Explaining symmetry elevation in InGaAs quantum dots through bulk symmetry-structure symmetry interaction

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Introduction

An outline of the problem

- Master's project (MSci) under Professor Dimitri Vvedensky at Imperial College London
- Collaboration with Professor Stefan Schulz and Professor Emanuele Pelucchi
- Problem specifics:
  - Quantum dots with high spatial symmetry: photoluminiscence
  - Fine-structure splitting of excitonic energy levels
  - Resolvable peaks within major features of the photoluminiscence spectrum
  - Symmetry elevation
- Motivation:
  - Artificial atoms
  - Programmable structural and spectral properties
  - Usage in quantum computing, medical imagining, lasing, photovoltaic engineering, and other areas.

Introduction

The quantum dot in question

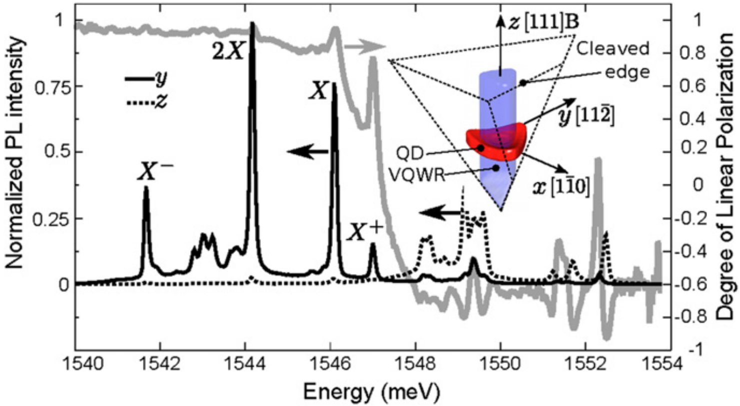
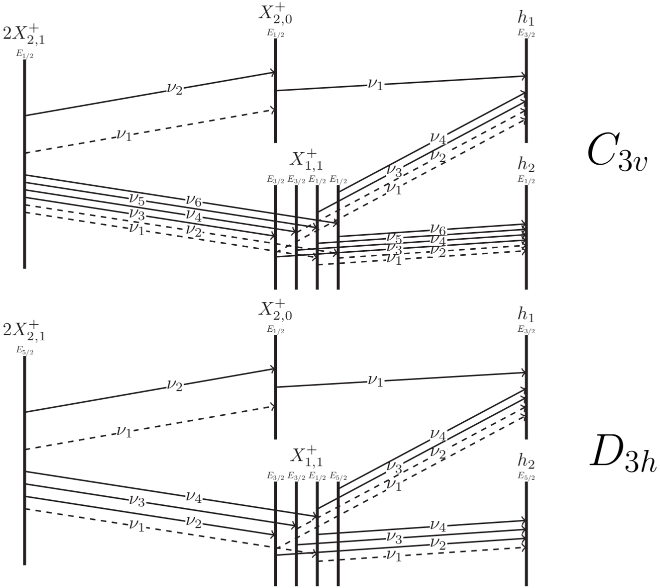


Figure: Gross spectrum of a C_{3v} InGaAs QD. Image credit: Karlsson, K. F. et al (2015), Spectral signatures of high-symmetry quantum dots and effects of symmetry breaking. New Journal of Physics, 17 103017

Introduction

Exciton energy levels and transitions



Results

Framework for automatic energy level splitting and selection rules calculation

- Structure point group is a subgroup of $SU(2) \otimes C_i$
- Single fermions are j-eigenstates, hence we can use subduction
- Multiplication tables of double groups can be constructed from the double covering of $O(3)$ by $SU(2) \otimes C_i$ (quaternion approach)
- The faithful irrep of $SO(3)$ is the Cartesian rep, which, subdued into the double group, identifies the Cartesian basis vector transformation laws.
- By considering subtraces of Wigner D-matrices, we can identify the irreps and basis partners of any j-state $|j, m\rangle$.
- A careful treatment of parity under l- and j-coupling is introduced.
- The entire group-theoretical analysis as performed by Karlsson et al. is automated in our Python package AReTDoG (Algorithms for Representation Theory of Double Groups).

Results

Symmetry suppression theory

- Symmetry elevation can be understood as partial symmetry breaking from a higher-symmetry Hamiltonian $\hat{H}_+$ which approximates the true Hamiltonian $\hat{H}$.
- Every eigenstate of $\hat{H}$ decomposable into an eigenstate of $\hat{H}_+$ and a residual component.
- Surjection of basis vectors $\rightarrow$ transformation properties of the elevated symmetry component
- Selection rules can allow a transition from the lower symmetry eigenstate but forbid it from the elevated symmetry component, suppressing the rate.

Results

Evidence for symmetry suppression in InGaAs QDs grown in inverted tetrahedrons

- Symmetry elevation matches the bulk symmetry (C_{6v}) on a sample dataset.
- Differently-sized quantum wires in the growth mode result in a hexagonal structure.
- By considering only the envelope functions, we model exciton complexes as a many-body particle system in a box with j-coupling and Coulomb interactions.
- Wavefunction localisation around the centre–approximate elevation from structure symmetry to bulk symmetry.
- Due to breakage of exchange symmetry, mixed-hole excitons are predicted to probe for structure symmetry.
- Pure light-hole excitons empirically probe for structure symmetry, presumably due to weak localisation in the centre.

Results

Evidence for symmetry suppression in InGaAs QDs grown in inverted tetrahedrons

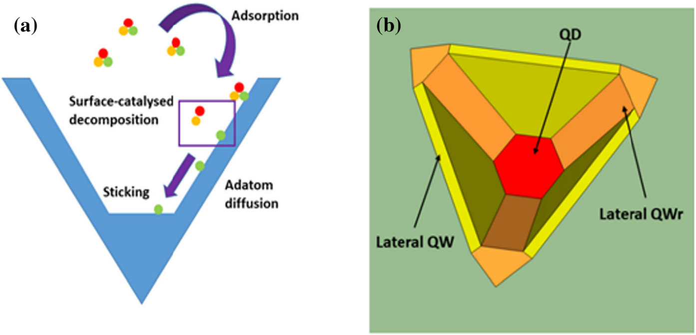


Figure: The epitaxy growth process and the sketch of a QD with large-scale QWs. Smaller QWs may result in an irregular hexagon with 3+3 structure. Image credit: Holsgrove, K. M. et al (2022), Towards 3D characterisation of site-controlled InGaAs pyramidal QDs at the nanoscale. J Mater Sci., 57:16383–16396

Predictions and outlook

- We predict only pure heavy-hole excitons to undergo symmetry elevation to bulk symmetry (weakly supported by Karlsson data)
- An error in Karlsson analysis of C_{6v} selection rules–C_{6v} and D_{3h} do give different predictions regarding the z-polarised spectra.
- We predict one weak z-polarised emission line for every pure heavy-hole exciton complex (challege in identification).
- We also predict pure light-hole excitons to be delocalised in the QD.
- These predictions will be compared to experimental data (Pelucchi) as well as simulation (Schulz).

References

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