A stable discretization method for "Dirac-like" effective Hamiltonians

Z. Stanojević, O. Baumgartner, H. Kosina
Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, 1040 Vienna, Austria
stanojevic@iue.tuwien.ac.at

In the context of quantum cascade (QC) structure design the analysis of (quasi-)bound states and their corresponding energies is an important tool. The analysis is done by numerically solving the Schrödinger equation based on an effective $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. The common materials used for QC structures in infra-red applications (AlGaAs, InGaSb, ...) can be described by an eight band Hamiltonian, which for layered structures reduces to three bands for $k_{\|} \approx 0$ approximation. The three bands can further be approximated by two bands, if one is interested in the conduction band only[1].

The problem with this kind of Hamiltonian is that it contains terms only up to first order in momentum, p_z. A discretization scheme based on central differences fails to give any results for this coupled first-order problem. A one-sided differencing scheme was already proposed by Stier et al.[2]. The method is numerically stable and preserves the Hermiticity of the Hamiltonian, but requires a fine spatial grid and can give significant deviations at domain boundaries and interfaces where material properties change abruptly.

It can be shown that the Schrödinger equation containing the effective Hamiltonian is structurally similar to the Dirac equation known from relativistic quantum mechanics. This similarity is also responsible for peculiarities found in the wavefunctions (cusps at heterointerfaces, non-zero values at boundaries)[3]. The Dirac equation is the "square root" of the Klein-Gordon equation, which is of second order. Our approach exploits this property and uses a similarity transform on the Hamiltonian. The similarity transform ensures that the Hamiltonian's spectrum (i.e. its eigenvalues) is preserved. It converts the first-order terms to zeroth and second order, thereby eliminating the stability problem. This comes at the cost of losing the Hermiticity of the Hamiltonian, which somewhat limits the choice of the eigenvalue solver but poses no further problem. In fact, the approximate eigenstates of the untransformed Hamiltonian can be extracted from the ones computed for the transformed one in a post-processing step.

$$H = \begin{pmatrix} E_\mathrm{c}(z) & \frac{p_{cv}p_z}{m_e} \\ -\frac{p_{cv}p_z}{m_e} & E_\mathrm{v}(z) \end{pmatrix} \mapsto \begin{pmatrix} E_\mathrm{c}(z) & \frac{p_{cv}p_z}{m_e}\sigma_z \\ \frac{p_{cv}p_z}{m_e}\sigma_z & E_\mathrm{v}(z) \end{pmatrix} \mapsto \begin{pmatrix} E_\mathrm{c}(z) & \frac{p_{cv}^2}{m_e} \\ \frac{p_z^2}{m_e} & E_\mathrm{v}(z) \end{pmatrix}$$

The usability of this method extends beyond the two-band Hamiltonian by Sirtori et al. The same $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian structure can be also found in narrow-gap materials such as lead-salts[4] and graphene[5]. Numerical results for example QC structures will be discussed.

[1] C. Sirtori *et al.*, Phys. Rev. B **50**, 8663 (1994).

[2] O. Stier *et al.*, Phys. Rev. B **55**, 7726 (1997).

[3] V. Alonso *et al.*, European Journal of Physics **18**, 315 (1997).

[4] M. Kriechbaum *et al.*, Phys. Rev. B **30**, 3394 (1984).

[5] P. Marconcini *et al.*, ArXiv e-prints (2011).