Variational Formulation of Stable Discrete $\mathbf{k}\cdot\mathbf{p}$ Models

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The longstanding problem of spurious states in $\mathbf{k}\cdot\mathbf{p}$ models of semiconductor nanostructures has been shown to be an artifact of the use of the centered-difference approximation to the gradient, and it has been shown that stable models may be constructed on the basis of lower-order one-sided differences [1]–[4]:

$$\left(\hat{K}_L f\right)_n = \left(\hat{K}_R^\dagger f\right)_n = (-i/\Delta)\left(f_n - f_{n-1}\right). \quad (1)$$

Key results are illustrated in Figs. 1–3. These demonstrate that the conventional approach of deriving the formulation in the continuum and then invoking approximation theory to obtain the discrete model is seriously flawed. The flaws should be obvious: the bandstructures produced by the $\mathbf{k}\cdot\mathbf{p}$ approximation can never be periodic functions, and their results are therefore nonphysical at short distances. Approximation theory then emphasizes fidelity to these nonphysical results by focusing on short-distance behavior. Every discrete formulation will yield a periodic bandstructure; thus discrete models may be approximations, but they can be far more credible descriptions of the physical systems than continuum $\mathbf{k}\cdot\mathbf{p}$ approximations.

Variational Formulation

To avoid approximation theory we invoke a more fundamental formulation and separately derive the continuum and discrete models from it. A $\mathbf{k}\cdot\mathbf{p}$ model of the form:

$$\hat{H}_{\alpha\beta} = \gamma_{\alpha\beta}k_z^2 + P_{\alpha\beta}k_z + V_{\alpha\beta}, \quad (2)$$

can be derived by minimizing the action:

$$S = \int dz\, \left[\gamma_{\alpha\beta}\partial_z\psi_\alpha^*\partial_z\psi_\beta + P_{\alpha\beta}\psi_\alpha^*\partial_z\psi_\beta + V_{\alpha\beta}\psi_\alpha^*\psi_\beta - E\psi_\alpha^*\psi_\beta\right]. \quad (3)$$

To derive the discrete Schrödinger equation, we must make explicit assumptions about how the wavefunction and material parameters vary within each mesh interval, as illustrated in Fig. 4. The best choice is to assume that the $\psi_\beta(z)$ vary linearly within a mesh interval. The action (3) then becomes a sum over mesh intervals of bilinear expressions in the discrete wavefunctions $\psi_{\alpha;j}^*$ and $\psi_{\beta;j}$. For this discrete formulation, the functional derivative reduces to the set of all derivatives $\partial S/\partial\psi_{\alpha;j}^*$, and each derivative yields a row of the discrete Schrödinger equation.

The γ terms produce variations on the three-point difference formula for the Laplacian that are well known in the study of single-band effective-mass models [5]. The P terms require special attention. Straightforward evaluations of the action produce centered-difference discretizations, which result in spurious states. We must therefore impose a form which produces a one-sided difference, such as:

$$iP_{\alpha\beta}\left[\psi_{\alpha;j}^*\left(\psi_{\beta;j} - \psi_{\beta;j+1}\right) - \psi_{\beta;j}\left(\psi_{\alpha;j}^* - \psi_{\alpha;j+1}^*\right)\right]. \quad (4)$$

The variational treatment of the V terms produces an unexpectedly rich structure, and leads to the elimination of a major cause of slope anomalies [2] in the resulting wavefunctions. Let $B_{\alpha;j}$ be the energy of band α for the material associated with meshpoint j. Then we normally assume $V_{\alpha\alpha;jj} = B_{\alpha;j}$. A calculation using this assumption is shown in Fig. 5, and shows a slope anomaly. But, if we take the model of Fig. 4(a) that associates a material with a mesh interval $j + 1/2$, the crudest approximation to the functional (ψ piecewise constant) gives $V_{\alpha\alpha;jj} = (B_{\alpha;j-1/2} + B_{\alpha;j+1/2})/2$. Fig. 6 uses this form. Ma *et al.* [3] found this remedy, but could only attribute it to a grading of the heterojunction. We see that it is a natural consequence of modeling an abrupt heterojunction within the detailed description demanded by the variational formulation. Evaluating the functional under the assumption of piecewise-linear ψ_α^* and ψ_β yields a weakly nonlocal V matrix, with small super- and sub-diagonal terms. The implications of this form are still being explored.

In summary, the variational approach provides a systematic procedure for deriving discrete envelope-function models. Abstract discussions of operator ordering and symmetrization are replaced by concrete considerations of how the wavefunctions and material parameters vary between meshpoints.

References

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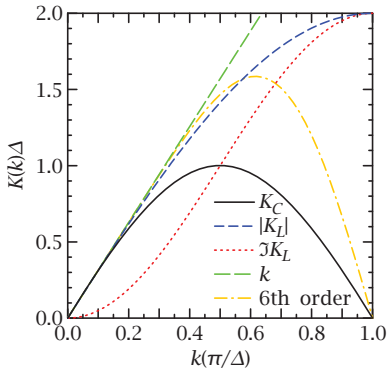

Fig. 1. Dispersion relations for the different $\hat{K}$ operators.

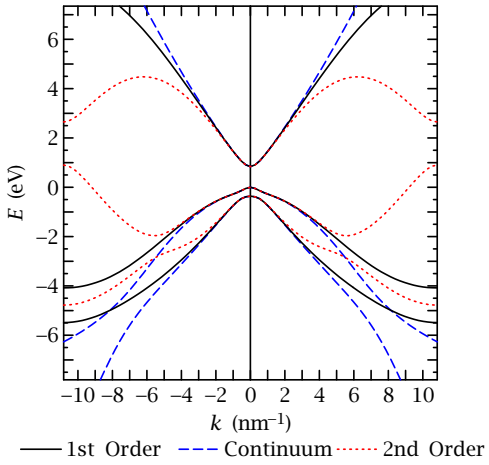

Fig. 2. Band structure resulting from the first-order and centered-difference models, compared to the continuum solution. The Hamiltonian is the 3-band model employed by Cartoixà applied to $In_{0.53}Ga_{0.47}As$ with a mesh spacing of 0.29 nm which equals $a/2$.

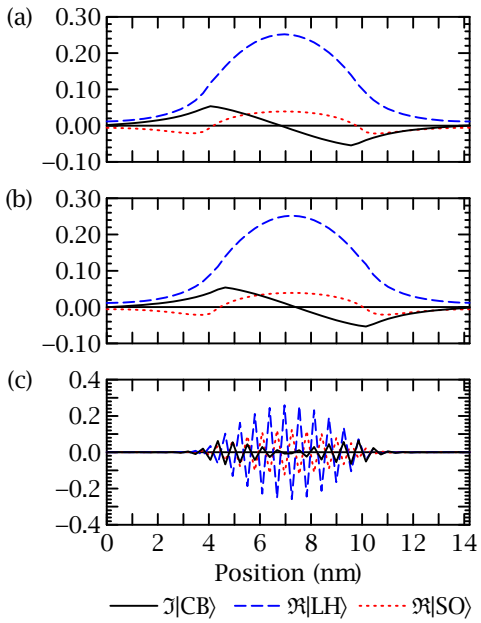

Fig. 3. The state which should be the highest-energy hole state of a model superlattice. The discrete formulations are: (a) left-hand, (b) right-hand and (c) centered difference. Case (c) is clearly spurious.

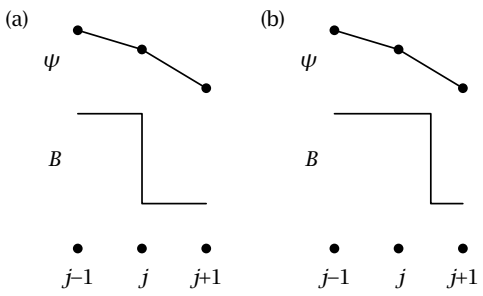

Fig. 4. Assumed details of a discrete model within a mesh interval. B represents a band-edge energy. Heterojunctions are taken to be either coincident with a mesh point (a), or centered within an interval (b).

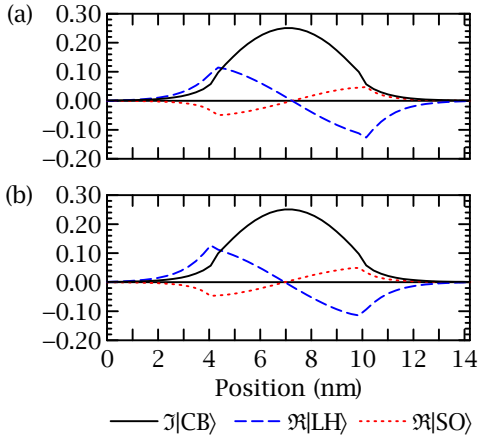

Fig. 5. Lowest-energy conduction band state of an InAs-AlSb structure showing slope anomaly due to simplistic treatment of V terms. (a) left-hand difference, (b) right-hand difference.

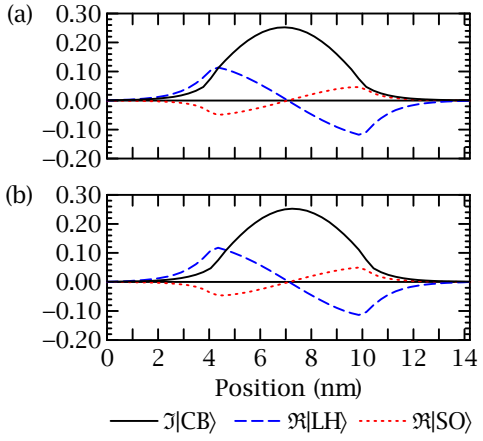

Fig. 6. Calculation of Fig. 5 but using material-averaged V terms.