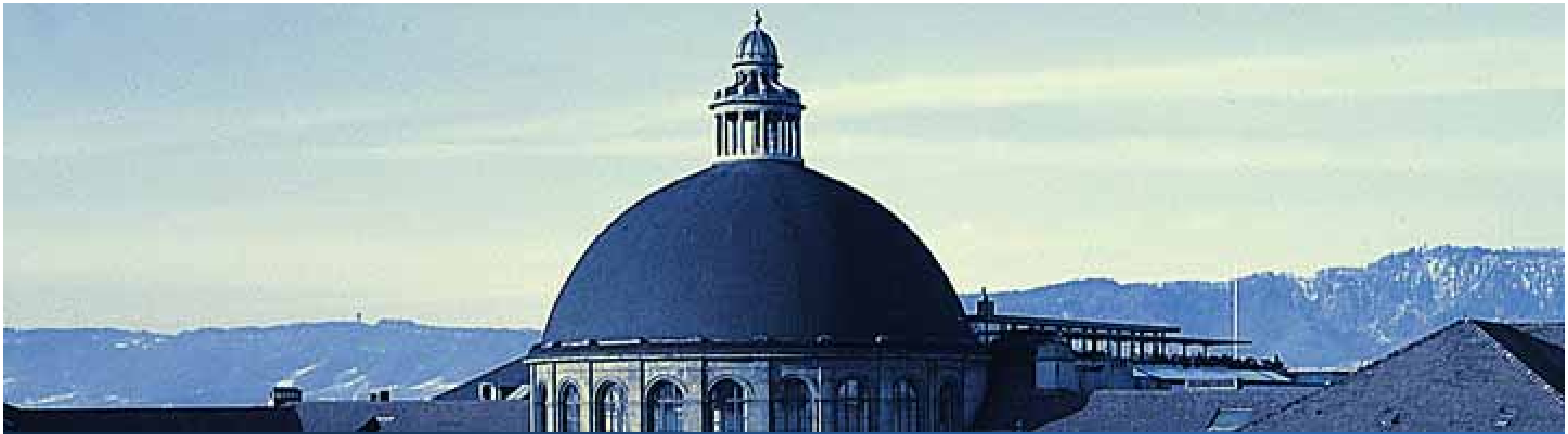
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Ellipticity and Spurious Solutions in k·p Calculations of III-Nitride Nanostructures

Ratko G. Veprek, Sebastian Steiger, Bernd Witzigmann

Computational Optoelectronics Group

Integrated Systems Laboratory, ETH Zurich



Sept 4th, 2008

Outline

- Introduction to **k·p** envelope function method
- Operator ordering
- Effect of operator ordering / spurious solutions in III-Nitrides
- Ellipticity analysis of Wurtzite **k·p** Hamiltonian
- Conclusions and Outlook

Introduction I:
k·p Envelope Function Method I

k·p in Heterostructure

- Bloch function

$$\Psi(\mathbf{x}) = \sum_n u_{n0}(\mathbf{x}, z) e^{i\mathbf{k}\cdot\mathbf{x}} f_n(z)$$

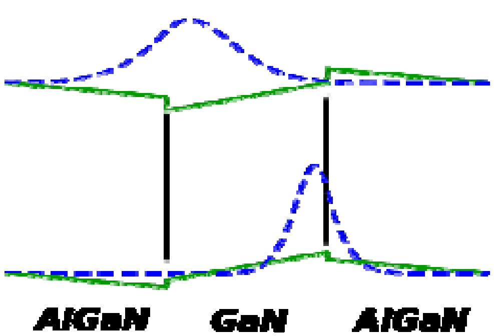
- Equation for $f_n(z)$: $k_i \rightarrow -i\hbar\partial_i$

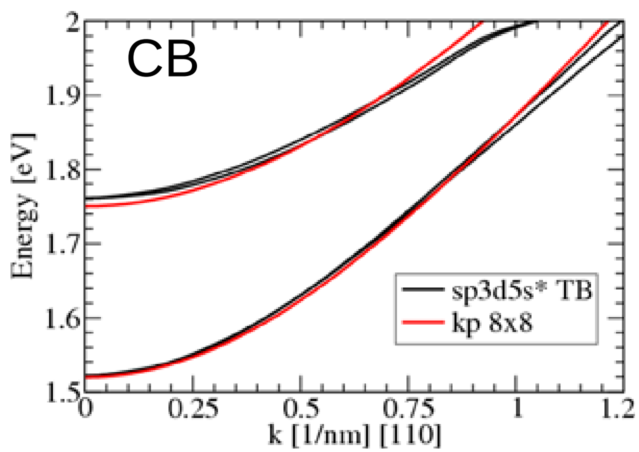
$$-\mathbf{H}_{ij}^{(2)} k_i k_j + \mathbf{H}_i^{(1)} k_i + \mathbf{H}^{(0)}$$

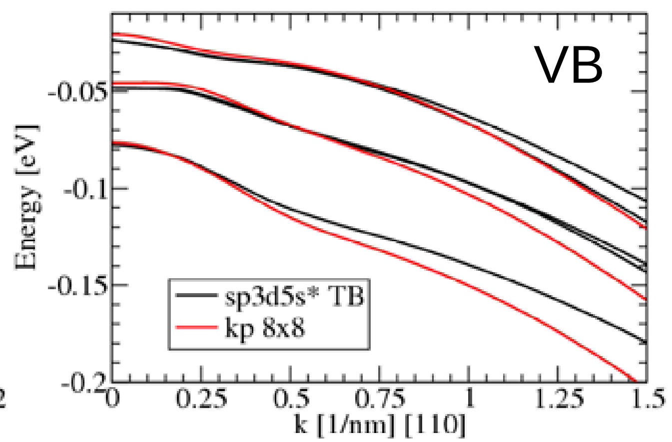
k·p 8x8 compared to Empirical Tight Binding Method

- cb / vb bandstructure 5 nm GaAs / $Al_{0.3}Ga_{0.7}As$ quantum well [1]

[1] Veprek, Steiger, Witzigmann, Proc. IWCE 12 (2007)



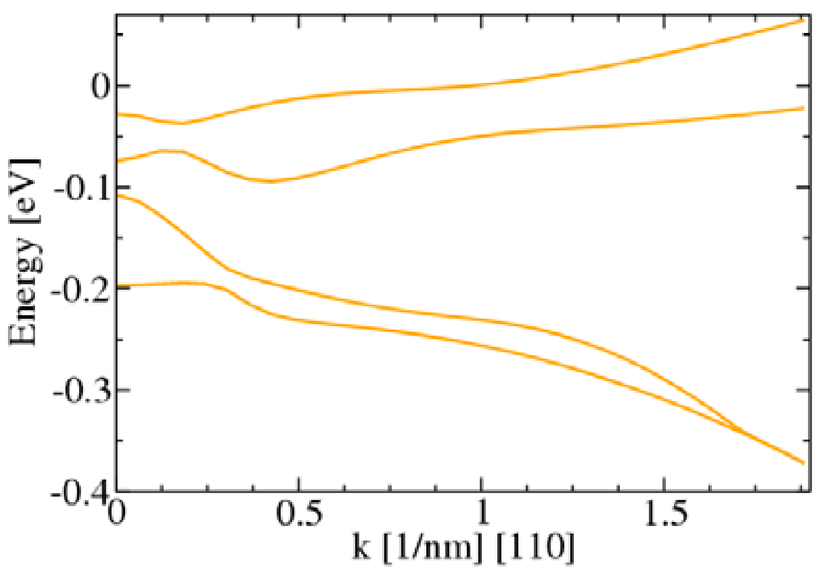




Introduction I:
k·p Envelope Function Method II

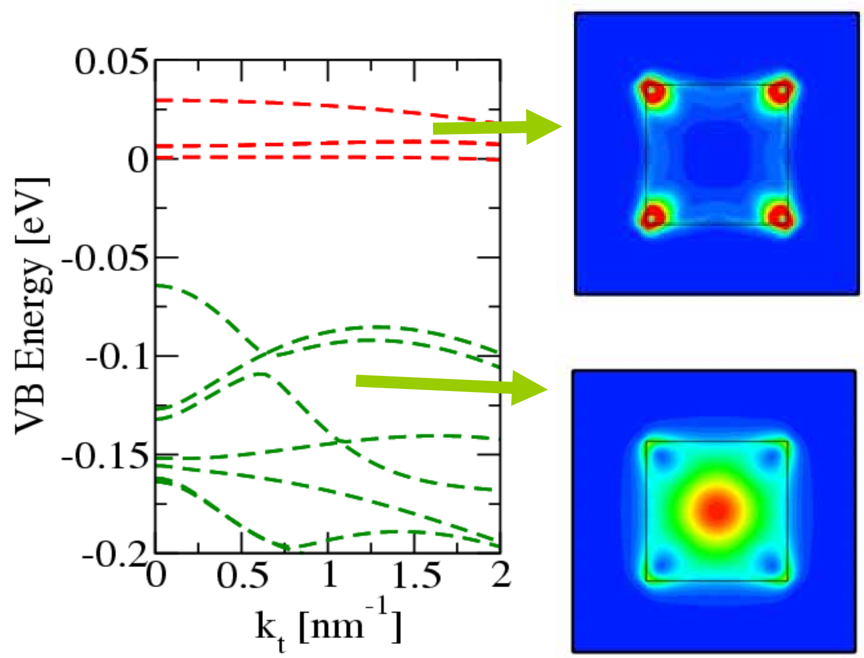
Spurious Solutions

Bandstructure of 5 nm InAs / GaAs quantum well, **k·p** 4x4



Spurious Solutions

Bandstructure of $GaN/Al_{0.7}Ga_{0.3}N$ quantum wire



Introduction II:
Burt-Foreman Operator Ordering I

Second Order Terms

- Hermitian equation:

$$-\mathbf{H}_{ii}^{(2)} k_i^2 \rightarrow \partial_i \mathbf{H}_{ii}^{(2)} \partial_i$$

- Distribution in cross-terms:

$$-\mathbf{H}_{ij}^{(2)} k_i k_j \rightarrow \partial_i \mathbf{H}_{ij}^{+} \partial_j + \partial_j \mathbf{H}_{ji}^{-} \partial_i$$

- Usual approach: symmetrize

$$\mathbf{H}_{ij}^{+} = \mathbf{H}_{ji}^{-} = \frac{1}{2} \mathbf{H}_{ij}^{(2)}$$

Derived Ordering

- Burt-Foreman [2,3]: Derived EFT and operator ordering
- Distribution is not necessarily symmetric
- Important at interfaces
- Terms caused by perturbative treatment of remote bands

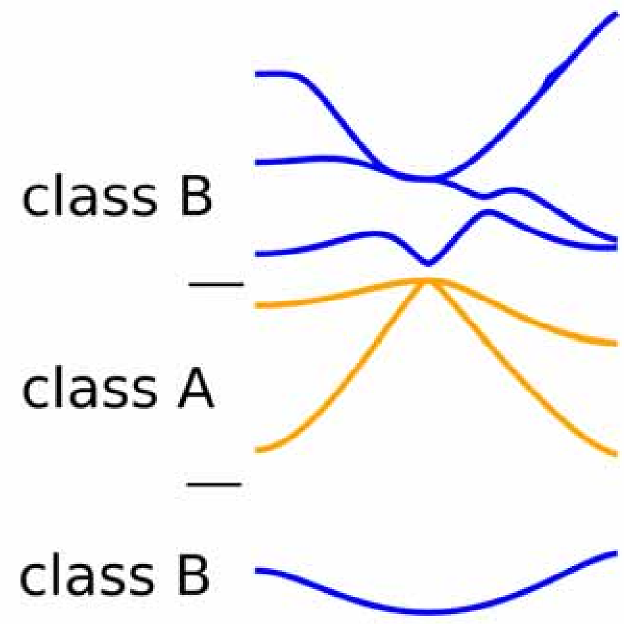
[2]: M.G. Burt, J. Phys: Condens. Matter 4 (1992)
[3]: B.A. Foreman, Phys. Rev. B 54 (1997)

Introduction II:
Burt-Foreman Operator Ordering II

Löwdin - Perturbation

- Restrict calculation to small set of bands (class A)
- Treat remaining bands (class B) using perturbation theory.
- Notation of Stavrinou [4]:

$$\frac{\hbar^2}{m_0^2} \sum_{\alpha,\beta=x,y,z} \hat{k}_\alpha \left(\sum_\nu \frac{\langle j|\hat{p}_\alpha|\nu\rangle\langle\nu|\hat{p}_\beta|j'\rangle}{E - E_\nu} \right) \hat{k}_\beta$$



(example: GaAs **k·p** 6x6)

[4]: P.N. Stavrinou et al., Phys. Rev. B 55 (1997)

Operator Ordering in III-Nitride Systems

k·p 6x6 Hamiltonian for Wurtzite

- Introduces splitting in A_5, A_6
  $A_i = A_i^+ + A_i^-$
- Virtual terms on diagonal
- Reduces to standard Hamiltonian for bulk crystals

$$\begin{pmatrix} F+\varrho & \kappa^* & \xi & 0 & 0 & 0 \\ \kappa & G-\varrho & -\xi^* & 0 & 0 & \Delta \\ \eta^* & -\eta & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F-\varrho & \kappa & -\xi^* \\ 0 & 0 & \Delta & \kappa^* & G+\varrho & \xi \\ 0 & \Delta & 0 & -\eta & \eta^* & \lambda \end{pmatrix}$$

$$F = \Delta_1 + \Delta_2 + \lambda + \theta \qquad G = \Delta_1 - \Delta_2 + \lambda + \theta$$
$$\lambda = \hat{k}_z A_1 \hat{k}_z + \hat{k}_x A_2 \hat{k}_x + \hat{k}_y A_2 \hat{k}_y \qquad \theta = \hat{k}_z A_3 \hat{k}_z + \hat{k}_x A_4 \hat{k}_x + \hat{k}_y A_4 \hat{k}_y$$
$$\kappa = -\hat{k}_x A_5 \hat{k}_x + \hat{k}_y A_5 \hat{k}_y + i(\hat{k}_x A_5 \hat{k}_y + \hat{k}_y A_5 \hat{k}_x) \qquad (4)$$
$$\eta = -\hat{k}_z A_6^+ (\hat{k}_x + i\hat{k}_y) - (\hat{k}_x + i\hat{k}_y) A_6^- \hat{k}_z \qquad \xi = -\hat{k}_z A_6^- (\hat{k}_x + i\hat{k}_y) - (\hat{k}_x + i\hat{k}_y) A_6^+ \hat{k}_z$$
$$\varrho = i\hat{k}_y (A_5^+ - A_5^-) \hat{k}_x - i\hat{k}_x (A_5^+ - A_5^-) \hat{k}_y \qquad \Delta = \sqrt{2}\Delta_3 .$$

Effects of Operator Ordering: Quantum Well

tdkp: a **k·p** Solver

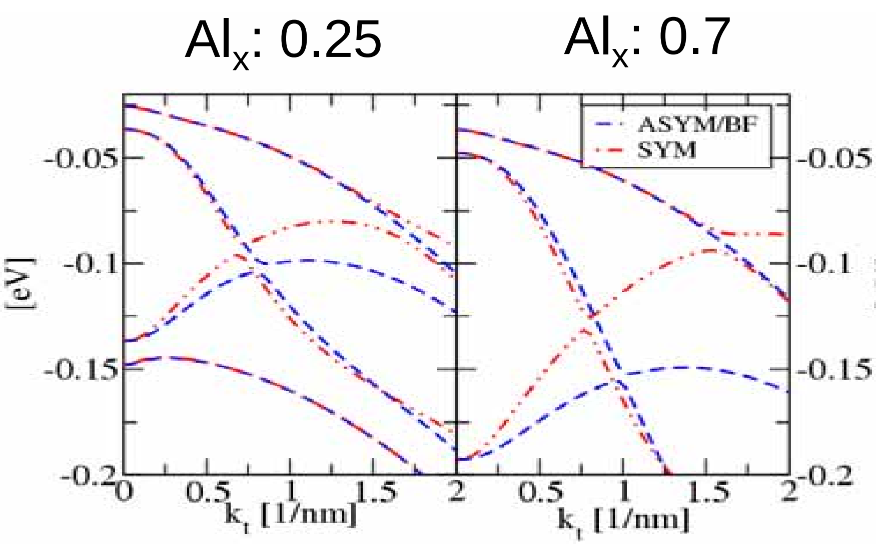
- Examples solved using *tdkp*
- *tdkp* solves envelope equations for wells, wires and dots (incl. strain and piezo-electric effects) using finite elements.

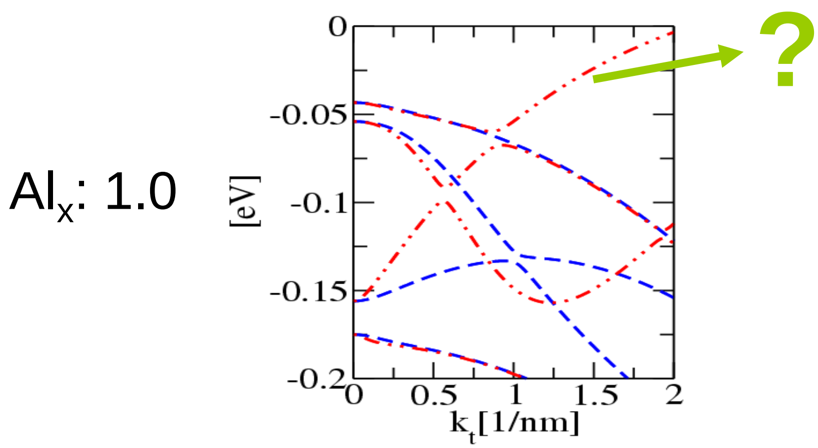
Bandstructure of GaN-$Al_xGa_{1-x}N$ Quantum Well

- Both operator orderings used:

SYMMETRIC

BURT-FOREMAN (ASYMMETRIC)

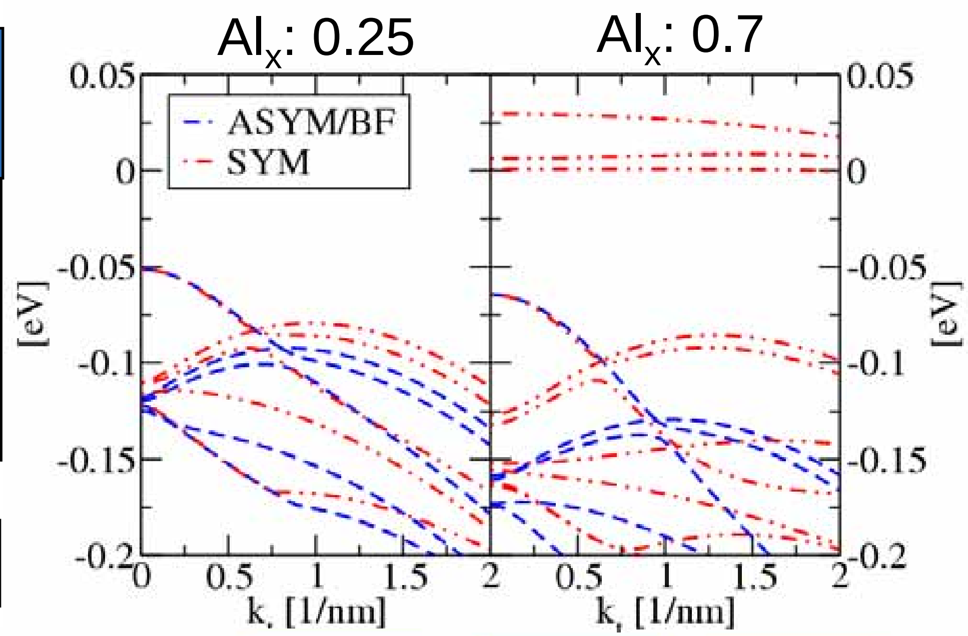




Effect of Operator Ordering: Quantum Wire

Bandstructure of GaN-AlGaN Quantum Wire

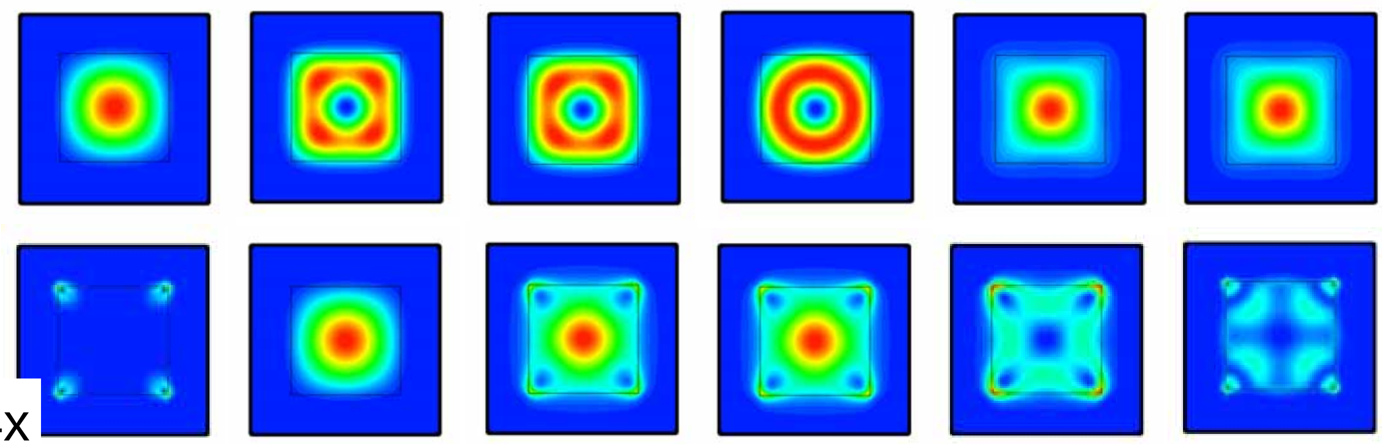
- Model square quantum wire
- Same setup as well
- VB edge is at 0.0156 eV!



Probability density at k = 0, x = 0.7

BURT-FOREMAN

SYMMETRIC



4x

Ellipticity Analysis I: Motivation

Equation Types

- Parabolic

  $$\left(\partial_t + \nabla^2\right) u(\mathbf{x}, t)$$

  (Heat equation)
- Hyperbolic

  $$\left(-\partial_t^2 + \nabla^2\right) u(\mathbf{x}, t)$$

  (Wave equation)
- Elliptic

  $$\nabla^2 u(\mathbf{x})$$

  (Time indep. Schroedinger)

General Expression

- General expression for scalar 2nd order partial differential eq.:

$$\left(\nabla \cdot \mathbf{K}(\mathbf{x})\nabla + \mathbf{b}(\mathbf{x}) \cdot \nabla + c(\mathbf{x})\right) u(\mathbf{x})$$

- Elliptic if matrix $\mathbf{K}(\mathbf{x})$ is definite.
- If non-elliptic: **not a boundary value problem!**

  → **Improperly posed.**

(see: D.Braess, Finite Elemente, Springer-Verlag Berlin Heidelberg 1992/1997)

Ellipticity Analysis II: Coefficient Matrix of III-Nitrides

III-Nitride Coefficient Matrix

$$\begin{pmatrix}
A_2+A_4 & -A_5 & 0 & i(A_5^- - A_5^+) & -i(A_5^- + A_5^+) & 0 & 0 & 0 & -A_6^+ \\
-A_5 & A_2+A_4 & 0 & i(A_5^- + A_5^+) & -i(A_5^- - A_5^+) & 0 & 0 & 0 & A_6^+ \\
0 & 0 & A_2 & 0 & 0 & 0 & -A_6^- & A_6^- & 0 \\
-i(A_5^- - A_5^+) & -i(A_5^- + A_5^+) & 0 & A_2+A_4 & A_5 & 0 & 0 & 0 & -iA_6^+ \\
i(A_5^- + A_5^+) & i(A_5^- - A_5^+) & 0 & A_5 & A_2+A_4 & 0 & 0 & 0 & -iA_6^+ \\
0 & 0 & 0 & 0 & 0 & A_2 & iA_6^- & iA_6^- & 0 \\
0 & 0 & -A_6^- & 0 & 0 & -iA_6^- & A_1+A_3 & 0 & 0 \\
0 & 0 & A_6^- & 0 & 0 & -iA_6^- & 0 & A_1+A_3 & 0 \\
-A_6^+ & A_6^+ & 0 & iA_6^+ & iA_6^+ & 0 & 0 & 0 & A_1
\end{pmatrix}$$

Non-Ellipticity Ratio ρ

- Estimate needed to visualize non-ellipticity
- Estimate defined by

  ratio of positive to negative eigenvalues.
- Equation is elliptic for $\rho = 0$

$$\rho = \left| \frac{\sum_{i,\lambda_i>0} \lambda_i}{\sum_{j,\lambda_j<0} \lambda_j} \right|$$

λ_i = eigenvalue of $\mathbf{K}(\mathbf{x})$

Ellipticity Analysis III: Material Parameter Dependence I

Vurgaftman 2003 Parameter

- Distribution in A_5, A_6

$$A_i^- = A_i - A_i^+$$

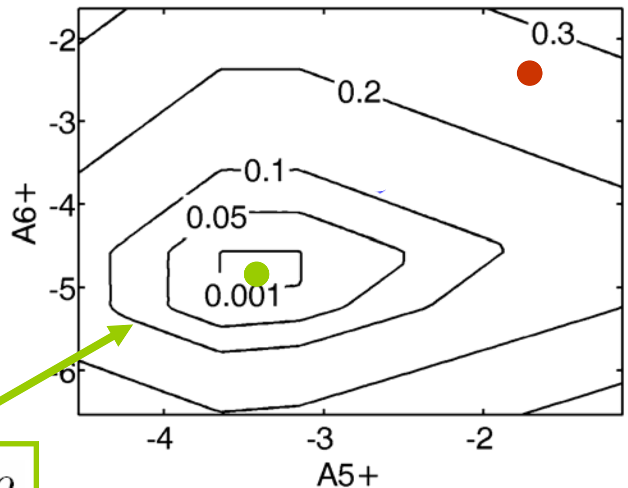
- Green Point: Asymmetric/BF

$$A_i^+ = A_i, \quad A_i^- = 0$$

- Red Point: Symmetric

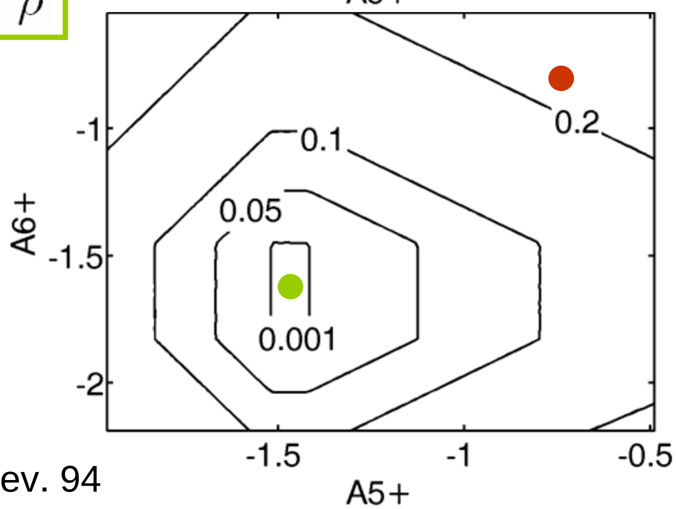
$$A_i^+ = A_i^- = \frac{1}{2} A_i$$

GaN:



Iso-lines for ρ

AlN:



•

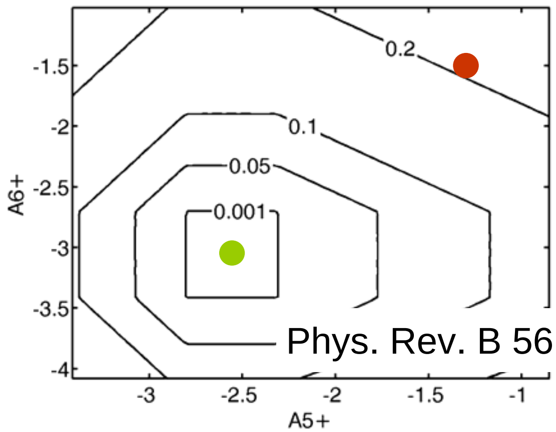
Vurg.2003: Appl. Phys. Rev. 94

Ellipticity Analysis III: Material Parameter Dependence II

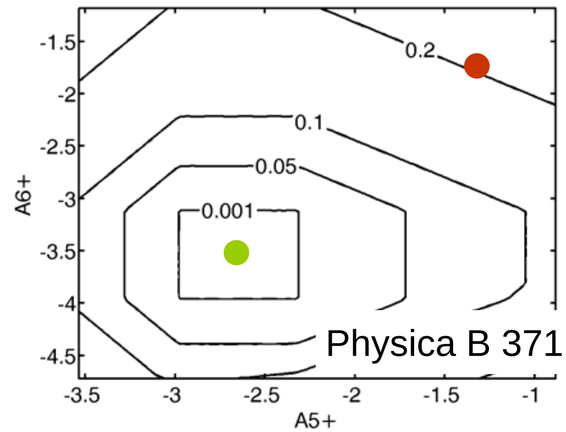
Other Parameter sets:

Asymmetric splitting is elliptic for various parameter sets found in the literature

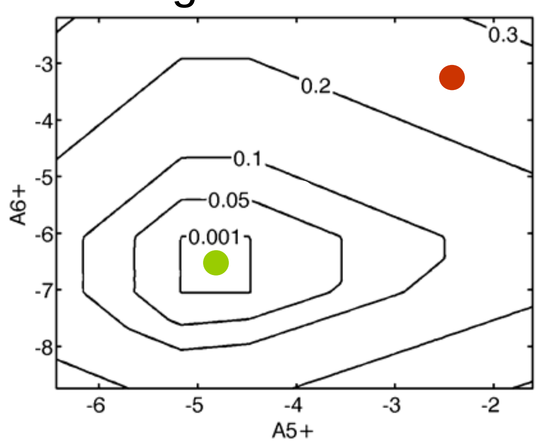
Kim et al. GaN



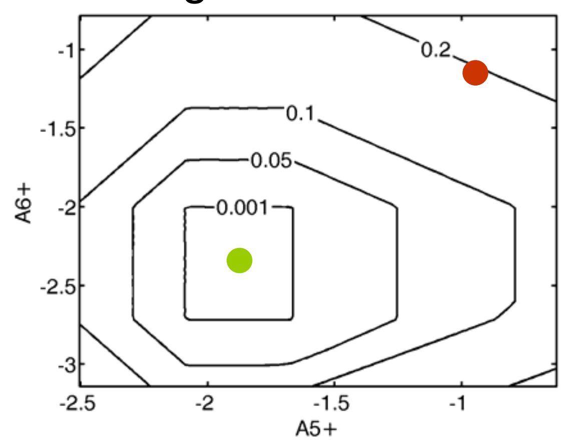
Rezeai et al. GaN



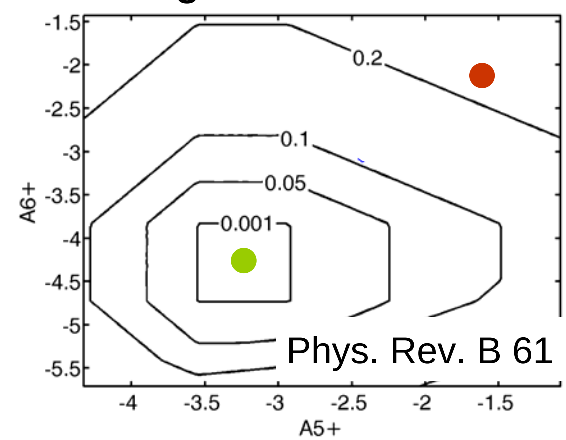
Dugdale et al. InN



Dugdale et al. AlN



Dugdale et al. GaN



Conclusions and Outlook

- Ellipticity basic criterion for equation stability
- Elliptic equations are stable: We have never obtained spurious solutions if equation is elliptic.
- Applies to Zinc-blende* and Wurtzite
- Wurtzite: Complete asymmetric splitting required by all available parameter sets; Mathematical criterion
- Agreement with first principle parameter determination?

*Zinc-blende ellipticity: R.G. Veprek, S. Steiger, B. Witzigmann, Phys. Rev. B 76, 165320 (2007)