Lanczos Method for Eigensystems

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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, $\lambda_1[A] \le \ldots \le \lambda_n[A]$ its eigenvalues in ascending order, $x \in R^n$, & the Rayleigh quotient

$$\rho(\mathbf{x};\mathbf{A}) = \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \quad \text{then} \quad \begin{cases} \lambda_1[\mathbf{A}] = \min\limits_{\mathbf{x}\in\Re^n} \rho(\mathbf{x};\mathbf{A}) \\ \lambda_n[\mathbf{A}] = \max\limits_{\mathbf{x}\in\Re^n} \rho(\mathbf{x};\mathbf{A}) \end{cases}$$

Proof

Let $q^{(k)}$ be the k-th orthonormalized eigenvector of 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 $Q^TQ = I$), 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 $\{q_1,\ldots,q_m\}$ ($q_j \in R^n$; $j = 1,\ldots,m$; $m < n$) be an orthonormal set, so that any vector $x \in R^n$ in the range is expressed as a linear combination of $q_1,\ldots,q_m$:

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

then the best approximations for $\lambda_1[A]$ & $\lambda_n[A]$ 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 $\lambda_1[H]$ & $\lambda_m[H]$.

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

the minimum of which is $\lambda_1[H]$ (*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 = [$s_1 \ldots s_m$] ($s_j \in R^n$) as (see supplementary note):**

$$
\begin{aligned}
&\mathbf{q}_1 = \mathbf{s}_1 / |\mathbf{s}_1| \\
&\text{for} \quad i = 2 \quad \text{to} \quad m \\
&\qquad \mathbf{q}'_i = \mathbf{s}_i - \sum_{j=1}^{i-1} \mathbf{q}_j \left(\mathbf{q}_j \bullet \mathbf{s}_i \right) \\
&\qquad \mathbf{q}_i = \mathbf{q}'_i / |\mathbf{q}'_i| \\
&\text{endfor}
\end{aligned}
$$

Projection!

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

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

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

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

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 $\mathbf{H} = \mathbf{Q}^\mathrm{T}\mathbf{AQ}$

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

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, $\mathbf{y}_k = \mathbf{Q}\mathbf{g}_k$ ($k = 1$ & m).

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

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

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

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

Krylov Subspace

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

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 $i < j-1$.

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

- **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, Aq_i is a linear combination of q_{i-1}, q_i & q_{i+1}:**

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

If we define $q_0 = 0$, the above equation is valid for $i = 1$ as well. Let $r_i \equiv \beta_i q_{i+1}$ (r_i is a component of Aq_i orthogonal to q_j for $j \le i$), then

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

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

- **Lanczos algorithm:**

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

Keep increasing *m* until $\lambda_1[T_m]$ 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)

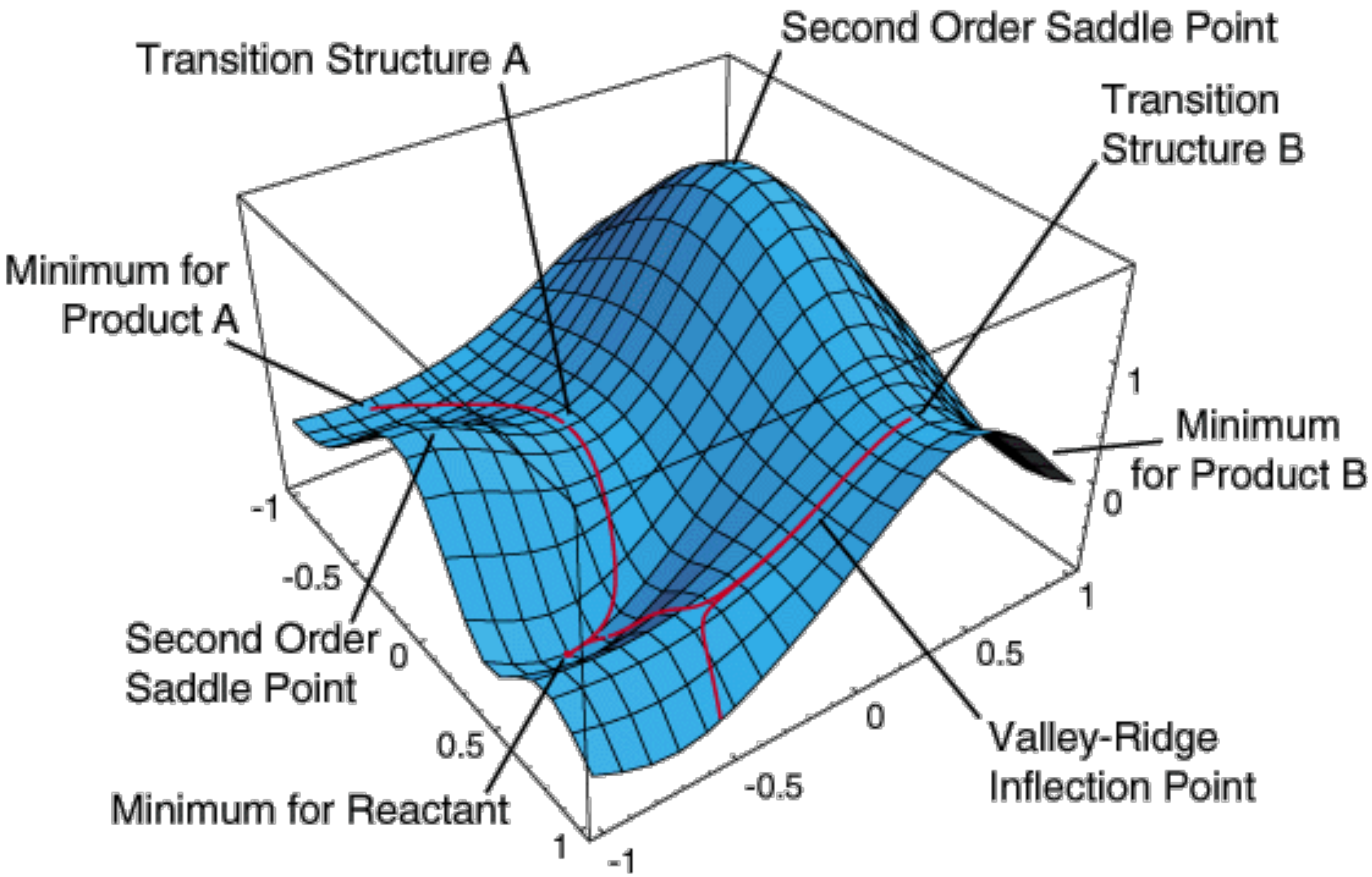


Figure from Prof. H. B. Schlegel; http://chem.wayne.edu/schlegel

Lanczos Algorithm for Hessian Calculation

A. Nakano / Computer Physics Communications 176 (2007) 292–299

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
$s \leftarrow s + 1$
$\mathbf{Q}^s \leftarrow \Delta/\beta^{s-1}$
$c_{\mathrm{fd}} \leftarrow \max_{i\alpha}\{|q^s_{i\alpha}| \mid i = 1, \ldots, N; \alpha = x, y, z\}/\delta_{\mathrm{fd}}$
$\Delta \leftarrow c_{\mathrm{fd}}[-\mathbf{F}(\mathbf{R} + \mathbf{Q}^s/c_{\mathrm{fd}}) + \mathbf{F}(\mathbf{R})] - \beta^{s-1}\mathbf{Q}^{s-1}$
$\alpha^s \leftarrow \mathbf{Q}^{s\mathrm{T}}\Delta$
$\Delta \leftarrow \Delta - \alpha^s \mathbf{Q}^s$
$\beta^s \leftarrow \|\Delta\|$

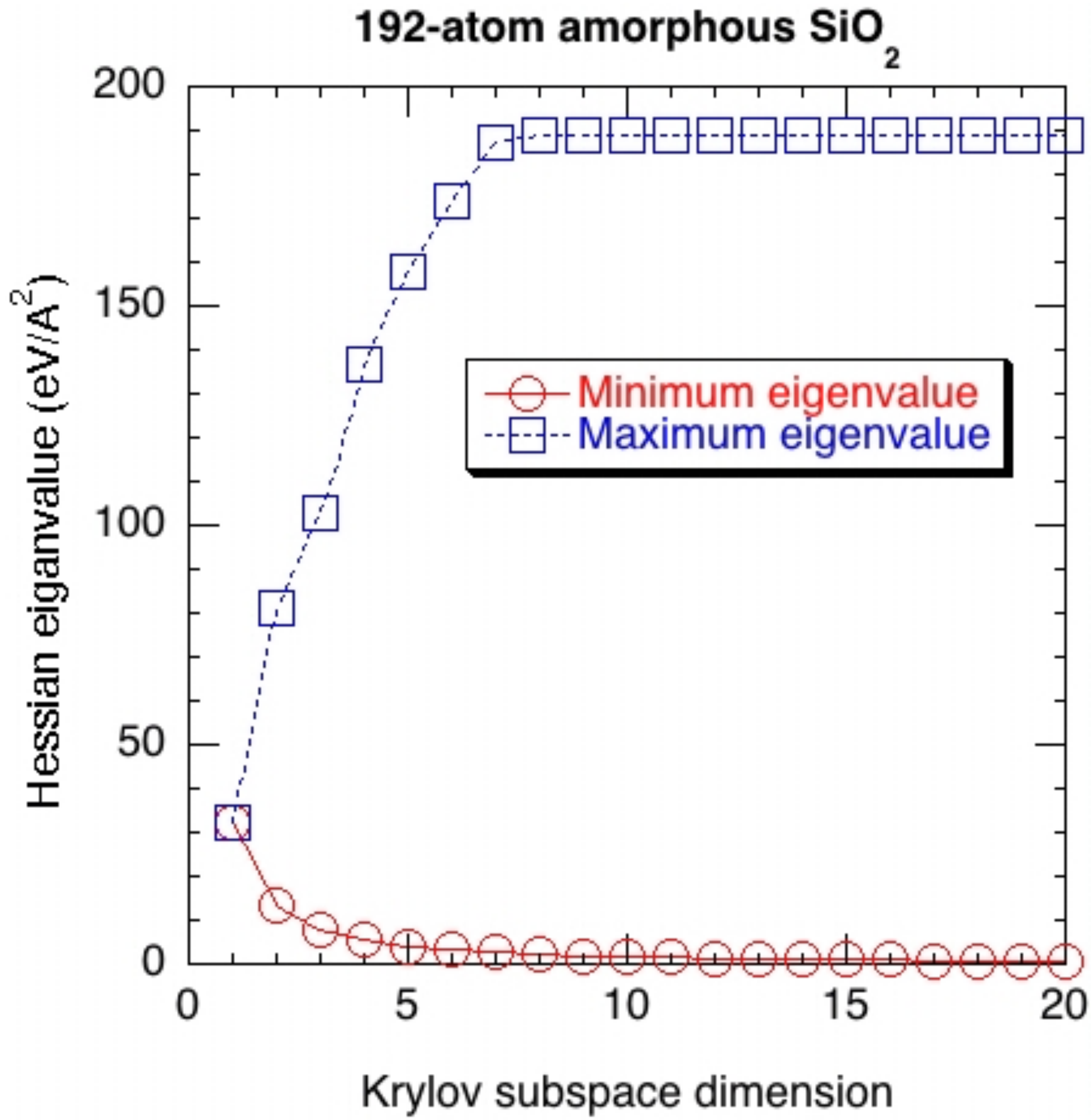
$$\text{diagonalize } \mathbf{T}_s = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{s-2} & \alpha_{s-1} & \beta_{s-1} \\ & & & \beta_{s-1} & \alpha_s \end{bmatrix}, \quad \text{so that } \tilde{\mathbf{Q}}_s^{\mathrm{T}} \mathbf{T}_s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

$tqli() — O(N)$

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

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

Sample Run of Lanczos Program



Electronic Energy Bands of GaAs

- **8-band k•p model**

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

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

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

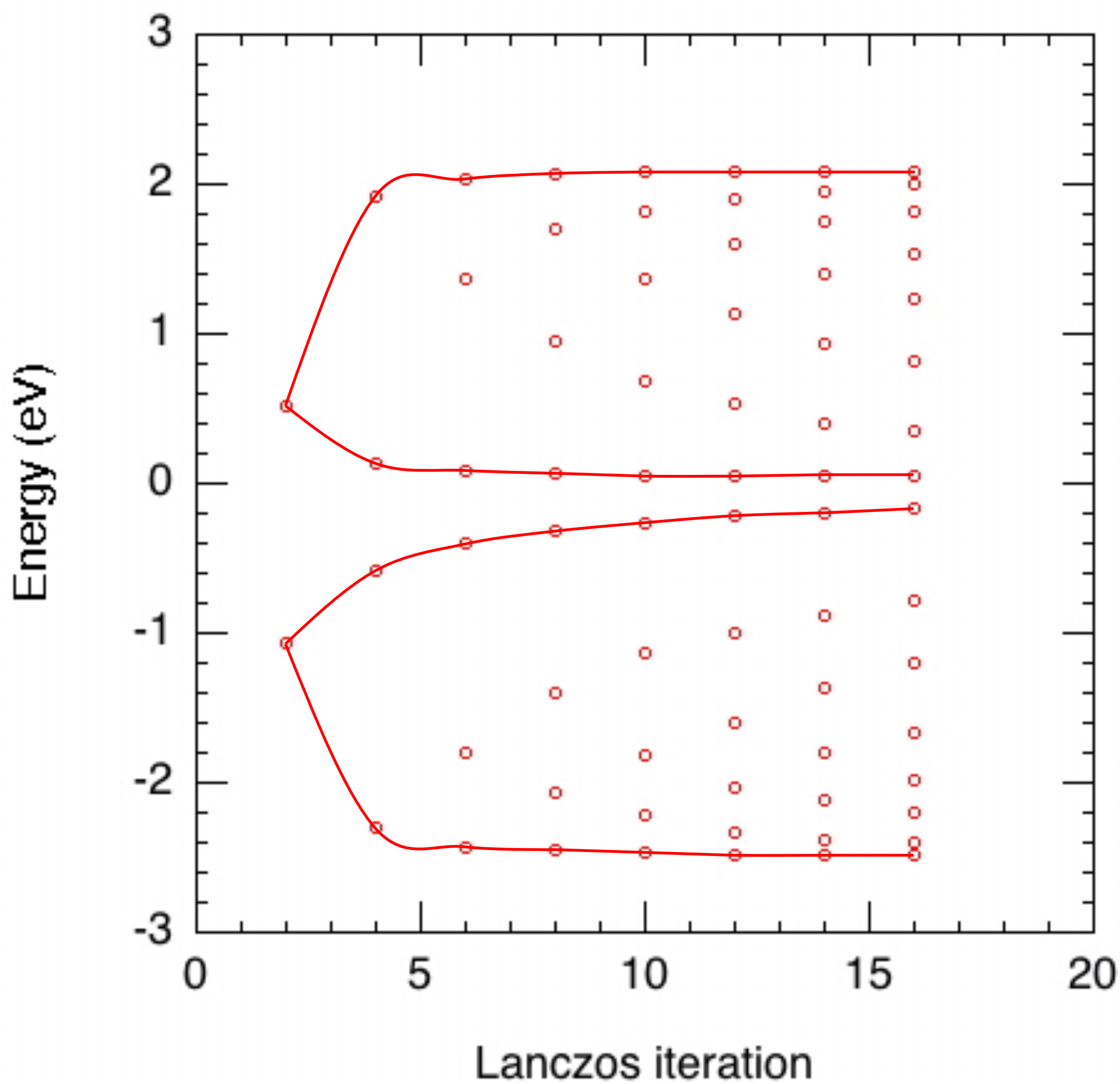
$$Q=-\gamma_2\frac{\hbar^2}{2m_0}(\partial_x^2+\partial_y^2-2\partial_z^2),$$

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

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

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

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



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

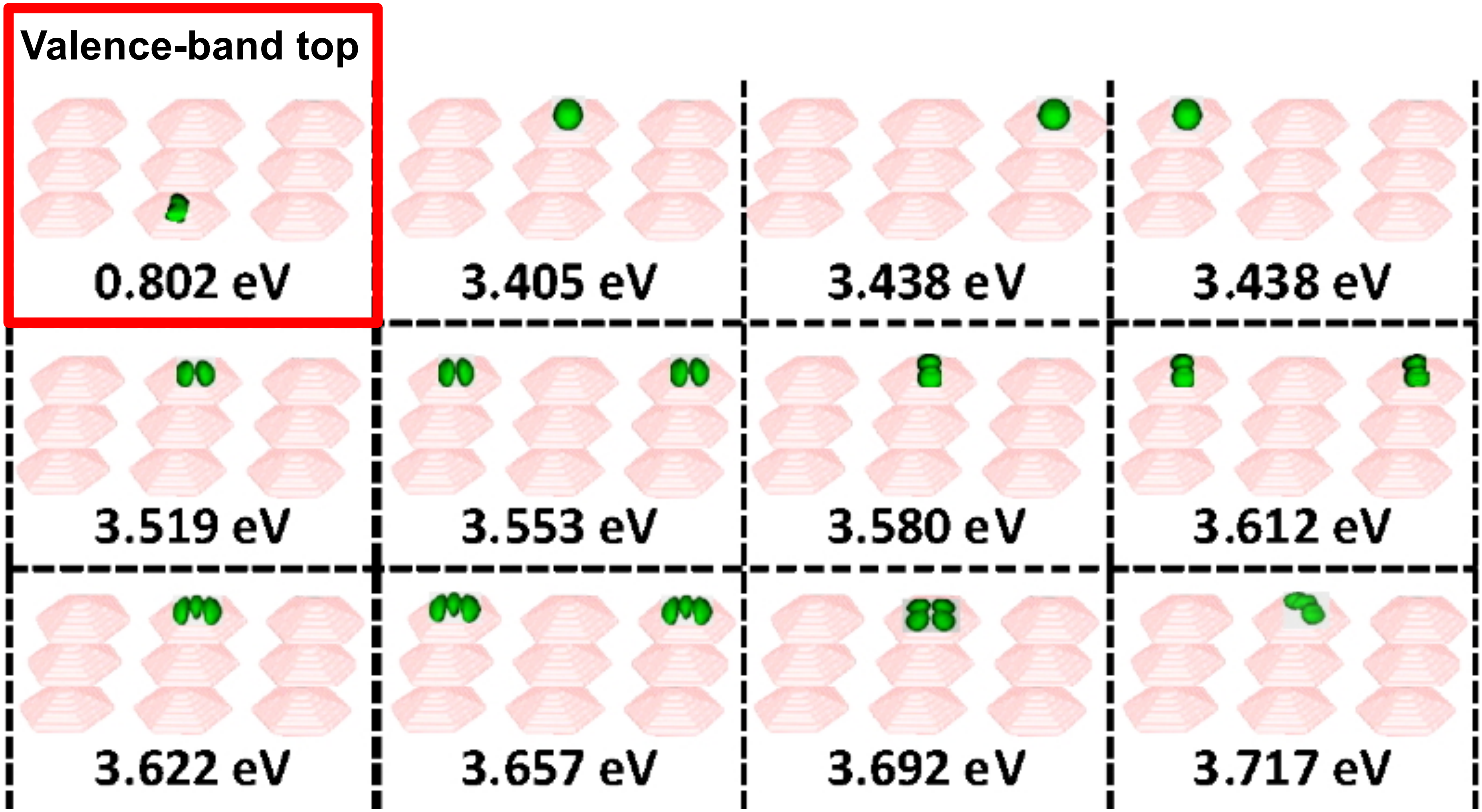
Lanczos Program in Fortran

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

Band-edge Wave Functions

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



Conduction-band states

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