Jacobi Davidson method and its applications

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Outline

Some basic theorems

Eigenproblems

- Standard eigenproblems: $Ax = \lambda x$
- Generalized eigenproblems: $Ax = \lambda Bx$
- Higher order poly. eigenproblems: $(A_0 + \lambda A_1 + ... + \lambda^n A_n)x = 0$
- Eigenproblems of λ-matrices: $F(\lambda)x = 0$

What do we care ?

(i) In theory: eigenstructure, spectrum decomposition, canonical form, . . . , etc.

(ii) In computation: eigenvalues, eigenvectors, invariant subspaces, . . . , etc.

Theorem (Fischer)

Let the Hermitian matrix A have eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

Then

$$\lambda_i = \min_{dim(\mathcal{W})=n-i+1} \left\{ \max_{w\in\mathcal{W}, \|w\|_2=1} w^H A w \right\}$$

and

$$\lambda_i = \max_{dim(\mathcal{W})=i} \left\{ \min_{w\in\mathcal{W}, \|w\|_2=1} w^H A w \right\}.$$

Theorem

Let $\mathcal{X}$ be an eigenspace of A and let X be a basis for $\mathcal{X}$. Then there is a unique matrix L such that

$$AX = XL.$$

The matrix L is given by

$$L = X^I AX,$$

where X^I is a matrix satisfying $X^I X = I$.
If (λ, x) is an eigenpair of A with $x \in \mathcal{X}$, then $(\lambda, X^I x)$ is an eigenpair of L.
Conversely, if (λ, u) is an eigenpair of L, then (λ, Xu) is an eigenpair of A.

Proof:

Let

$$X = [x_1 \cdots x_k] \quad \text{and} \quad Y = AX = [y_1 \cdots y_k].$$

Since $y_i \in \mathcal{X}$ and X is a basis for $\mathcal{X}$, there is a unique vector ℓ_i such that

$$y_i = X\ell_i.$$

If we set $L = [\ell_1 \cdots \ell_k]$, then $AX = XL$ and

$$L = X^I XL = X^I AX.$$

Now let (λ, x) be an eigenpair of A with $x \in \mathcal{X}$. Then there is a unique vector u such that $x = Xu$. However, $u = X^I x$. Hence

$$\lambda x = Ax = AXu = XLu \quad \Rightarrow \quad \lambda u = \lambda X^I x = Lu.$$

Conversely, if $Lu = \lambda u$, then

$$A(Xu) = (AX)u = (XL)u = X(Lu) = \lambda(Xu),$$

so that (λ, Xu) is an eigenpair of A.

Theorem (Optimal residuals)

Let $[X \ X_\perp]$ be unitary. Let

$$R = AX - XL \quad \text{and} \quad S^H = X^H A - LX^H.$$

Then $\|R\|$ and $\|S\|$ are minimized when

$$L = X^H AX,$$

in which case

$$\begin{array}{ll} (a) & \|R\| = \|X_\perp^H AX\|, \\ (b) & \|S\| = \|X^H AX_\perp\|, \\ (c) & X^H R = 0. \end{array}$$

Proof:

Set

$$\begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} A \begin{bmatrix} X & X_\perp \end{bmatrix} = \begin{bmatrix} \hat{L} & H \\ G & M \end{bmatrix}.$$

Then

$$\begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} R = \begin{bmatrix} \hat{L} & H \\ G & M \end{bmatrix} \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} X - \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} XL = \begin{bmatrix} \hat{L} - L \\ G \end{bmatrix}.$$

It implies that

$$\|R\| = \left\| \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} R \right\| = \left\| \begin{bmatrix} \hat{L} - L \\ G \end{bmatrix} \right\|,$$

which is minimized when $L = \hat{L} = X^H AX$ and

$$\min \|R\| = \|G\| = \|X_\perp^H AX\|.$$

The proof for S is similar. If $L = X^H AX$, then

$$X^H R = X^H AX - X^H XL = X^H AX - L = 0.$$

Definition

Let X be of full column rank and let X^I be a left inverse of X. Then $X^I AX$ is a Rayleigh quotient of A.

Theorem

Let X be orthonormal, A be Hermitian and

$$R = AX - XL.$$

If $\ell_1, \ldots, \ell_k$ are the eigenvalues of L, then there are eigenvalues $\lambda_{j_1}, \ldots, \lambda_{j_k}$ of A such that

$$|\ell_i - \lambda_{j_i}| \leq \|R\|_2 \quad \text{and} \quad \sqrt{\sum_{i=1}^{k} (\ell_i - \lambda_{j_i})^2} \leq \sqrt{2}\|R\|_F.$$

Jacobi's orthogonal component correction (JOCC), 1846

Consider the eigenvalue problem

$$A \begin{bmatrix} 1 \\ z \end{bmatrix} \equiv \begin{bmatrix} \alpha & c^T \\ b & F \end{bmatrix} \begin{bmatrix} 1 \\ z \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ z \end{bmatrix}, \quad (1)$$

where A is diagonal dominant and α is the largest diagonal element. (1) is equivalent to

$$\begin{cases} \lambda = \alpha + c^T z, \\ (F - \lambda I)z = -b. \end{cases}$$

Jacobi iteration : (with $z_1 = 0$)

$$\begin{cases} \theta_k = \alpha + c^T z_k, \\ (D - \theta_k I)z_{k+1} = (D - F)z_k - b \end{cases} \quad (2)$$

where $D = \mathrm{diag}(F)$.

Davidson's method (1975)

Algorithm (Davidson's method)

Given unit vector v, set $V = [v]$
Iterate until convergence
  Compute desired eigenpair (θ, s) of $V^T AV$.
  Compute $u = Vs$ and $r = Au - \theta u$.
  If $(\| r \|_2 < \varepsilon)$, stop.
  Solve $(D_A - \theta I)t = r$.
  Orthog. $t \perp V \rightarrow v$, $V = [V, v]$
end

Let $u_k = (1, z_k^T)^T$. Then

$$r_k = (A - \theta_k I)u_k = \begin{bmatrix} \alpha - \theta_k + c^T z_k \\ (F - \theta_k I)z_k + b \end{bmatrix}$$

Substituting the residual vector r_k into linear systems

$$(D_A - \theta_k I)t_k = -r_k, \quad \text{where} \quad D_A = \begin{bmatrix} \alpha & 0 \\ 0 & D \end{bmatrix},$$

we get

$$\begin{aligned} (D - \theta_k I)y_k &= -(F - \theta_k I)z_k - b \\ &= (D - F)z_k - (D - \theta_k I)z_k - b \end{aligned}$$

From (2) and above equality, we see that

$$(D - \theta_k I)(z_k + y_k) = (D - F)z_k - b = (D - \theta_k I)z_{k+1}$$

This implies that $z_{k+1} = z_k + y_k$ as one step of JOCC starting with z_k.

Polynomial eigenvalue problems

- Polynomial eigenvalue problems:

$$\mathbf{A}(\lambda)x \equiv \left(\lambda^\tau A_\tau + \cdots + +\lambda^2 A_2 + \lambda A_1 + A_0\right) x = 0. \tag{3}$$

- Enlarged linear eigenvalue problem: (e.g. cubic polynomial)

$$\begin{bmatrix} 0 & I & 0 \\ 0 & 0 & I \\ A_0 & A_1 & A_2 \end{bmatrix} \begin{bmatrix} x \\ \lambda x \\ \lambda^2 x \end{bmatrix} = \lambda \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -A_3 \end{bmatrix} \begin{bmatrix} x \\ \lambda x \\ \lambda^2 x \end{bmatrix}.$$

- Disadvantages:
  - The order of the larger matrices are tripled
  - The condition number of eigenvalues and eigenvectors may increase

- Consider the quadratic eigenvalue problem[1]

$$Q(\lambda)x \equiv \left(\lambda^2 M + \lambda C + K\right) x = 0$$

with

$$M = \frac{1}{2} I_n,\ \ K = \mathrm{diag}_{1\le j\le n}\left(j^2\pi^2(j^2\pi^2 + \tau - \kappa v^2)/2\right),$$

$$C = -C^T = (c_{ij}) \ \text{ with } \ c_{ij} = \begin{cases} \frac{4ij}{j^2-i^2} v & \text{if } i+j \text{ is odd} \\ 0 & \text{otherwise.} \end{cases}$$

Take $v = 10, \kappa = 0.8$ and $\tau = 77.9$.

- Enlarged linear eigenvalue problem:

$$\begin{bmatrix} K & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ \lambda x \end{bmatrix} = \lambda \begin{bmatrix} -C & -M \\ I & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda x \end{bmatrix}$$

[1] F. Tisseur and K. Meerbergen, SIAM Rev. Vol. 43, pp. 235-286, 2001

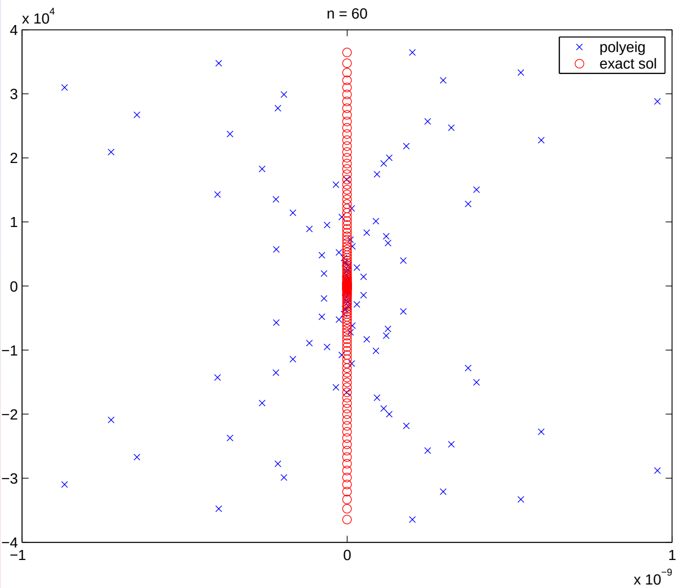


Figure: The spectrum of $Q(\lambda)$

Polynomial Jacobi-Davidson method

(θ_k, u_k): approx. eigenpair of $\mathbf{A}(\lambda)$, $\theta_k \approx \lambda$, with

$$u_k = V_k s_k, \quad V_k^T \mathbf{A}(\lambda) V_k s_k = 0 \quad \text{and} \quad \| s_k \|_2 = 1.$$

Let

$$r_k = \mathbf{A}(\theta_k) u_k.$$

Then

$$u_k^T r_k = u_k^T \mathbf{A}(\theta_k) u_k = s_k^T V_k^T \mathbf{A}(\theta_k) V_k s_k = 0 \;\Rightarrow\; r_k \perp u_k$$

Find the correction t such that

$$\mathbf{A}(\lambda)(u_k + t) = 0.$$

That is

$$\mathbf{A}(\lambda) t = -\mathbf{A}(\lambda) u_k = -r_k + (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda)) u_k.$$

Let

$$p_k = \mathbf{A}'(\theta_k)u_k \equiv \left(\sum_{i=1}^{\tau} i\theta_k^{i-1} A_i \right) u_k.$$

- $\mathbf{A}(\lambda) = A - \lambda I$:

$$\begin{aligned} p_k &= -u_k, \\ (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= (\lambda - \theta_k)u_k = (\theta_k - \lambda_k)p_k \end{aligned}$$

- $\mathbf{A}(\lambda) = A - \lambda B$:

$$\begin{aligned} p_k &= -Bu_k, \\ (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= (\lambda - \theta_k)Bu_k = (\theta_k - \lambda)p_k \end{aligned}$$

- $\mathbf{A}(\lambda) = \sum_{i=0}^{\tau} \lambda^i A_i$ with $\tau \geq 2$:

$$\begin{aligned} (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= \left[(\theta_k - \lambda)\mathbf{A}'(\theta_k) - \frac{1}{2}(\theta_k - \lambda)^2 \mathbf{A}''(\xi_k) \right] u_k \\ &= (\theta_k - \lambda)p_k - \frac{1}{2}(\theta_k - \lambda)^2 \mathbf{A}''(\xi_k)u_k \end{aligned}$$

Hence

$$\mathbf{A}(\lambda)t = -r_k + (\theta_k - \lambda)p_k - \frac{1}{2}(\theta_k - \lambda)^2 \mathbf{A}''(\xi_k)u_k$$

Since $r_k \perp u_k$, we have

$$\left(I - \frac{p_k u_k^T}{u_k^T p_k}\right)\mathbf{A}(\lambda)t = -r_k - \frac{1}{2}(\theta_k - \lambda)^2 \left(I - \frac{p_k u_k^T}{u_k^T p_k}\right)\mathbf{A}''(\xi_k)u_k.$$

Correction equation:

$$\left(I - \frac{p_k u_k^T}{u_k^T p_k}\right)\mathbf{A}(\theta_k)(I - u_k u_k^T)t = -r_k \quad \text{and} \quad t \perp u_k,$$

or

$$\left(I - \frac{p_k u_k^T}{u_k^T p_k}\right)(A - \theta_k B)\left(I - \frac{u_k p_k^T}{p_k^T u_k}\right)t = -r_k \quad \text{and} \quad t \perp_B u_k,$$

with symmetric positive definite matrix B.

Solving correction vector t

Correction equation:

$$\left(I - \frac{p_k u_k^T}{u_k^T p_k}\right) \mathbf{A}(\theta_k)(I - u_k u_k^T)t = -r_k. \tag{4}$$

Method I:

- Use preconditioning iterative approximations, e.g., GMRES, to solve (4).
- Use a preconditioner

$$\mathcal{M}_p \equiv \left(I - \frac{p_k u_k^T}{u_k^T p_k}\right) \mathcal{M} \left(I - u_k u_k^T\right) \approx \left(I - \frac{p_k u_k^T}{u_k^T p_k}\right) \mathbf{A}(\theta_k) \left(I - u_k u_k^T\right),$$

  where $\mathcal{M}$ is an approximation of $\mathbf{A}(\theta_k)$.
- In each of the iterative steps, it needs to solve the linear system

$$\mathcal{M}_p t = y, \quad t \perp u_k \tag{5}$$

  for a given y.

- Since $t \perp u_k$, Eq. (5) can be rewritten as

$$\left(I - \frac{p_k u_k^T}{u_k^T p_k}\right)\mathcal{M}t = y \;\Rightarrow\; \mathcal{M}t = \frac{u_k^T \mathcal{M}t}{u_k^T p_k} p_k + y \equiv \eta_k p_k + y.$$

Hence

$$t = \mathcal{M}^{-1}y + \eta_k \mathcal{M}^{-1} p_k,$$

where

$$\eta_k = -\frac{u_k^T \mathcal{M}^{-1} y}{u_k^T \mathcal{M}^{-1} p_k}.$$

- SSOR preconditioner: Let $\mathbf{A}(\theta_k) = L + D + U$. Then

$$\mathcal{M} = (D + \omega L)D^{-1}(D + \omega U).$$

Method II: Since $t \perp u_k$, Eq. (4) can be rewritten as

$$\mathbf{A}(\theta_k)t = \frac{u_k^T \mathbf{A}(\theta_k)t}{u_k^T p_k} p_k - r_k \equiv \varepsilon p_k - r_k. \tag{6}$$

- Let t_1 and t_2 be approximated solutions of the following linear systems:

$$\mathbf{A}(\theta_k)t = -r_k \quad \text{and} \quad \mathbf{A}(\theta_k)t = p_k,$$

respectively. Then the approximated solution $\tilde{t}$ for (6) is

$$\tilde{t} = t_1 + \varepsilon t_2 \quad \text{for} \quad \varepsilon = -\frac{u_k^T t_1}{u_k^T t_2}.$$

- The approximated solution $\tilde{t}$ for (6) is

$$\tilde{t} = -\mathcal{M}^{-1} r_k + \varepsilon \mathcal{M}^{-1} p_k \quad \text{for} \quad \varepsilon = \frac{u_k^T \mathcal{M}^{-1} r_k}{u_k^T \mathcal{M}^{-1} p_k},$$

where $\mathcal{M}$ is an approximation of $\mathbf{A}(\theta_k)$.

Method III:

- Eq. (6) implies that

$$t = \varepsilon \mathbf{A}(\theta_k)^{-1} p_k - \mathbf{A}(\theta_k)^{-1} r_k = \varepsilon \mathbf{A}(\theta_k)^{-1} p_k - u_k.$$

Let t_1 be approximated solution of the following linear system:

$$\mathbf{A}(\theta_k) t = p_k.$$

Then the approximated solution $\tilde{t}$ for (6) is

$$\tilde{t} = \varepsilon t_1 - u_k \quad \text{for} \quad \varepsilon = \left(u_k^T t_1 \right)^{-1}.$$

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

Choose an n-by-m orthonormal matrix V_0

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

Compute all the eigenpairs of $V_k^T \mathbf{A}(\lambda) V_k = 0$.

Select the desired (target) eigenpair (θ_k, s_k) with $\|s_k\|_2 = 1$.

Compute $u_k = V_k s_k$, $r_k = \mathbf{A}(\theta_k) u_k$ and $p_k = \mathbf{A}'(\theta_k) u_k$.

If $(\|r_k\|_2 < \varepsilon)$, $\lambda = \theta_k$, $x = u_k$, Stop

Solve (approximately) a $t_k \perp u_k$ from

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

Orthogonalize $t_k \perp V_k \rightarrow v_{k+1}$, $V_{k+1} = [V_k, v_{k+1}]$

Restarting

- A double precision real variable needs to 8 bytes to save in Memory.
- 125 double precision real variables $\approx$ 1 KB
- $125,000$ double precision real variables $\approx$ 1 MB
- Keep the locked Schur vectors as well as the Schur vectors of interest in the subspace and throw away those we are not interested.

(v) Solve correct equation (approximately) to obtain a $t \perp u_k$ by the method determined below.

If ($\|r_k\|_2 > 0.1$ and $k \leq 9$) then

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

else

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

End if

Figure: The heuristic strategy for computing the first target eigenvalue.

Locking for $Ax = \lambda x$

V_k with $V_k^* V = I_k$ are convergent Schur vectors, i.e.,

$$AV_k = V_k T_k$$

for some upper triangular T_k. Set $V = [V_k, V_q]$ with $V^* V = I_{k+q}$ in $k+1$-th iteration of Jacobi-Davidson Algorithm. Then

$$\begin{aligned} V^* AV &= \begin{bmatrix} V_k^* AV_k & V_k^* AV_q \\ V_q^* AV_k & V_q^* AV_q \end{bmatrix} = \begin{bmatrix} T_k & V_k^* AV_q \\ V_q^* V_k T_k & V_q^* AV_q \end{bmatrix} \\ &= \begin{bmatrix} T_k & V_k^* AV_q \\ 0 & V_q^* AV_q \end{bmatrix}. \end{aligned}$$

Locking Polynomial Jacobi–Davidson Method

(0) Given $\mathbf{A}(\lambda) = \sum_{i=0}^{\tau} \lambda^i A_i$ and the number of desired eigenvalues σ.

(1) Initialize $V = [V_{ini}]$ as an orthonormal matrix and $V_x = []$.

(2) For $j = 1, 2, ..., \sigma$

- (2.1) Iterate until convergence
  - (i) Compute the jth desired eigenpairs (θ, s) of $V^T \mathbf{A}(\theta) V$.
  - (ii) Compute $u = Vs$, $p = \mathbf{A}'(\theta)u$, and $r = \mathbf{A}(\theta)u$.
  - (iii) If $(||r||_2 < \varepsilon)$, Set $\lambda_j = \theta$, $x_j = u$, Goto Step (2.2).
  - (iv) Solve (approximately) a $t \perp u$ from $(I - \frac{pu^T}{u^T p})\mathbf{A}(\theta)(I - uu^T)t = -r$.
  - (v) Orthogonalize $t \perp V \to v$, $V = [V, v]$
- (2.2) Orthogonalize $x_j \perp V_x \to x_j$; $V_x = [V_x, x_j]$
- (2.3) Choose an orthonormal matrix $V_{ini} \perp V_x$; Set $V = [V_x, V_{ini}]$

Ref: G. L. G. Sleijpen, G. L. Booten, D. R. Fokkema and H. A. van der Vorst, BIT, 36:595-633, 1996

(v) Solve correct equation (approximately) to obtain a $t \perp u_k$ 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

Figure: The heuristic strategy for computing eigenvalues other than the first convergent eigenvalue.

Non-equivalence deflation of quadratic eigenproblems

Let λ_1 be a real eigenvalue of $\mathbf{Q}(\lambda)$ and x_1, z_1 be the associated right and left eigenvectors, respectively, with $z_1^T K x_1 = 1$. Let

$$\theta_1 = (z_1^T M x_1)^{-1}.$$

We introduce a deflated quadratic eigenproblem

$$\widetilde{\mathbf{Q}}(\lambda)x \equiv \left[\lambda^2 \widetilde{M} + \lambda \widetilde{C} + \widetilde{K}\right] x = 0,$$

where

$$\begin{aligned}
\widetilde{M} &= M - \theta_1 M x_1 z_1^T M, \\
\widetilde{C} &= C + \frac{\theta_1}{\lambda_1}(M x_1 z_1^T K + K x_1 z_1^T M), \\
\widetilde{K} &= K - \frac{\theta_1}{\lambda_1^2} K x_1 z_1^T K.
\end{aligned}$$

Complex deflation

Let $\lambda_1 = \alpha_1 + i\beta_1$ be a complex eigenvalue of $\mathbf{Q}(\lambda)$ and $x_1 = x_{1R} + ix_{1I}$, $z_1 = z_{1R} + iz_{1I}$ be the associated right and left eigenvectors, respectively, such that

$$Z_1^T K X_1 = I_2,$$

where $X_1 = [x_{1R}, x_{1I}]$ and $Z_1 = [z_{1R}, z_{1I}]$. Let

$$\Theta_1 = (Z_1^T M X_1)^{-1}.$$

Then we introduce a deflated quadratic eigenproblem with

$$\begin{aligned}
\widetilde{M} &= M - MX_1\Theta_1 Z_1^T M, \\
\widetilde{C} &= C + MX_1\Theta_1\Lambda_1^{-T} Z_1^T K + KX_1\Lambda_1^{-1}\Theta_1^T Z_1^T M, \\
\widetilde{K} &= K - KX_1\Lambda_1^{-1}\Theta_1\Lambda_1^{-T} Z_1^T K
\end{aligned}$$

in which $\Lambda_1 = \begin{bmatrix} \alpha_1 & \beta_1 \\ -\beta_1 & \alpha_1 \end{bmatrix}$.

Theorem

(i) *Let* λ_1 *be a simple real eigenvalue of* $\mathbf{Q}(\lambda)$*. Then the spectrum of* $\widetilde{\mathbf{Q}}(\lambda)$ *is given by*

$$\left(\sigma(\mathbf{Q}(\lambda))\diagdown\{\lambda_1\}\right) \cup \{\infty\}$$

provided that $\lambda_1^2 \neq \theta_1$.

(ii) *Let* λ_1 *be a simple complex eigenvalue of* $\mathbf{Q}(\lambda)$*. Then the spectrum of* $\widetilde{\mathbf{Q}}(\lambda)$ *is given by*

$$\left(\sigma(\mathbf{Q}(\lambda))\diagdown\{\lambda_1, \bar{\lambda}_1\}\right) \cup \{\infty, \infty\}$$

provided that $\Lambda_1 \Lambda_1^T \neq \Theta_1$.

Furthermore, in both cases (i) and (ii), if $\lambda_2 \neq \lambda_1$ *and* (λ_2, x_2) *is an eigenpair of* $\mathbf{Q}(\lambda)$ *then the pair* (λ_2, x_2) *is also an eigenpair of* $\widetilde{\mathbf{Q}}(\lambda)$.

Ref: T.-M. Hwang, W.-W. Lin and V. Mehrmann, SIAM J. Sci. Comput.

Suppose that M, C, K are symmetric. Given an eigenmatrix pair $(\Lambda_1, X_1) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}$ of $Q(\lambda)$, where Λ_1 is nonsingular and X_1 satisfies

$$X_1^T K X_1 = I_r, \qquad \Theta_1 := (X_1^T M X_1)^{-1}.$$

We define $\tilde{Q}(\lambda) := \lambda^2 \tilde{M} + \lambda \tilde{C} + \tilde{K}$, where

$$\begin{aligned} \tilde{M} &:= M - MX_1\Theta_1 X_1^T M, \\ \tilde{C} &:= C + MX_1\Theta_1\Lambda_1^{-T}X_1^T K + KX_1\Lambda_1^{-1}\Theta_1 X_1^T M, \\ \tilde{K} &:= K - KX_1\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}X_1^T K. \end{aligned}$$

Theorem

Suppose that $\Theta_1 - \Lambda_1\Lambda_1^T$ is nonsingular. Then the eigenvalues of the real symmetric quadratic pencil $\tilde{Q}(\lambda)$ are the same as those of $Q(\lambda)$ except that the eigenvalues of Λ_1, which are closed under complex conjugation, are replaced by r infinities.

Proof:

Since (Λ_1, X_1) is an eigenmatrix pair of $Q(\lambda)$, i.e.,

$$MX_1\Lambda_1^2 + CX_1\Lambda_1 + KX_1 = 0,$$

we have

$$\begin{aligned}\tilde{Q}(\lambda) &= Q(\lambda) + [MX_1(\lambda I_r + \Lambda_1) + CX_1]\,\Theta_1\Lambda_1^{-T}(X_1^T K - \lambda\Lambda_1^T X_1^T M) \\ &= Q(\lambda) + Q(\lambda)X_1(\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(X_1^T K - \lambda\Lambda_1^T X_1^T M).\end{aligned}$$

By using the identity

$$\det(I_n + RS) = \det(I_m + SR),$$

where $R, S^T \in \mathbb{R}^{n\times m}$, we have

$$\begin{aligned}&\det[\tilde{Q}(\lambda)] \\ =\ & \det[Q(\lambda)]\det[I + X_1(\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(X_1^T K - \lambda\Lambda_1^T X_1^T M)] \\ =\ & \det[Q(\lambda)]\det[I_r + (\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(I_r - \lambda\Lambda_1^T\Theta_1^{-1})] \\ =\ & \frac{\det[Q(\lambda)]}{\det(\lambda I_r - \Lambda_1)}\det(\Theta_1\Lambda_1^{-T} - \Lambda_1).\end{aligned}$$

Since $(\Theta_1 - \Lambda_1 \Lambda_1^T) \in \mathbb{R}^{r \times r}$ is nonsingular, we have

$$\det(\Theta_1 \Lambda_1^{-T} - \Lambda_1) \neq 0.$$

Therefore, $\tilde{Q}(\lambda)$ has the same eigenvalues as $Q(\lambda)$ except that r eigenvalues of Λ_1 are replaced by r infinities. $\square$

Non-equivalence deflation for cubic polynomial eigenproblems

Let $(\Lambda, V_u) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}$ be an eigenmatrix pair of $\mathbf{A}(\lambda)$ with $V_u^T V_u = I_r$ and $0 \notin \sigma(\Lambda)$, i.e.,

$$A_3 V_u \Lambda^3 + A_2 V_u \Lambda^2 + A_1 V_u \Lambda + A_0 V_u = 0. \tag{7}$$

Define a new deflated cubic eigenvalue problem by

$$\widetilde{\mathbf{A}}(\lambda) u = (\lambda^3 \tilde{A}_3 + \lambda^2 \tilde{A}_2 + \lambda \tilde{A}_1 + \tilde{A}_0) u = 0, \tag{8}$$

where

$$\begin{cases} \tilde{A}_0 = A_0, \\ \tilde{A}_1 = A_1 - (A_1 V_u V_u^T + A_2 V_u \Lambda V_u^T + A_3 V_u \Lambda^2 V_u^T), \\ \tilde{A}_2 = A_2 - (A_2 V_u V_u^T + A_3 V_u \Lambda V_u^T), \\ \tilde{A}_3 = A_3 - A_3 V_u V_u^T. \end{cases} \tag{9}$$

Lemma

Let $\mathbf{A}(\lambda)$ *and* $\widetilde{\mathbf{A}}(\lambda)$ *be cubic pencils given by (3) and (8), respectively. Then it holds*

$$\widetilde{\mathbf{A}}(\lambda) = \mathbf{A}(\lambda)\left(I_n - \lambda V_u(\lambda I_r - \Lambda)^{-1} V_u^T\right). \tag{10}$$

Theorem

Let (Λ, V_u) *be an eigenmatrix pair of* $\mathbf{A}(\lambda)$ *with* $V_u^T V_u = I_r$. *Then*

(i) $(\sigma(\mathbf{A}(\lambda)) \setminus \sigma(\Lambda)) \cup \{\infty\} = \sigma(\widetilde{\mathbf{A}}(\lambda))$.

(ii) *Let* (μ, z) *be an eigenpair of* $\mathbf{A}(\lambda)$ *with* $\| z \|_2 = 1$ *and* $\mu \notin \sigma(\Lambda)$. *Define*

$$\tilde{z} = (I_n - \mu V_u \Lambda^{-1} V_u^T) z \equiv T(\mu) z. \tag{11}$$

Then $(\mu, \tilde{z})$ *is an eigenpair of* $\widetilde{\mathbf{A}}(\lambda)$.

Proof of Lemma:

Using (9) and (7), and the fundamental matrix calculation, we have

$$\begin{aligned}
\widetilde{\mathbf{A}}(\lambda) &= \mathbf{A}(\lambda) - \lambda\Big(\lambda^2 A_3 V_F V_F^T + \lambda A_2 V_F V_F^T + \lambda A_3 V_F \Lambda V_F^T + A_1 V_F V_F^T \\
&\quad + A_2 V_F \Lambda V_F^T + A_3 V_F \Lambda^2 V_F^T\Big) \\
&= \mathbf{A}(\lambda) - \lambda\Big(A_3 V_F (\lambda I_r - \Lambda)^3 (\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + 3A_3 V_F \Lambda (\lambda I_r - \Lambda)^2 (\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + 3A_3 V_F \Lambda^2 (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + A_2 V_F (\lambda I_r - \Lambda)^2 (\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + 2A_2 V_F \Lambda (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + A_1 V_F (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T\Big)
\end{aligned}$$

$$
\begin{aligned}
\widetilde{\mathbf{A}}(\lambda) &= \mathbf{A}(\lambda) - \lambda \left\{ \left[A_3 V_F(\lambda^3 I_r - \Lambda^3) + A_2 V_F(\lambda^2 I_r - \Lambda^2) \right.\right. \\
&\quad \left.\left. + A_1 V_F(\lambda I_r - \Lambda) + A_0 V_F - A_0 V_F \right] (\lambda I_r - \Lambda)^{-1} V_F^T \right\} \\
&= \mathbf{A}(\lambda) - \lambda \left[\mathbf{A}(\lambda) V_F (\lambda I_r - \Lambda)^{-1} V_F^T \right] \\
&= \mathbf{A}(\lambda) \left[I_n - \lambda V_F (\lambda I_r - \Lambda)^{-1} V_F^T \right].
\end{aligned}
$$

□

Proof of Theorem

: (i) Using the identity

$$\det(I_n + RS) = \det(I_m + SR)$$

and Lemma 8, we have

$$\begin{aligned} \det(\widetilde{\mathbf{A}}(\lambda)) &= \det(\mathbf{A}(\lambda)) \det \left(I_n - \lambda V_F (\lambda I_r - \Lambda)^{-1} V_F^T \right) \\ &= \det(\mathbf{A}(\lambda)) \det \left(I_n - \lambda (\lambda I_r - \Lambda)^{-1} \right) \\ &= \det(\mathbf{A}(\lambda)) \det(\lambda I_r - \Lambda)^{-1} \det(-\Lambda). \end{aligned}$$

Since $0 \notin \sigma(\Lambda)$, $\det(-\Lambda) \neq 0$. Thus, $\widetilde{\mathbf{A}}(\lambda)$ and $\mathbf{A}(\lambda)$ have the same finite spectrum except the eigenvalues in $\sigma(\Lambda)$. Furthermore, dividing Eq. (8) by λ^3 and using the fact that

$$\widetilde{\mathbf{A}}_3 V_F = (A_3 - A_3 V_F V_F^T) V_F = 0,$$

we see that $(\text{diag}_r\{\infty, \cdots, \infty\}, V_F)$ is an eigenmatrix pair of $\widetilde{\mathbf{A}}(\lambda)$ corresponding to infinite eigenvalues.

(ii) Since $\mu \notin \sigma(\Lambda)$, the matrix $T(\mu) = (I - \mu V_F \Lambda^{-1} V_F^T)$ in (11) is invertible with the inverse

$$T(\mu)^{-1} = I_n - \mu V_F (\mu I_r - \Lambda)^{-1} V_F^T. \tag{12}$$

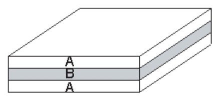
From Lemma 8, we have

$$\widetilde{\mathbf{A}}(\mu)\tilde{z} = \mathbf{A}(\mu)\left[I_n - \mu V_F(\mu I_r - \Lambda)^{-1} V_F^T\right]\left[I_n - \mu V_F \Lambda^{-1} V_F^T\right] z = 0.$$

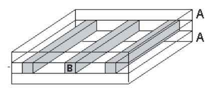
This completes the proof. $\square$

Applications

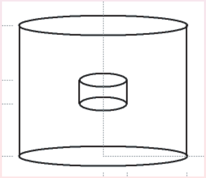
- Quantum well (2 dim.)



- Quantum wire (1 dim.)

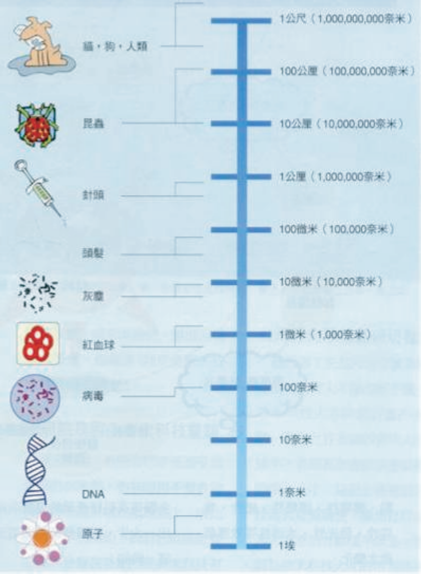


- Quantum dot (0 dim.)



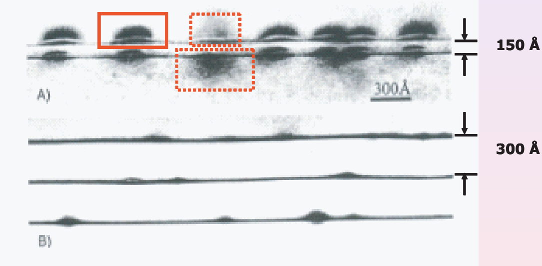
Nanometer

- $1nm = 10^{-9}m$
  Nano-scale ≈ 1–100 nm
- A semiconductor QD ≈ 10 nm
- QD : hair ≈ 1 : 10000
- Why consider quantum effects?
  Small devices imply significant quantum effect

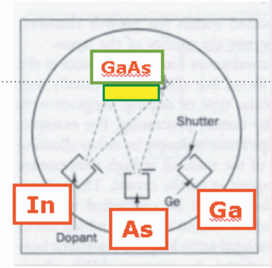


Quantum dot

- Cross-sections of hetero-structure InAs/GaAs QDs by Transmission Electron Microscope [Schoenfeld, 00]



Molecular beam epitaxy



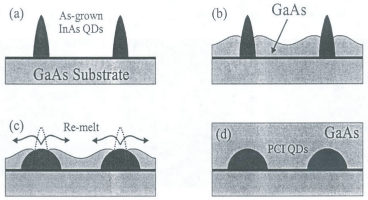
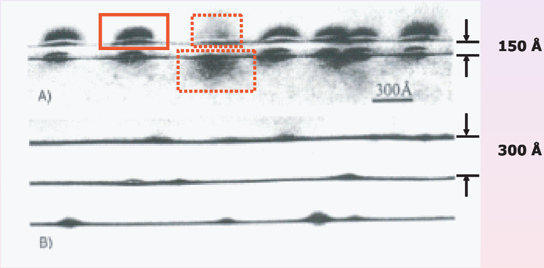


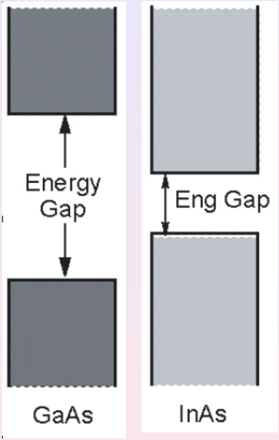
Figure 2.2-1: Schematic of the PCI growth process: (a) As-grown InAs QDs, (b) partial coverage of islands, (c) re-melt, and (c) overgrowth by GaAs.

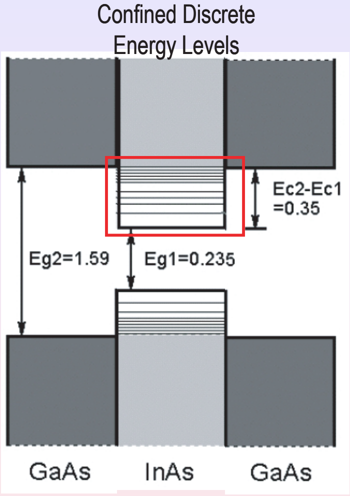
Quantum dot

- Cross-sections of hetero-structure InAs/GaAs QDs by Transmission Electron Microscope [Schoenfeld, 00]



Energy levels (eigenvalues)





Numerical experiments for linear eigenproblems

- The Schrödinger equation for Semiconductor:

$$-\nabla \cdot (\alpha \nabla u) + Vu = \lambda u,$$

where

$$\alpha = \begin{cases} \alpha^- \equiv \frac{\hbar^2}{2m_1} & \text{inside}, \\ \alpha^+ \equiv \frac{\hbar^2}{2m_2} & \text{outside}, \end{cases} \qquad V = \begin{cases} V^- = V_1 & \text{inside}, \\ V^+ = V_2 & \text{outside} \end{cases}$$

$\hbar$:	Plank constant	m_ℓ:	parabolic effective mass
V_ℓ:	confinement potential	λ:	total energy

- Interface condition:

$$\alpha^- \frac{\partial u}{\partial n}\Big|_{\partial D_-} = \alpha^+ \frac{\partial u}{\partial n}\Big|_{\partial D_+}$$

- Dirichlet boundary conditions

Symmetric eigenvalue problem

$$Ax = \lambda x$$

where A is a symmetric matrix.

Reference:

- Tsung-Min Hwang, Wen-Wei Lin, Wei-Cheng Wang and Weichung Wang, Numerical simulation of three dimensional pyramid quantum dot, Journal of Computational Physics, Vol 196, pp. 208-232, 2004.

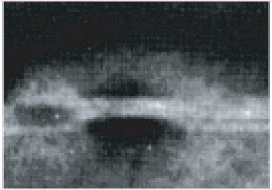
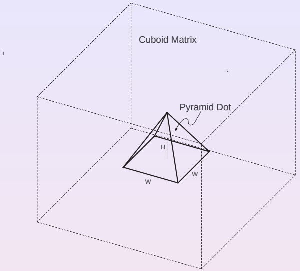
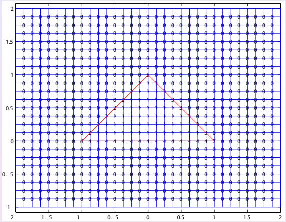
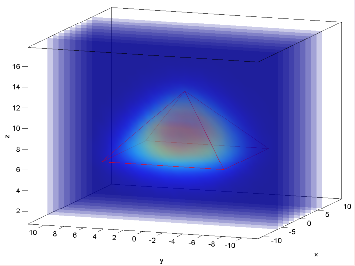


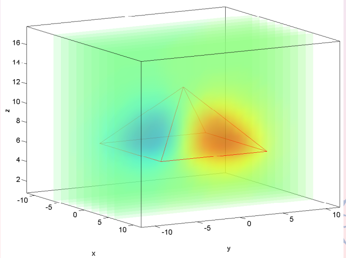
Figure: PRB, 54, 8743, (1996)

Three dimensional pyramid quantum dot









- Finite volume discretized scheme
- Symmetric eigenvalue problems: $Ax = \lambda x$
- Second order convergent rate
- Correction vector with SSOR preconditioner:

$$t = -M_A^{-1} r + \varepsilon M_A^{-1} p$$

with

$$\varepsilon = \frac{u^T M_A^{-1} r}{u^T M_A^{-1} p},$$

where $M_{\mathbf{A}} = (D + \omega L) D^{-1} (D + \omega U)$.

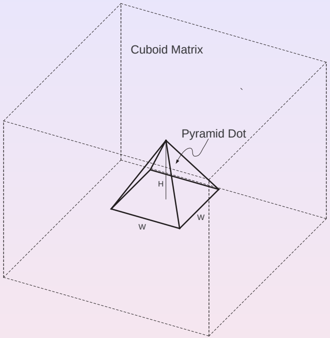


Figure: Structure schema of a pyramid quantum dot.

- The width of the QD (matrix) base is 12.4 nm (24.8 nm); the height of the QD (matrix) is 6.2 nm (18.6 nm).
- InAs QD: $\alpha_1 = 0.024 m_e$ and $V_1 = 0.0$
  GaAs matrix: $\alpha_2 = 0.067 m_e$ and $V_2 = 0.70$.
- Stopping criteria: residual $< 10^{-10}$
- Convergent rate

(L,M,N)	Mtx. dim.	λ_1	Rate	λ_2	Rate
(16, 16, 12)	2,475	0.4226	-	0.6527	-
(32, 32, 24)	22,103	0.4001	-	0.6423	-
(64, 64, 48)	186,543	0.3934	1.744	0.6391	1.708
(128,128, 96)	1,532,255	0.3916	1.905	0.6383	1.866
(256,256,192)	12,419,775	0.3911	1.954	0.6380	1.912

Table: Convergent rate = $\log_2 \left((\lambda^{(4h)} - \lambda^{(2h)}) / (\lambda^{(2h)} - \lambda^{(h)}) \right)$

- $\dim(A) = 1,532,255$ on PC with P4 1.8 GHz CPU and 1 GB of main memory.

	Value	Ite. no.	CPU time (sec.)
λ_1	0.3916	72	278.0
λ_2	0.6383	72	284.3
λ_3	0.6383	125	521.4

- $\dim(A) = 32,401,863$ on HP workstation with a 1.0 GHz Intel Itanium II CPU and 12 GBs of main memory.

	Value	Ite. no.	CPU time (sec.)
λ_1	0.3910	138	5,852
λ_2	0.6380	133	5,354
λ_3	0.6380	220	8,511

Unsymmetric eigenvalue problem

$$Ax = \lambda x$$

where A is a unsymmetric matrix.

Reference:

- Tsung-Min Hwang, Wei-Hua Wang and Weichung Wang, Efficient numerical schemes for electronic states in coupled quantum dots, accepted for publication in Journal of Nanoscience and Nanotechnology.

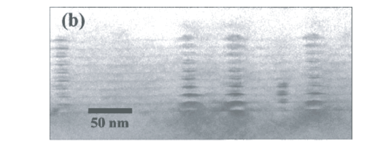
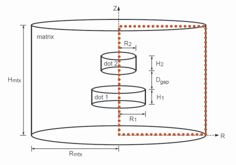
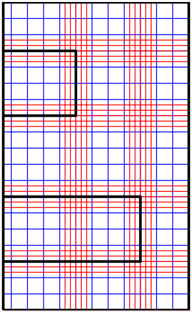


Figure: JAP, 90-12, (2001)

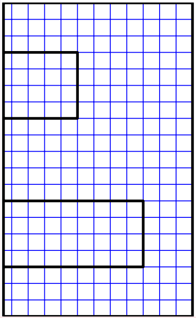
Vertically aligned quantum dot array



(a) Nonuniform mesh



(b) Uniform mesh



- Reduce three-dimensional systems to two-dimensional systems by Fourier transformation.
- Finite volume discretized scheme
- Unsymmetric eigenvalue problems: $Ax = \lambda x$
- Second order convergent rate
- Method II with SSOR preconditioner:

$$M_{\mathbf{A}} = (D + \omega L) D^{-1} (D + \omega U).$$

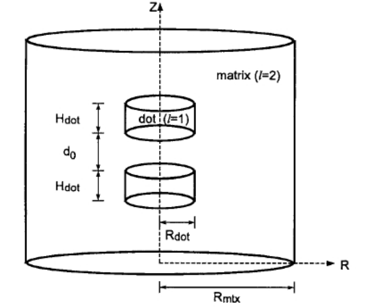


Figure: Structure schema of a cylindrical vertically aligned quantum dot array.

- Reduce three-dimensional systems to two-dimensional systems by Fourier transformation.
- Finite volume discretized scheme
- Unsymmetric eigenvalue problems: $Ax = \lambda x$
- Second order convergent rate
- Method II with SSOR preconditioner:

$$M_{\mathbf{A}} = (D + \omega L) D^{-1} (D + \omega U).$$

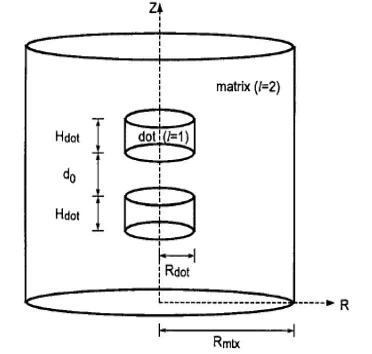


Figure: Structure schema of a cylindrical vertically aligned quantum dot array.

- Reduce three-dimensional systems to two-dimensional systems by Fourier transformation.
- Finite volume discretized scheme
- Unsymmetric eigenvalue problems: $Ax = \lambda x$
- Second order convergent rate
- Method II with SSOR preconditioner:

$$M_{\mathbf{A}} = (D + \omega L) D^{-1} (D + \omega U).$$

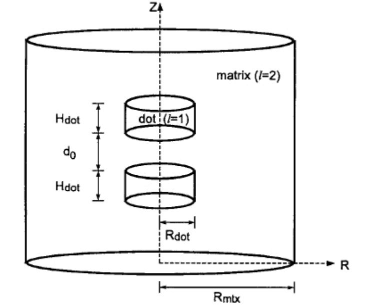


Figure: Structure schema of a cylindrical vertically aligned quantum dot array.

- gap = 6nm and $\dim(A) = 12,288,000$ on HP workstation with a 1.0 GHz Intel Itanium II CPU and 12 GBs of main memory.

	$r_2 = 3.198$			$r_2 = 3.223$		
	Value	Ite. no.	Time (sec.)	Value	Ite. no.	Time (sec.)
λ_1	0.1587	83	20,287	0.1587	84	23,840
λ_2	0.35553	109	26,030	0.3526	91	31,612
λ_3	0.3558	53	13,831	0.3555	61	25,706

- gap = 3nm and $\dim(A) = 11,059,200$ on HP workstation with a 1.0 GHz Intel Itanium II CPU and 12 GBs of main memory.

	$r_2 = 3.198$			$r_2 = 3.223$		
	Value	Ite. no.	Time (sec.)	Value	Ite. no.	Time (sec.)
λ_1	0.1586	85	20,072	0.1586	83	18,455
λ_2	0.3540	257	56,811	0.3515	130	29,506
λ_3	0.3564	53	12,257	0.3558	54	13,082

Generalized eigenvalue problem

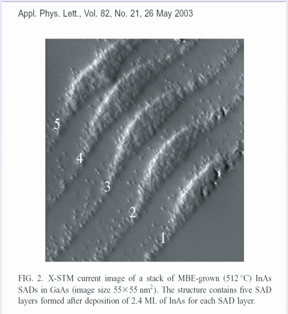
$$Ax = \lambda Bx$$

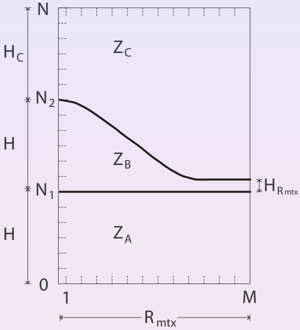
where A is symmetric positive definite and B is a positive diagonal matrix.

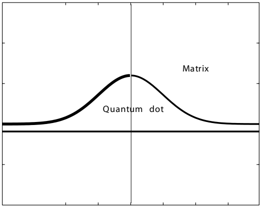
Reference:

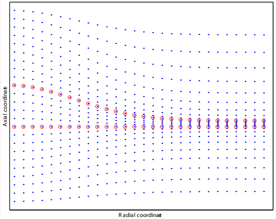
- Tsung-Min Hwang, Wei-Cheng Wang and Weichung Wang, Numerical schemes for three dimensional irregular shape quantum dots over curvilinear coordinate systems, accepted for publication in Journal of Computational Physics.

Three dimensional arbitrary shape quantum dots









- Curvilinear coordinate system
- Reduce three-dimensional systems to two-dimensional systems by Fourier transformation.
- Jump condition capturing scheme (nine points)
- Generalized eigenvalue problems: $Ax = \lambda Bx$, A is symmetric positive definite and B is a positive diagonal matrix.
- Second order convergent rate
- Method I with SSOR preconditioner:

$$M_{\mathbf{A}} = (D + \omega L)D^{-1}(D + \omega U).$$

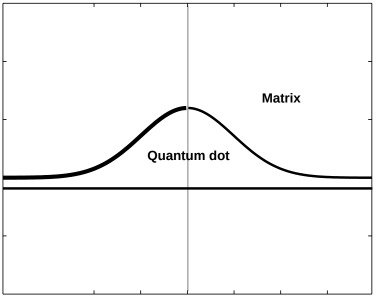


Figure: Structure schema of the quantum dot model.

- $\dim(A) = 1,935,090$ on HP workstation with a 1.3 GHz Intel Itanium II CPU and 24 GBs of main memory.

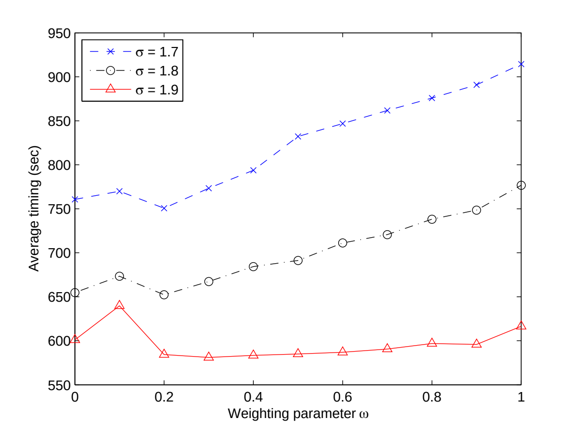


Figure: Average timing results for computing all the target eigenvalues by using three different SSOR preconditioner parameter σ.

Numerical experiments for polynomial eigenproblems

- The Schrödinger equation for Semiconductor:

$$-\nabla \cdot (\alpha \nabla u) + Vu = \lambda u,$$

where

$$\alpha = \begin{cases} \alpha^- \equiv \frac{\hbar^2}{2m_1} & \text{inside}, \\ \alpha^+ \equiv \frac{\hbar^2}{2m_2} & \text{outside}, \end{cases} \qquad V = \begin{cases} V^- = V_1 & \text{inside}, \\ V^+ = V_2 & \text{outside} \end{cases}$$

- non-parabolic effective mass

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

- Interface condition:

$$\alpha^- \frac{\partial u}{\partial n}\Big|_{\partial D_-} = \alpha^+ \frac{\partial u}{\partial n}\Big|_{\partial D_+}$$

- Dirichlet boundary conditions

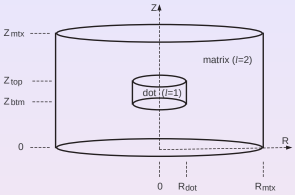
Cubic polynomial eigenvalue problem

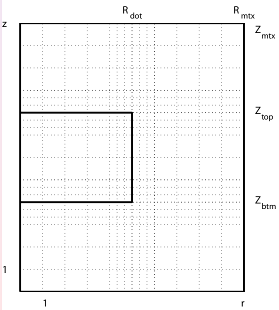
$$(\lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)x = 0.$$

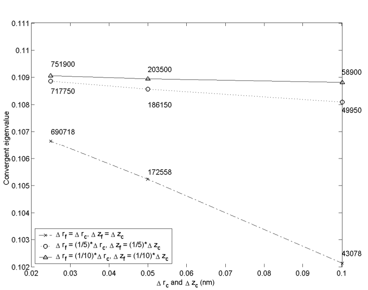
Reference:

- Weichung Wang, Tsung-Min Hwang, Wen-Wei Lin and Jinn-Liang Liu, Numerical methods for semiconductor heterostructures with band nonparabolicity, Journal of Computational Physics, Vol. 190, pp. 141-158, 2003.
- Tsung-Min Hwang, Wen-Wei Lin, Jinn-Liang Liu and Weichung Wang, Fixed point methods for a semiconductor quantum dot model, Mathematical and Computer Modelling, Vol 40, pp. 519-533, 2004.
- Tsung-Min Hwang, Wen-Wei Lin, Jinn-Liang Liu and Weichung Wang, Jacobi-Davidson methods for cubic eigenvalue problems, Numerical Linear Algebra with Applications, Vol. 12, pp. 585-682, 2005.

Three dimensional cylindrical quantum dot







- non-parabolic effective mass

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

- Central finite difference scheme with nonuniform grid points
- Multiply the common denominator for all grid points
- A cubic polynomial eigenvalue problem:

$$(\lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)x = 0.$$

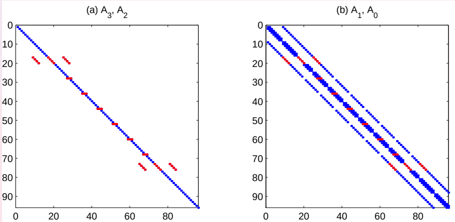


Figure: Sparsity patterns of matrices A_i.

- The diameter and the height of the cylindrical QD (matrix) are 15 (75) and 2.5 (12.5) nm, respectively.
- $V_1 = 0.000$, $g_1 = 0.235$, $\delta_1 = 0.81$, $P_1 = 0.2875$, $V_2 = 0.350$, $g_2 = 1.590$, $\delta_2 = 0.80$, and $P_2 = 0.1993$.
- Correction vector with SSOR preconditioner:

$$t = -M_A^{-1} r + \varepsilon M_A^{-1} p$$

with

$$\varepsilon = \frac{u^T M_A^{-1} r}{u^T M_A^{-1} p},$$

where $M_{\mathbf{A}} = (D + \omega L) D^{-1} (D + \omega U)$.

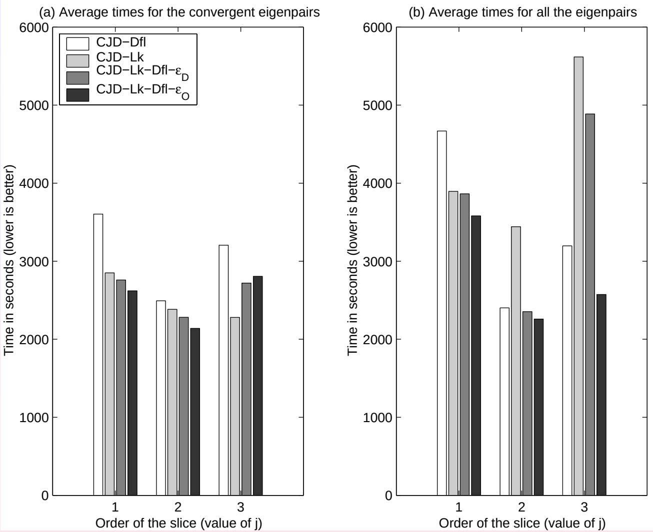
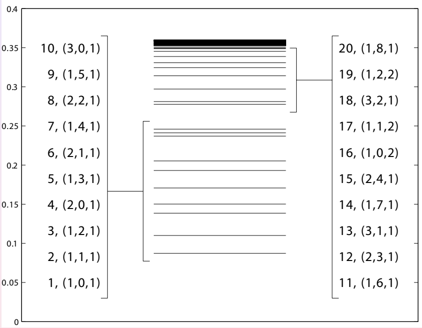
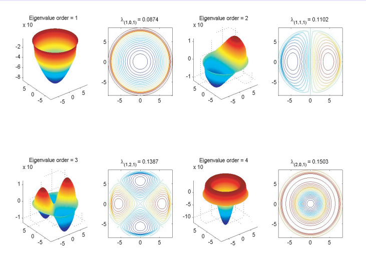
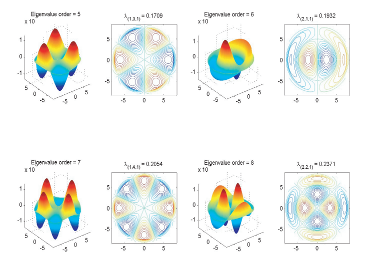


Figure: Comparison of efficiency. Average timing results calculated by two ways are compared for the four methods.

Energy states and wave functions





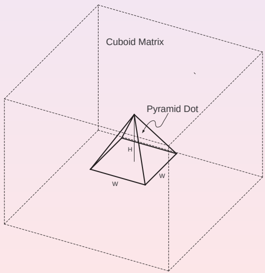


Quintic polynomial eigenvalue problem

$$(\lambda^5 A_5 + \lambda^4 A_4 + \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0)x = 0.$$

Reference:

- Tsung-Min Hwang, Wen-Wei Lin, Wei-Cheng Wang and Weichung Wang, Numerical simulation of three dimensional pyramid quantum dot, Journal of Computational Physics, Vol 196, pp. 208-232, 2004.



Three dimensional pyramid quantum dot

- non-parabolic effective mass

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

- Finite volume discretized scheme with uniform grid points
- Multiply the common denominator for all grid points
- A quintic polynomial eigenvalue problem:

$$\left(\sum_{i=0}^{5} \lambda^i A_i\right) x = 0.$$

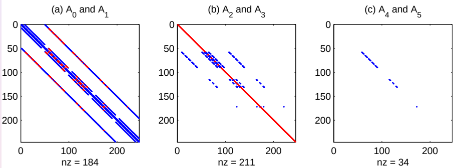


Figure: Sparsity patterns of matrices A_i.

- Second order convergent rate.

- $\dim(A) = 1,532,255$ on PC with P4 1.8 GHz CPU and 1 GB of main memory.

	Value	Ite. no.	CPU time (sec.)
λ_1	0.4165	47	447.4
λ_2	0.5993	45	460.7
λ_3	0.5993	50	544.7

- $\dim(A) = 32,401,863$ on HP workstation with a 1.0 GHz Intel Itanium II CPU and 12 GBs of main memory.

	Value	Ite. no.	CPU time (sec.)
λ_1	0.4162	84	4,856
λ_2	0.5991	74	4,835
λ_3	0.5991	113	8,280

Reference

Z. Bai, J. Demmel, J. Dongarra, A. Ruhe and H. van der Vorst.
Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide.
SIAM, Philadelphia, 2000.

T.-M. Hwang, W.-W. Lin and V. Mehrmann.
Numerical solution of quadratic eigenvalue problems with structure preserving methods,
SIAM J. Sci. Comput. Vol. 24, No. 4, pp. 1283-1302, 2003.

T.-M. Hwang, W.-W. Lin, W.-C. Wang and W. Wang.
Numerical simulation of three dimensional pyramid quantum dot,
Journal of Computational Physics, Vol 196, 208-232, 2004.

T.-M. Hwang, W.-W. Lin, J.-L. Liu and W. Wang.
Jacobi-Davidson methods for cubic eigenvalue problems,
Numerical Linear Algebra with Applications, Vol. 12, pp. 605-624, 2005.

Reference

T.-M. Hwang, W.-C. Wang and W. Wang.
Numerical schemes for three dimensional irregular shape quantum dots over curvilinear coordinate systems,
Journal of Computational Physics, Vol. 226, pp. 754–773, 2007.

K. Meerbergen,
Locking and restarting quadratic eigenvalue solvers,
SIAM J. Sci. Comput., Vol. 22, pp. 1814–1839, 2001.

G. L. G. Sleijpen, A. G. L. Booten, D. R. Fokkema and H. A. van der Vorst,
Jacobi-Davidson type methods for generalized eigenproblems and polynomial eigenproblems.
BIT, Vol. 36, pp. 595–633, 1996.

G. L. G. Sleijpen and H. A. van der Vorst,
A Jacobi-Davidson iteration method for linear eigenvalue problems,
SIAM J. Matrix Anal. Appl., Vol. 17, pp. 401–425, 1996.