle = (1/\sqrt{3})(|1, 0, +\rangle - \sqrt{2}|1, 1, -\rangle) \\
|1/2, -1/2\rangle = (1/\sqrt{3})(|1, 0, +\rangle - \sqrt{2}|1, -1, -\rangle)
\end{cases}
\]
Bandstructure With Spin-Orbit Interaction

- degeneracy partially lifted
- splitting of the valence band dependent on materials
  - GaAs $\sim$ 0.34 eV
  - Si $\sim$ 0.05 eV
- Bandgap GaAs $\sim$ 1.42 eV

We restrict our attention further only to the $j = 3/2$ states.
So far we can describe the holes in a bulk crystal. How do we describe the quantum dot?

**External Potentials**

The quantum dot is described by additional, slow varying potential. For a heterojunction:

\[ U(x, y) = \frac{K_0}{m} (x^2 + y^2) \]

\[ U(z) = \begin{cases} \infty & : z < 0 \\ z & : z \geq 0 \end{cases} \]

Crystal potential \( V \) varies at \( \sim 1 \, \text{Å} \)

External potential \( U \) varies at \( \sim 100 - 200 \, \text{Å} \)
We start again with:

\[
\left( \frac{\hbar^2 k^2}{2m_e} + \frac{\hbar}{m_e} \mathbf{k} \cdot \mathbf{p} + \frac{p^2}{2m_e} + V_{cr}(\mathbf{r}) + U_{ex}(\mathbf{r}) \right) \psi(\mathbf{r}) = E_n k \psi(\mathbf{r})
\]

Bloch functions at the zone center form an orthonormal basis set:

\[
\psi(\mathbf{r}) = \sum_{n'} \psi_{n'}(\mathbf{r}) u_{n'0}(\mathbf{r})
\]

The \( \psi_{n'} \) are space-dependent coefficients.

To take an external magnetic field into account we substitute:

\[
k \rightarrow \frac{1}{\hbar} (\mathbf{p} + e\mathbf{A})
\]
After multiplying with $u_{n0}^*$ and integrating over one unit cell we get the:

### Envelope Function Hamiltonian

\[
\sum_{n'} \left\{ \left( \frac{(p + eA(r))^2}{2m_e} + E_n(0) + U_{ex}(r) \right) \delta_{nn'} + P_{nn'} \cdot (p + eA(r)) \right\} \psi_{n'}(r) = E \psi_n(r)
\]

Because the $\psi_n(r)$ are nearly constant in one unit cell, we can tread them like constants during the integration.

The $P_{nn'}$ are once again determined by symmetry considerations.
Kohn-Lüuttinger Hamiltonian

\[
\begin{pmatrix}
P + Q + \frac{3}{2} \kappa B \\
\gamma_1 \frac{1}{2m_e} (\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) \\
S^\dagger & P - Q + \frac{3}{2} \kappa B \\
0 & 0 \\
R^\dagger & 0 \\
0 & R \\
\end{pmatrix}
\]

- \( \gamma \)-s Determined by Crystal
- \( \hat{p} = (p + eA) \)
- \( \frac{m_e}{\gamma_1 + \gamma_2} \) : "Heavy" Holes
- \( \frac{m_e}{\gamma_1 - \gamma_2} \) : "Light" Holes
- \( \frac{3}{2} \kappa B \) Spin Splitting
Envelope Functions

\[ \psi(r) = \sum_{\nu n} C_{\nu n} \zeta_\nu(z) R_{nm}(\rho) e^{im\phi} \]

The envelope functions are just the Fock-Darwin states in the plane

\[ R_n(\rho) e^{im\phi} \]

and Airy functions perpendicular to it

\[ \zeta_\nu(z) \]

Diagonalizing the Kohn-Lüttinger matrix with this functions gives us the energy eigenvalues and eigenstates!
The $\mathbf{k} \cdot \mathbf{p}$ -Theory has been presented.
The Envelope Function Approximation has been introduced.
The Kohn-Lüttinger Matrix for hole-states in crystals with zinc-blende structure was presented.

To Do...

- finally get the Matrix diagonalized properly
- identificate the ground states in terms of Fock-Darwin states
- describe the interaction with the manganese
- ...

Summary and Outlook
Thank You for your attention!!!