# 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, $\lambda_1[\mathbf{A}] \le \ldots \le \lambda_n[\mathbf{A}]$ its eigenvalues in ascending order, $\mathbf{x} \in \mathbf{R}^n$, & 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 $\mathbf{q}^{(k)}$ 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 $\mathbf{x} = \mathbf{Q}\mathbf{z}$ (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 $\mathbf{z}^T = (1,0,\ldots,0) = \mathbf{e}_1$ & $\mathbf{x} = \mathbf{Q}\mathbf{e}_1 = \mathbf{q}_1$.

# Rayleigh-Ritz Procedure

**Theorem**

Let $\{\mathbf{q}_1,\ldots,\mathbf{q}_m\}$ ($\mathbf{q}_j \in \mathbf{R}^n$; $j = 1,\ldots,m$; $m < n$) be an orthonormal set, so that any vector $\mathbf{x} \in \mathbf{R}^n$ in the range is expressed as a linear combination of $\mathbf{q}_1,\ldots,\mathbf{q}_m$:

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

$\mathbf{x} \in$ rank-$m$ subspace $\subset \mathbf{R}^n$

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

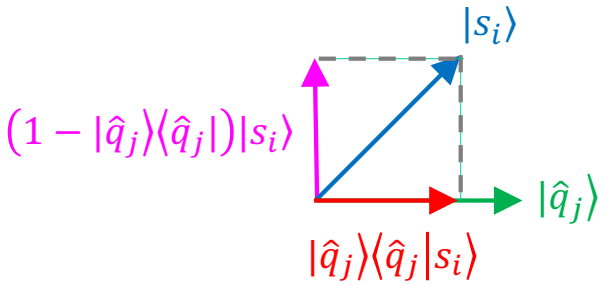
then $$\rho(\mathbf{x};\mathbf{A}) = \frac{\mathbf{z}^T\mathbf{Q}^T\mathbf{A}\mathbf{Q}\mathbf{z}}{\mathbf{z}^T\mathbf{Q}^T\mathbf{Q}\mathbf{z}} = \frac{\mathbf{z}^T\mathbf{H}\mathbf{z}}{\mathbf{z}^T\mathbf{z}} = \frac{z_1^2\lambda_1(\mathbf{H}) + \cdots + z_m^2\lambda_m(\mathbf{H})}{z_1^2 + \cdots +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

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 = $[\mathbf{s}_1 \ldots \mathbf{s}_m]$ ($\mathbf{s}_j \in \mathbf{R}^n$) as (see supplementary note):**

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




**Project out!**

$$\begin{pmatrix} & \sum_{j=1}^{i-1} |\hat{q}_j\rangle\langle\hat{q}_j| \\ 1 - & \overbrace{\quad\quad}^{\hat{P}} \end{pmatrix} |s_i\rangle$$

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

$$\underset{n}{\overset{m}{\begin{bmatrix} \mathbf{s}_1 & \mathbf{s}_2 & \mathbf{s}_3 & \mathbf{s}_4 \end{bmatrix}}} = \underset{n}{\overset{m}{\begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \mathbf{q}_4 \end{bmatrix}}} \overset{m}{\begin{bmatrix} |\mathbf{q}'_1| & \mathbf{q}_1 \bullet \mathbf{s}_2 & \mathbf{q}_1 \bullet \mathbf{s}_3 & \mathbf{q}_1 \bullet \mathbf{s}_4 \\ 0 & |\mathbf{q}'_2| & \mathbf{q}_2 \bullet \mathbf{s}_3 & \mathbf{q}_2 \bullet \mathbf{s}_4 \\ 0 & 0 & |\mathbf{q}'_3| & \mathbf{q}_3 \bullet \mathbf{s}_4 \\ 0 & 0 & 0 & |\mathbf{q}'_4| \end{bmatrix}}_{i-1} m$$

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

*cf.* QR decomposition
$A = Q[\blacktriangleright]$

- **For higher parallelization, Cholesky decomposition (BLAS3) is used instead**
  https://aiichironakano.github.io/phys516/Cholesky.pdf

Hasegawa *et al.*, *SC* ('11)

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

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

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

$$\mathbf{A}\,\overbrace{\mathbf{Q}\mathbf{g}_k}^{\mathbf{y}_k} \cong \lambda_k(\mathbf{H})\,\overbrace{\mathbf{Q}\mathbf{g}_k}^{\mathbf{y}_k}$$

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

*cf.* $\mathbf{Q}^T\mathbf{Q} \neq \mathbf{I}^{m\times m}$ — orthonormal in $\mathbf{R}^m$ subspace but not complete in total $\mathbf{R}^n$ space

Davidson method augments the vector subspace by residual, $\mathbf{r}_k = \mathbf{A}\mathbf{y}_k - \lambda_k\,\mathbf{y}_k$.

See Tkachenko *et al.*, *Quant. Sci. Tech.* **9**, 035012 ('24)

# 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 $i < j-1$.**

$$\mathbf{T}_m = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{m-2} & \alpha_{m-1} & \beta_{m-1} \\ & & & \beta_{m-1} & \alpha_m \end{bmatrix}$$

$$\begin{cases} \alpha_j = \mathbf{q}_j^T \mathbf{A} \mathbf{q}_j & j = 1, \dots, m \\ \beta_j = \mathbf{q}_{j+1}^T \mathbf{A} \mathbf{q}_j & j = 1, \dots, m-1 \end{cases}$$

- **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, $\mathbf{Aq}_i$ is a linear combination of $\mathbf{q}_{i-1}$, $\mathbf{q}_i$ & $\mathbf{q}_{i+1}$:**

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

**If we define $\mathbf{q}_0 = 0$, 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 $\mathbf{Aq}_i$ orthogonal to $\mathbf{q}_j$ for $j \le i$), then**

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

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

- **Lanczos algorithm:**

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

**Keep increasing $m$ until $\lambda_1[\mathbf{T}_m]$ 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)

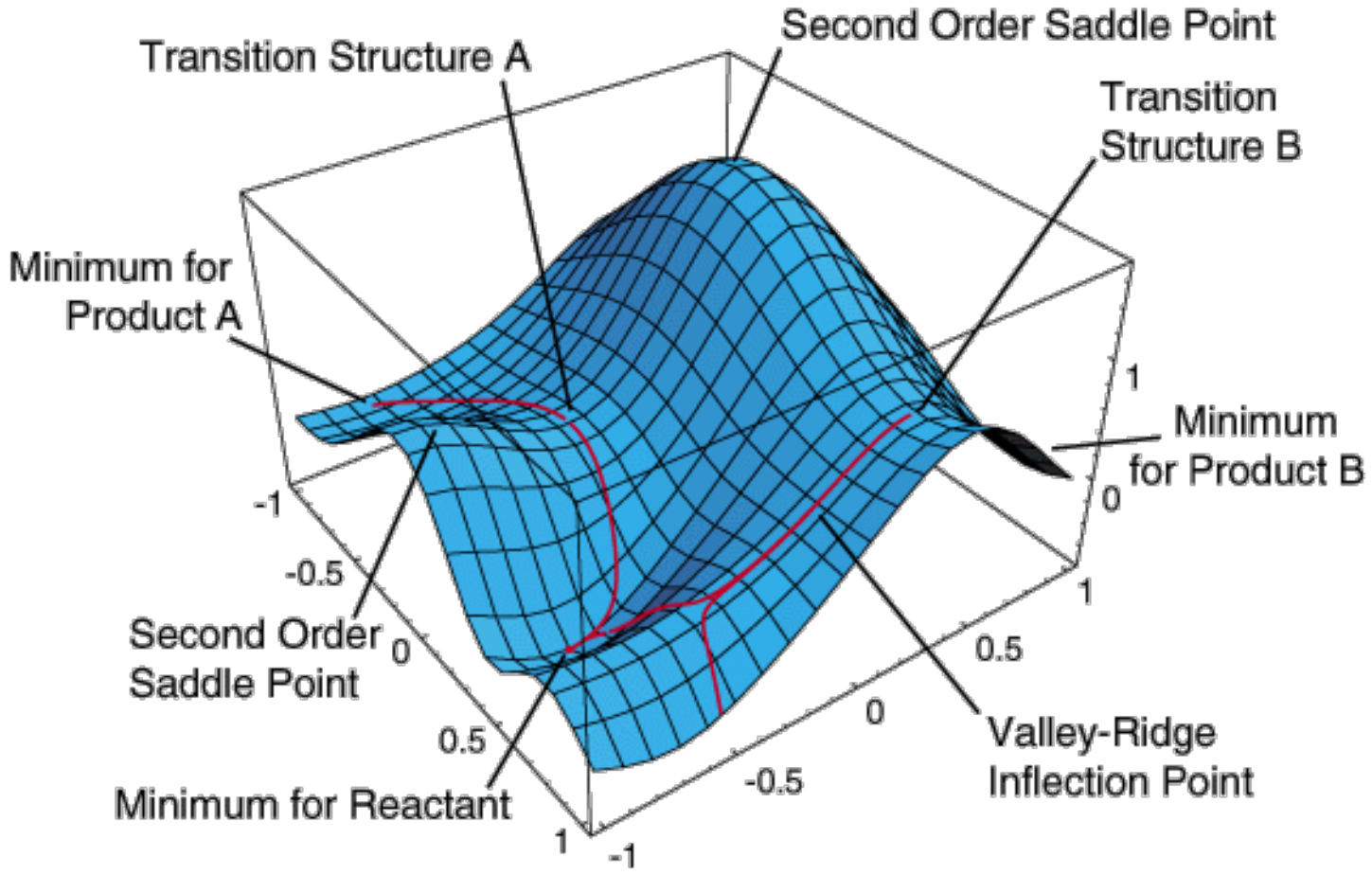



Figure from Prof. H. B. Schlegel; http://chem.wayne.edu/schlegel

# 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:**

$\lambda_1$: 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 $\lambda_1$

**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

$s \leftarrow s + 1$

$\mathbf{Q}^s \leftarrow \Delta / \beta^{s-1}$

$c_{\mathrm{fd}} \leftarrow \max_{i\alpha}\{|q^s_{i\alpha}| \mid i = 1, \ldots, N; \alpha = x, y, z\}/\delta_{\mathrm{fd}}$

$\Delta \leftarrow c_{\mathrm{fd}}[-\mathbf{F}(\mathbf{R} + \mathbf{Q}^s/c_{\mathrm{fd}}) + \mathbf{F}(\mathbf{R})] - \beta^{s-1}\mathbf{Q}^{s-1}$

$\alpha^s \leftarrow \mathbf{Q}^{s\mathrm{T}}\Delta$

$\Delta \leftarrow \Delta - \alpha^s \mathbf{Q}^s$

$\beta^s \leftarrow \|\Delta\|$

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 $\tilde{\mathbf{Q}}_s^{\mathrm{T}} \mathbf{T}_s \tilde{\mathbf{Q}}_s = \mathrm{diag}(\tilde{\lambda}^s_1, \ldots, \tilde{\lambda}^s_s)^*$

while $|(\tilde{\lambda}^s_1 - \tilde{\lambda}^{s-1}_1)/\tilde{\lambda}^{s-1}_1| > \Delta_{\mathrm{eigen}}$

$\lambda_1 \leftarrow \tilde{\lambda}^s_1$

$\mathbf{V}^1 \leftarrow \sum_{k=1}^{s} \mathbf{Q}^k \tilde{q}^1_k$

$\mathbf{V}^1 \leftarrow \mathbf{V}^1 / \|\mathbf{V}^1\|$

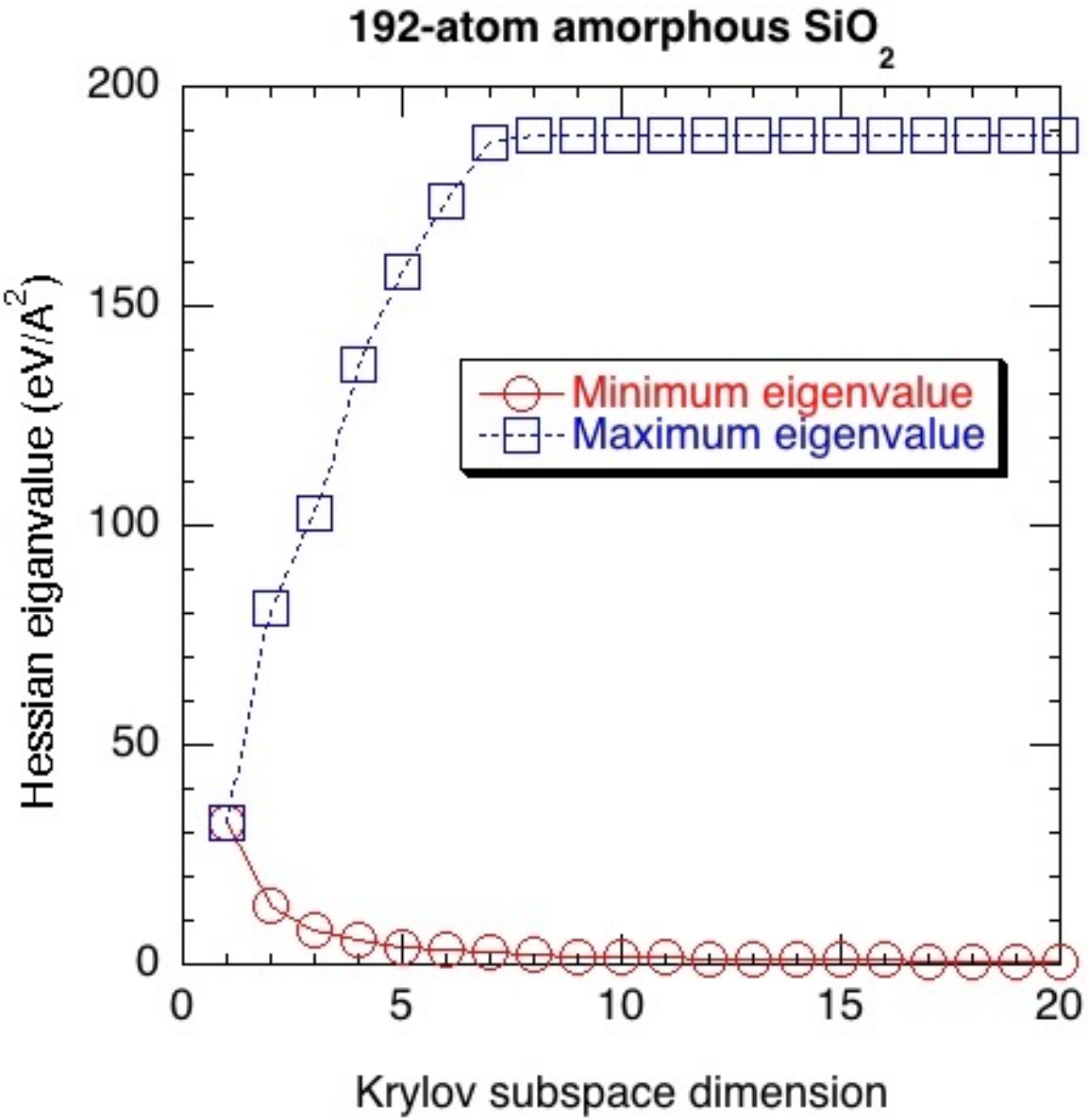
$$\vec{F}(\vec{R} + \vec{Q}) = \vec{F}(\vec{R}) + \overbrace{\partial \vec{F}/\partial \vec{R}}^{-\vec{\vec{H}}(\vec{R})} \bullet \vec{Q}$$

$$\therefore \vec{\vec{H}}(\vec{R}) \bullet \vec{Q} = -\vec{F}(\vec{R} + \vec{Q}) + \vec{F}(\vec{R})$$

$tqli() - O(N)$

* $\mathrm{diag}(\tilde{\lambda}^s_1, \ldots, \tilde{\lambda}^s_s)$ is an $s$ by $s$ diagonal matrix, with its diagonal elements given by $\tilde{\lambda}^s_1, \ldots, \tilde{\lambda}^s_s$. $\tilde{\mathbf{Q}}^s = [\tilde{\mathbf{q}}^1, \ldots, \tilde{\mathbf{q}}^s]$ is an $s$ by $s$ orthogonal matrix, with $\tilde{\mathbf{q}}^m \in \mathbb{R}^s$ is the $m$th eigenvector of $\mathbf{T}_s$.

# Sample Run of Lanczos Program



# Electronic Energy Bands of GaAs

- **8-band k•p model**

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

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

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

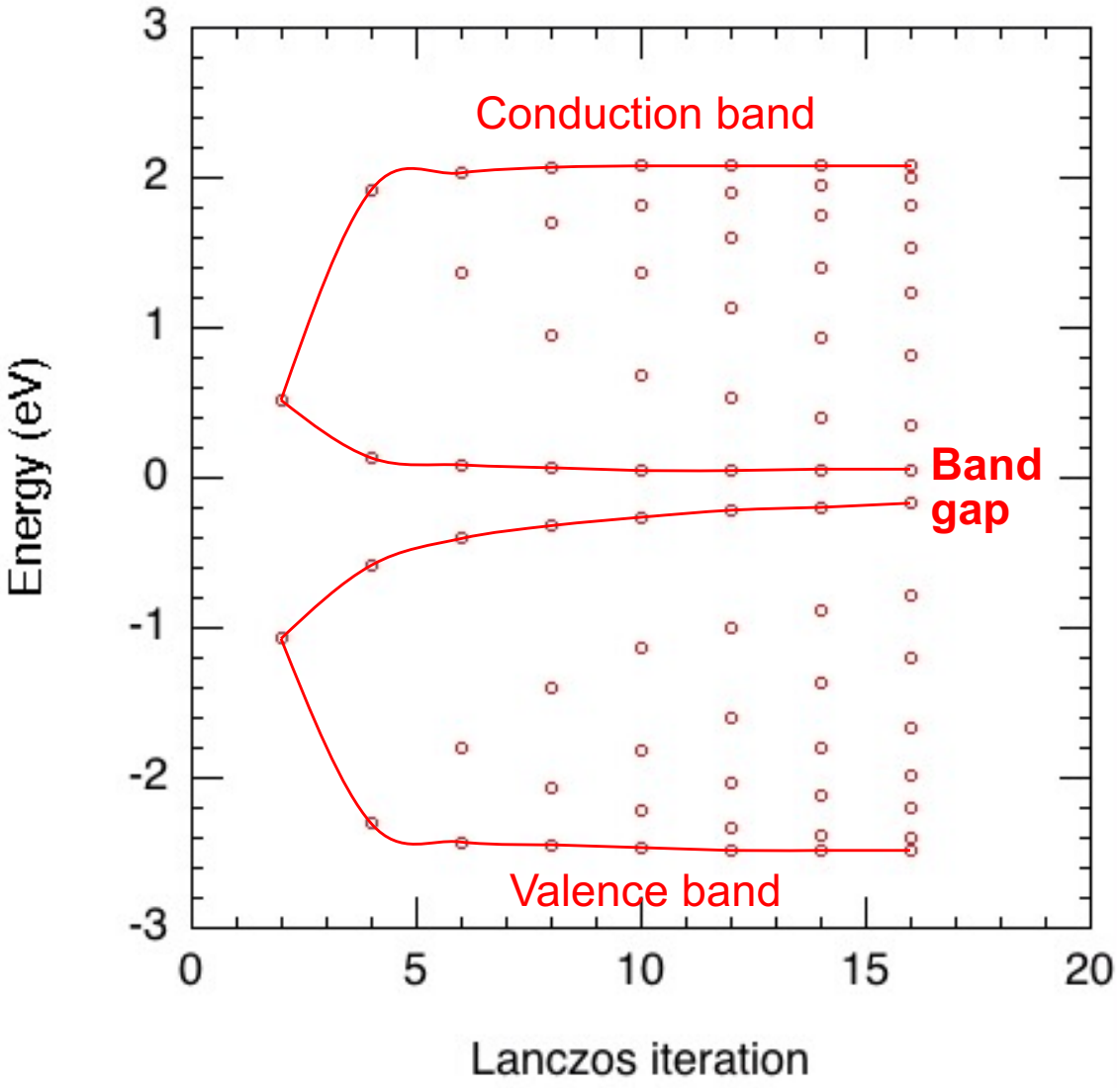
$$Q = -\gamma_2\frac{\hbar^2}{2m_0}(\partial_x^2+\partial_y^2-2\partial_z^2),$$

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

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

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

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




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

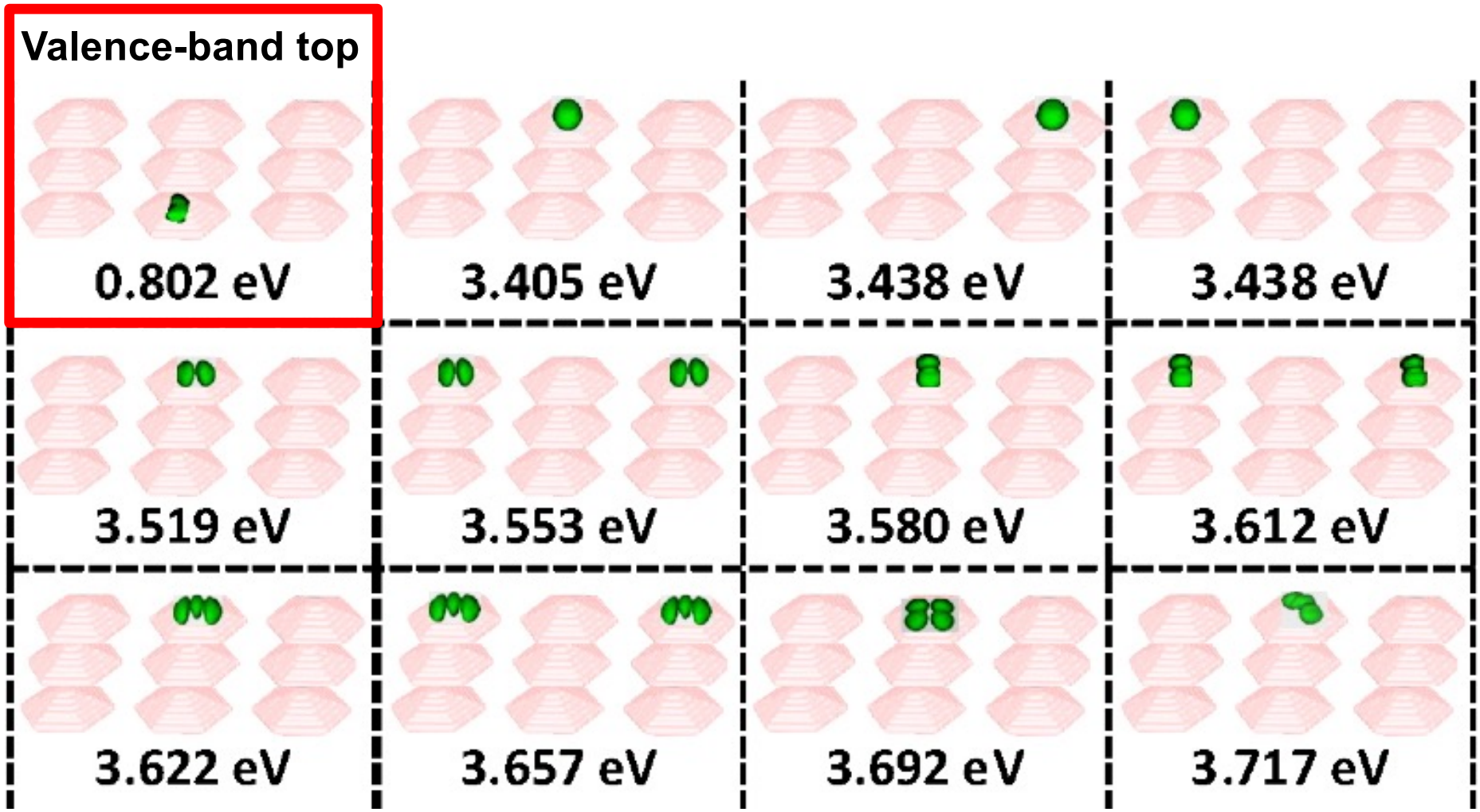
# Lanczos Program in Fortran

```
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

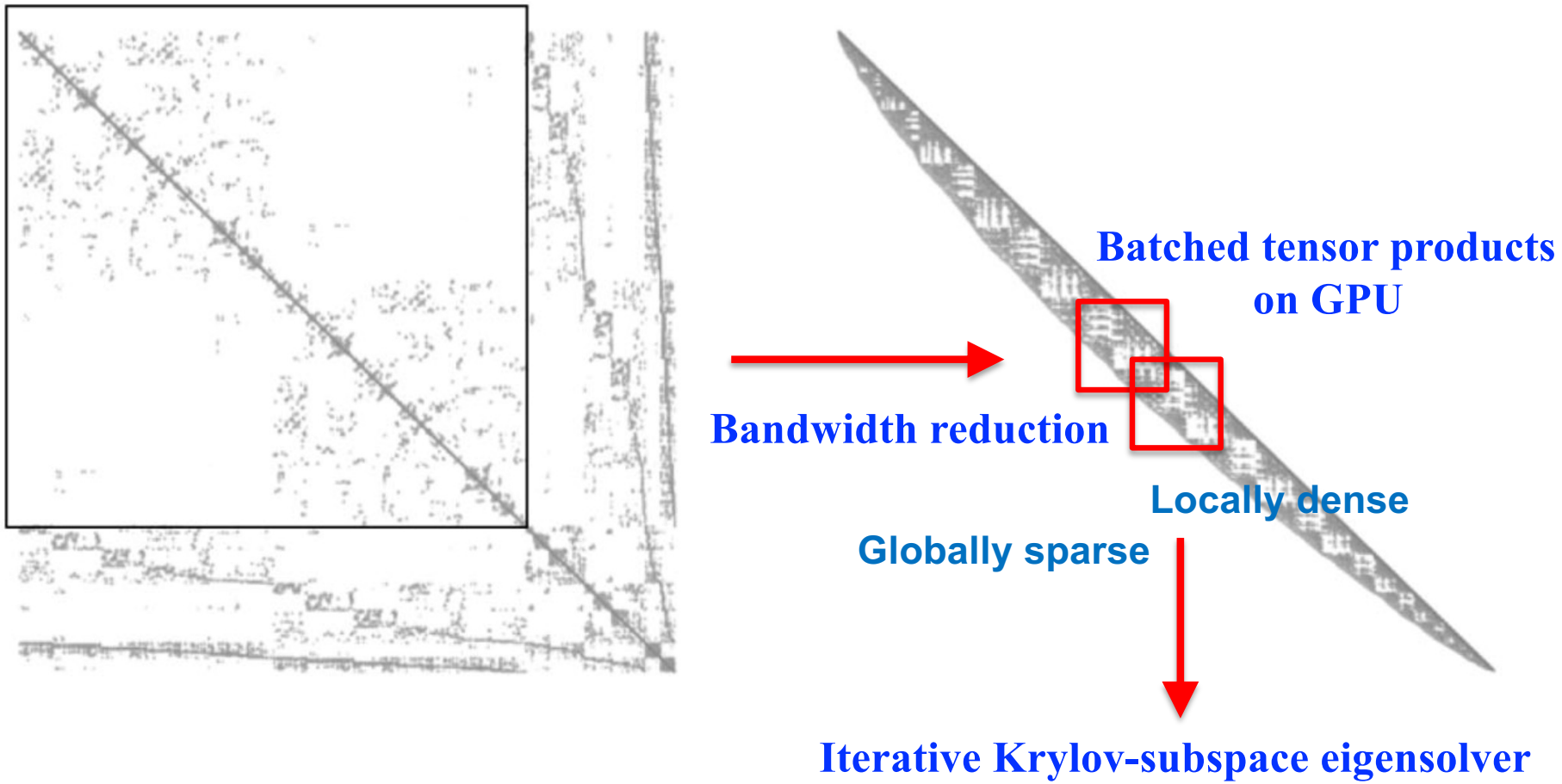
- **Band-edge states in an array of GaN quantum dots in AlN matrix**




**Conduction-band states**

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

# Globally-Sparse Yet Locally-Dense Eigensolver




- **250-fold speed-up over state-of-the-art for 2.4M atom molecular vibrational modes**

J. H. Lam *et al.*, *Nature Commun.* **15**, 3479 ('24)

# Top 10 Algorithms in History

In putting together this issue of *Computing in Science & Engineering*, we knew three things: it would be difficult to list just 10 algorithms; it would be fun to assemble the authors and read their papers; and, whatever we came up with in the end, it would be controversial. We tried to assemble the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century. Following is our list (here, the list is in chronological order; however, the articles appear in no particular order):

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

PHYS 516
CSCI 596
CSCI 653

*IEEE CiSE*, Jan/Feb (2000)