Solving Polynomial Eigenvalue Problems Arising in Simulations of Nanoscale Quantum Dots

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- Wei-Hua Wang (University of California, Riverside)
- National Science Council
- National Center for Theoretical Science
• Motivation:
  • Nano-physics and engineering

• 3D Models: The Schrödinger equations
  • Geometries
    • Cylinder, pyramid, and irregular types
  • Effective mass
    • Constant effective mass
    • Non-parabolic effective mass
Challenges for the 3D quantum dot models

- Neither analytical nor experimental techniques provide enough useful information
- Lack of efficient 3D numerical simulation tools
- Only several interior eigenvalues are of interest
• Main results:
  • Discretization schemes
    • Simple (finite diff./ finite-vol.); efficient (2nd order conv.)
    • Interface conditions are incorporated
    • Various geometries and various effective mass models
  • Polynomial eigenvalue problem solvers
    • Jacobi-Davidson Methods
    • Deflation/Locking/Restart for the interior eigenpairs
    • Heuristics for correction vectors
    • Efficient and solve large problem (up to 32 million)
  • Physics predictions
Motivation and Model
Nanometer

- $1 \text{ nm} = 10^{-9} \text{ m}$
  
  Nano-scale $\approx 1$-100 nm

- A semiconductor QD $\approx 10$ nm

- QD:hair $\approx 1:10,000$

- Why consider quantum effects?
  
  Small devices imply significant quantum effect.

- “Plenty of Room at the Bottom”
  Richard P. Feynman, 1959
Quantum mechanism

• Quantum dot (0 dim.):
  • An artificial structure that carriers are confined in all three-dimensions (carriers have 0-dim freedom)
  • The carriers exhibit wavelike properties and discrete energy states exist
  • To understand fundamental physics and to inspire applications

• Quantum wire (1 dim.):

• Quantum well (2 dim.):
QD cross-section in Transmission Electron Microscope

- Cross-sections of hetero-structure InAs/GaAs QDs by Transmission Electron Microscope [Schoenfeld, 00]
Nano-scale quantum dot fabrication

- E-beam, chemical solution,… (bigger QDs)
- Molecular beam epitaxy (smaller QDs)

Figure 2.2-1: Schematic of the PCI growth process: (a) As-grown InAs QDs, (b) partial coverage of islands, (c) re-melt, and (d) overgrowth by GaAs.
Energy levels (eigenvalue):

- Each chemical element is associated with a unique energy level.
Wave function (eigenvector)

- Wave function $\varphi$ (eigenvector):
  
  \[ p(x, y, z) = |\varphi(x, y, z)|^2. \]

  (The square of wave function is the probability of finding the particle at a certain location.)

  - Thus $\varphi$ should be normalized.

- Superposition of state (various states exist simultaneously)
  \[ \psi(x, t) = C_1(t) \varphi_2(x) + C_2(t) \varphi_2(x) \]
Mathematics Model:
The Schrödinger equations
(A single electron confined in a 3D quantum dot)
The Schrödinger equation for single particle:

\[-\nabla \cdot \left( \frac{\hbar^2}{2m} \nabla u \right) + V u = \lambda u\]

- \(\lambda\): energy (eigenvalue);  \(u(x,y,z)\): wave function (eigenvector);
- \(m\): effective mass;  \(V\): confinement potential;
- \(\hbar\): reduced Plank constant;

- \(m\) and \(V\) are discontinuous across the heterojunction

\[m = \begin{cases} 
m_1 & \text{in the dot}, \\
m_2 & \text{in the matrix}, 
\end{cases} \quad V = \begin{cases} 
V_1 & \text{in the dot}, \\
V_2 & \text{in the matrix}.
\end{cases}\]
• Effective mass models
  • Constant model
  • Non-parabolic model

\[ \frac{1}{m_\ell(\lambda)} = \frac{P_\ell^2}{\hbar^2} \left( \frac{2}{\lambda + g_\ell - V_\ell} + \frac{1}{\lambda + g_\ell - V_\ell + \delta_\ell} \right), \quad \ell = 1, 2 \]

• \( P_\ell, g_\ell, \delta_\ell \): the momentum, main energy gap, and spin-orbit splitting in the \( l \)-th region, respectively.

\[ E_{c1} = 0.000, \quad E_{c2} = 0.350, \quad E_{g1} = 0.235, \quad E_{g2} = 1.590 \]
\[ \Delta_1 = 0.81, \quad \Delta_2 = 0.80, \quad P_1 = 0.28750, \quad P_2 = 0.19930. \]
The Schrödinger equation (cont.)

- BenDaniel-Duke interface condition

\[ [u] = 0, \quad \frac{1}{m_2} \frac{\partial u}{\partial \vec{n}} \bigg|_{\partial D^+} = \frac{1}{m_1} \frac{\partial u}{\partial \vec{n}} \bigg|_{\partial D^-} \]

- Dirichlet boundary condition

\[
\begin{align*}
-\hbar^2 \frac{\partial F}{2m_1(\lambda) \partial Z} \bigg|_{Z_{\text{top}}^{-}} &= -\hbar^2 \frac{\partial F}{2m_2(\lambda) \partial Z} \bigg|_{Z_{\text{top}}^{t+}} \\
-\hbar^2 \frac{\partial F}{m_1(\lambda) \partial R} \bigg|_{R_{\text{det}}^{-}} &= -\hbar^2 \frac{\partial F}{m_2(\lambda) \partial R} \bigg|_{R_{\text{det}}^{t+}} \\
-\hbar^2 \frac{\partial F}{2m_2(\lambda) \partial Z} \bigg|_{Z_{\text{bom}}^{-}} &= -\hbar^2 \frac{\partial F}{2m_1(\lambda) \partial Z} \bigg|_{Z_{\text{bom}}^{t+}}
\end{align*}
\]

\[ F(R, \theta, Z_{\text{tx}}) = 0 \]

\[ F(R_{\text{tx}}, \theta, Z) = 0 \]

\[ F(R, \theta, 0) = 0 \]
Structure schema of quantum dots

WHLL, JCP (2003)

HW, CMA (2005)

HWW, JNN (2008)

JAP, 90-12, (2001)

HLWW, JCP (2004)

WHC, CPC (2006)

PRB, 54, 8743, (1996)


HWW, JCP, (2007)

Corresponding eigenvalue problems

- \( Ax = \lambda x \)  \( A \): unsymmetric

- \( Ax = \lambda x \)  \( A \): symmetric

- \( Ax = \lambda Bx \)  \( A \): s.p.d. and \( B \): pos. diag.

- **Cubic:** \( (\lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)x = 0 \)

- **Quintic:** \( (\lambda^5 A_5 + \lambda^4 A_4 + \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)x = 0 \)
Numerical schemes

• Large-scale eigensolver for polynomial eigenvalue problems
  • Jacobi-Davidson methods (HLLW, NLAA, 2005)
  • Fixed Point Methods (HLLW, MCM, 2004)
Extreme Large-scale Eigenvalue Problems
Polynomial eigenvalue problems

- General form:

\[
A(\lambda)F = \left( \sum_{i=0}^{\tau} \lambda^i A_i \right) F = 0
\]

- Constant effective mass model

\[
A_0 F = -\lambda A_1 F
\]
Polynomial eigenvalue problems (cont.)

- Non-parabolic effective mass model

\[-\nabla \cdot \left( \frac{\hbar^2}{2m} \nabla u \right) + Vu = \lambda u\]

\[
\frac{1}{m_\ell(\lambda)} = \frac{p_\ell^2}{\hbar^2} \left( \frac{2}{\lambda + g_\ell - V_\ell} + \frac{1}{\lambda + g_\ell - V_\ell + \delta_\ell} \right), \quad \ell = 1, 2
\]

- multiply the common denominator

\[
(\lambda + g_1 - V_1)(\lambda + g_1 - V_1 + \delta_1)
\]

\[
(\lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)F = 0
\]

or

\[
(\lambda + g_1 - V_1)(\lambda + g_1 - V_1 + \delta_1)(\lambda + g_2 - V_2)(\lambda + g_2 - V_2 + \delta_2)
\]

\[
(\lambda^5 A_5 + \lambda^4 A_4 + \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)F = 0
\]
Enlarged linear eigenvalue problem

• Cubic example

\[
\begin{bmatrix}
0 & I & 0 \\
0 & 0 & I \\
A_0 & A_1 & A_2
\end{bmatrix}
\begin{bmatrix}
F \\
\lambda F \\
\lambda^2 F
\end{bmatrix}
= \lambda
\begin{bmatrix}
I & 0 & 0 \\
0 & I & 0 \\
0 & 0 & -A_3
\end{bmatrix}
\]

• Larger size, maybe larger condition number
• Issues on efficiency, accuracy, convergence
• Shifted and invert
Spectrum of the (968) eigenvalues

Spectrum of the fifth order eigenvalue problem

- $\lambda_1 = 0.4408$
- $\lambda_2 = 0.6170$
- $\lambda_3 = 0.6170$

Eigenvalues

-2 -1 0 1 2
Cylindrical quantum dot and quantum dot array
• Discretization
• Eigensolver
• Physics
Discretization scheme

- Seven-point finite difference
- 2-point finite difference at the heterojunction
Mesh points

- Left: Half-mesh shifted in r-dir. No pole condition. [Lai 01]
- Right: Uniform/Non-uniform mesh on a $r$-$z$ plane
The non-uniform meshes
Problem reduction

- Transform the 3D problem to a sequence of 2D problems
- Matrix viewpoint (WHLL 03, JCP)
  - 7-point finite difference
  - Block diagonalizing the coef. matrix by the Fourier matrix
  - Reordering
• Discretization
• Eigensolver
• Physics
The resulting (2D) eigenvalue problems

- Matrix polynomial eigenvalue problems

\[ A(\lambda)F = \left( \sum_{i=0}^{\tau} \lambda^i A_i \right) F = 0 \]

- Linear (\( \tau = 1 \)) for constant effective mass

- Cubic (\( \tau = 3 \)) for non-parabolic effective mass

\[ \frac{1}{m_\ell(\lambda)} = \frac{P_\ell^2}{\hbar^2} \left( \frac{2}{\lambda + g_\ell - c_\ell} + \frac{1}{\lambda + g_\ell - c_\ell + \delta_\ell} \right) \]

where \( P_\ell, g_\ell, \) and \( \delta_\ell \) are the momentum, main energy gap, and spin–orbit splitting in the \( \ell \)th region, respectively. In our numerical experiments, the values of these parameters are \( c_1 = 0.000, g_1 = 0.235, \delta_1 = 0.81, P_1 = 0.2875, c_2 = 0.350, g_2 = 1.590, \delta_2 = 0.80, \) and \( P_2 = 0.1993. \)
Deflation scheme for success eigenvalues

- Explicit non-equivalence deflation

- Original: \( \mathbf{A}(\lambda) = \lambda^3 \mathbf{A}_3 + \lambda^2 \mathbf{A}_2 + \lambda \mathbf{A}_1 + \mathbf{A}_0 \)

- Deflated: \( \tilde{\mathbf{A}}(\lambda) = \lambda^3 \tilde{\mathbf{A}}_3 + \lambda^2 \tilde{\mathbf{A}}_2 + \lambda \tilde{\mathbf{A}}_1 + \tilde{\mathbf{A}}_0 \)

\[
\begin{align*}
\tilde{\mathbf{A}}_0 &= \mathbf{A}_0, \\
\tilde{\mathbf{A}}_1 &= \mathbf{A}_1 - (\mathbf{A}_1 + \lambda_1 \mathbf{A}_2 + \lambda_1^2 \mathbf{A}_3) y_1 y_1^T, \\
\tilde{\mathbf{A}}_2 &= \mathbf{A}_2 - (\mathbf{A}_2 + \lambda_1 \mathbf{A}_3) y_1 y_1^T, \\
\tilde{\mathbf{A}}_3 &= \mathbf{A}_3 - \mathbf{A}_3 y_1 y_1^T,
\end{align*}
\]

where \((\lambda_1, y_1)\) is an eigenpair of \(\mathbf{A}(\lambda)\).
Deflation scheme (cont.)

• Theorem 1.

Let \((\lambda_1, y_1)\) be a simple eigenpair of \(A(\lambda)\) with \(y_1^T y_1 = 1\).

\[
[ \sigma(A(\lambda)) \setminus \{\lambda_1\} ] \cup \{\infty\} = \sigma(\widetilde{A}(\lambda)).
\]
• Theorem 2.

Suppose $\lambda_2 \neq \lambda_1$ and $(\lambda_2, y_2)$ is an eigenpair of $A(\lambda)$.

Let $\tilde{y}_2 = (I - \frac{\lambda_2}{\lambda_1} y_1 y_1^T) y_2$.

Then $(\lambda_2, \tilde{y}_2)$ is an eigenpair of $\tilde{A}(\lambda)$. 

• Discretization
• Eigensolver
• Physics
- Discretization
- Eigensolver
- Physics
Simplification of explicit deflation

- Recursive explicit deflation formula is replaced by representation of original matrices

\[ A_i^{(j+1)} = A_i - \sum_{k=1}^{j} y_i^{(k)} y_k^T, \]

\[ y_i^{(1)} = \sum_{k=i}^{3} \lambda_1^{k-i} A_k y_1, \]

\[ y_i^{(j)} = \sum_{k=i}^{3} \lambda_j^{k-i} \left[ A_k - \sum_{\ell=1}^{j-1} y_k^{(\ell)} y_{\ell}^T \right] y_j, \]
- Discretization
- Eigensolver
- Physics
Energy states spectrum

\[(n_r, n_\theta, n_z)\]

- no. of nodal lines of the wave fits in \( r, \theta, z \) dir.

\( \lambda_{1,2,3} = 0.13 \)
• Discretization
• Eigensolver
• Physics
• The solution is periodical in angle and thus can be approximated by truncated Fourier series

\[ u(r, z, \theta) = \sum_{\ell=-L/2}^{L/2-1} u_\ell(r, z) e^{i\ell\theta}. \]

• The eq. associated with the \( \ell \text{th} \) Fourier mode

\[ -m \left[ \frac{\partial^2 u_\ell}{\partial r^2} + \frac{1}{r} \frac{\partial u_\ell}{\partial r} + \frac{\partial^2 u_\ell}{\partial z^2} - \frac{\ell^2}{r^2} u_\ell \right] + cu_\ell = \lambda u_\ell. \]
Uniform mesh
Finite volume formulas with

- $O(h^2)$ for interior and exterior points
- $O(h)$ for boundary points
The 2D problem

- To simplify the notations, use the following form

\[-m \left[ \partial_r (r \partial_r u) + r \partial_z^2 u \right] + \left( cr + \frac{m\ell^2}{r} \right) u = \lambda ru.\]

- The integral form

\[-\int_{\partial \Omega} m \left[ (-r \partial_z u)dr + r \partial_r udz \right] = \iint_{\Omega} \left( \lambda r - cr - \frac{m\ell^2}{r} \right) u.\]
Top interface points (1/2)

\[
\int_{\partial \Omega_E} m \left[ (-r \partial_z u) dr + r \partial_r u dz \right] = \int_{z_{k-1/2}}^{z_k} m^i r \partial_r u dz + \int_{z_k}^{z_{k+1/2}} m^o r \partial_r u dz
\]

\[
= \frac{m^i}{2} \left[ (r \partial_r u)_{i+1/2, k-1/2} + (r \partial_r u)_{i+1/2, k+1/2} \right] \Delta z
\]

\[
+ \frac{m^o}{2} \left[ (r \partial_r u)_{i+1/2, k-1/2} + (r \partial_r u)_{i+1/2, k+1/2} \right] \Delta z + O(h^3)
\]

\[
= \frac{m^i r_{i+1/2}}{2} \left[ (\partial_r u)_{i+1/2, k} + \frac{1}{2} \left[ (\partial_r u)_{i+1/2, k-1/2} - (\partial_r u)_{i+1/2, k+1/2} \right] \right] \Delta z
\]

\[
+ \frac{m^o r_{i+1/2}}{2} \left[ (\partial_r u)_{i+1/2, k} + \frac{1}{2} \left[ (\partial_r u)_{i+1/2, k-1} - (\partial_r u)_{i+1/2, k+1} \right] \right] \Delta z + O(h^3)
\]

\[
= \frac{m^i r_{i+1/2}}{2} \left[ (\partial_r u)_{i+1/2, k} - \frac{\Delta z}{4} (\partial_z (\partial_r u))_{i+1/2, k} \right] \Delta z
\]

\[
+ \frac{m^o r_{i+1/2}}{2} \left[ (\partial_r u)_{i+1/2, k} + \frac{\Delta z}{4} (\partial_z (\partial_r u))_{i+1/2, k} \right] \Delta z + O(h^3)
\]

\[
= \frac{(m^i + m^o) r_{i+1/2}}{2} (\partial_r u)_{i+1/2, k} \Delta z + O(h^3)
\]

(From interface condition (6))

\[
= \frac{(m^i + m^o) r_{i+1/2}}{2} \frac{u_{i+1, k} - u_{i, k}}{\Delta r} \Delta z + O(h^3).
\]

(21)
- Discretization
- Eigensolver
- Physics
Numerical results

- Campaq AlphaServer DS20E; Dual 667MHz CPUs; 1 GB memory; Tru64 Unix ver. 5.0; Fortran 90;

- Domain [Liu, Voskoboynikov, Li, 01], [Schoenfeld, 00]
  - InAs dot: diameter: 15 nm, height: 2.5 nm
  - GaAs matrix: diameter: 75 nm, height: 12.5 nm

- Matrix size:
  - 3D: 755x280x360 ≈ 76,000,000
  - 2D: 755x280 ≈ 211,000
## Energy states (eigenvalues)

<table>
<thead>
<tr>
<th>j-Ord</th>
<th>$\lambda$</th>
<th>Ite.</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-1</td>
<td>0.0874</td>
<td>1922</td>
<td>2445</td>
</tr>
<tr>
<td>1-2</td>
<td>0.1503</td>
<td>479</td>
<td>661</td>
</tr>
<tr>
<td>1-3</td>
<td>0.2460</td>
<td>815</td>
<td>1231</td>
</tr>
<tr>
<td>1-4</td>
<td>0.3305</td>
<td>1273</td>
<td>2080</td>
</tr>
<tr>
<td>2-1</td>
<td>0.1102</td>
<td>631</td>
<td>799</td>
</tr>
<tr>
<td>2-2</td>
<td>0.1932</td>
<td>524</td>
<td>723</td>
</tr>
<tr>
<td>2-3</td>
<td>0.2972</td>
<td>666</td>
<td>1007</td>
</tr>
<tr>
<td>2-4</td>
<td>0.3385</td>
<td>851</td>
<td>1394</td>
</tr>
<tr>
<td>3-1</td>
<td>0.1387</td>
<td>1727</td>
<td>2204</td>
</tr>
<tr>
<td>3-2</td>
<td>0.2371</td>
<td>525</td>
<td>735</td>
</tr>
<tr>
<td>3-3</td>
<td>0.3454</td>
<td>2091</td>
<td>3191</td>
</tr>
<tr>
<td>3-4</td>
<td>0.3486</td>
<td>759</td>
<td>1252</td>
</tr>
</tbody>
</table>
Structure schema of a QD array

Non-uniform mesh
Ground state energies

- Ground state energies for various spacer layer distances $d_0$
- Number of quantum dots.
Bifurcation for two quantum dots.
When the bifurcation happens
Uniform mesh with 2nd order convergence rate

Non-uniform mesh

Uniform mesh
All bounded state energy levels

![Diagram showing energy levels](image)

<table>
<thead>
<tr>
<th>Figure 2 part</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
<th>(f)</th>
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<tbody>
<tr>
<td>$R_2$ (nm)</td>
<td>8</td>
<td>8</td>
<td>-</td>
<td>-</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>$R_1$ (nm)</td>
<td>8</td>
<td>8</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>$H_1 = H_2$ (nm)</td>
<td>6</td>
<td>6</td>
<td>-</td>
<td>-</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>$D_{gap}$ (nm)</td>
<td>3</td>
<td>6</td>
<td>-</td>
<td>-</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>$R$ (nm)</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>4</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$H$ (nm)</td>
<td>-</td>
<td>-</td>
<td>6</td>
<td>6</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Dynamics of the wave functions
Effect of pile-up dots

- More interactions are found in higher energy levels
Effect of pile-up dots (cont.)

- More interactions are found in higher energy levels
Effect of gap distance

- Smaller gap distance leads to stronger interactions

![Graph showing effect of gap distance](image)
Effect of different size QDs

• Larger dot results in more interactions
Effect of different size QDs

- Larger dots result in more interactions
The bottom QD is fixed as $R_1 = 8$ nm and $H_1 = 6$ nm. The height of the top QD is fixed as $H_2 = 6$ nm. The top dot size $R_2$ is changed from 2 to 8 nm.
Bifurcation for two same size quantum dots.
A close look of the crossing and anti-crossing

Fine mesh \((2560 \times 4320 = 11,059,200)\) with \(\Delta r = \Delta z = 0.0063 \text{ nm}\)
Wave functions in crossing and anti-crossing areas

- **Crossing**
  - 2nd E.V.
  - 3rd E.V.

- **Anti-Crossing**
  - 2nd E.V.
  - 3rd E.V.

Top figures: $R_2 = 3.1981$ nm; Bottom figures: $R_2 = 3.2044$ nm

$(\Delta r = 0.0063$ nm)$
Pyramid quantum dot
- Discretization
- Eigensolver
- Physics
A finite volume discretization

• 3D scheme:

\[-\nabla_h \cdot (\bar{\alpha} \nabla_h u) + \bar{V} u = \lambda u,\]

\(\bar{\alpha}\) and \(\bar{V}\) denote surface and volume average over the control element

• uniform mesh due to the geometric structure

• automatically builds in the interface condition
The 3D scheme

- Exterior/interior points: local truncation error $O(h^2)$
- Interface points: local truncation error $O(h)$
  - Surfaces (N, W, S, E, B)
  - Edges (NW, WS, SE, EN, NB, WB, SB, EB)
  - Corners (NW, WS, SE, EN, Tip)
2nd order convergence rate

\[ \log_2 \left( \frac{\lambda^{(4h)}}{\lambda^{(2h)} - \lambda^{(h)}} \right) \]

<table>
<thead>
<tr>
<th>( (L,M,N) )</th>
<th>Mtx. dim.</th>
<th>( \lambda_1 )</th>
<th>Rate</th>
<th>( \lambda_2 )</th>
<th>Rate</th>
<th>( \lambda_3 )</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>(16, 16, 12)</td>
<td>2,475</td>
<td>0.4226</td>
<td>-</td>
<td>0.6527</td>
<td>-</td>
<td>0.6527</td>
<td>-</td>
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<tr>
<td>(32, 32, 24)</td>
<td>22,103</td>
<td>0.4001</td>
<td>-</td>
<td>0.6423</td>
<td>-</td>
<td>0.6423</td>
<td>-</td>
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<tr>
<td>(64, 64, 48)</td>
<td>186,543</td>
<td>0.3934</td>
<td>1.744</td>
<td>0.6391</td>
<td>1.708</td>
<td>0.6391</td>
<td>1.708</td>
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<tr>
<td>(128,128, 96)</td>
<td>1,532,255</td>
<td>0.3916</td>
<td>1.905</td>
<td>0.6383</td>
<td>1.866</td>
<td>0.6383</td>
<td>1.866</td>
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<tr>
<td>(256,256,192)</td>
<td>12,419,775</td>
<td>0.3911</td>
<td>1.954</td>
<td>0.6380</td>
<td>1.912</td>
<td>0.6380</td>
<td>1.912</td>
</tr>
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</table>

Non-parabolic effective mass model

<table>
<thead>
<tr>
<th>( (L,M,N) )</th>
<th>Mtx. dim.</th>
<th>( \lambda_1 )</th>
<th>Rate</th>
<th>( \lambda_2 )</th>
<th>Rate</th>
<th>( \lambda_3 )</th>
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<td>0.4314</td>
<td>-</td>
<td>0.6101</td>
<td>-</td>
<td>0.6101</td>
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<tr>
<td>(32, 32, 24)</td>
<td>22,103</td>
<td>0.4204</td>
<td>-</td>
<td>0.6022</td>
<td>-</td>
<td>0.6022</td>
<td>-</td>
</tr>
<tr>
<td>(64, 64, 48)</td>
<td>186,543</td>
<td>0.4173</td>
<td>1.813</td>
<td>0.5999</td>
<td>1.793</td>
<td>0.5999</td>
<td>1.793</td>
</tr>
<tr>
<td>(128,128, 96)</td>
<td>1,532,255</td>
<td>0.4165</td>
<td>1.948</td>
<td>0.5993</td>
<td>1.938</td>
<td>0.5993</td>
<td>1.938</td>
</tr>
<tr>
<td>(256,256,192)</td>
<td>12,419,775</td>
<td>0.4163</td>
<td>1.986</td>
<td>0.5991</td>
<td>1.983</td>
<td>0.5991</td>
<td>1.983</td>
</tr>
</tbody>
</table>
• Discretization
• Eigensolver
• Physics
Efficiency on a ordinary PC

- Matrix size: 1,532,255
- Pentium 4 (1.8GHz) and 800MB of main memory

<table>
<thead>
<tr>
<th></th>
<th>Constant effective mass model (Linear eigenvalue problem)</th>
<th>Non-parabolic effective mass model (Quintic eigenvalue problem)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>It. no.</td>
<td>CPU time (sec.)</td>
</tr>
<tr>
<td>$\lambda_1$</td>
<td>0.3916</td>
<td>72</td>
</tr>
<tr>
<td>$\lambda_2$</td>
<td>0.6383</td>
<td>72</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>0.6383</td>
<td>125</td>
</tr>
</tbody>
</table>
**Efficiency on a decent workstation**

- Matrix size: 32,401,863 (352×352 × 264)
- Intel Itanium II (1.0GHz) and 12 GB of main memory.

<table>
<thead>
<tr>
<th></th>
<th>Constant effective mass model</th>
<th>Non-parabolic effective mass model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Linear eigenvalue problem)</td>
<td>(Quintic eigenvalue problem)</td>
</tr>
<tr>
<td>Value</td>
<td>Value</td>
<td>Value</td>
</tr>
<tr>
<td>Ite. no.</td>
<td>Ite. no.</td>
<td>Ite. no.</td>
</tr>
<tr>
<td>CPU time (sec.)</td>
<td>CPU time (sec.)</td>
<td>CPU time (sec.)</td>
</tr>
<tr>
<td>(\lambda_1)</td>
<td>0.3910</td>
<td>0.4162</td>
</tr>
<tr>
<td></td>
<td>138</td>
<td>84</td>
</tr>
<tr>
<td></td>
<td>5,852</td>
<td>4,856</td>
</tr>
<tr>
<td>(\lambda_2)</td>
<td>0.6380</td>
<td>0.5991</td>
</tr>
<tr>
<td></td>
<td>133</td>
<td>74</td>
</tr>
<tr>
<td></td>
<td>5,354</td>
<td>4,835</td>
</tr>
<tr>
<td>(\lambda_3)</td>
<td>0.6380</td>
<td>0.5991</td>
</tr>
<tr>
<td></td>
<td>220</td>
<td>113</td>
</tr>
<tr>
<td></td>
<td>8,511</td>
<td>8,280</td>
</tr>
</tbody>
</table>

(5000 sec ~ 1 hr 20 min; 8600 sec ~ 2 hr 20 min)
Sparsity patterns \((L, M, N) = (8, 8, 6)\)
### Matrices properties

<table>
<thead>
<tr>
<th></th>
<th>$A_0$</th>
<th>$A_1, A_2, A_3$</th>
<th>$A_4, A_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetry</td>
<td>▲ (partial)</td>
<td>▲ (partial)</td>
<td>● yes (Diag. mtx.)</td>
</tr>
<tr>
<td>Diagonal Dominance</td>
<td>● (yes)</td>
<td>▲ (partial)</td>
<td>● yes (Diag. mtx.)</td>
</tr>
</tbody>
</table>

▲ : except the row entries involving interface grids

- **Asymptotic structure**

\[
A_0 F = -\lambda A_1 F + O(h^2) + B,
\]

$B$ is a low rank matrix.
• Discretization
• Eigensolver
• Physics
Wave fts. assoc. w/ $\lambda_1$ and $\lambda_2$
Computational results in energy states

Changes of energy states in terms of truncated QD heights
(Dimension: 63 x 63 x N)
Computational results in wave functions

Figure 8: 3D-Wavefunctions in Truncated Pyramid Quantum Dots (truncated 12.5%)

Figure 9: 3D-Wavefunctions in Truncated Pyramid Quantum Dots (truncated 25%)

Figure 10: 3D-Wavefunctions in Truncated Pyramid Quantum Dots (truncated 50%)

Figure 11: 3D-Wavefunctions in Truncated Pyramid Quantum Dots (truncated 62.5%)
Irregular shape quantum dot
• Discretization
• Eigensolver
• Physics
FIG. 2. X-STM current image of a stack of MBE-grown (512 °C) InAs SADs in GaAs (image size 55×55 nm²). The structure contains five SAD layers formed after deposition of 2.4 ML of InAs for each SAD layer.
Scheme 1: Curvilinear coordinate

\[ A_L \hat{F} = \lambda B_L \hat{F}, \]

- Matrix $A_L$: Sym. Pos. Def.; 9 nonzeros each row
- Matrix $B_L$: diagonal matrix
Scheme 2: The skewed coordinate

\[ A_S \hat{F} = \lambda B_S \hat{F} \]

- Matrix \( A_S \): Sym. Pos. Def.; 9 nonzeros each row
- Matrix \( B_S \): diagonal matrix
Scheme 3: Mixed coordinate

\[ A_M \hat{F}^n = \lambda B_M \hat{F}^n \]

\[ A_M = wA_L + (1 - w)A_S, \quad B_M = B_L = B_S \]

- Symmetry preserving average
- Not clear how \( \omega \) affects the convergence of the eigenvalue solver analytically
- Numerical investigation provides some clues
Effect of the symmetry average parameter

Fig. 11. The timing results for computing eigenvalues. Scheme $S_s$ and $S_c$ are corresponding to the cases that $\omega = 0$ and 1, respectively. Results for scheme $S_m$ are shown in the part that $\omega \neq 0$. Part (a) and (b) demonstrate the total and average timing in seconds for various $\omega$, respectively.
Fig. 12. The eigenvalue convergence rates for schemes $S_c$, $S_s$, and $S_m$ are shown in part (a), (b) and (c), respectively.
## Summary of the proposed schemes

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Formula</th>
<th>False Eigenpair</th>
<th>Timing</th>
<th>Conv. Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_c$</td>
<td>In between</td>
<td>None</td>
<td>Slow</td>
<td>$\approx 2$</td>
</tr>
<tr>
<td>$S_s$</td>
<td>Simple</td>
<td>Several</td>
<td>Quick</td>
<td>$\approx 2$ (with variation)</td>
</tr>
<tr>
<td>$S_m$</td>
<td>Complex</td>
<td>None</td>
<td>Quickest (for $\omega = 0.1$)</td>
<td>$\approx 2$</td>
</tr>
</tbody>
</table>
• Discretization
• Eigensolver
• Physics
A Jacobi-Davidson method with locking (and restarting)

Algorithm (Jacobi-Davidson Algorithm for solving $A(\lambda)x = 0$)

Choose an $n$-by-$m$ orthonormal matrix $V_0$

Do $k = 0, 1, 2, \ldots$

- Compute all the eigenpairs of $V_k^T A(\lambda) V_k = 0$.
- Select the desired (target) eigenpair $(\theta_k, s_k)$ with $\|s_k\|_2 = 1$.
- Compute $u_k = V_k s_k$, $r_k = A(\theta_k) u_k$ and $p_k = A'(\theta_k) u_k$.
- If ($\|r_k\|_2 < \varepsilon$), $\lambda = \theta_k$, $x = u_k$, Stop.
- Solve (approximately) a $t_k \perp u_k$ from

$$
(l - \frac{p_k u_k^T}{u_k^T p_k}) A(\theta_k) (I - u_k u_k^T) t = -r_k.
$$

- Orthogonalize $t_k \perp V_k \rightarrow v_{k+1}$, $V_{k+1} = [V_k, v_{k+1}]$
Solving the correction equation

- Sleijpen and van der Vorst (SIMA96)

\[
\left( I - \frac{p_k}{u^*_k p_k} \right) \left( A - \theta_k B \right) \left( I - \frac{u_k p_k^*}{u^*_k p_k} \right) t = -r_k
\]

\[
\mathcal{M}_p = \left( I - \frac{p_k}{u^*_k p_k} \right) \mathcal{M}_p \left( I - \frac{u_k p_k^*}{u^*_k p_k} \right) \approx \left( I - \frac{p_k}{u^*_k p_k} \right) \left( A - \theta_k B \right) \left( I - \frac{u_k p_k^*}{u^*_k p_k} \right)
\]

\[
\mathcal{M}_p t = y
\]

\[
t = \mathcal{M}^{-1} y - \zeta \mathcal{M}^{-1} Bu_k
\]

where

\[
\zeta = \frac{u_k^T B \mathcal{M}^{-1} y}{u_k^T B \mathcal{M}^{-1} Bu_k}.
\]
Computing the smallest positive eigenvalue

(v) Solve Eq. (33) (approximately) to obtain a \( t \perp_B u_k \) by the method determined below.

If \( k \leq 9 \) then

Use \{BiCGSTAB, No precond., 7, 10^{-3}\}

else

Use \{GMRES, SSOR, 30, 10^{-3}\}

End if

Fig. 5. The heuristic strategy for computing the smallest positive eigenvalue.

- **SSOR:** \( M = (D + \sigma L)D^{-1}(D + \sigma U) \)
Computing the successive eigenvalues

(v) Solve Eq. (33) (approximately) to obtain a $t \perp_B u_k$
by the method determined below.
If ($\| r_k \|_2 > 0.1$ and $k < 10$) then
  Use \{BiCGSTAB, No precond., 7, $10^{-3}$\}
else if ($\| r_k \|_2 \geq 0.1$ and $k > 14$) then
  Use \{GMRES, SSOR, 30, $10^{-3}$\}
else if ($\| r_k \|_2 < 0.1$ and $\| r_{k-1} \|_2 / \| r_k \|_2 < 4$) then
  Set $j = \min(30, j + 2)$ and use \{GMRES, SSOR, $j$, $10^{-3}$\}
else
  Use \{GMRES, SSOR, $j$, $10^{-3}$\}
End if

Fig. 6. The heuristic strategy for computing eigenvalues other than the smallest positive one.
Performance of SSOR preconditioner

- Dimension: 1,935,090
- HP workstation with 1.3GHz Intel Itanium II CPU with 24 GB memory
- Average timing for computing all target eigenpairs
• Discretization
• Eigensolver
• Physics
Fig. 9. The spectrums of energy levels (eigenvalues) computed by schemes $S_c$, $S_s$, and $S_m$ are shown in part (a), (b), and (c), respectively. Scheme $S_s$ has produced several extra eigenvalues due to the discretization scheme. These false eigenvalues are plotted by dashed lines in part (b).
• Ground state ($\lambda_1=0.3869$ eV), 1st excited ($\lambda_2=0.6670$ eV), and 2nd excited ($\lambda_3=0.7410$ eV) state energy

• The first three eigenvectors associated with the first three smallest positive eigenvalues.
Conclusion
A “computational science” approach

- Discretization scheme
  - non-uniform mesh, uniform mesh
  - finite-diff. on cylindrical cord.
  - finite-volume on Cartesian and curvilinear coordinate

- Large-scale matrix computation
  - matrix reduction
  - nonlinear eigenvalue solver
  - deflation scheme
  - accelerator

- The 3D model: Schrödinger eqs. with constant or non-parabolic effective mass approx.

- Concerning issues: eng. level & wave ft.

- Computed results verifications, explanations, applications

- Practical algorithms (for a certain architecture and language)

- Robust & efficient implementations

- Numerical experiments

- Computational and visual results
Thank you.