Block-Tridiagonal Divide-and-Conquer for Electronic-Structure Calculation

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[W.N. Gansterer, R.C. Ward, R.P. Muller, ACM Trans. Math. Software 28, 45 ('02)]

- Problem: block-tridiagonal Hamiltonian

$$
H = \begin{array}{c|ccccc|c}
 & k_1 & k_2 & \cdots & & & \\
\hline
k_1 & B_1 & E_1^T & & & & \\
k_2 & E_1 & B_2 & E_2^T & & & \\
\vdots & & E_2 & B_3 & \ddots & & \vdots \\
 & & & \ddots & \ddots & E_{p-1}^T & k_{p-1} \\
 & & & & E_{p-1} & B_p & k_p \\
\hline
 & & & \cdots & k_{p-1} & k_p &
\end{array} \qquad (1)
$$

$E_1^T \rightarrow$ environment

$B_p \rightarrow$ disjoint-partition clusters

where $B_i \in \mathbb{R}^{k_i \times k_i}$ $(i = 1, \ldots, p)$ are diagonal blocks and $E_i \in \mathbb{R}^{k_{i+1} \times k_i}$ $(i = 1, \ldots, p-1)$ are off-diagonal "environment" blocks that couple B_i and B_{i+1}.

- Rank-1 (mean-field) environment approximation

$$
\underset{k_{i+1}\times k_i}{E_i} \simeq \sigma_i \underset{k_{i+1}\times 1}{u_i} \underset{1\times k_i}{v_i^T} \quad (i = 1, \ldots, p-1) \qquad (2)
$$

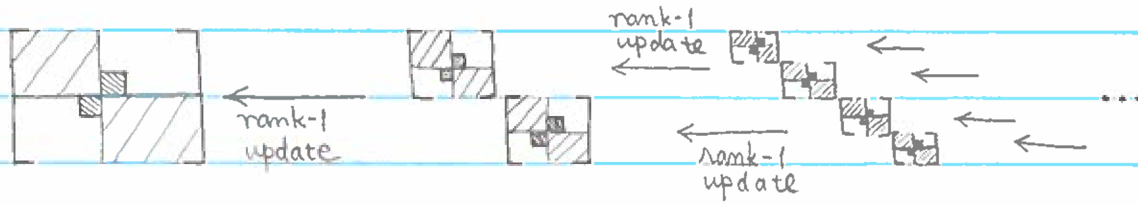
The mean field σ_i and self-energy vectors $u_i \in \mathbb{R}^{k_{i+1} \times 1}$ and $v_i \in \mathbb{R}^{k_i \times 1}$, which are optimal in the 2-norm (least-square) sense, are obtained by the singular value decomposition (SVD) of E_i,

$$
E_i = \sum_\alpha u_i^{(\alpha)} \sigma_i^{(\alpha)} v_i^{(\alpha)T}, \qquad (3)
$$

where $\sigma_i^{(1)} \geq \sigma_i^{(2)} \geq \cdots$, and retaining the largest singular value, $\sigma_i \equiv \sigma_i^{(1)}$.

– Recursive (successive) rank-1 updates

The block-tridiagonal Hamiltonian (1) is diagonalized by recursively applying rank-1 updates (perturbations), each time for two coupled blocks.



In the following, we consider two-block coupling, which is the building block of the recursive divide-&-conquer procedure.

– D&C algorithm step 1 : Subdivision

$$H = \begin{array}{cc} & \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{array}{c} k_1 \\ k_2 \end{array} & \begin{bmatrix} B_1 & E_1^T \\ E_1 & B_2 \end{bmatrix} \end{array} = \begin{array}{cc} & \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{array}{c} k_1 \\ k_2 \end{array} & \begin{bmatrix} B_1 & \sigma_1 \overset{k_1\,1}{v_1} \overset{1\,k_2}{u_1^T} \\ \sigma_1 \underset{k_2\,1}{u_1} \underset{1\,k_1}{v_1^T} & B_2 \end{bmatrix} \end{array} \tag{4}$$

Let's rewrite Eq.(4) as

$$H = \begin{bmatrix} B_1 - \sigma_1 v_1 v_1^T & 0 \\ 0 & B_2 - \sigma_1 u_1 u_1^T \end{bmatrix} + \begin{array}{cc} & \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{array}{c} k_1 \\ k_2 \end{array} & \begin{bmatrix} \sigma_1 v_1 v_1^T & \sigma_1 v_1 u_1^T \\ \sigma_1 u_1 v_1^T & \sigma_1 u_1 u_1^T \end{bmatrix} \end{array}$$

$$= \begin{bmatrix} \tilde{B}_1 & 0 \\ 0 & \tilde{B}_2 \end{bmatrix} + \sigma_1 \begin{array}{cc} & 1 \\ \begin{array}{c} k_1 \\ k_2 \end{array} & \begin{bmatrix} v_1 \\ u_1 \end{bmatrix} \end{array} \begin{array}{cc} & \begin{array}{cc} k_1 & k_2 \end{array} \\ 1 & \begin{bmatrix} v_1^T & u_1^T \end{bmatrix} \end{array}$$

$$= \tilde{H} + \sigma_1 \begin{bmatrix} v_1 \\ u_1 \end{bmatrix} \begin{bmatrix} v_1^T & u_1^T \end{bmatrix} \tag{5}$$

where $\tilde{B}_1 = B_1 - \sigma_1 v_1 v_1^T$ and $\tilde{B}_2 = B_2 - \sigma_1 u_1 u_1^T$ are dressed (environment-modified) particles with self-energy, and $\sigma_1 \begin{bmatrix} v_1 \\ u_1 \end{bmatrix} [v_1^T u_1^T]$ is the rank-1 perturbation.

— D&C algorithm step 2: "Independent" solutions of subprograms.

Diagonalize each dressed sub-Hamiltonian with self-energy corrections.

$$\sum_{\nu=1}^{k_1} (\tilde{B}_1)_{\mu\nu} \underbrace{q_\nu^{(n)}}_{(Q_1)_{\nu n}} = q_\nu^{(n)} d_n = \sum_{m=1}^{k_1} \underbrace{q_\nu^{(m)}}_{(Q_1)_{\nu m}} \underbrace{(d_m \delta_{mn})}_{(D_1)_{mn}}$$

$$\therefore \quad \tilde{B}_1 Q_1 = Q_1 D_1$$

Therefore

$$\tilde{B}_1 = Q_1 D_1 Q_1^T \in \mathbb{R}^{k_1 \times k_1} \qquad (6)$$

$$\tilde{B}_2 = Q_2 D_2 Q_2^T \in \mathbb{R}^{k_2 \times k_2} \qquad (7)$$

where D_1 and D_2 are diagonal eigenvalue matrices, and Q_1 and Q_2 are orthogonal: $\sum_{\mu=1}^{k_1} \underbrace{q_\mu^{(m)}}_{(Q_1^T)_{m\mu}} \underbrace{q_\mu^{(n)}}_{(Q_1)_{\mu n}} = \delta_{mn}$, or

$$Q_1^T Q_1 = I_{k_1} \qquad (8)$$

$$Q_2^T Q_2 = I_{k_2} \qquad (9)$$

Substitute the spectral decompositions (6) & (7) into Eq. (5)

$$H = \begin{bmatrix} Q_1 D_1 Q_1^T & 0 \\ 0 & Q_2 D_2 Q_2^T \end{bmatrix} + \sigma_1 \begin{bmatrix} v_1 \\ u_1 \end{bmatrix} [v_1^T \; u_1^T]$$

$$= \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix}$$

$$+ \sigma_1 \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \underbrace{\begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix} \begin{bmatrix} v_1 \\ u_1 \end{bmatrix}}_{\begin{bmatrix} Q_1^T v_1 \\ Q_2^T u_1 \end{bmatrix} = \begin{bmatrix} z_1 \end{bmatrix}} \underbrace{[v_1^T \; u_1^T] \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix}}_{[v_1^T Q_1 \;\; u_1^T Q_2] = [z_1^T \; z_2^T]} \begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix}$$

$$\therefore H = \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \left\{ \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} + \sigma_1 \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \begin{bmatrix} z_1^T & z_2^T \end{bmatrix} \right\} \begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix} \tag{10}$$

$$= Q \left(D + \sigma_1 z z^T \right) Q^T \tag{11}$$

where

$$Q = \begin{bmatrix} Q_1 & 0 \\ 0 & Q_2 \end{bmatrix} \tag{12}$$

$$D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \tag{13}$$

$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \tag{14}$$

$$z_1 = Q_1^T v_1 \tag{15}$$

$$z_2 = Q_2^T u_1 \tag{16}$$

- D&C algorithm step 3: Synthesize the sub-solutions

Rank-1 update of the eigenvalues $d_1, \dots, d_{k_1+k_2}$.

$$\underset{k1}{(D} + \sigma_1 \underset{k1}{z} \underset{1k}{z^T}) \underset{k1}{u} = \lambda \underset{k1}{u}$$

$$k = k_1 + k_2$$

$$(D - \lambda I) \underset{k1}{u} + \sigma_1 \underset{k1}{z} \underbrace{(\underset{1k}{z^T} \underset{k1}{u})}_{\text{contracted}} = 0$$

$$\therefore \quad u + \sigma_1 (D - \lambda I)^{-1} z \, (z^T u) = 0 \tag{17}$$

$z^T \times$ Eq. (17)

$$(\overset{1k}{z^T} \overset{k1}{u}) + \sigma_1 \overset{1k}{z^T} \overset{kk}{(D - \lambda I)^{-1}} \overset{k1}{z} \, (\overset{1k}{z^T} \overset{k1}{u}) = 0$$

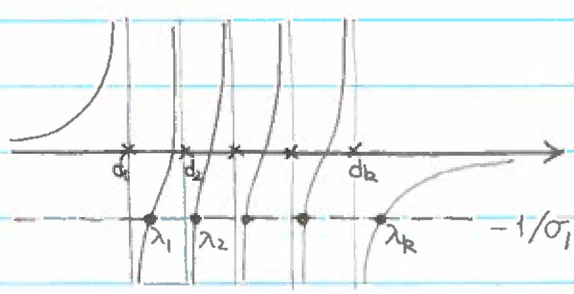
$$\left[1 + \sigma_1 z^T (D - \lambda I)^{-1} z \right] (z^T u) = 0 \tag{18}$$

For this to have a nontrivial ($u = 0$) solution, the secular equation must be satisfied:

$$1 + \sigma_1 \underbrace{z^T (D - \lambda I)^{-1} z}_{\sum_{\mu=1}^{k} \sum_{\nu=1}^{k} z_\mu (d_\mu - \lambda)^{-1} \delta_{\mu\nu} z_\nu} = 0 \tag{19}$$

$$= \sum_{\mu=1}^{k} z_\mu (d_\mu - \lambda)^{-1} z_\mu$$

$$\therefore \quad 1 + \sigma_1 \sum_{\mu=1}^{k} \frac{z_\mu^2}{d_\mu - \lambda} = 0 \tag{20}$$



To obtain the corresponding eigenvectors, let's assume

$$\mathcal{U}^{(n)} = C\,(D - \lambda_n I)^{-1} z \qquad (21)$$

Substituting Eq. (21) into the eigen equation (17),

$$C(D-\lambda_n I)^{-1} z + \cancel{\sigma_1}\,(D-\lambda_n I)^{-1} z\, C\, \underbrace{z^T (D-\lambda_n I)^{-1} z}_{-\frac{1}{\cancel{\sigma_1}}} = 0$$

from the eigenvalue equation (19)

$$C(D-\lambda_n I)^{-1} z - C\,(D-\lambda_n I)^{-1} z = 0$$

Therefore, Eq. (21) is indeed the eigenvector.

From the normalization condition,

$$1 = \sum_{\mu=1}^{k} \mathcal{U}^{(n)2} = C^2 \sum_{\mu=1}^{k} \frac{z_\mu^2}{(d_\mu - \lambda_n)^2}$$

$$\therefore\ C = \left[\sum_{\mu=1}^{k} \left(\frac{z_\mu}{d_\mu - \lambda_n}\right)^2\right]^{-1/2}$$

Therefore,

$$\mathcal{U}^{(n)} = \left[\sum_{\mu=1}^{k} \left(\frac{z_\mu}{d_\mu - \lambda_n}\right)^2\right]^{-1/2} (D - \lambda_n I)^{-1} z \qquad (22)$$

Spectral decomposition in terms of these eigenstates are

$$D + \sigma_1 z z^T = U \Lambda U^T \qquad (23)$$

where using the solutions of Eq. (20),

$$\Lambda = \mathrm{diag}\,(\lambda_1, \ldots, \lambda_k) \qquad (24)$$

and in terms of the eigenvectors Eq. (22)

$$U_{\mu n} = \mathcal{U}_\mu^{(n)} = \left[\sum_{\mu=1}^{k} \left(\frac{z_\mu}{d_\mu - \lambda_n}\right)^2\right]^{-1/2} (d_\mu - \lambda_n)^{-1} z_\mu \qquad (25)$$

Finally, substituting Eq. (23) in (11),

$$H = Q U \Lambda U^T Q^T$$

$$= (QU)\,\Lambda\,(QU)^T \qquad (26)$$