Finite Difference Schemes for $\mathbf{k} \cdot \mathbf{p}$ Models: A Comparative Study

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Multi-band $\mathbf{k} \cdot \mathbf{p}$ models discretized with finite difference method (FDM) have been widely used to study electronic properties of semiconductor nanostructures. However, different schemes of FDM exist in the literature, some of them are numerically unstable leading to spurious states [1][2], while others are stable but require special treatment of the boundary conditions and/or the material interfaces [3][4][5][6]. Therefore, a comparison of their numerical behaviors (and implementation tricks) will be very helpful for selecting a suitable scheme and obtaining reliable results. To this end, we have implemented into NEMO5 simulation software [7] the following options, (a) centered difference for symmetrized (SYM) Hamiltonian [1], (b) centered difference for Burt-Foreman (BF) Hamiltonian [8], (c) one-sided differences for SYM Hamiltonian [3], and (d) one-sided differences for BF Hamiltonian [6]. For all cases, eight-band and six-band models for both zincblende and wurtzite type materials are available.

In Fig. 1, we compare the dispersion relations of bulk InAs (operator ordering is irrelevant here) discretized with centered and one-sided differences. Note that Foreman's Ac=0 strategy [8] has been applied. It is clear that centered difference causes the bowing down of the conduction band, implying that when the structure is confined there will be high-k oscillating states polluting the low energy window. The one-sided difference instead approximates the original continuum band structure quite well.

This has been confirmed by plotting the band structure of a GaAs-InAs quantum well with SYM operator ordering (Fig. 2). The centered difference produces spurious bands appearing almost everywhere around the band gap, whereas the one-sided difference is free of any of those unphysical bands. For BF operator ordering, the one-sided difference also gives results free of spurious bands (not shown here). The convergence behaviors of the one-sided differences for both SYM and BF ordering are plotted in Fig. 3. It can be observed that the error decreases with the mesh size and thus they are numerically stable.

The implementation is simple and straightforward for the centered difference case, but a bit complicated for the one-side difference case. For the latter case, in order to avoid artificial spin splitting, interchange of forward and backward schemes is required when one goes from one spin group to the other spin group (Fig. 4). In addition, the imposing of Dirichlet and Neumann boundary conditions is tricky. As illustrated in Fig. 5, to enforce Dirichlet (Neumann) boundaries at the two ends, one needs to eliminate one row and one column corresponding to the spin-down (up) conduction band of the first node, and those corresponding to the spin-up (down) conduction band of the last node.

For BF ordering, further cares are needed in order to preserve the geometric symmetry and eliminate slope anomalies of the wave functions. In particular, averaged band edges should be used at the heterojunction interfaces and the mesh points where they should be placed matter [6]. As a result, the electron wave function is smooth at the material interfaces, but shifted forward (backward) by half a mesh for the first (second) spin group, shown in Fig. 6. As a comparison, the wave functions of the SYM Hamiltonian using one-sided difference [3] are also plotted, it is observed that they are not shifted but there are slope discontinuities around the interfaces.

In summary, centered difference produces spurious solution; one-sided difference gives stable results but it needs proper cares regarding its im-

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plementation and interpretation.

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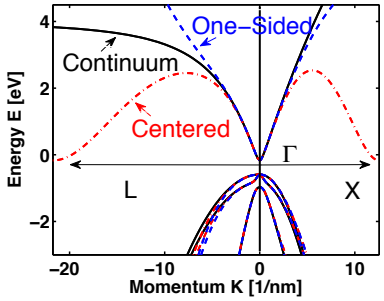

Fig. 1. Eight-band E-k relations of bulk InAs. For discrete E-k relations, $\Delta X = \Delta Y = \Delta Z = 0.25nm$.

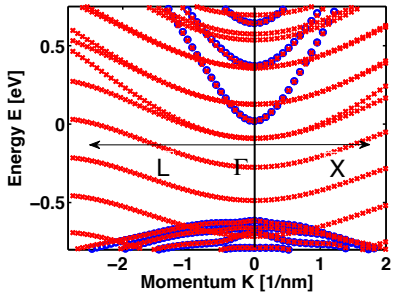

Fig. 2. E-k relations of a GaAs-InAs quantum well. The crosses (circles) are results of centered (one-sided) difference.

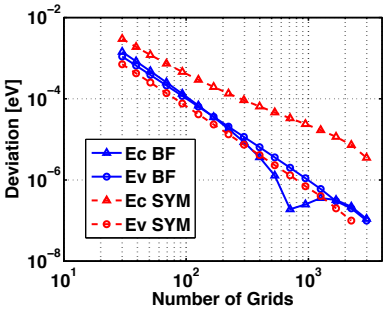

Fig. 3. Deviation of the 1st conduction and valence band energies with respect to number of grids.

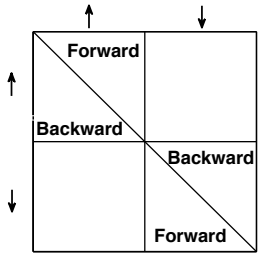

Fig. 4. Interchange of forward and backward schemes for different spin groups of the eight-band model.

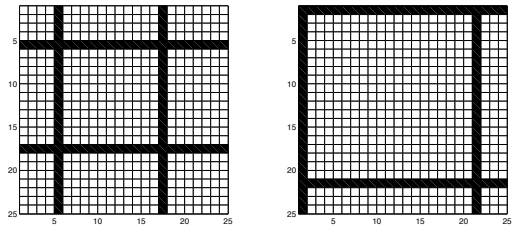

Fig. 5. An example of enforcing Dirichlet (left) and Neumann (right) boundary conditions for a matrix with 3 nodes (the matrix size is thus 24). The discretization scheme for each node is shown in Fig. 4.

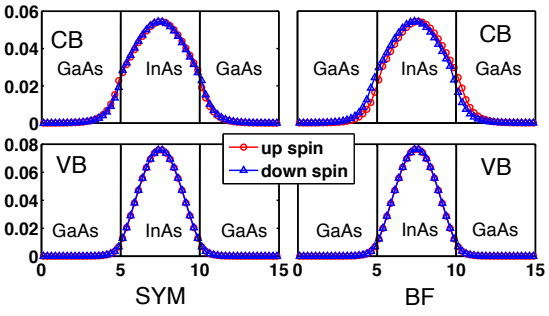

Fig. 6. Wave functions of the lowest (highest) electron (hole) states, using one-sided differences, for both SYM and BF Hamiltonian. The spin up and down states are degenerate.