On Eigenvalue Problems Arising from the Modeling of Semiconductor Nanostructures

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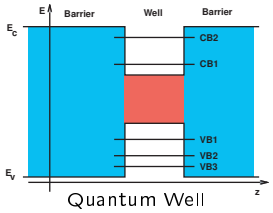

Quantum Well

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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* $\mathbf{k}_\parallel = (k_1, k_2) \in \mathbb{R}^2$.

$k\cdot p$ Schrödinger operators for d states

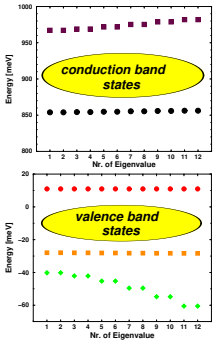
Ordinary differential operator defined on $L^2([0,L];\mathbb{C}^d)$:

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

Piecewise constant $d\times d$ matrix-valued functions $\mathrm{m},\mathrm{e},\mathrm{V},\mathrm{M},\mathrm{U}$:
m,e: real, diagonal, same signature
e: spatial variation of the band edges
V, M,U: complex and selfadjoint

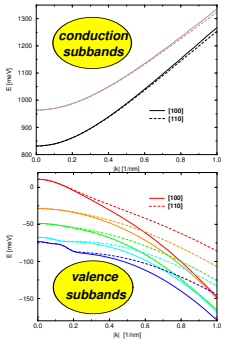
Typically $d = 4, 6, 8, 14$

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 $\mathbf{k}_\parallel$ 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.

Eigenvalue Problem

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

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

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

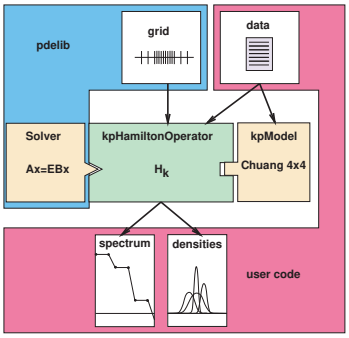
Results

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

In dependence on the data, there is a certain range for $\mathbf{k}_\parallel \neq 0$, 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 $\mathbf{k}_\parallel$-plane, while asymptotically preserving the spectral properties of $\mathrm{H}_{\mathbf{k}_\parallel}|_{L^2}$.

Code: KPLIB

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



k·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].

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:

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

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 $E(\mathbf{k}_\parallel)$ of the matrix family $\{A(\mathbf{k}_\parallel)\}$ doesn't explode in the finite $\mathbf{k}_\parallel$-plane. The family $\{A(\mathbf{k}_\parallel)\}$ has asymptotically the same spectral properties as $\mathrm{H}_{\mathbf{k}_\parallel}|_{L^2}$ [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.

Questions

- Continuation methods for $E(\mathbf{k}_\parallel)$ and $f(\mathbf{k}_\parallel)$?
- 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