Lanczos Method for Eigensystems

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California

Email: anakano@usc.edu

1. *$O(N)$* (*vs.* conventional *$O(N^3)$*) eigensolver
2. **Krylov subspace**

B. N. Parlett
The Symmetric Eigenvalue Problem
(Prentice-Hall, '80) Secs. 11-13

Rayleigh Quotient

Theorem

Let A be an $n \times n$ real symmetric matrix, $\lambda_1[A] \leq \ldots \leq \lambda_n[A]$ its eigenvalues in ascending order, $x \in R^n$, & the Rayleigh quotient

$$\rho(\mathbf{x}; \mathbf{A}) = \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \quad \text{then} \quad \begin{cases} \lambda_1[\mathbf{A}] = \min_{\mathbf{x} \in \mathfrak{R}^n} \rho(\mathbf{x}; \mathbf{A}) \\ \lambda_n[\mathbf{A}] = \max_{\mathbf{x} \in \mathfrak{R}^n} \rho(\mathbf{x}; \mathbf{A}) \end{cases}$$

Proof

Let $\mathbf{q}^{(k)}$ be the k-th orthonormalized eigenvector of $\mathbf{A}$, $\mathbf{A}\mathbf{q}_k = \lambda_k \mathbf{q}_k$, & orthogonal transformation matrix, $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n]$, then

$$\mathbf{Q}^T \mathbf{A} \mathbf{Q} = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Let x = Qz (note $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$), then

$$\rho(\mathbf{x}; \mathbf{A}) = \frac{\mathbf{z}^T \mathbf{Q}^T \mathbf{A} \mathbf{Q} \mathbf{z}}{\mathbf{z}^T \mathbf{Q}^T \mathbf{Q} \mathbf{z}} = \frac{z_1^2 \lambda_1 + \cdots + z_n^2 \lambda_n}{z_1^2 + \cdots + z_n^2}$$

which is a weighted average of $\lambda_1, \ldots, \lambda_n$, & the minimum is when $z^T = (1,0,\ldots,0) = e_1$ & $x = Qe_1 = q_1$.

Rayleigh-Ritz Procedure

Theorem

Let $\{q_1,...,q_m\}$ ($q_j \in \mathbf{R}^n$; $j = 1,...,m$; $m < n$) be an orthonormal set, so that any vector $x \in \mathbf{R}^n$ in the range is expressed as a linear combination of $q_1,...,q_m$:

$$\mathbf{x} = z_1\mathbf{q}_1 + \cdots + z_m\mathbf{q}_m \quad \text{or} \quad n\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = n\overset{1}{\begin{bmatrix} \mathbf{q}_1 & \cdots & \overset{m}{\mathbf{q}_m} \end{bmatrix}}\overset{1}{\begin{bmatrix} z_1 \\ \vdots \\ z_m \end{bmatrix}}m = \mathbf{Qz}$$

then the best approximations for $\lambda_1[\mathbf{A}]$ & $\lambda_n[\mathbf{A}]$ are obtained by diagonalizing

$$\underset{m \times m}{\mathbf{H}} = \underset{m \times n}{\mathbf{Q}^T} \ \underset{n \times n}{\mathbf{A}} \ \underset{n \times m}{\mathbf{Q}}$$

as $\lambda_1[\mathbf{H}]$ & $\lambda_m[\mathbf{H}]$.

Proof

Note $(\mathbf{Q}^T\mathbf{Q})_{ij} = \sum_{k=1}^{n} Q_{ki}Q_{kj} = \mathbf{q}_i \bullet \mathbf{q}_j = \delta_{ij}$

then

$$\rho(\mathbf{x}; \mathbf{A}) = \frac{\mathbf{z}^T\mathbf{Q}^T\mathbf{A}\mathbf{Qz}}{\mathbf{z}^T\mathbf{Q}^T\mathbf{Qz}} = \frac{\mathbf{z}^T\mathbf{Hz}}{\mathbf{z}^T\mathbf{z}} = \frac{z_1^2\lambda_1(\mathbf{H}) + \cdots + z_m^2\lambda_m(\mathbf{H})}{z_1^2 + \cdots + z_m^2}$$

the minimum of which is $\lambda_1[\mathbf{H}]$ (*cf.* proof in the previous page).

Orthogonalization by QR Decomposition

- **Gram-Schmidt orthonormalization:** The orthonormal set Q required for the Rayleigh-Ritz procedure is obtained starting from an arbitrary set of m vectors, $S = [s_1 \ldots s_m]$ ($s_j \in \mathbf{R}^n$) as (see supplementary note):

$$\mathbf{q}_1 = \mathbf{s}_1 / |\mathbf{s}_1|$$

$$\text{for} \quad i = 2 \quad \text{to} \quad m$$

$$\mathbf{q}'_i = \mathbf{s}_i - \sum_{j=1}^{i-1} \mathbf{q}_j (\mathbf{q}_j \bullet \mathbf{s}_i)$$

Projection!

$$\underbrace{\hat{P}}_{\sum_{j=1}^{i-1} |q_j\rangle\langle q_j|} \quad |s_i\rangle$$

$$\mathbf{q}_i = \mathbf{q}'_i / |\mathbf{q}'_i|$$

$$\text{endfor}$$

- **The Gram-Schmidt procedure amounts to QR decomposition, $S = QR$, where R is an $m \times m$ right-triangle matrix:**

$$n \begin{bmatrix} \mathbf{s}_1 & \mathbf{s}_2 & \mathbf{s}_3 & \mathbf{s}_4 \end{bmatrix} = n \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \mathbf{q}_4 \end{bmatrix} \begin{bmatrix} |\mathbf{q}'_1| & \mathbf{q}_1 \bullet \mathbf{s}_2 & \mathbf{q}_1 \bullet \mathbf{s}_3 & \mathbf{q}_1 \bullet \mathbf{s}_4 \\ 0 & |\mathbf{q}'_2| & \mathbf{q}_2 \bullet \mathbf{s}_3 & \mathbf{q}_2 \bullet \mathbf{s}_4 \\ 0 & 0 & |\mathbf{q}'_3| & \mathbf{q}_3 \bullet \mathbf{s}_4 \\ 0 & 0 & 0 & |\mathbf{q}'_4| \end{bmatrix} m$$

$$\therefore \mathbf{s}_i = |\mathbf{q}'_i|\mathbf{q}_i + \sum_{j=1}^{i-1} \mathbf{q}_j (\mathbf{q}_j \bullet \mathbf{s}_i)$$

Rayleigh-Ritz Algorithm

1. Start from $\mathbf{S} = [\mathbf{s}_1 \ldots \mathbf{s}_m]$ ($\mathbf{s}_j \in \mathbf{R}^n$) & do Gram-Schmidt orthonormalization, $\mathbf{S} = \mathbf{QR}$, to obtain an orthonormal set $\mathbf{Q} = [\mathbf{q}_1 \ldots \mathbf{q}_m]$

2. Form $\mathbf{H} = \mathbf{Q}^T\mathbf{AQ}$

3. Diagonalize $\mathbf{H}$ to get $\lambda_1[\mathbf{H}], \ldots, \lambda_m[\mathbf{H}]$: $\mathbf{Hg}_k = \lambda_k[\mathbf{H}]\mathbf{g}_k$ ($k = 1, \ldots, m$)

4. Approximations of $\lambda_1[\mathbf{A}]$ & $\lambda_n[\mathbf{A}]$ are given by $\lambda_1[\mathbf{H}]$ & $\lambda_m[\mathbf{H}]$ with the corresponding eigenvectors, $\mathbf{y}_k = \mathbf{Qg}_k$ ($k = 1$ & m).

$$\underbrace{\mathbf{Q}^T\mathbf{AQ}}_{\mathbf{H}}\,\mathbf{g}_k = \lambda_k(\mathbf{H})\mathbf{g}_k$$

$$* \quad \downarrow \quad \mathbf{Q}\times$$

$$\therefore \mathbf{A}\underbrace{\mathbf{Qg}_k}_{\mathbf{y}_k} = \lambda_k(\mathbf{H})\underbrace{\mathbf{Qg}_k}_{\mathbf{y}_k}$$

$^*\mathbf{QQ}^T \neq \mathbf{I}^{N\times N}$ but spans a subspace of the N-dimensional space

Krylov Subspace

- **Krylov subspace S_m is spanned by a Krylov matrix, $K^m(f) = [f \ Af \ \dots \ A^{m-1}f]$ ($f \in R^n$)**

Theorem

Let Q_m be the orthonormal basis obtained by QR factorization, $K_m(f) = Q_m R$, then $T_m = Q_m^T A Q_m$ is a tridiagonal matrix

Proof (see [supplementary note](#))

For $i > j+1$, $q_i^T(Aq_j) = 0$, since $Aq_j \subset S_{j+1}$ by construction & $q_i \perp S_{j+1}$ by Gram-Schmidt orthonormalization for $i > j+1$. By the symmetry of A, $q_i^T(Aq_j) = q_j^T(A^T q_i) = q_j^T(Aq_i) = 0$ for $j > i+1$ or $i < j-1$.

$$\mathbf{T}_m = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & & \ddots \\ & & \beta_{m-2} & \alpha_{m-1} & \beta_{m-1} \\ & & & \beta_{m-1} & \alpha_m \end{bmatrix} \quad \begin{cases} \alpha_j = \mathbf{q}_j^T \mathbf{A} \mathbf{q}_j & j = 1, \dots, m \\ \beta_j = \mathbf{q}_{j+1}^T \mathbf{A} \mathbf{q}_j & j = 1, \dots, m-1 \end{cases}$$

- **Tridiagonal matrix can be diagonalized in $O(N)$ time**
  cf. tqli() in Numerical Recipes

Alexei Krylov with daughter Anna, later Anna Kapitsa, wife of Pyotr Kapitsa (1904)

Recursion Formula

- **Due to the tridiagonality, $A\mathbf{q}_i$ is a linear combination of $\mathbf{q}_{i-1}$, $\mathbf{q}_i$ & $\mathbf{q}_{i+1}$:**

$$A\mathbf{q}_i = \beta_{i-1}\mathbf{q}_{i-1} + \alpha_i\mathbf{q}_i + \beta_i\mathbf{q}_{i+1} \quad 2 \leq i \leq m-1$$

If we define $\mathbf{q}_0 = 0$, the above equation is valid for $i = 1$ as well. Let $\mathbf{r}_i \equiv \beta_i\mathbf{q}_{i+1}$ ($\mathbf{r}_i$ is a component of $A\mathbf{q}_i$ orthogonal to $\mathbf{q}_j$ for $j \leq i$), then

$$\mathbf{r}_i = A\mathbf{q}_i - \beta_{i-1}\mathbf{q}_{i-1} - \alpha_i\mathbf{q}_i \quad 1 \leq i \leq m-1$$

$$A\mathbf{q}_i = \beta_{i-1}\mathbf{q}_{i-1} + \alpha_i\mathbf{q}_i + \beta_i\mathbf{q}_{i+1} \quad 2 \leq i \leq m-1$$

- **Lanczos algorithm:**

Given $\mathbf{r}_0, \beta_0 = \|\mathbf{r}_0\|$ ($\mathbf{q}_0 = 0$)
for $i = 1, \dots, m$
  $\mathbf{q}_i \leftarrow \mathbf{r}_{i-1}/\beta_{i-1}$
  $\mathbf{r}_i \leftarrow A\mathbf{q}_i - \beta_{i-1}\mathbf{q}_{i-1}$
  $\alpha_i \leftarrow \mathbf{q}_i^T\mathbf{r}_i$ $\because \mathbf{q}_i^T(A\mathbf{q}_i - \beta_{i-1}\mathbf{q}_{i-1}) = \mathbf{q}_i^T A\mathbf{q}_i = \alpha_i$ (orthogonality)
  $\mathbf{r}_i \leftarrow \mathbf{r}_i - \alpha_i\mathbf{q}_i$
  $\beta_i = \|\mathbf{r}_i\|$ (only when $i \leq m-1$)
endfor

Keep increasing m until $\lambda_1[\mathrm{T}_m]$ converges

Application of Rayleigh-Ritz/Lanczos

- **Search for transition states (with a negative eigenvalue of the Hessian matrix, $\partial^2 E/\partial r_i \partial r_j$, by following the eigenvector with the smallest eigenvalue**
  - **Rayleigh-Ritz:** Kumeda, Wales & Munro, *Chem. Phys. Lett.* **341**, 185 ('01)
  - **Lanczos:** Mousseau *et al.*, *J. Mol. Graph. Model.* **19**, 78 ('01)
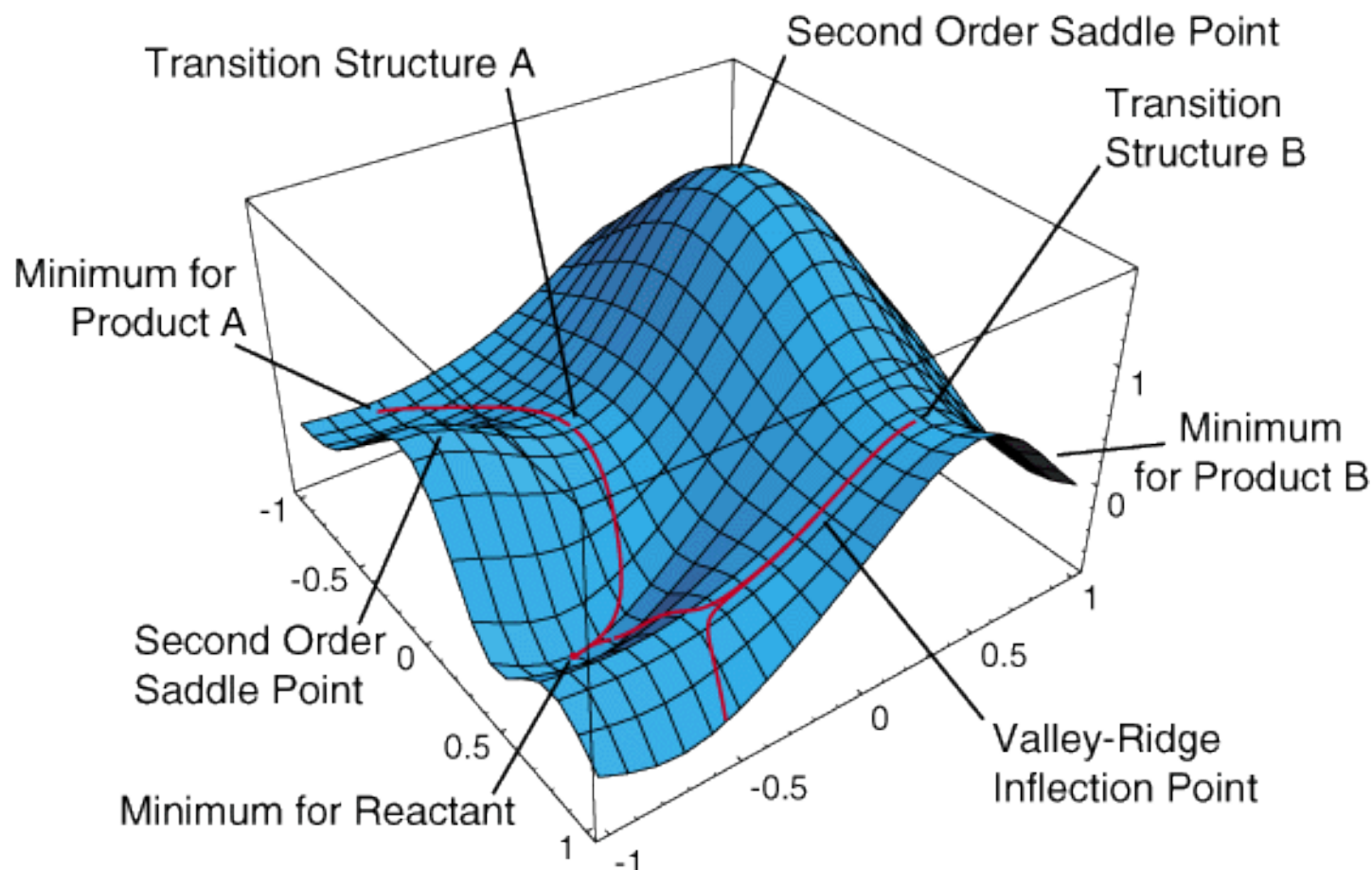

Figure from Prof. H. B. Schlegel; http://chem.wayne.edu/schlegel

Lanczos Algorithm for Hessian Calculation

Algorithm Lanczos

Input:
$\mathbf{R} \in \mathbb{R}^{3N}$: a state
logical *initialize*: TRUE for the first call in each event generation; FALSE otherwise

Output:
λ_1: the minimum eigenvalue of the Hessian matrix, $\mathbf{H}(\mathbf{R}) = \partial^2 V / \partial \mathbf{R}^2$
$\mathbf{V}^1 \in \mathbb{R}^{3N}$: the Hessian eigenvector corresponding to λ_1

Steps:
if *initialize*
    randomize $\Delta \in \mathbb{R}^{3N}$, such that it contains no translational motion
$s \leftarrow 0$
$\beta^s \leftarrow \|\Delta\|$
$\mathbf{Q}^s \ (\in \mathbb{R}^{3N}) \leftarrow 0$
do
    $s \leftarrow s + 1$
    $\mathbf{Q}^s \leftarrow \Delta / \beta^{s-1}$
    $c_{\text{fd}} \leftarrow \max_{i\alpha}\{|q_{i\alpha}^s| \,|\, i = 1, \ldots, N; \alpha = x, y, z\} / \delta_{\text{fd}}$
    $\Delta \leftarrow c_{\text{fd}}[-\mathbf{F}(\mathbf{R} + \mathbf{Q}^s / c_{\text{fd}}) + \mathbf{F}(\mathbf{R})] - \beta^{s-1}\mathbf{Q}^{s-1}$
    $\alpha^s \leftarrow \mathbf{Q}^{s\text{T}}\Delta$
    $\Delta \leftarrow \Delta - \alpha^s \mathbf{Q}^s$
    $\beta^s \leftarrow \|\Delta\|$

diagonalize $\mathbf{T}_s = \begin{bmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{s-2} & \alpha_{s-1} & \beta_{s-1} \\ & & & \beta_{s-1} & \alpha_s \end{bmatrix}$, so that $\tilde{\mathbf{Q}}_s^{\text{T}} \mathbf{T}_s \tilde{\mathbf{Q}}_s = \text{diag}(\tilde{\lambda}_1^s, \ldots, \tilde{\lambda}_s^s)^*$ *tqli()* $- O(N)$

while $|(\tilde{\lambda}_1^s - \tilde{\lambda}_1^{s-1})/\tilde{\lambda}_1^{s-1}| > \Delta_{\text{eigen}}$
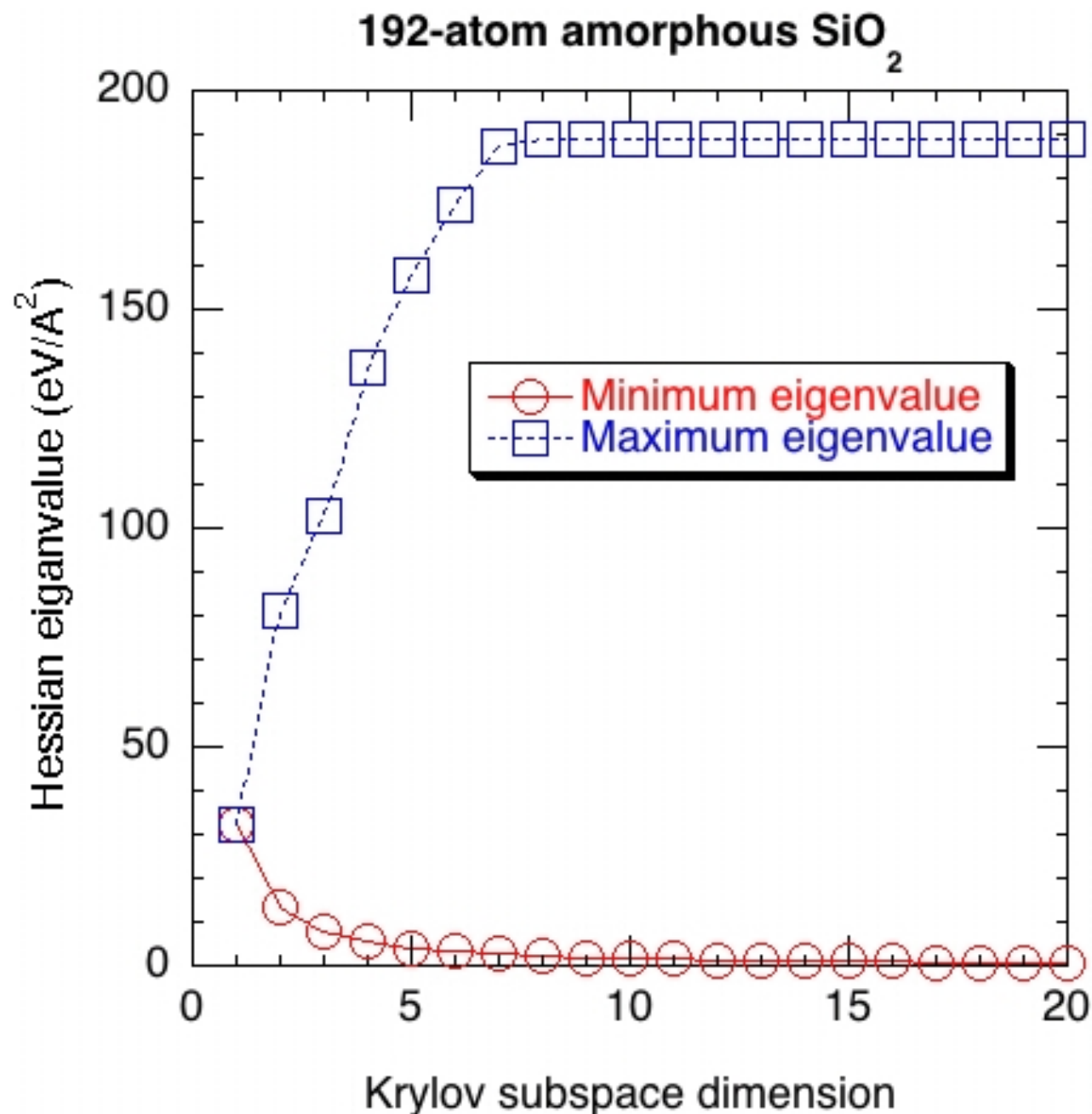$\lambda_1 \leftarrow \tilde{\lambda}_1^s$
$\mathbf{V}^1 \leftarrow \sum_{k=1}^s \mathbf{Q}^k \tilde{q}_k^1$
$\mathbf{V}^1 \leftarrow \mathbf{V}^1 / \|\mathbf{V}^1\|$

* $\text{diag}(\tilde{\lambda}_1^s, \ldots, \tilde{\lambda}_s^s)$ is an s by s diagonal matrix, with its diagonal elements given by $\tilde{\lambda}_1^s, \ldots, \tilde{\lambda}_s^s$. $\tilde{\mathbf{Q}}^s = [\tilde{q}^1, \ldots, \tilde{q}^s]$ is an s by s orthogonal matrix, with $\tilde{q}^m \in \mathbb{R}^s$ is the mth eigenvector of $\mathbf{T}_s$.

Sample Run of Lanczos Program

192-atom amorphous SiO$_2$

Electronic Energy Bands of GaAs

- **8-band k•p model**

$$H_k = \begin{pmatrix}
A & 0 & V^* & 0 & \sqrt{3}V & -\sqrt{2}U & -U & \sqrt{2}V^* \\
0 & A & -\sqrt{2}U & -\sqrt{3}V^* & 0 & -V & \sqrt{2}V & U \\
V & -\sqrt{2}U & -P+Q & -S^* & R & 0 & \sqrt{\tfrac{3}{2}}S & -\sqrt{2}Q \\
0 & -\sqrt{3}V & -S & -P-Q & 0 & R & -\sqrt{2}R & \frac{1}{\sqrt{2}}S \\
\sqrt{3}V^* & 0 & R^* & 0 & -P-Q & S^* & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R^* \\
-\sqrt{2}U & -V^* & 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{\tfrac{3}{2}}S^* \\
-U & \sqrt{2}V^* & \sqrt{\tfrac{3}{2}}S^* & -\sqrt{2}R^* & \frac{1}{\sqrt{2}}S & \sqrt{2}Q & -P-\Delta & 0 \\
\sqrt{2}V & U & -\sqrt{2}Q & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R & \sqrt{\tfrac{3}{2}}S & 0 & -P-\Delta
\end{pmatrix}$$

$$A = E_c - \frac{\hbar^2}{2m_0}(\partial_x^2 + \partial_y^2 + \partial_z^2),$$

$$P = -E_v - \gamma_1 \frac{\hbar^2}{2m_0}(\partial_x^2 + \partial_y^2 + \partial_z^2),$$

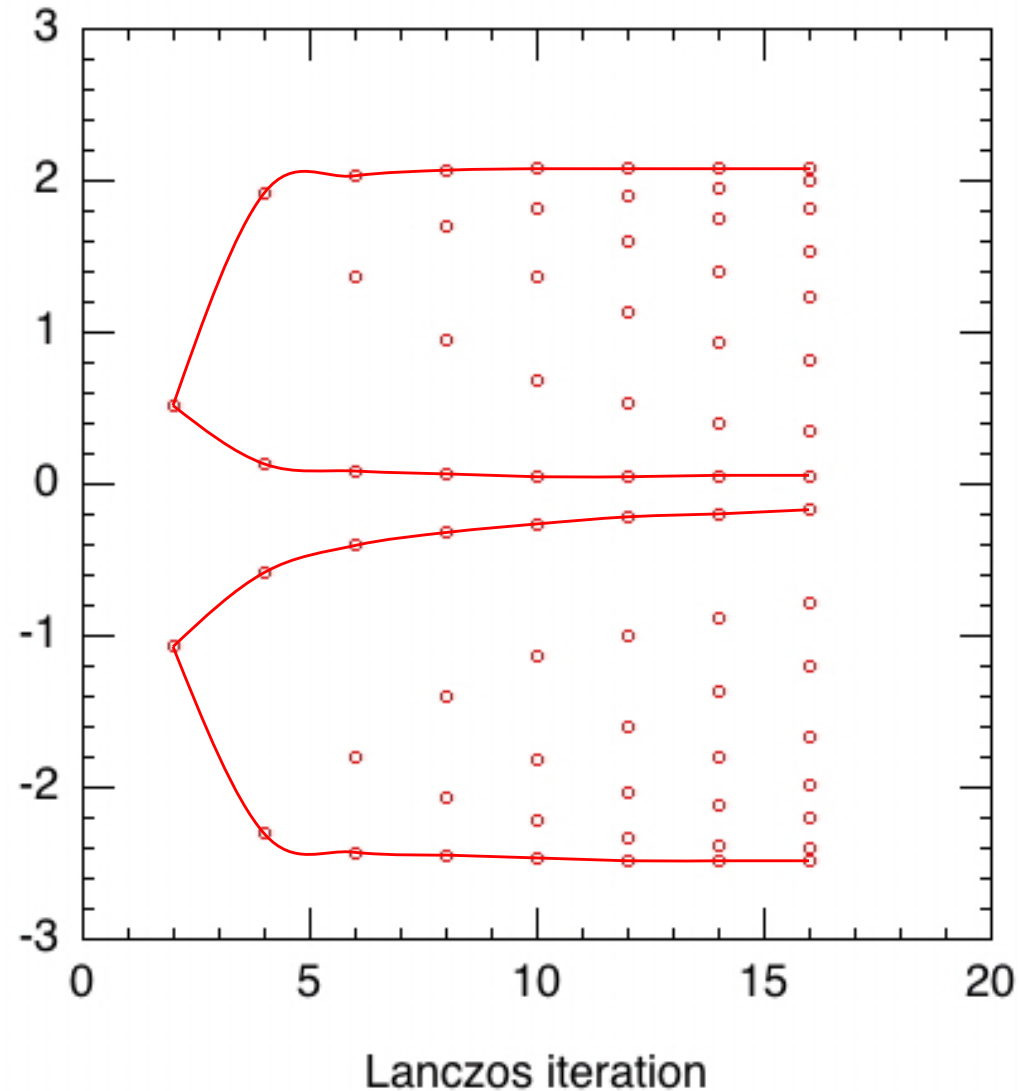$$Q = -\gamma_2 \frac{\hbar^2}{2m_0}(\partial_x^2 + \partial_y^2 - 2\partial_z^2),$$

$$R = \sqrt{3}\frac{\hbar^2}{2m_0}[\gamma_2(\partial_x^2 - \partial_y^2) - 2i\gamma_3\partial_x\partial_y],$$

$$S = -\sqrt{3}\gamma_3 \frac{\hbar^2}{m_0}\partial_z(\partial_x - i\partial_y),$$

$$U = \frac{-i}{\sqrt{3}}P_0\partial_z,$$

$$V = \frac{-i}{\sqrt{6}}P_0(\partial_x - i\partial_y).$$

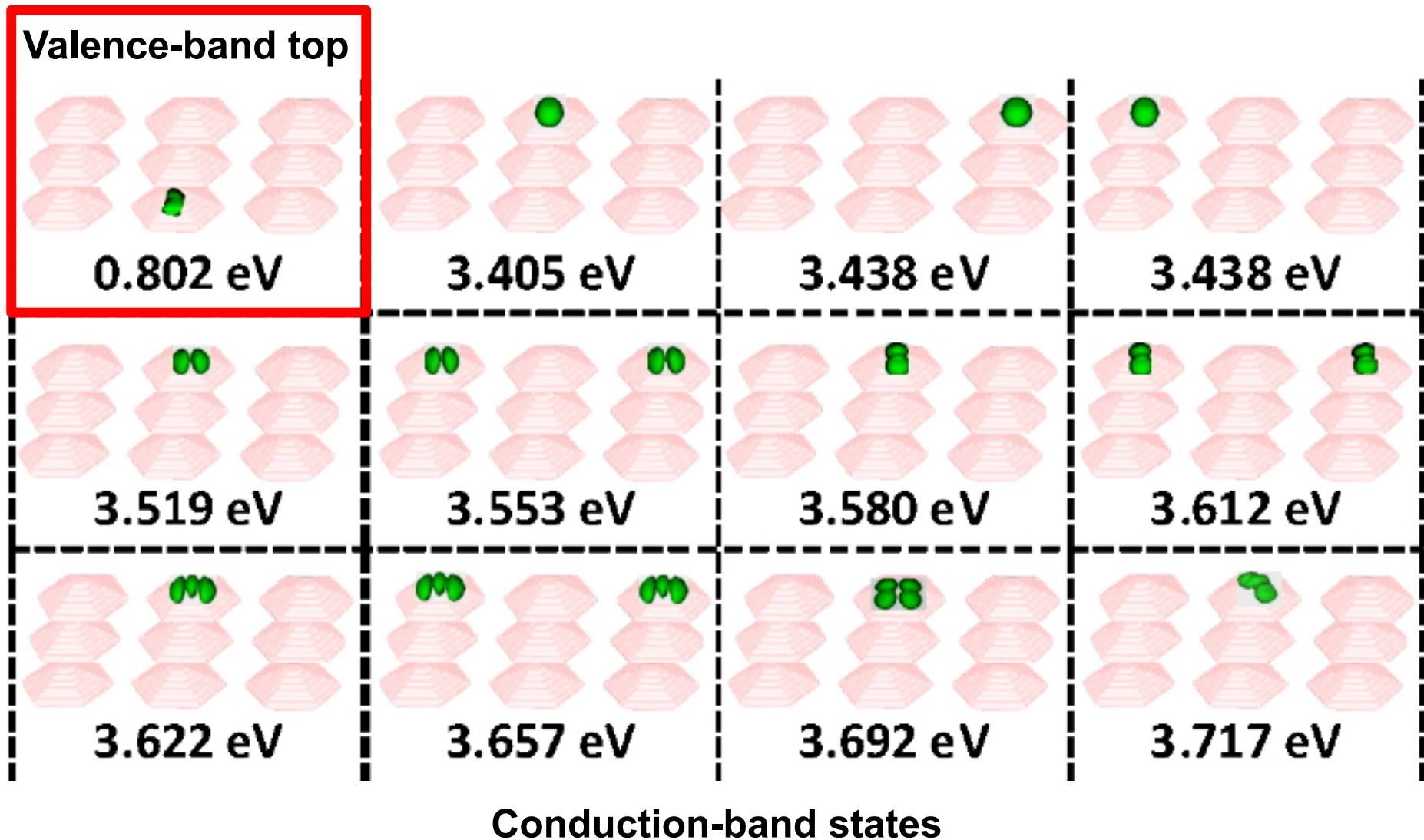C. Pryor, *Phys. Rev. B* **57**, 7190 ('98)

Lanczos Program in Fortran

```fortran
do s = 1,NWF
  q(:,:,:,s) = v/bet(s-1)
  call hamiltonian_op(q(:,:,:,s),hv)  ! Operates Hamiltonian H on Q(S)
  v = hv-bet(s-1)*q(:,:,:,s-1)
  alp(s) = inner_product(q(:,:,:,s),v)
  v = v-alp(s)*q(:,:,:,s)
  bet(s) = sqrt(inner_product(v,v))
  call tridiag(eval,s)  ! Diagonalize the S by S tridiagonal matrix
end do  ! Lanczos iteration over s
```

Given $\mathbf{r}_0, \beta_0 = \|\mathbf{r}_0\|$ ($\mathbf{q}_0 = 0$)
for $i = 1, \ldots, m$
$\quad \mathbf{q}_i \leftarrow \mathbf{r}_{i-1}/\beta_{i-1}$
$\quad \mathbf{r}_i \leftarrow \mathbf{A}\mathbf{q}_i - \beta_{i-1}\mathbf{q}_{i-1}$
$\quad \alpha_i \leftarrow \mathbf{q}_i^T \mathbf{r}_i$
$\quad \mathbf{r}_i \leftarrow \mathbf{r}_i - \alpha_i \mathbf{q}_i$
$\quad \beta_i = \|\mathbf{r}_i\|$ (only when $i \leq m - 1$)
endfor

Band-edge Wave Functions

- **Band-edge states in an array of GaN quantum dots in AlN matrix**

Valence-band top

0.802 eV   3.405 eV   3.438 eV   3.438 eV

3.519 eV   3.553 eV   3.580 eV   3.612 eV

3.622 eV   3.657 eV   3.692 eV   3.717 eV

Conduction-band states

S. Sburlan, Ph.D. dissertation, USC ('13)