On Eigenvalue Problems Arising from the Modeling of Semiconductor Nanostructures

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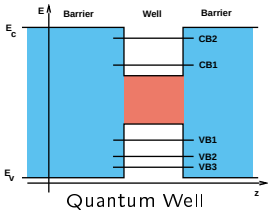

Quantum Well

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Introduction

The $k \cdot p$-method in combination with the *envelope function approximation* is a widely used tool for the near-bandedge modeling of electronic states in one-dimensional semiconductor nanostructures like Quantum Wells (QW) and Multi Quantum Wells (MQW). Within the nanostructure the wave function is represented in terms of *envelope functions*, which are eigenfunctions of matrix-valued $k \cdot p$ Schrödinger operators with *discontinous* coefficients. The $k \cdot p$ Schrödinger operators describe the *mixing* of the near-bandedge states of the semiconductor materials. They parameterically depend on the *reduced wave vector* $\mathbf{k}_| = (k_1, k_2) \in \mathbb{R}^2$.

$k \cdot p$ Schrödinger operators for d states

Ordinary differential operator defined on $L^2([0,L];\mathbb{C}^d)$:

$$\begin{aligned}\mathsf{H}_{\mathbf{k}_|} = &-\frac{d}{dz}\mathbf{m}(z)\frac{d}{dz} + \mathbf{e}(z) + \mathbf{V}(z)\\ &+ \mathbf{M}_0(z)\, i\frac{d}{dz} + i\frac{d}{dz}(\mathbf{M}_0(z)\cdot)\\ &+ \sum_{r=1,2} k_r\left(\mathbf{M}_r(z)\, i\frac{d}{dz} + i\frac{d}{dz}(\mathbf{M}_r(z)\cdot)\right)\\ &+ \sum_{r=1,2} k_r\, \mathbf{U}_r(z) + \sum_{r,s=1,2} k_r k_s\, \mathbf{U}_{r,s}(z) + \text{b.c.}\end{aligned}$$

Piecewise constant $d \times d$ matrix-valued functions $\mathbf{m}, \mathbf{e}, \mathbf{V}, \mathbf{M}, \mathbf{U}$:

$\mathbf{m}, \mathbf{e}$: real, diagonal, same signature
$\mathbf{e}$: spatial variation of the band edges
$\mathbf{V}$, $\mathbf{M}, \mathbf{U}$: complex and selfadjoint

Typically $d = 4, 6, 8, 14$

Eigenvalue Problem

Calculation of eigenvalue dispersions $E_n(\mathbf{k}_|)$ and corresponding eigenfunctions $F_n(z;\mathbf{k}_|)$ of $k \cdot p$ Schrödinger operators:

$$\mathsf{H}_{\mathbf{k}_|} F_n(z;\mathbf{k}_|) = E_n(\mathbf{k}_|) F_n(z;\mathbf{k}_|), \quad F_n = (F_{n,1}, \ldots, F_{n,d})^T$$

- conditions for the persistance of a spectral gap, the band gap in semiconductors, at $\mathbf{k}_| = 0$ for $\mathbf{k}_| \neq 0$
- spurious modes (band gap solutions) can appear for $k \cdot p$ Schrödinger operators modeling the mixing between conduction and valence bands

Results

We have proven general properties of the operator familiy $\{\mathsf{H}_{\mathbf{k}_|}\}_{\mathbf{k}_| \in \mathbb{C}^2}$ [1]. In particular, the spectral properties of $\{\mathsf{H}_{\mathbf{k}_|}\}$ depend *analytically* on $\mathbf{k}_|$. The operators H_k are not self-adjoint on $W^{-1,2}$. The restriction $\mathsf{H}_{\mathbf{k}_|}|_{L^2}$ for $\mathbf{k}_| \in \mathbb{R}^2$ is a selfadjoint operator. However, the operators $\mathsf{H}_{\mathbf{k}_|}$ behave in the L^2-context much more irregulary then over $W^{-1,2}$. In particular, the domain of $\mathsf{H}_{\mathbf{k}_|}|_{L^2}$ usually depends on $\mathbf{k}_|$.

In dependence on the data, there is a certain range for $\mathbf{k}_| \neq 0$, where a spectral gap exists [1]. If the interband coupling between the conduction and valence bands remains weak enough, spurious solutions don't appear [1]. We introduced a *regularization* of the problem, such that the eigenvalue curves *cannot* explode in the finite $\mathbf{k}_|$-plane, while asymptotically preserving the spectral properties of $\mathsf{H}_{\mathbf{k}_|}|_{L^2}$.

Discretization

The numerical solution of the eigenvalue problem for the $k \cdot p$ Schrödinger operators requires a suitable finite dimensional approximation of the problem. This can be done by defining the operators in the sense of forms on finite dimensional subspaces of $W^{1,2}([0,L];\mathbb{C}^d)$. We consider a discretization by piecewise linear finite elements, leading to matrix eigenvalue problems:

$$A(\mathbf{k}_|) \cdot f(\mathbf{k}_|) = E(\mathbf{k}_|) B \cdot f(\mathbf{k}_|)$$

with A complex and selfadjoint, B real, symmetric and postive definite.

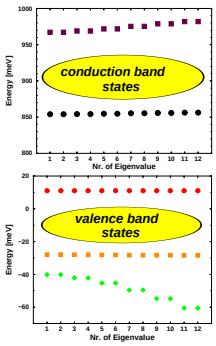
This finite element discretization acts as a regularization of the problem in the sense mentioned above. Thus the eigenvalue curves $E(\mathbf{k}_|)$ of the matrix family $\{A(\mathbf{k}_|)\}$ doesn't explode in the finite $\mathbf{k}_|$-plane. The family $\{A(\mathbf{k}_|)\}$ has asymptotically the same spectral properties as $\mathsf{H}_{\mathbf{k}_|}|_{L^2}$ [1].

Block structure of the matrix A:

$$A = \begin{pmatrix} a_1 & b_1 & & & \\ b_1^+ & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{N-2}^+ & a_{N-1} & b_{N-1} \\ & & & b_{N-1}^+ & a_N \end{pmatrix}$$

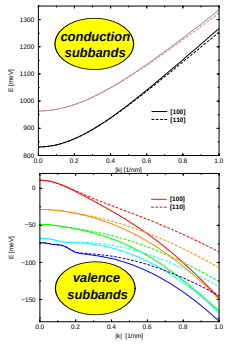
with dense $d \times d$ matrix blocks a_i, b_i: $a_i = a_i^+$, N is the number of grid points.

Eigenvalue distribution



Eigenvalue spectrum for a MQW structure consisting of 6 Quantum Wells. Due to symmetry all eigenvalues are twice degenerate, yielding groups of 12 eigenvalues.

Eigenvalue dispersion

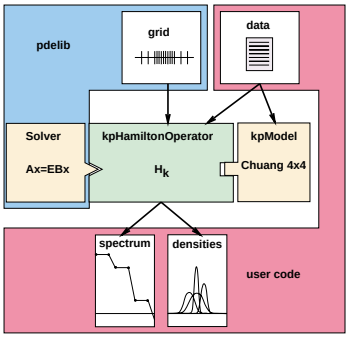


Subband dispersion and warping (angluar dependence) in a strained single Quantum Well for different crystallographic directions in the $\mathbf{k}_|$ plane.

In both examples an 8×8 $k \cdot p$ Schrödinger operator has been used, modeling the *mixing* of valence and conduction bands in InGaAsP Quantum Wells.

Code: KPLIB

KPLIB: **Template Methods** for the numerical handling of $k \cdot p$ Schrödinger operators



$\mathbf{k}\cdot\mathbf{p}$ Models: one single conduction band, four valence bands eight mixed conduction and valence bands

Solver: LAPACK, ARPACK (shift-invert mode)

Based on PDELIB [3].

Questions

- Continuation methods for $E(\mathbf{k}_\|)$ and $f(\mathbf{k}_\|)$?
- Specifically adapted eigenvalue solvers (e.g. point-blockorientied iterative methods)?

References:

[1] U. Bandelow, H.-Chr. Kaiser, Th. Koprucki, J. Rehberg: Spectral properties of $k \cdot p$ Schrödinger operators in one space dimension, to appear in *Numer. Func. Anal. Optim.*, 21 (2000).

[2] U. Bandelow, H.-Chr. Kaiser, Th. Koprucki, J. Rehberg: Modeling and Simulation of Strained Quantum Wells in Semiconductor Lasers, WIAS-Preprint No. 582, Berlin.

[3] http://www.wias-berlin.de/products/pdelib