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2nd International Conference and Exhibition on
Lasers, Optics & Photonics
September 08-10, 2014 Philadelphia, USA

A meshless k·p method for analyzing electronic structures of quantum dots

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Introduction

Formulation of FT-based k·p method

Control of computation error

Case study: strain effect

Optical gain calculation

Control of Spurious solutions

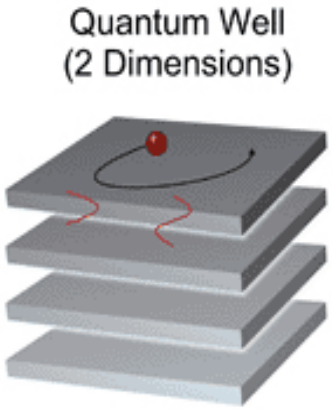
Summary

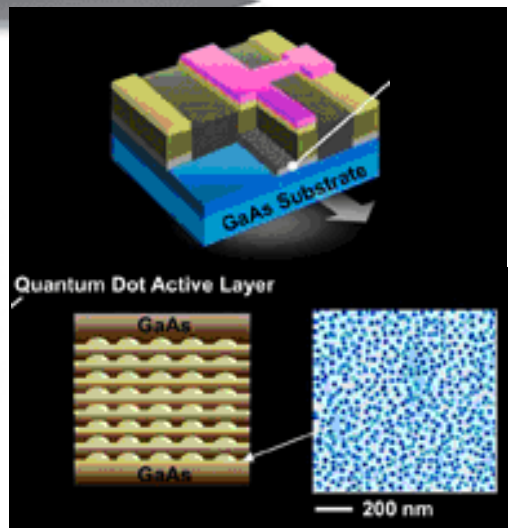
"Lasers Gone Dotty"

QW Laser

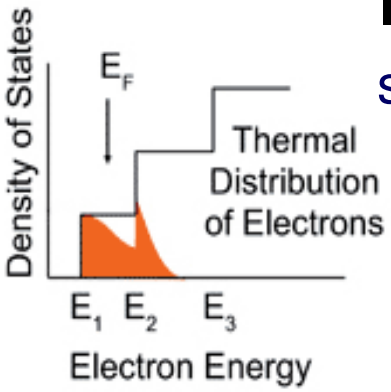
Evolution

QD laser

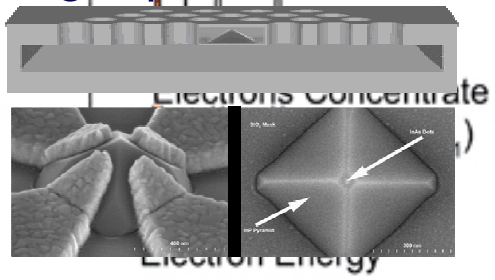




QW LED



single-photon source



It is crucial to understand electronic structures and optical properties

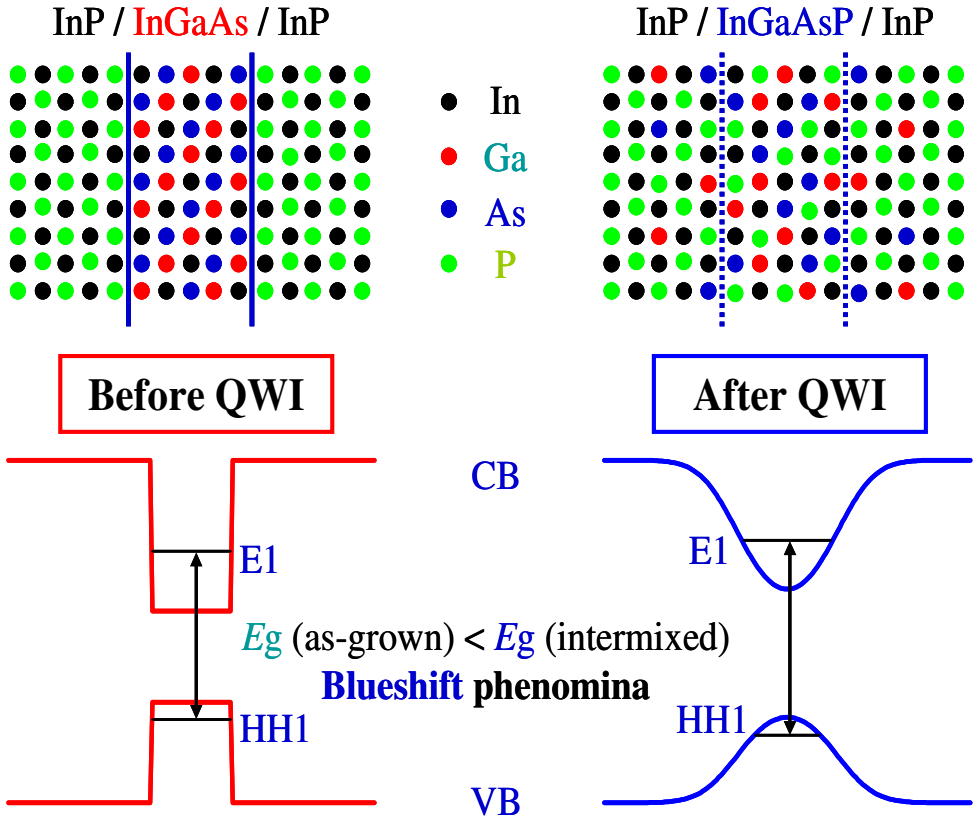
- relatively temperature-insensitive

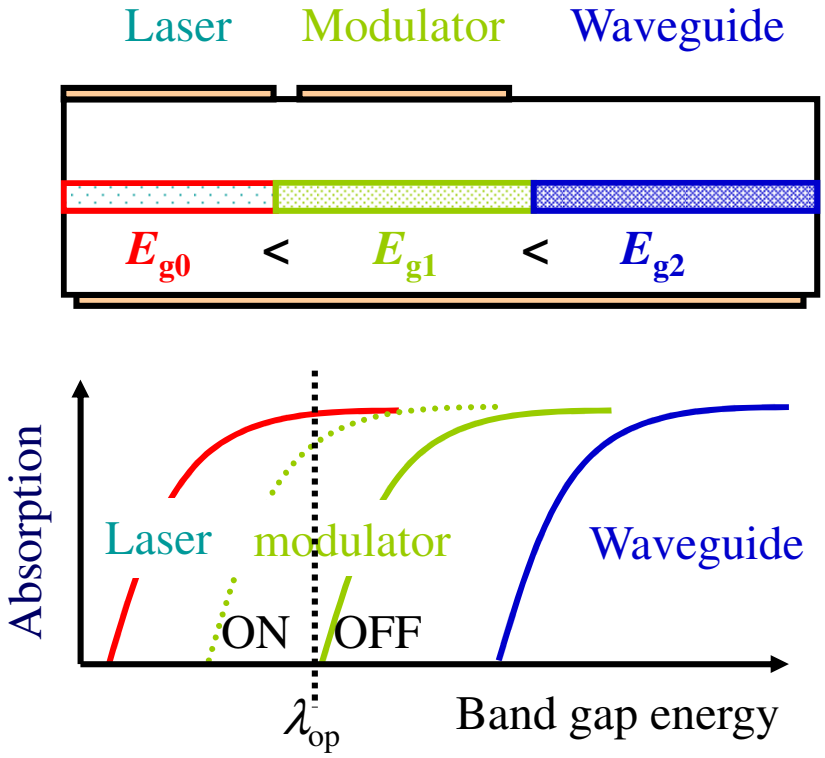
They are all about band-edge transitions!

A practical demand for electronic structure calculation

Intermixing Technique

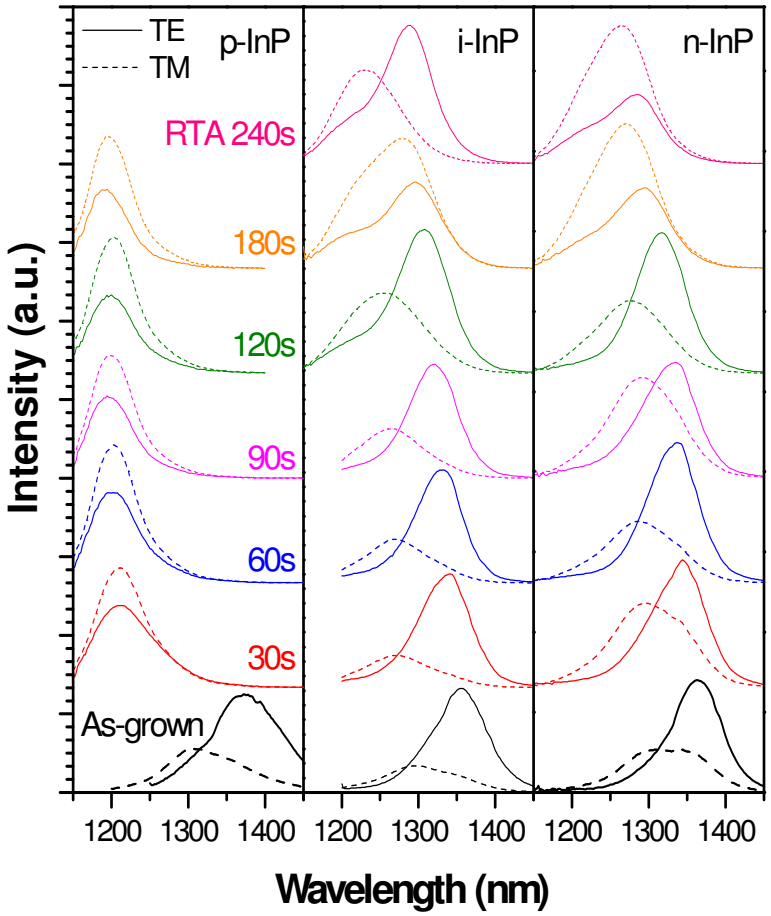
- Core technique for fabrication of Photonic Integrated Circuits
- Local band gap modification after growth
- Control of interdiffusion process

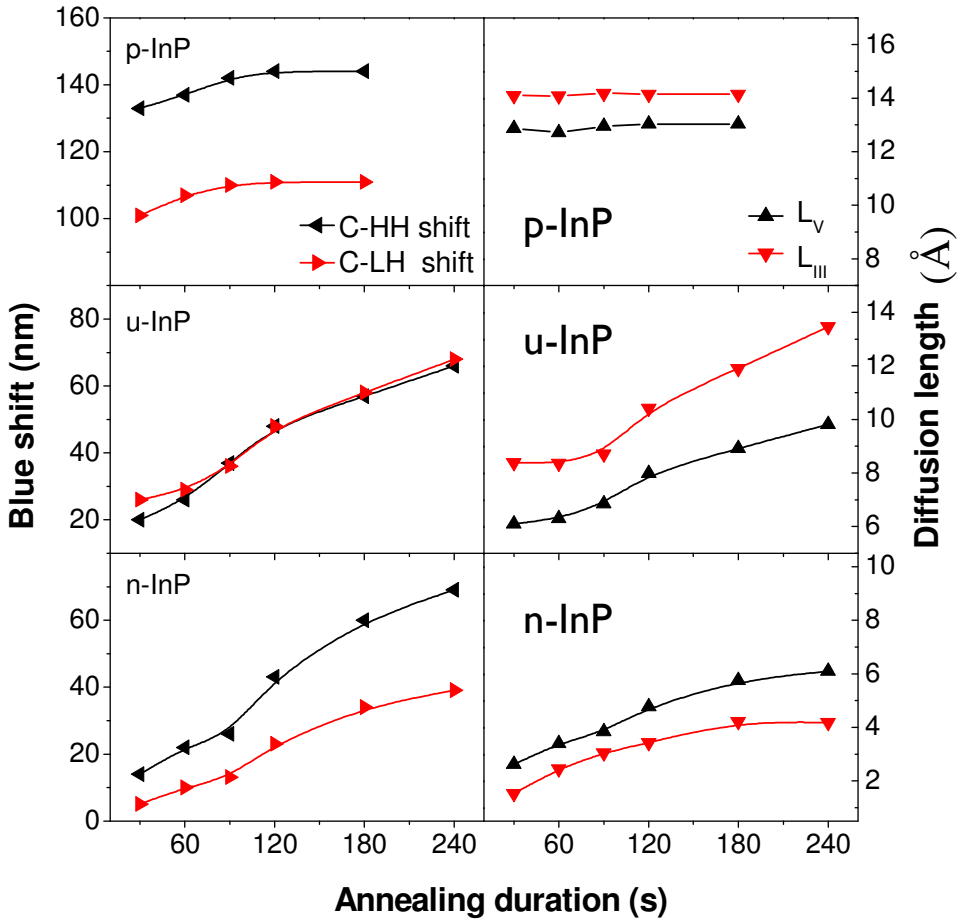




Photonic Integrated Circuits

A practical demand for electronic structure calculation





Deriving diffusion lengths from photoluminescence data need calculate of electronic structures

- Appl. Phys. Lett. 91, 181111, 2007

Practicability - Expected features of calculation method

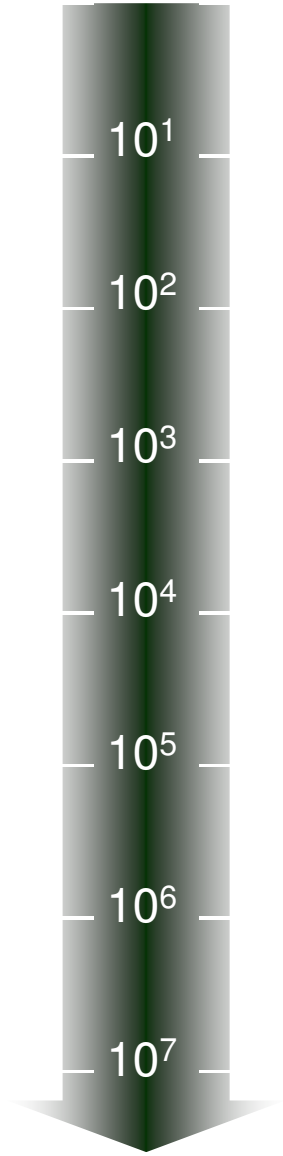
- Time efficient
- Easy programming
- Allowing parametric investigation
  i.e. study of Influence of structural shape

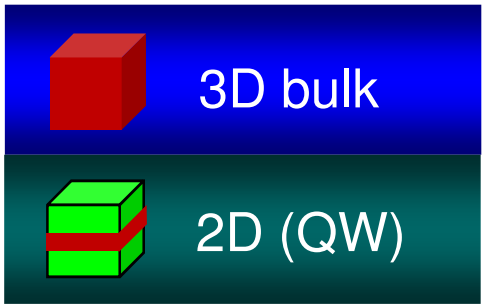
Modeling electronic structures

The first principles
atomistic, ab initial
most accurate
challenging in handling
excited states properties

Tight Binding
atomistic, empirical

The k·p method
continuum, empirical
applicable near the Γ point of
Brillouin zone (k=0)
good enough for optical
property





Nature of the Bands Near Bandedges

In semiconductors we are primarily interested in the valence band and conduction band. Moreover, for most applications we are interested in what happens near the top of the valence band and the bottom of the conduction band. These states originated from the atomic levels of the valence shell in the elements making up the semiconductor

IV Semiconductors

C $1s^2 2s^2 2p^2$

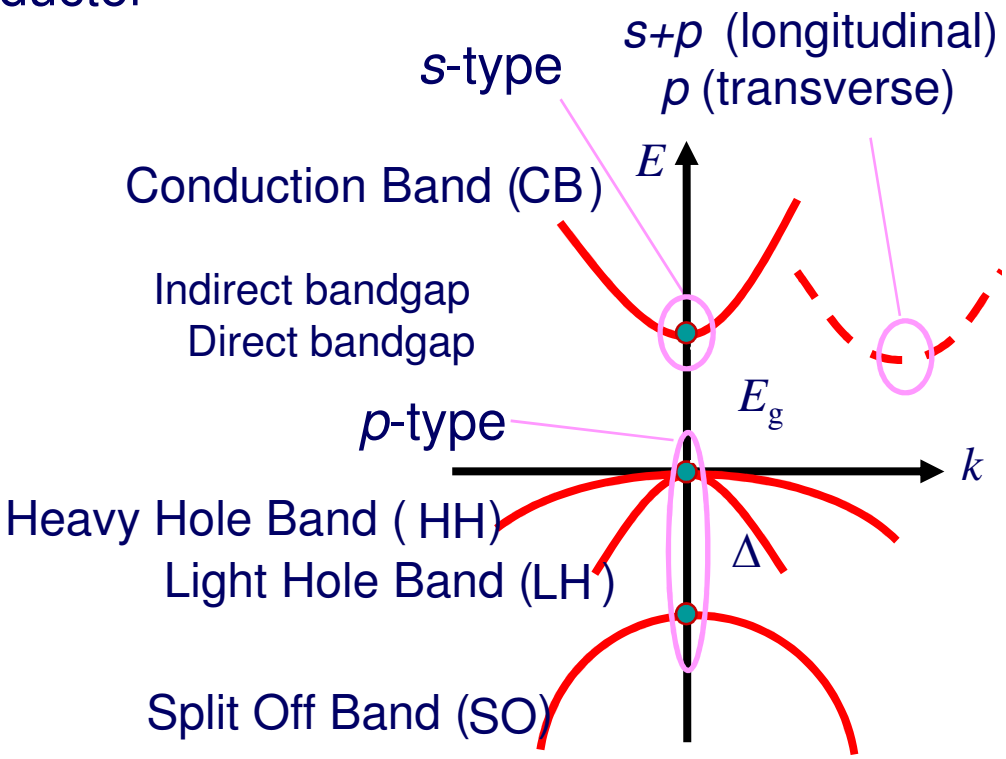
Si $1s^2 2s^2 2p^6 3s^2 3p^2$

Ge $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 4p^2$

III-V Semiconductors

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$

As $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$



Outmost atomic levels are either *s*-type or *p*-type

Basic theory of k·p method

Fundamentals

Time-independent Schrödinger equation

$$\left[\frac{-\hbar}{2m_0}\nabla^2 + V_L(\mathbf{r})\right]\psi_n(\mathbf{r}) = E(\mathbf{k})\psi_n(\mathbf{r})$$

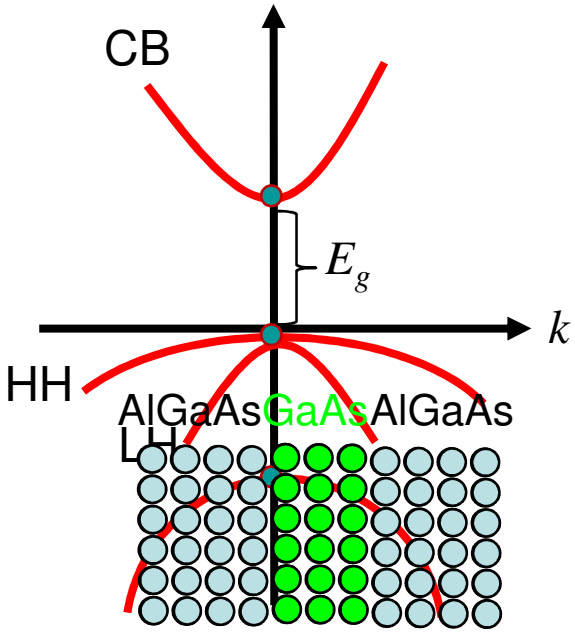
Symmetry of bulk crystal

Crystal potential $V_L(R+\mathbf{r}) = \psi_L(\mathbf{r})$

Wave function $\psi(R+\mathbf{r}) = \psi(\mathbf{r})$

Bloch wave $\psi_n(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$ — $u_{n,\mathbf{k}}$: unit cell function; $e^{i\mathbf{k}\cdot\mathbf{r}}$: plane wave

$$\mathbf{H}(\mathbf{k}) = \begin{bmatrix}
A & 0 & T^*+V^* & 0 & -\sqrt{3}(T-V) & \sqrt{2}(W-U) & W-U & \sqrt{2}(T^*+V^*) \\
0 & A & \sqrt{2}(W-U) & -\sqrt{3}(T^*+V^*) & 0 & T-V & -\sqrt{2}(T-V) & W^*+U \\
cc & cc & -P+Q & -S^* & R & 0 & \sqrt{3/2}S & -\sqrt{2}Q \\
cc & cc & cc & -P-Q & 0 & R & -\sqrt{2}R & \sqrt{1/2}S \\
cc & cc & cc & cc & -P-Q & S^* & \sqrt{1/2}S^* & \sqrt{2}R^* \\
cc & cc & cc & cc & cc & -P+Q & \sqrt{2}Q & \sqrt{3/2}S^* \\
cc & cc & cc & cc & cc & cc & Z & 0 \\
cc & cc & cc & cc & cc & cc & cc & Z
\end{bmatrix}
\begin{matrix} \text{CB} \\ \text{CB} \\ \text{LH} \\ \text{HH} \\ \text{HH} \\ \text{LH} \\ \text{SO} \\ \text{SO} \end{matrix}$$



Hamiltonian equations $\sum_j \mathbf{H}_{n,j}(\mathbf{k})a_j = E_n(\mathbf{k})a_n$

Knowing $u_{j,0}$ and $E_n(\mathbf{k}=0)$ → Solving $E_n(\mathbf{k})$ and ψ_n

- N. W. Ashcroft and N. D. Mermin, *Solid state physics*. New York: Holt, Rinehart and Winston, 1976
- J. Callaway, *Quantum theory of the solid state*. Boston: Academic Press, 1991
- J. M. Luttinger, and W. Kohn, *Phys. Rev.* **97**, 869 (1955)
- E. O. Kane, *J. Phys. Chem. Solids*. 1, 249 (1957).

Bulk crystal → low-dimensional structure

Bulk crystal

Envelope function theory

Low-dimensional structure

$$\psi_n(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$$

unit cell function

plane wave

$$u_{n,\mathbf{k}}(\mathbf{r}) = \sum_j a_j(\mathbf{k}) u_{j,\mathbf{k}_0=0}(\mathbf{r})$$

$$\psi(\mathbf{r}) = \sum_j^V F_j(\mathbf{r}) u_{j,0}(\mathbf{r})$$

Number of bands

Envelope function

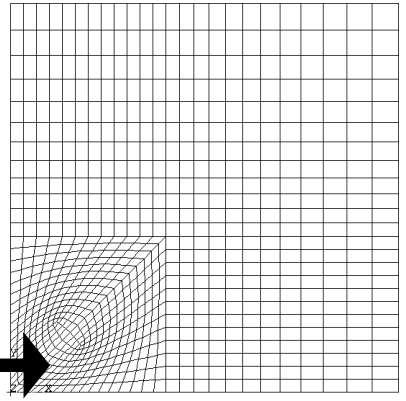
Bloch basis

Band index

Position-dependent Hamiltonian

$$\mathbf{H}(\mathbf{r};\mathbf{k}): \quad k_\alpha \to -i\partial_\alpha;\ \gamma k_\alpha^2 \to -\partial_\alpha(\gamma\partial_\alpha)$$

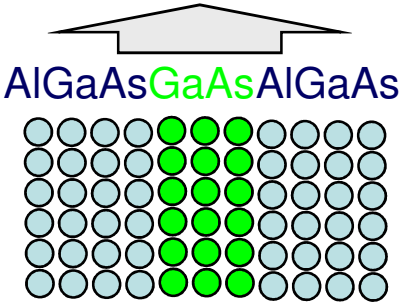
3D mesh for QDs



Coupling equations on the 3D mesh

Finite element method (FEM)

Finite difference method (FDM)



- C. Pryor, *Phys. Rev. B.* **57**, 7190 (1998)
- S. F. Tsay, et al. *Phys. Rev. B.* **56**, 13242 (1997)

Numerical approaches for the k·p method

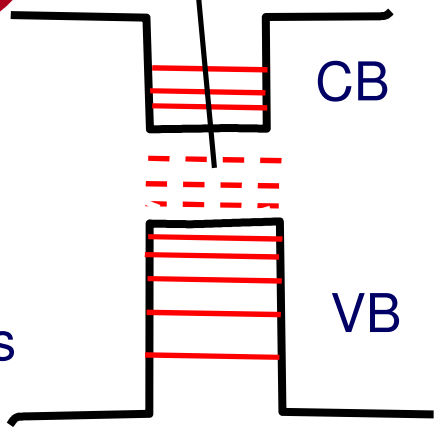
Finite element method (FEM)

- Cumbersome mesh process
- Finite element to deal with coupling equations
- Numerical integration
- Computationally intensive

Finite difference method (FDM)

- Simple structures only
- 8 couple equations on every point
- Numerical differentiation
- Programming challenge for QDs

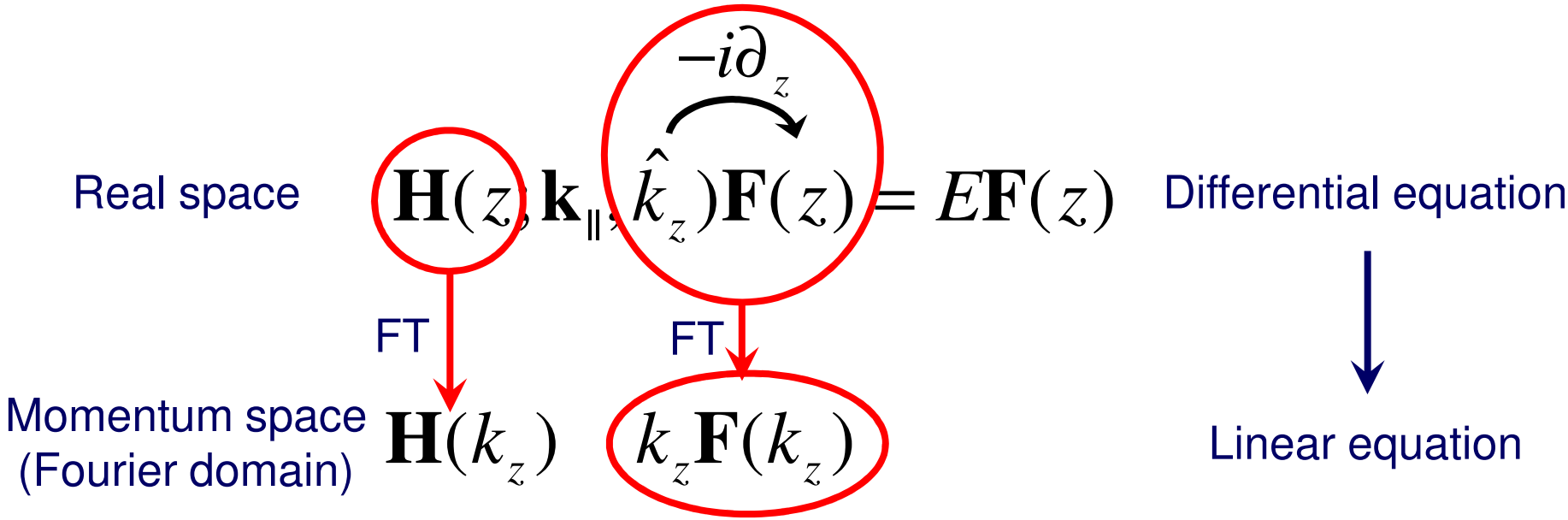
More serious issue in common – poor control of spurious solutions



Can We?

- discard the 3D mesh
- skip numerical integration/differentiation
- ease the programming job
- have better control on spurious solutions

Fourier-transform k·p method (FTM)



The use of Fourier series $\xrightarrow{\text{truncation}}$ excellent control of spurious solutions!

- T. Mei, J. App. Phys. 102, 053708 (2007)
- Q. J. Zhao, and T. Mei, J. Appl. Phys., 109, 063101 (2011)
- Q. J. Zhao, T. Mei, D. H. Zhang, and O. Kurniawan, Opt. Quant. Electron., 42, 705(2011)
- Q. J. Zhao, T. Mei, and D. H. Zhang, J. Appl. Phys., 111,053702 (2012)

Detailed FTM formulation for QW superlattice

$$\psi(\mathbf{r}) = \sum_{j}^{V} F_j(\mathbf{r}) u_{j,0}(\mathbf{r}) \qquad F_z(\mathbf{r}) = \left(1/\sqrt{L}\right) e^{ik_z z} \sum_n \mathbf{c}_n e^{in\kappa z}$$

Waver vector $-\kappa/2 \le k_z \le \kappa/2$

Fourier Frequency $\kappa = 2\pi/L$

$\mathbf{c}_n = [c_1, c_2, ..., c_8]_n^T$

Periodical length

Boundary condition for N QW superlattice periods $k_z = -\frac{\kappa}{2} + \frac{2\pi j}{NL}, 0 \le j \le N$

Hamiltonian in Fourier series expansion

$$\mathbf{H} = \mathbf{H}^{(zz)}(z)\hat{k}_z^2 + \mathbf{H}^{(z)}(z)\hat{k}_z + \mathbf{H}^{(0)}(z)$$

$$= \left[\sum_q \tilde{H}^{(zz)}(q) e^{iq\kappa z}\right]\hat{k}_z^2 + \left[\sum_q \tilde{H}^{(z)}(q) e^{iq\kappa z}\right]\hat{k}_z + \sum_q \tilde{H}^{(0)}(q) e^{iq\kappa z}$$

$H(\square)$ $H(\square)$ $H(\square)$

Complex exponential functions' orthogonality

Operator: $H(Q) = \sum_q \left\langle e^{i(k_z+m\kappa)z} \middle| Q \middle| e^{i(k_z+n\kappa)z} \right\rangle$

$$\left(\frac{\kappa m + \kappa n}{2} + k_z\right)\tilde{H}_{uv}^{(z)}(q = m-n) \qquad \tilde{H}_{uv}^{(0)}(q = m-n)$$

$$(\kappa m + k_z)(\kappa n + k_z)\tilde{H}_{uv}^{(zz)}(q = m-n)$$

Eigen-equation

Transformation of Hamiltonian

$$[M_{st}][c_t] = E[c_t]$$

$$s = j + V(m + N_{tr}) \qquad j, j' = 1, 2, \cdots V$$

$$t = j' + V(n + N_{tr}) \qquad m, n = -N_{tr}, \cdots 0, \cdots N_{tr}$$

$$q = -2N_{tr}, \cdots 0, \cdots 2N_{tr}$$

Order of Fourier truncation

Dimension of **M**: $V(2N_{tr}+1) \times V(2N_{tr}+1)$

T. Mei, *J. App. Phys.* **102**, 053708 (2007)

Hamiltonian matrix for QD (SYM & BF operator ordering)

Wavefunction $$\mathbf{F}(\mathbf{r}) = \frac{1}{\sqrt{d_x d_y d_z}} e^{ik_x x + ik_y y + ik_z z} \sum_{n_x} \sum_{n_y} \sum_{n_z} c_{n_x n_y n_z} e^{i\left(n_x \kappa_x x + n_y \kappa_y y + n_z \kappa_z z\right)}$$

Eigen equation $$[\mathbf{M}][\mathbf{c}] = E[\mathbf{c}]$$

Burt-Foreman (BF) Operator Ordering

$$\mathbf{H} = H^{(zz)} \hat{k}_z^2 + H_L^{(z)} \hat{k}_z + \hat{k}_z H_R^{(z)} + H^{(0)}$$

Symmetrical (SYM) Operator Ordering

$$\mathbf{H} = H^{(zz)} \hat{k}_z^2 + H^{(z)} \hat{k}_z + H^{(0)}$$

Hamiltonian matrix (SYM)

$$\mathbf{M}_{st} =$$

$$\frac{1}{2} \sum_{\alpha,\beta} \tilde{H}^{(\alpha\beta)}_{jj',q_i=m_i-n_i} \begin{bmatrix} \left(k_\beta + n_\beta \kappa_\beta\right)\left(k_\alpha + n_\alpha \kappa_\alpha\right) \\ +\left(k_\alpha + n_\alpha \kappa_\alpha\right)\left(k_\beta + n_\beta \kappa_\beta\right) \end{bmatrix}$$

$$+\frac{1}{2} \sum_{\alpha} \tilde{H}^{(\alpha)}_{jj',q_i=m_i-n_i} \left[2k_\alpha + \left(m_\alpha + n_\alpha\right)\kappa_\alpha\right]$$

$$+\tilde{H}^{(0)}_{jj',q_i=m_i-n_i}$$

Hamiltonian matrix (BF)

$$\mathbf{M}_{um,vn} =$$

$$\sum_{\alpha,\beta} \tilde{H}^{(\alpha\beta)}_{uv,q_i=m_i-n_i} \left(k_\alpha + m_\alpha \kappa_\alpha\right)\left(k_\beta + n_\beta \kappa_\beta\right) \quad 2^{\text{nd}} \text{ order}$$

$$+\sum_{\alpha} \begin{bmatrix} \tilde{H}^{(\alpha)}_{uv,q_i=m_i-n_i,L} \left(k_\alpha + n_\alpha \kappa_\alpha\right) \\ +\tilde{H}^{(\alpha)}_{uv,q_i=m_i-n_i,R} \left(k_\alpha + m_\alpha \kappa_\alpha\right) \end{bmatrix} \quad 1^{\text{st}} \text{ order}$$

$$+\tilde{H}^{(0)}_{uv,q_i=m_i-n_i} \quad 0^{\text{th}} \text{ order}$$

Dimensions of Hamiltonian $$V\prod_{\alpha}\left(2N_\alpha + 1\right) \times V\prod_{\alpha}\left(2N_\alpha + 1\right) \left(\alpha, \beta = x, y, z\right)$$

- Q. J. Zhao, and T. Mei, J. Appl. Phys., 109, 063101 (2011)
- Q. J. Zhao, T. Mei, and D. H. Zhang, J. Appl. Phys., 111,053702 (2012)

Finite Difference Method (FDM) v.s. Fourier Transform Method (FTM)

QW: Position-dependent Hamiltonian

$$\mathbf{H} = H^{(zz)} k_z^2 + H^{(z)} k_z + H^{(0)}$$

Differential operator: $\hat{k}_z = -i\partial_z$

FDM: finite difference in real space

$$\mathbf{H} = -H^{(zz)}\partial_z^2 - iH^{(z)}\partial_z + H^{(0)}$$

$$= -\partial_z \left(H^{(zz)} \partial_z f \right)\Big|_{z_i}$$

$$-\frac{i}{2}\left[H^{(z)}\partial_z f + \partial_z H^{(z)} f \right]\Big|_{z_i}$$

$$+ H^{(0)}\Big|_{z_i}$$

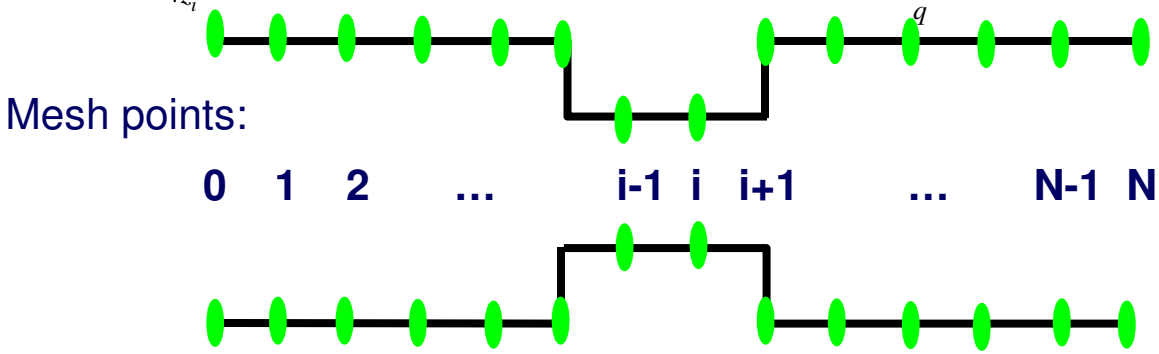
FTM: Fourier components in momentum space

$$\mathbf{H} = H^{(zz)}\hat{k}_z^2 + H^{(z)}\hat{k}_z + H^{(0)}$$

$$= \sum_q \tilde{H}^{(zz)}(q) e^{iq\kappa z}\hat{k}_z^2$$

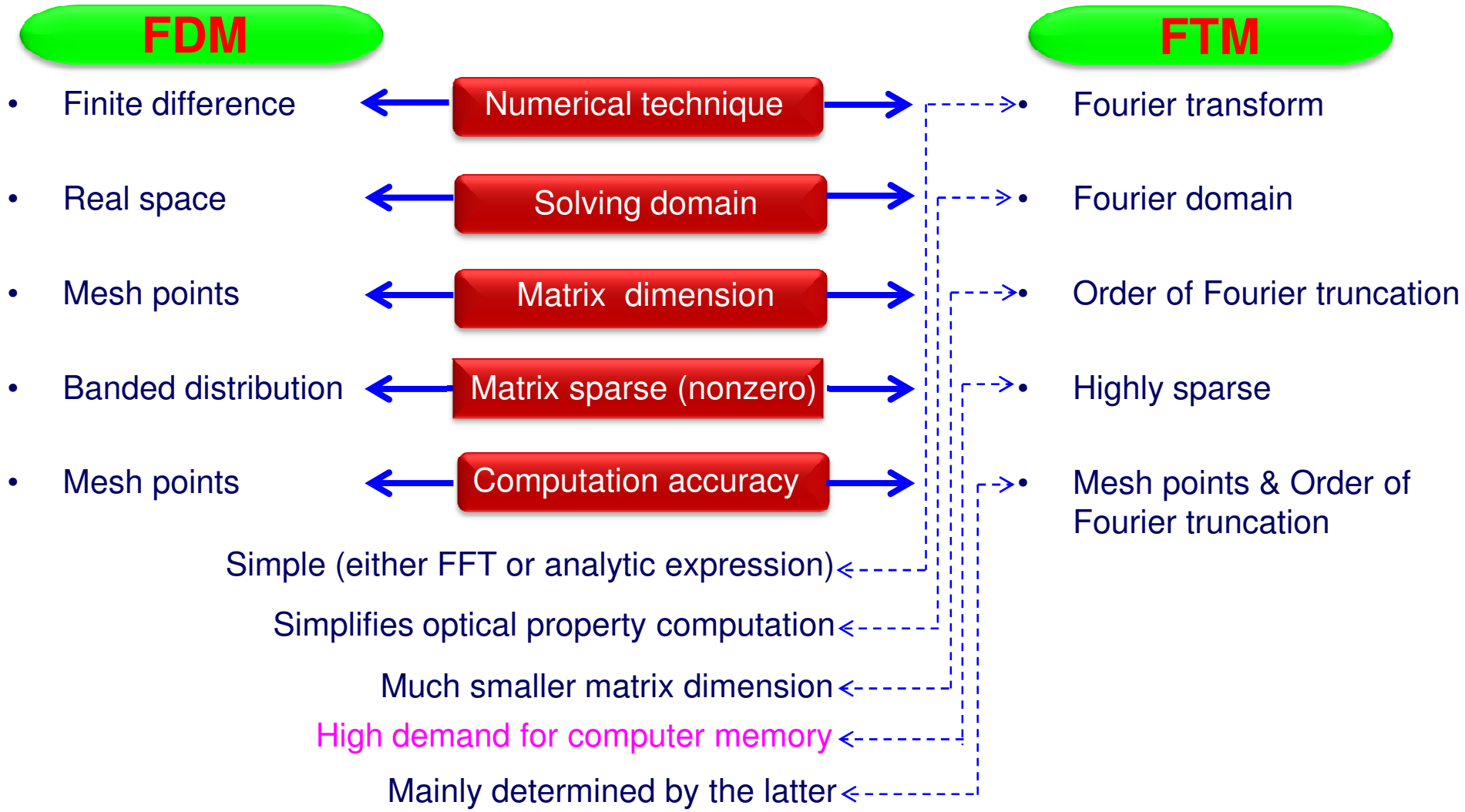
$$+ \sum_q \tilde{H}^{(z)}(q) e^{iq\kappa z}\hat{k}_z$$

$$+ \sum_q \tilde{H}^{(0)}(q)$$



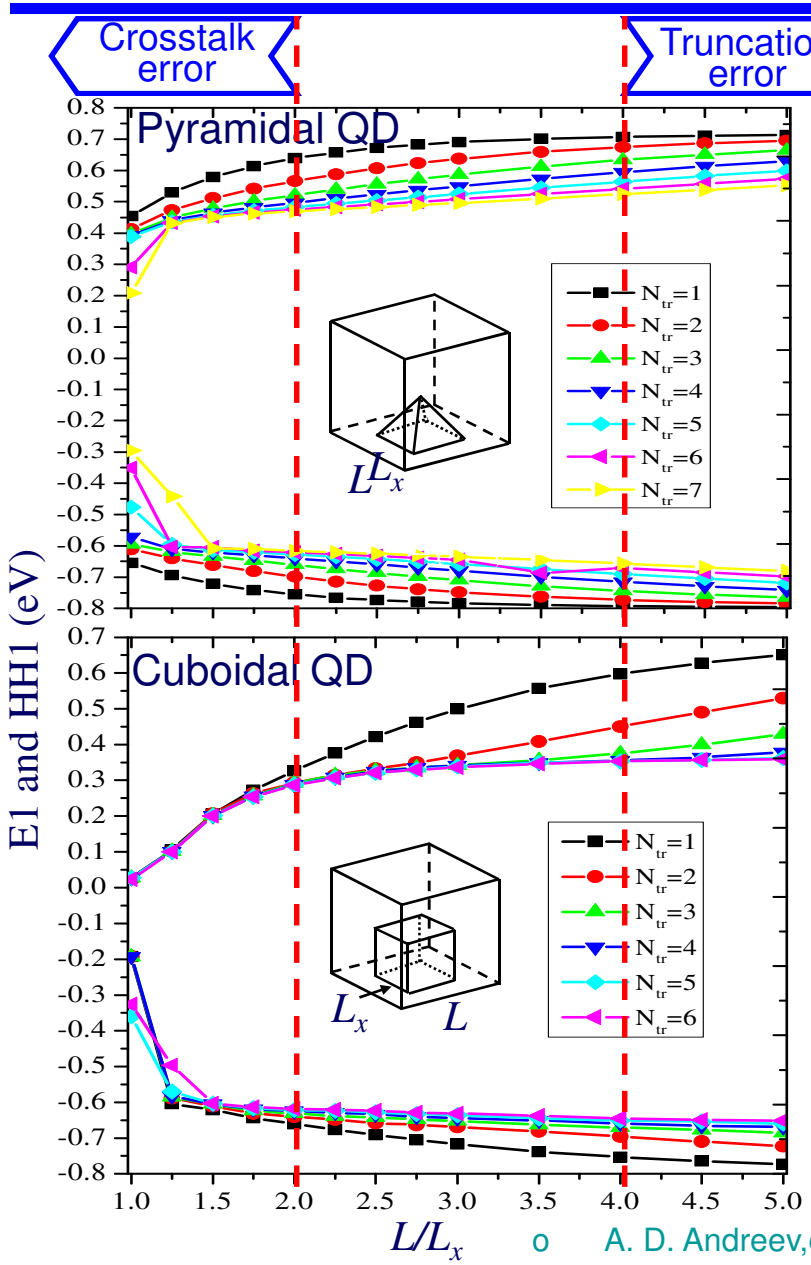
- X. Cartoxia, “Theoretical Methods for Spintronics in Semiconductor with Applications”, Doctor of Philosophy, Carliforlian Institute of Technology, Pasadena(2003)
- T. Mei, *J. Appl. Phys*. 102, 053708(2007).

Finite Difference Method (FDM) v.s. Fourier Transform Method (FTM)



- X. Cartoxia, et al *J. Appl. Phys*. 93, 3974(2003
- T. Mei, *J. Appl. Phys*. 102, 053708(2007).
- B. Lassen, *et al*, *Commun. Comput. Phys*. 6, 699 (2009)
- W. Liu, *et al*, *J. Appl. Phy*. 104, 053119 (2008)

Control of Computation errors in FTM (isolated QDs)



Truncation error ↑ ← ↓ **Fourier truncation** N_{tr} ↑ → ↑ **Volume of computation**

Crosstalk error ↑ ← ↓ **Periodical length** L

→ **Selection of Periodical length** L

$L = 3L_x$ is chosen by Andreev & Gunawan

Pyramidal QD

N_{tr}=7 by trading off the demand of higher order of Fourier truncation and the limit of computer capacity

Cuboidal QD

A smaller N_{tr} (= 6) is enough for smooth structures

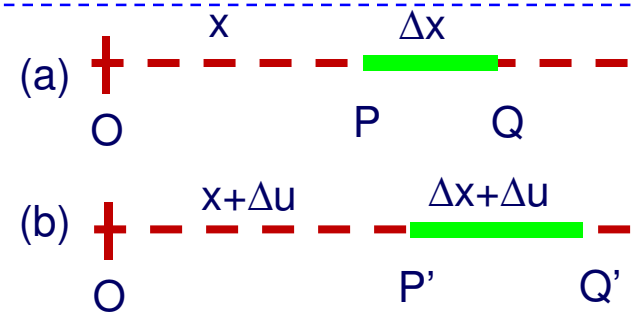
⇨ **Smooth structures possess narrow-span Fourier spectrum (Mei)**

→ **Selection of Fourier truncation N_{tr}**

Computation accuracy & Computer capacity

- A. D. Andreev,et al J. Appl. Phys., 86, 297(1999)
- O. Gunawan,et al, Phys. Rev. B, 71, 205319(2005)
- T. Mei, J. App. Phys. 102, 053708 (2007)

Strain definition & influence



Deformation of an extendible string: (a) unstreched and (b) stretched

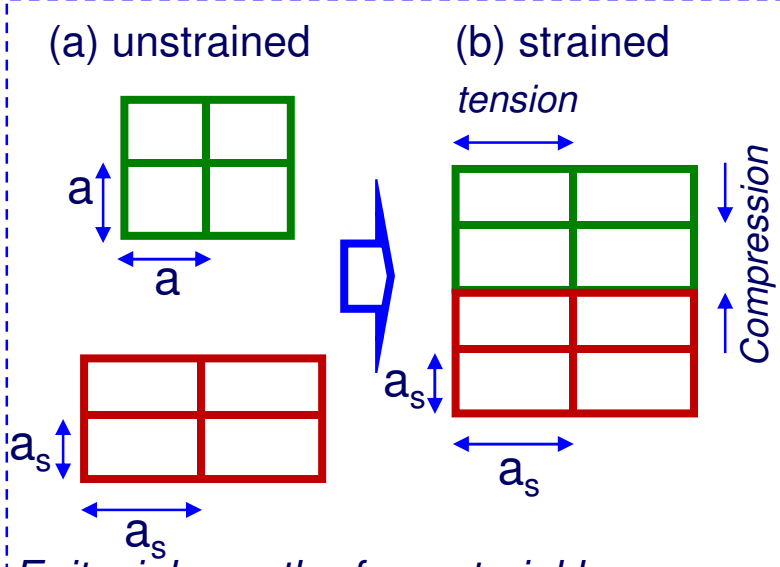
$$PQ: \frac{P'Q'-PQ}{PQ}=\frac{\Delta u}{\Delta x}$$

$$P: \quad e=\lim_{\Delta x\to 0}\frac{\Delta u}{\Delta x}=\frac{du}{dx}$$

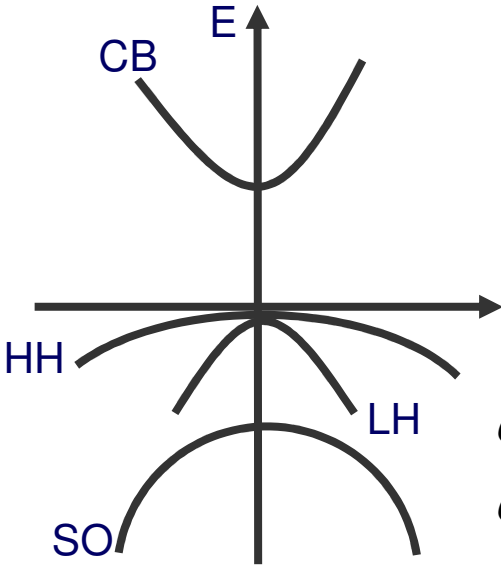
$$QDs: e_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$$

$$(i,j=1,2,3)$$

- Not a property of crystals
- A response of external force (Lattice mismatch)
- A balance of internal force (stress)
- Displacement



Epitaxial growth of a material layer on a substrate



$$\begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{13} & e_{22} & e_{23} \\ e_{23} & e_{13} & e_{33} \end{pmatrix}$$

$$e_h = e_{11}+e_{22}+e_{33}$$

$$e_b = e_{33}-(e_{11}+e_{22})/2$$

Strain influence on band structure

- J. F. Nye, *Physical properties of crystals: their representation by tensors and matrices*, Oxford University Press, Oxford, 1985
- S. L. Chuang, *Physics of optoelectronic device,* Wiley, New York, 1995, p. 144-154.

Strain computation

Fundamentals

Continuum Mechanical (CM) theory

- A microscopic physical theory
- Green's function method
  - Green's tensor is used to represent the response of the external force
  - Real space – integration
  - Fourier domain – Fourier-transform

Eshelby's inclusions theory

Real space

Stress

- Green's tensor
- QD shape function
- Young's modulus
- Poisson's ratio

Fourier domain

Displacement

- Green's tensor
- QD shape function
- Elastic constants

Strain tensor of a single QD in the Fourier domain

$$\tilde{e}_{ij}^{s}(\xi)=\varepsilon_0\tilde{\Lambda}(\xi)\left\{\delta_{ij}-\frac{(C_{11}+2C_{12})\xi_i\xi_j/\xi^2}{1+(C_{12}+C_{44})\sum_{p=1}^{3}\frac{\xi_p^{\,2}}{C_{44}+C_{an}\xi_p^{\,2}}}\left[\frac{1}{2\left(C_{44}+C_{an}\,\xi_i^{\,2}/\xi^2\right)}+\frac{1}{2\left(C_{44}+C_{an}\,\xi_j^{\,2}/\xi^2\right)}\right]\right\}$$

ξ : Cartesian coordinates in Fourier domain

$\tilde{\Lambda}(\xi)$: QD shape function in the Fourier domain

ε_0 : Initial lattice constant

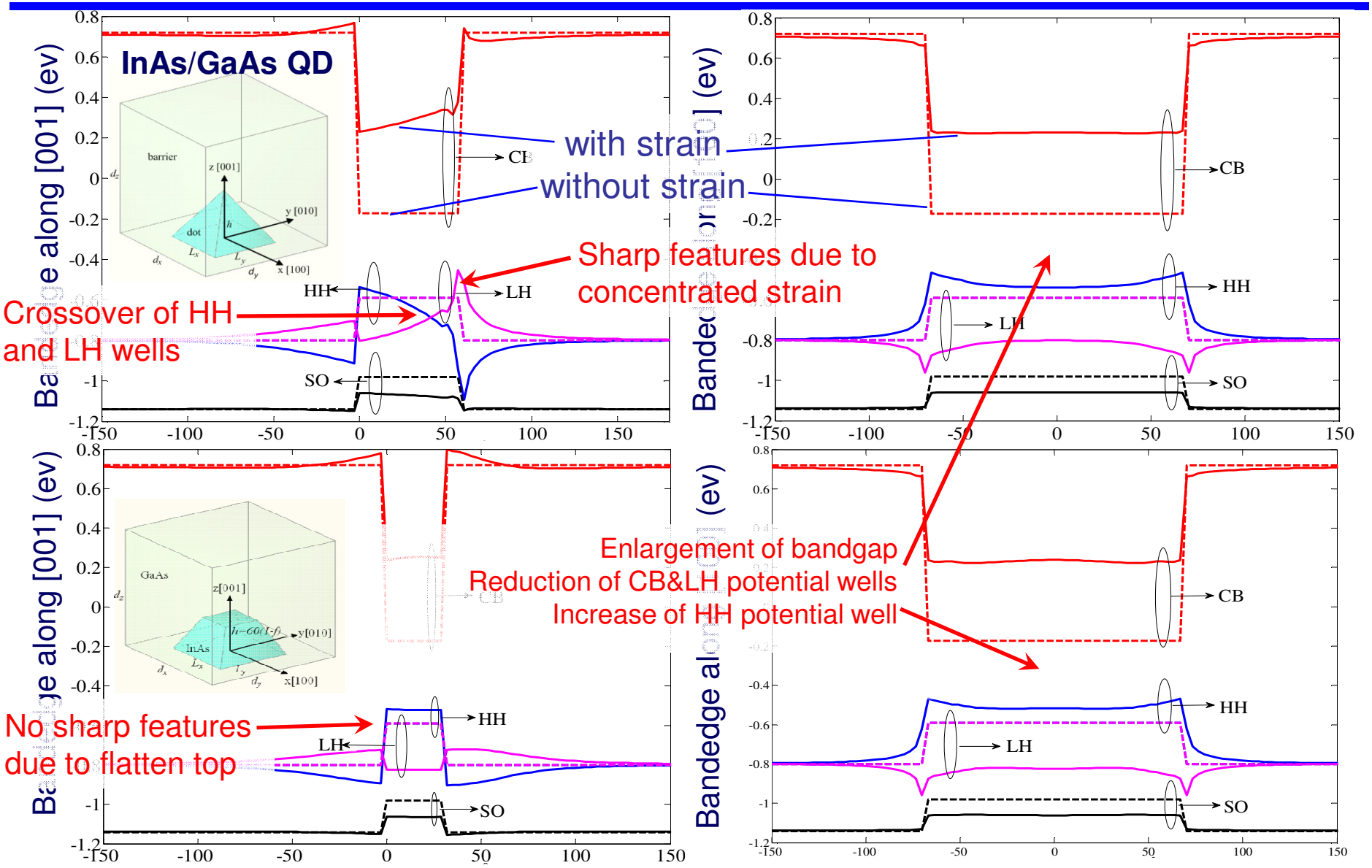
C_{ij} : Elastic constants $C_{an}=C_{11}-C_{12}-2C_{44}$

Analytical strain expression with linear elasticity

$$e_{ij}=\frac{(2\pi)^3}{d_1d_2d_3}\sum_{n_1,n_2,n_3}\tilde{e}_{ij}^{s}(\xi_n)\exp(i\xi_n\cdot\mathbf{r})$$

- J. R. Downes, D. A. Faux, and E. P. O'Reily, *J. Appl. Phys.* **81**, 6700 (1997).
- G. S. Pearson and D. A. Faux, *J. Appl. Phys.* **88**, 730 (2000).
- D. A. Faux and U. M. Christmas, *J. Appl. Phys.* **98**, 033534 (2005).
- D. Andreev, et al, *J. Appl. Phys.***86**, 297 (1999).

Effects of dimension and strain – Bandedge profiles

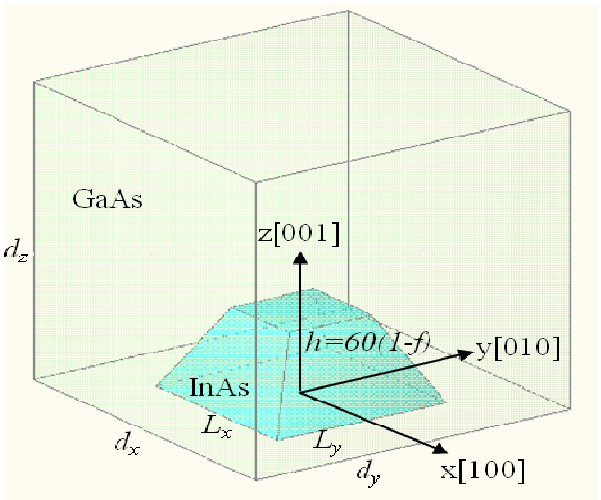


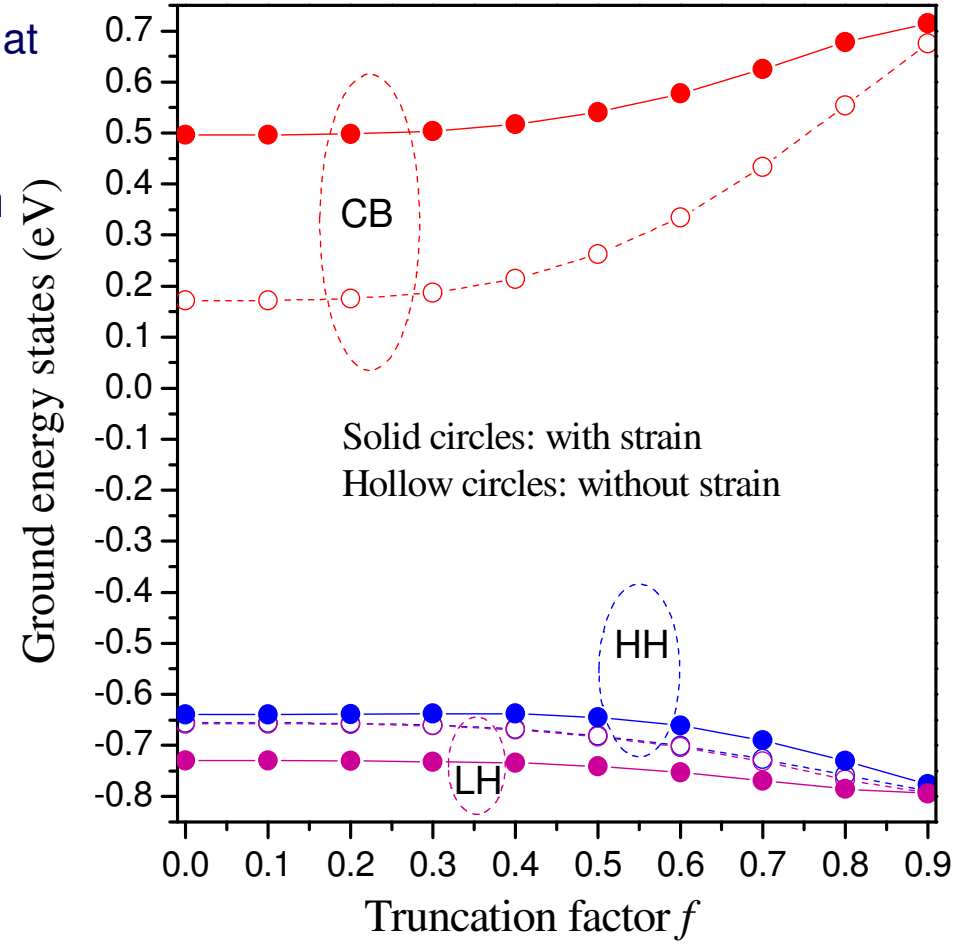
- Q. J. Zhao *et al, J. Appl. Phys.*, **109**, 063101-063113 (2011)
- C. Pryor, *Phys. Rev. B* **57**, 7190(1998)
- A. Schliwa, *et al. Phys. Rev. B* **76**, 205324(2007)

Effects of dimension and strain – Ground state energies

Variations of E1 , HH1, and LH1 v.s. truncation factor

- Strain effect (E1 and LH1) is more significant at small *f* (concentrated strain)
- Strain effect does not change HH1 much due to little change of band-edge profile
- The main contribution of CB-VB is the variation of E1 (consistent with the tight-binding work)

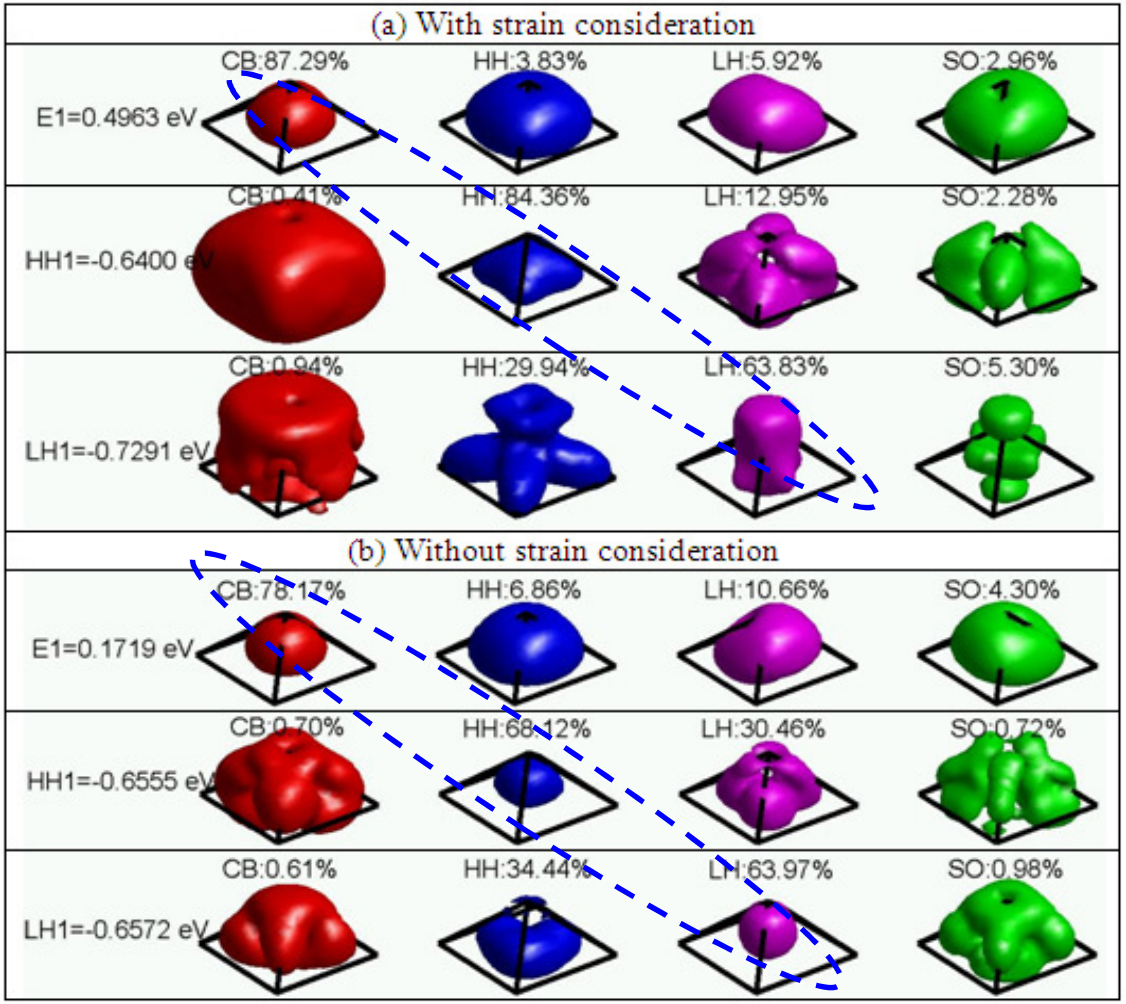


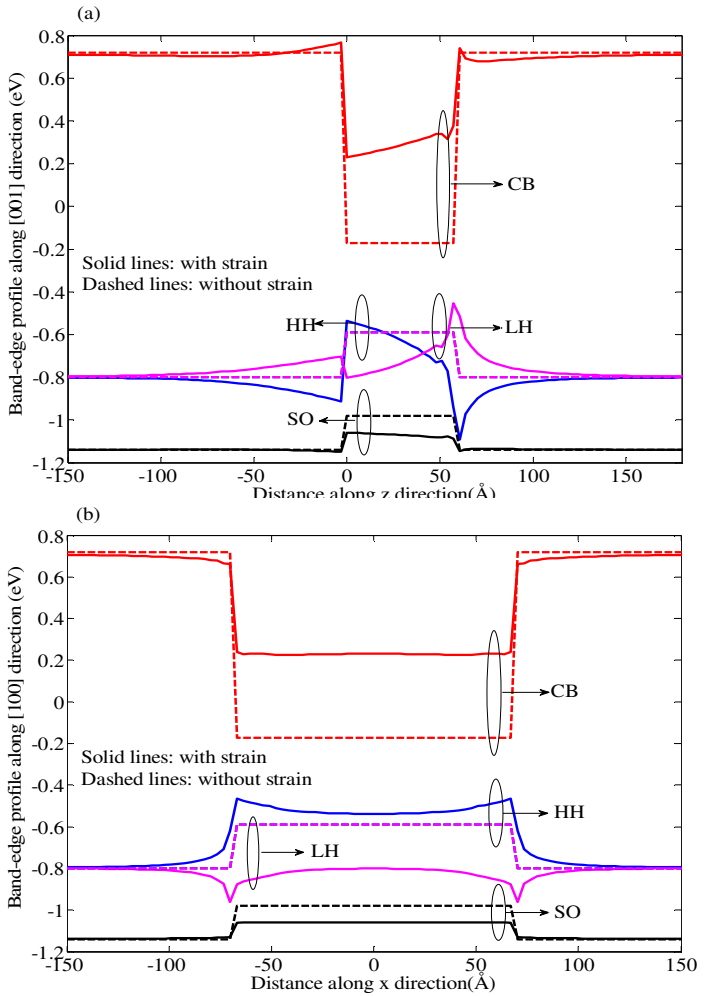


- Q. J. Zhao *et al, J. Appl. Phys.*, **109**, 063101-063113 (2011)
- R. Santoprete, *et al.*, Phys. Rev. B 68,235311(2003)

Effects of dimension and strain – 3D PDFs

3D Probability density functions (PDFs) of a pyramidal InAs/GaAs QD structure



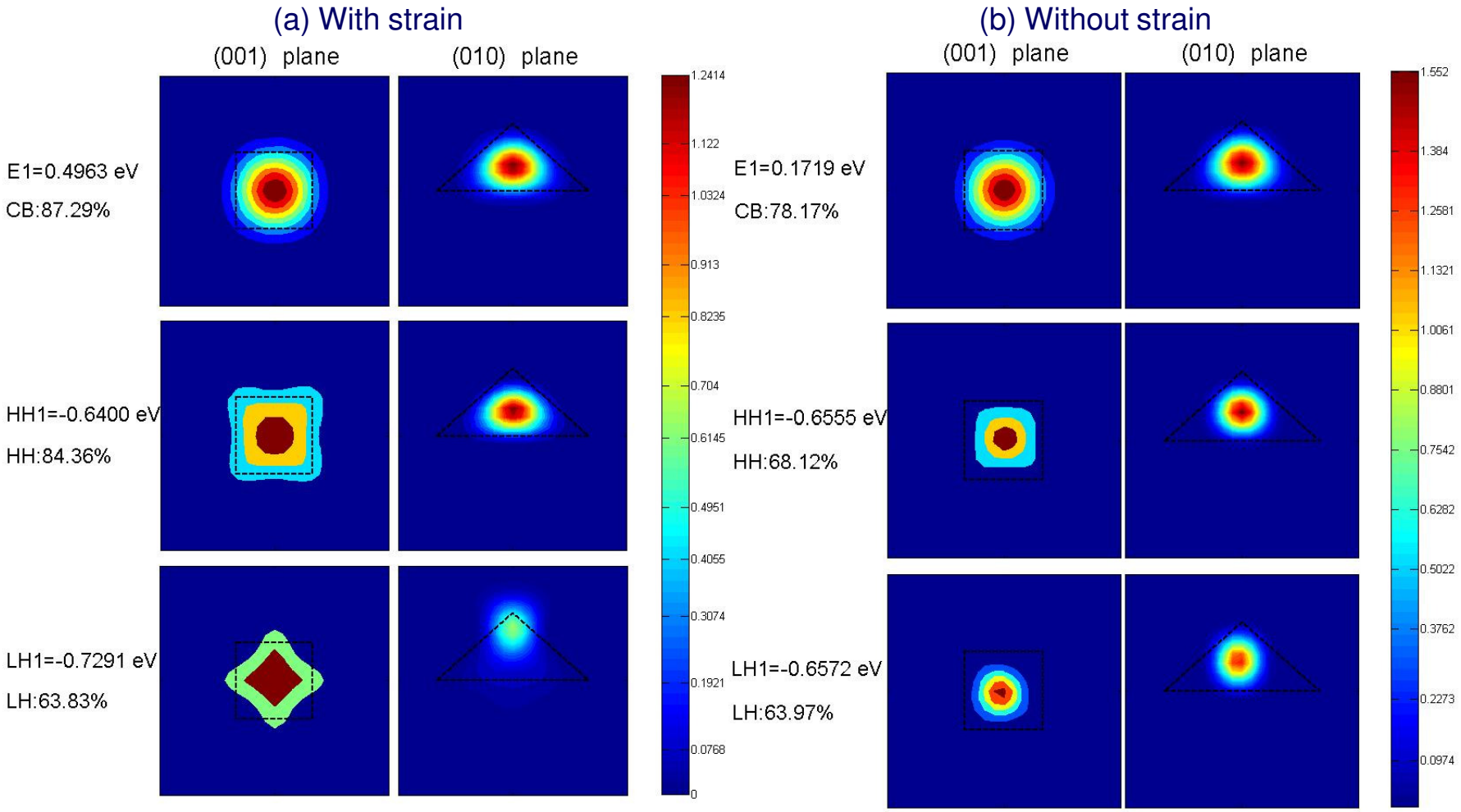


- Variation of CB's major PDF component is not as obvious as that of VB's
- Reduction of band mixing(CB and VB, HH and LH)
- Variations of PDFs' size, shape, and position

Q. J. Zhao *et al, J. Appl. Phys.*, **109**, 063101-063113 (2011)

Effects of dimension and strain – 2D PDFs

2D Probability density functions (PDFs) of a pyramidal InAs/GaAs QD structure



- Variations of PDFs' size, shape, position, and value
- Weaker confinement of carriers
- Consistent with band-edge profiles

Q. J. Zhao *et al, J. Appl. Phys.*, **109**, 063101-063113 (2011)

Optical gain calculation for QWs

Fundamentals

1. **Lorentzian/Sech line-shape function→ gain spectrum**
2. **Spontaneous emission coefficient→ gain spectrum**

Band mixing effect

Spontaneous emission

$$g_{sp}^{e}(\hbar\omega) = C_0 \sum_{n_c,n_v} \int \frac{dk_x dk_y}{4\pi^2} \left| M_{n_c,n_v}^{e}(k_x,k_y) \right|^2 f_{n_c}^{c}(k_x,k_y)\left[1 - f_{n_v}^{v}(k_x,k_y)\right]$$

$$\times \frac{(\hbar\gamma/\pi)}{\left[E_{n_c}^{c}(k_x,k_y) - E_{n_v}^{v}(k_x,k_y) - \hbar\omega\right]^2 + (\hbar\gamma)^2}$$

Lorentzian line-shape function

- W. W. Chow *et al.*, *Semiconductor-Laser Fundamentals*. Berlin: Springer, 1999
- S. L. Chuang *et al*, *IEEE J. Quantum Elect.*, 32, 1791(1996)
- D. Gershoni *et al.*, *IEEE J. Quantum Elect.*, **29**, 2433(1993)

Exact envelope function theory

$$\psi(\mathbf{r}) = \sum_j F_j(\mathbf{r}) u_{j,0}(\mathbf{r})$$

Basis function

Envelope function

Envelope function of QWs

$$F_j(\mathbf{k}) = e^{ik_x x + ik_y y} \sum_n c_j^n \phi_n(z)$$

Plane wave expansion

Fourier series

$$\phi_n(z) = 1/\sqrt{L} \exp\left[i\left(k_z + n2\pi/L\right)z\right]$$

$$M_{n_c,n_v}^{e} = \left\langle \psi_{n_v} \left| \hat{e}\cdot\mathbf{p} \right| \psi_{n_c} \right\rangle = \sum_j \sum_{j'} \sum_n \left[\left(c_j^{n_v,n}\right)^* \cdot c_{j'}^{n_c,n} \right] \left\langle u_j \left| \hat{e}\cdot\mathbf{p} \right| u_{j'} \right\rangle$$

- W. J. Fan, *et al.*, *J. Appl. Phys.*, **80**, 3471(1996)
- W. Liu, *et al*, *J. Appl. Phys*. **104**, 053119 (2008)

Optical gain calculation result by six-band FTM

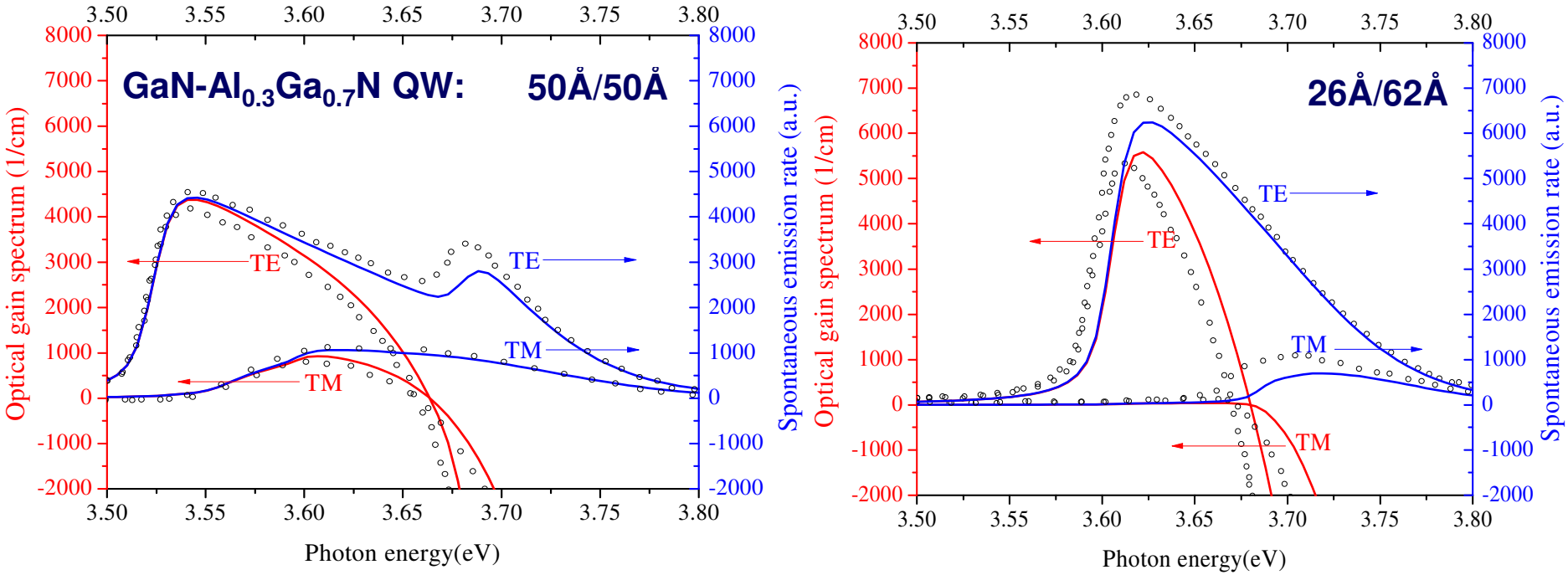
Relationship between gain and spontaneous coefficients (Chuang)

$$g(\hbar\omega) = g_{sp}^{e}(\hbar\omega)\left[1-\exp\left(\frac{\hbar\omega-\Delta F}{k_B T}\right)\right]; \quad (Separation\ of\ quasi-Fermi\ level)\,\Delta F = F_c - F_v$$

Band energies E_n

Fourier series C_n

FTM results → conveniently / accurately → **Optical gain**



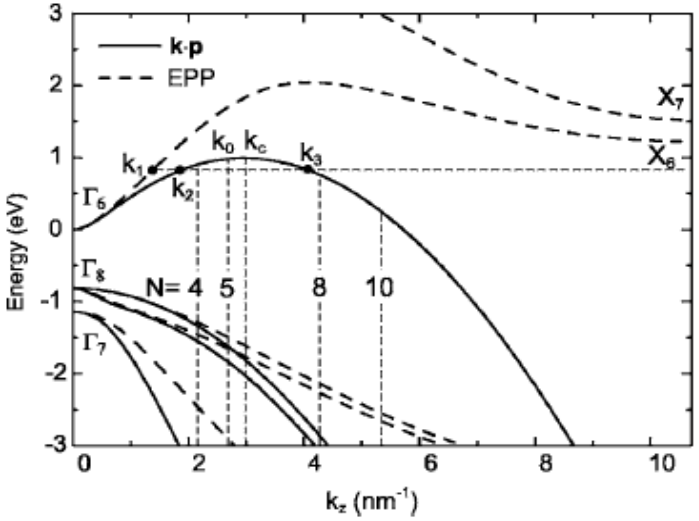
- S. L. Chuang *et al*, *IEEE J. Quantum Elect.*, 32, 1791(1996)

Spurious solutions issue

Fundamentals

Reasons

- Perturbative nature and incomplete set of basis →
- Adoption of SYM operator ordering →
- Fitting of bulk material parameters to experimental data →
- Satisfaction of boundary condition →



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Solutions

- Modifying Hamiltonian matrix → Cumbersome implement & Subsequent fixes
- Adoption of BF operator ordering → Effective for spurious solutions in VB but not CB in QWs & modification of some parameters
- Cut-off Method(Plane wave expansion) → Simple and effective

FTM → Cut-off ⟷ (Plane wave expansion) / (Fourier Transform) ← Lassen *et al*

→ Potential of FTM to eliminate spurious solutions

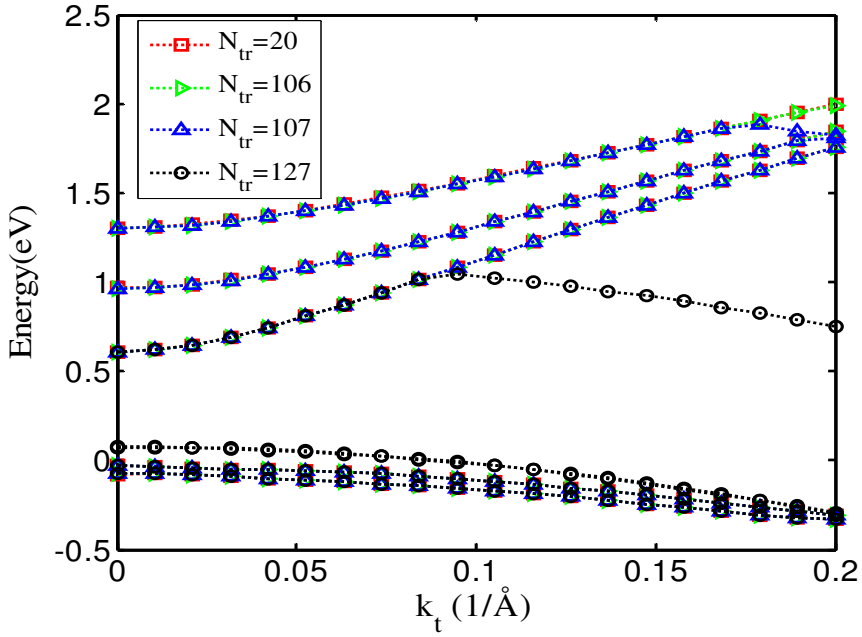
- R. Eppenga, *et al*, Phys. Rev. B 36, 1554(1987)
- K. I. Kolokolov, *et al*, *Phys*. Rev. B 68, 1613081 (2003)
- W. Yang, *et al*, Phys. Rev. B 72, 233309(2005)
- M. G. Burt, J, Phys. Condens. Mat. 4, 6651(1992)
- B. A. Foreman, *et al*, Phys. Rev. B 56, R12748(1997)

- R. G. Veprek, *et al*, Phys. Rev. B **76**, 165320(2007)
- B. Lassen, *et al*, *Commun. Comput. Phys*. **6**, 699 (2009)
- M. Holm, *et al*, *J. Appl. Phys.* **92**, 932 (2002)
- S. R. White *et al*, *Phys*. Rev. Lett. **47**, 879 (1981)
- A .T. Meney *et al*, *Phys*. Rev. B **50**, 10893(2003)

Eight-band calculation (QW)

Spurious solutions turn up in eight-band k·p computation (InAs/GaAs QW)

SYM & BF



BF operator ordering

$$H_4 = \begin{bmatrix} H_{cc} & iPk_x & iPk_y & iPk_z \\ -ik_xP & H_{xx} & H_{xy} & H_{xz} \\ -ik_yP & H_{yx} & H_{yy} & H_{yz} \\ -ik_zP & H_{zx} & H_{zy} & H_{zz} \end{bmatrix}$$

$$H_{xy} = k_x N_+^{'} k_y + k_y N_-^{'} k_x$$

$$H_{yx} = k_y N_+^{'} k_x + k_x N_-^{'} k_y$$

B. A. Foreman *et al*, Phys. Rev. B **56**,R12748(1997)

- No spurious solutions appear in VB
- Spurious solutions arise in CB since N_{tr}=107
- BF operator ordering fails to resist spurious solutions (CB and VB coupling)
- Intrinsic cut-off in FTM makes up this deficiency of BF operator ordering

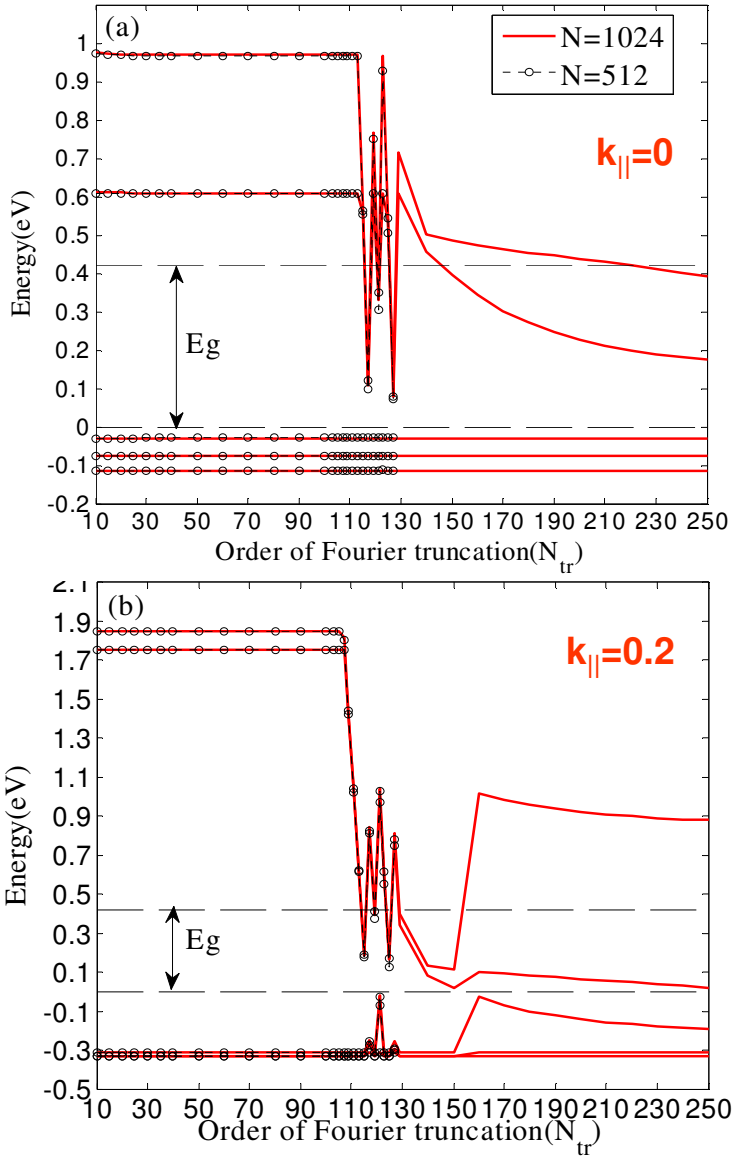
No requirement for manipulating material parameters

No setting for boundary conditions

Q. J. Zhao *et al, J. Appl. Phys.*, **111**, 053702-053708 (2012)

Control of spurious solutions in FTM

Influence of order of Fourier truncation N_{tr} and mesh point N (InAs/GaAs QW)



Comparison between $k_{||}$=0 and $k_{||}$=0.2

- Spurious solutions turn up ealier in CB at large wave vector ($k_{||}$=0)
- Spurious solutions in VB only present at large wave vector ($k_{||}$=0.2)
- It is the N_{tr} control the occurrence of spurious solutions in FTM but not step size of discretization in FDM (Cartoxia)

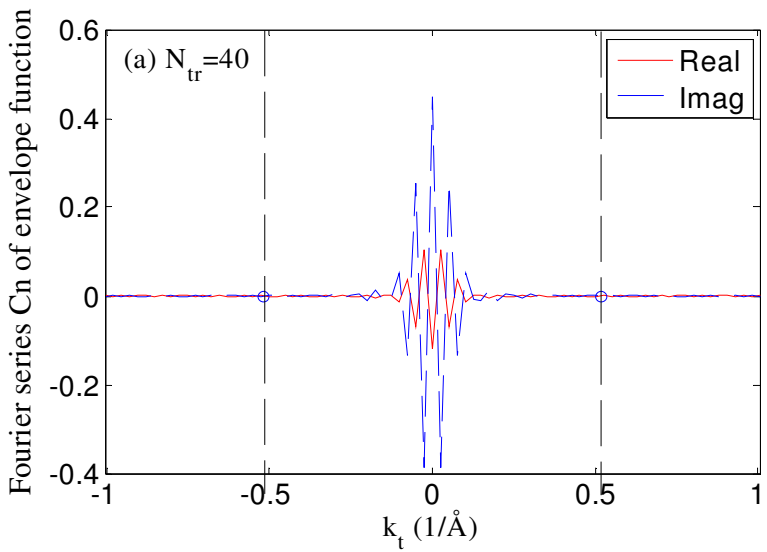
Rule of thumb

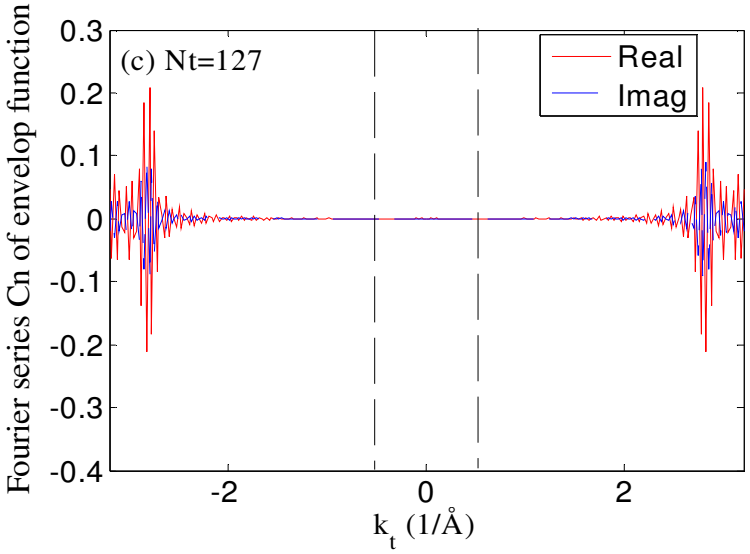
- Trade off (computation accuracy and elimination of spurious solutions)
- In practice, sufficient accuracy has been achieved before spurious solutions take place
- A smaller N_{tr} is demanded to resist spurious solutions for heterostructures with sharp interfaces, i.e., sharp geometry or drastic difference of material parameters

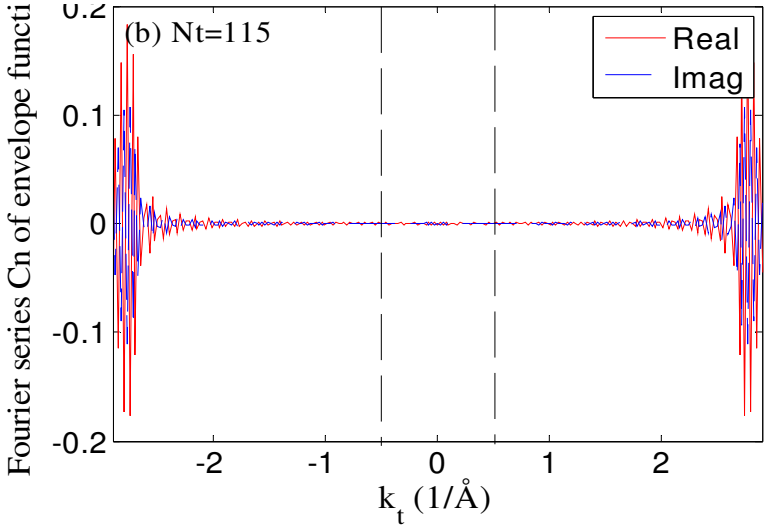
- Q. J. Zhao *et al, J. Appl. Phys.*, **111**, 053702-053708 (2012)
- X. Cartoxia, et al *J. Appl. Phys.* 93, 3974(2003)

Signature of Spurious solutions in FTM (QW)

Fourier expansion coefficients in FTM of CB component : InAs/GaAs QW







- N_{tr}=115 is the turning point
- The wild-spreading spectrum of the Fourier expansion coefficient C_n can be taken as the signature of spurious solutions

- Q. J. Zhao *et al, J. Appl. Phys.*, **111**, 053702-053708 (2012)
- B. Lassen, *et al*, *Commun. Comput. Phys.* 6, 699 (2009)

Six-band calculation (QWR)

Spurious solutions turn up in six-band k·p computation (GaN/AlN QWR)

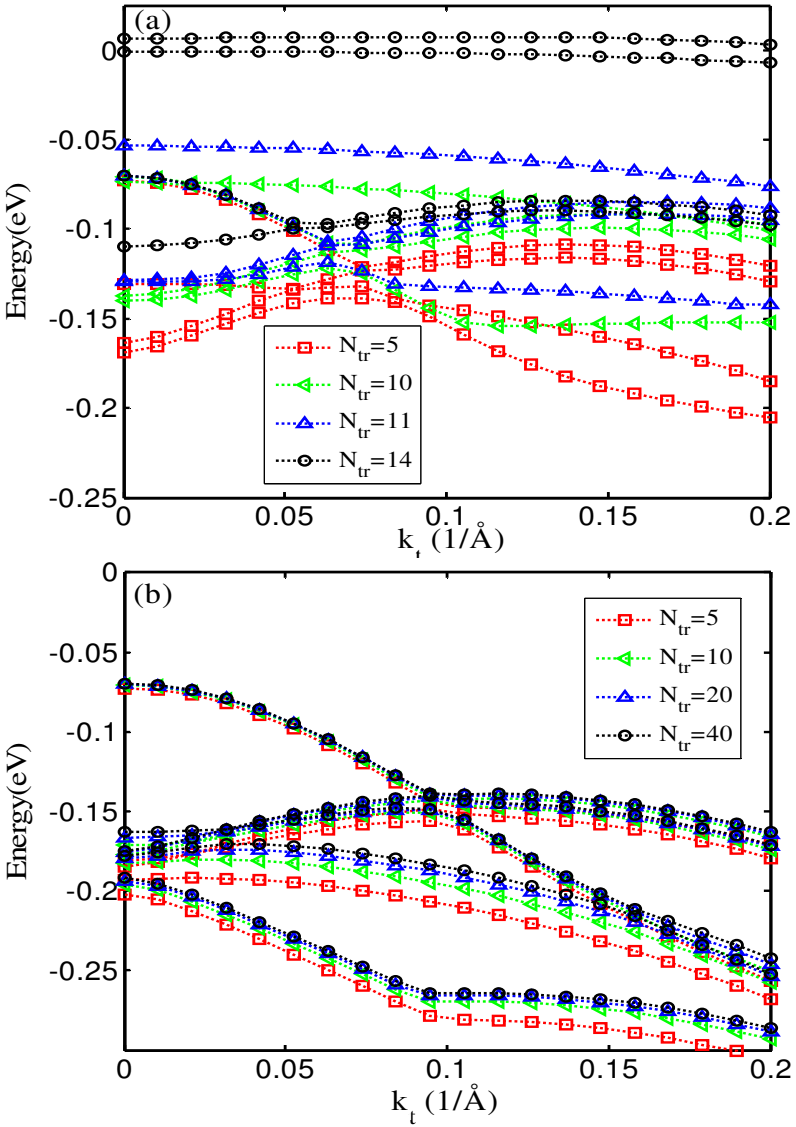


Fig. (a) SYM

- Solutions are not stable as varying N_{tr}
- Spurious solutions turn up quickly even at $k_{||}=0$
- $N_{tr}=5$ is a true solution with very poor computation accuracy

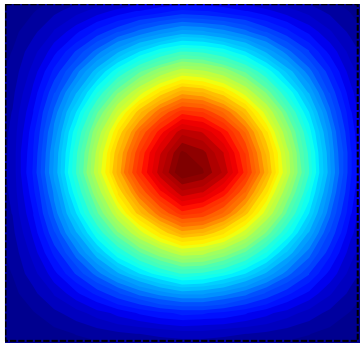
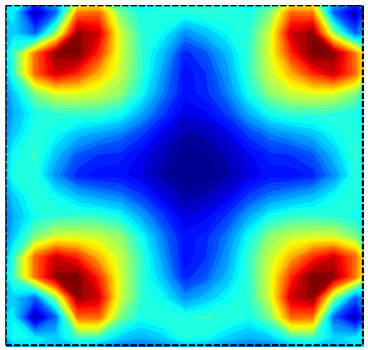
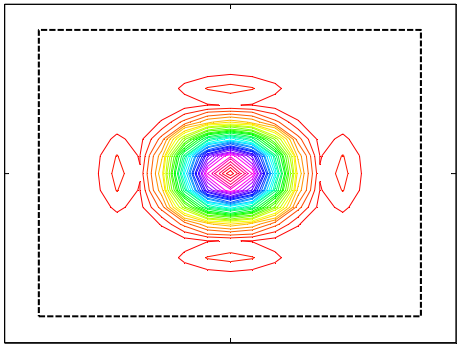
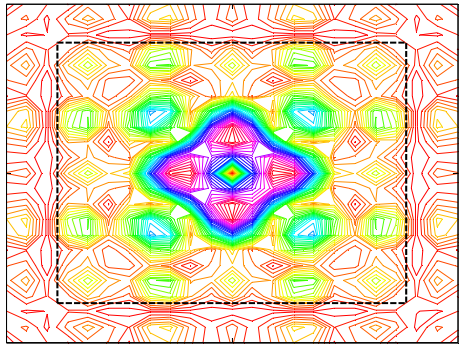
Fig. (b) BF

- Convergent solutions as varying Ntr, even at quite high order of Fourier truncation.
- BF operator ordering can resist the spurious solutions without any control of N_{tr}

➡ BF operator ordering is powerful to eliminate spurious solutions in the six-band calculation for any kind of heterostructure

Q. J. Zhao *et al, J. Appl. Phys.*, **111**, 053702-053708 (2012)

Signature of Spurious solutions in FTM (GaN/AlN QWR)

N_{tr}=10 (Major PDF component)	N_{tr}=11 (Major PDF component)
Eh=-0.0705eV 	Eh=-0.0535eV 
N_{tr}=10 (C_n)	N_{tr}=11 (C_n)
	

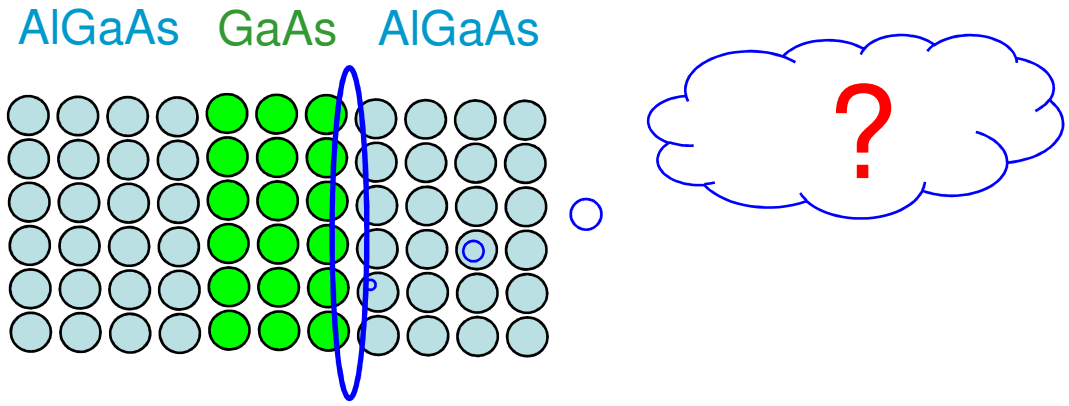
- N_{tr}=11 is the turning point
- The wild-spread distribution of C_n can be taken as the signature of spurious solutions

Q. J. Zhao *et al, J. Appl. Phys.*, **111**, 053702-053708 (2012)

Why is it easy for FTM to deal with spurious solution?

Spurious solution is the innate issue of the k·p method

The k·p method is developed in the BULK scenario, while has to work on heterostructures with discontinuity at interface



but the k·p method is continuum model and not atomistic model

Operating order reformation is effective for some case only(e.g. BF for 6-band)

Truncation of high-order Fourier frequencies eases the discontinuity issue

Merits of FTM with BF operator ordering

- Robust capability to resist spurious solutions
- No change to any material parameters
- No specific boundary condition
- Simple control using N_{tr}, which is much more convenient than other approaches

Summary

Pros of FTM

- No need for meshing
- No numerical differential or integration process
- Easy programming
- Natural control of spurious solutions
- Convenience for optical gain calculation
- Flexibility
  - Arbitrary QD shapes
  - Superlattices / isolated structures
  - Parametric variation

Cons of FTM

- Careful selection of N_{tr}
  - Memory→ limit N_{tr}
  - Spurious solutions → limit N_{tr}
  - Accuracy →large N_{tr}
- Careful selection of periodical length, considering
  - Truncation error
  - Crosstalk error
- Hunger for computer memory in QD calculation
  but not a problem nowadays
  32G→128G→960G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