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Spurious solutions and boundary conditions in $k \cdot p$ theory

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Abstract.
It is well known that the origin of one type of spurious solutions in multiband k·p theory is the failure to restrict the Fourier coefficients of the envelope functions to the first Brillouin zone. Often, the set of differential equations obtained is supplemented with interfacial boundary conditions derived by integrating the differential equations across the interface; however, this leads to a mathematically ill-posed problem as the envelope functions cannot simultaneously fulfill these boundary conditions and the requirement that the Fourier coefficients be restricted to the first Brillouin zone. We show, by way of an example, the origin of these spurious solutions and how to remove them.

Keywords: Exact envelope function theory, $k \cdot p$, spurious solutions, interfacial boundary conditions.
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EXACT ENVELOPE FUNCTION THEORY

The origin of certain spurious solutions can be found in the exact envelope function theory developed by Burt [1]. The starting point for this theory is the one-electron Schrödinger equation:

$$\Big[-\frac{\hbar^2}{2m}\Delta + V\Big]\psi = E\psi, \tag{1}$$

where $\hbar$ is Planck's constant divided by 2π, m is the mass of the electron, Δ is the Laplacian and V is a potential, e.g., the crystal potential. The central step is to make an envelope-function expansion:

$$\psi(\vec{r}) = \sum_n F_n(\vec{r}) U_n(\vec{r}), \tag{2}$$

where the Fourier expansion of F_n is restricted to the first Brillouin zone. We will see that it is the failure to restrict the envelope functions to the first Brillouin zone which is the origin of these spurious solutions. Based on this expansion and using certain approximations, multiband models can derived. In this paper we study the two-band model.

Two-Band Model without Restriction

The differential equations for the two-band model (conduction band + light hole) are given by:

$$\begin{bmatrix} -\frac{\partial}{\partial x}\left(\frac{\hbar^2}{2m_c} - \frac{P^2}{V_c - V_v}\right)\frac{\partial}{\partial x} + V_c & P\frac{\partial}{\partial x} \\ -P\frac{\partial}{\partial x} & -\frac{\partial}{\partial x}\left(\frac{\hbar^2}{2m_{lh}} + \frac{P^2}{V_c - V_v}\right)\frac{\partial}{\partial x} + V_v \end{bmatrix} \begin{pmatrix} F_1(x) \\ F_2(x) \end{pmatrix} = E \begin{pmatrix} F_1(x) \\ F_2(x) \end{pmatrix}, \tag{3}$$

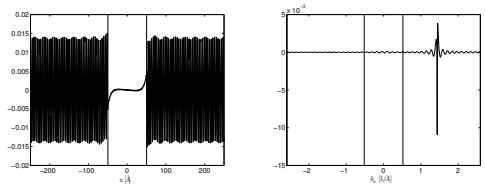

FIGURE 1. Left, conduction-band envelope function. Right, Fourier coefficients of the conduction-band envelope function.

where m_c (m_{lh}) is the conduction-band (light-hole) effective mass, V_c (V_v) is the conduction-band (valence-band) edge (all are step functions), $P = \sqrt{\hbar^2 E_p/(2m)}$, E_p is the Kane energy, and m is the free-electron mass.

We have solved this set of PDE's for an InAs/GaAs quantum-well system (material parameters are taken from Vurgaftman et al. [3]) without taking into account that the envelope functions should be restriced to the first Brillouin zone. We find that there are non-physical solutions (spurious solutions), e.g., the solution shown in Fig. 1 which has an energy located in the bandgap ($E = -0.259\,\mathrm{eV}$).

We see that this solution has considerable contributions outside the first Brillouin zone (inside black lines) and a similar behaviour is observed for all the other spurious solutions.

Two-Band Model with Restriction

The way to eliminate spurious solutions is to work in Fourier space and there to restrict the solution to the first

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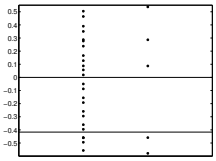

FIGURE 2. Left, the spectrum resulting from solving the differential equations. Right, the spectrum when the solutions are restricted to the first Brillouin zone.

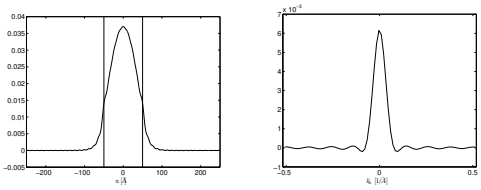

FIGURE 3. Left, the conduction-band envelope function (F_1). Right, the Fourier coefficients in the first Brillouin zone.

Brillouin zone, i.e., the so called cut-off method [2]. This is clearly seen from the two spectra shown in Fig. 2.

We see that all solutions located in the bandgap are removed by restricting the envelope functions to the first Brillouin zone and by inspection it is found that the solutions left are well-behaved in the sense that they are slowly varying (the central assumption in $k \cdot p$ theory). For example, the conduction-band ground state is shown in Fig. 3.

This clearly demonstrates that we can remove the spurious solutions by restricting the envelope functions to the first Brillouin zone.

INTERFACIAL BOUNDARY CONDITIONS

As many have pointed out, it appears to be inconsistent to use stepwise constant material parameters and at the same time restrict the envelope functions to the first Brillouin zone. This is seen from the fact that the envelope functions need out-of-zone contributions in order to satisfy boundary conditions at interfaces (found by integrating across the interface). One way to resolve this problem is to derive a reduced set of interfacial boundary conditions, see e.g., Rodina et al. [4]. It is important to note that spurious solutions are not removed by choosing appropriate boundary conditions, they are removed by restricting the envelope functions to the first Brillouin zone (see section the next section).

We would like to point out that it is the approximation that the material parameters are constant in each material which creates the apparent inconsistency and that by working in Fourier space there is no inconsistency as interfacial boundary conditions are not needed in this case because of the restriction to the first Brillouin zone.

Two-Band Model with Smooth Step Functions

To highlight that choosing the "right" interfacial boundary conditions do not remove the spurious solutions, we present results based on the two-band model where instead of using abrupt step functions we use the smooth step function given by:

$$S(x) = \frac{\tanh(a(x+b))\tanh(a(-x+b))+1}{2}, \quad (4)$$

where a controls how abrupt the step function is and b is the position of the interface (symmetric around 0). Solving the two-band model using $a = 2.5$ nm^{-1} and $b = 5$ nm we find that the ground state is well captured, however, we still find spurious solutions including states in the energy gap.

This clearly demonstrates that it is not the interfacial boundary conditions which creates the spurious solutions as interfacial boundary conditions are superfluous in this case as all material parameters are everywhere continuous.

CONCLUSION

We have shown the origin of one type of spurious solutions and how to remove them using the cut-off method. In addition, we have pointed out that it is the approximation of stepwise constant material parameters which is the origin of the ill-posedness in connection with boundary conditions and shown that choosing the "right" boundary conditions do not remove the spurious solutions.

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