



# Hartree-Fock Stability and its Relation to Strong Correlation

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# Background Information

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# Correlation Energy

- The Molecular Electronic S.E. in the Born-Oppenheimer approximation

$$\left( \hat{T}_{elec} + \hat{V}_{elec-nuc} + \hat{V}_{elec-elec} \right) \Psi = E_{exact} \Psi$$

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# Correlation Energy

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- The correlation energy is recovered by post Hartree-Fock methods (CC, MBPT) which perform better the closer the HF solution is to the exact.

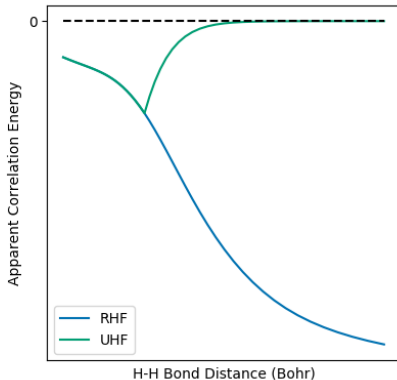
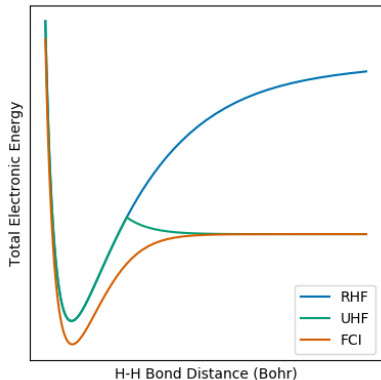
# Hartree-Fock Theory is Almost Always Restricted

Method	Spinorbital	DoF	Eigenfunction of
Restricted	$\chi_j^\alpha(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij} \phi_i(\vec{r}) \alpha(\sigma)$ $\chi_j^\beta(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij} \phi_i(\vec{r}) \beta(\sigma)$	N/2	$\hat{S}^2, \hat{S}_z$
Unrestricted	$\chi_j^\alpha(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij}^\alpha \phi_i(\vec{r}) \alpha(\sigma)$ $\chi_j^\beta(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij}^\beta \phi_i(\vec{r}) \beta(\sigma)$	N	$\hat{S}_z$
General	$\chi_j(\vec{r}, \sigma) = \sum_{i=1}^N [c_{ij}^\alpha \phi_i(\vec{r}) \alpha(\sigma) + c_{ij}^\beta \phi_i(\vec{r}) \beta(\sigma)]$	2N	Neither



# Case Study: $\text{H}_2$ Dissociation

Is this strong correlation or a bad reference?



# Project Questions

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- How can we improve our HF solutions?
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- Apply to systems (known molecules, periodic systems)

# Hartree-Fock Stability

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- This not the case if any **Orbital Hessian** (aka stability matrix, electronic Hessian) eigenvalues are **negative**

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = \omega \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} \quad (1)$$



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- Where

$$\begin{aligned} A_{ia,jb} &= \langle i^a | H - E_0 | j^b \rangle = (\epsilon_a - \epsilon_i) \delta_{ij} \delta_{ab} + \langle aj || ib \rangle \\ B_{ia,jb} &= \langle ij^a | H - E_0 | 0 \rangle = \langle ab || ij \rangle . \end{aligned} \quad (2)$$

# Hartree-Fock Stability Conditions

## The Matrix Equation Factorizes

Solution Type	Space Type					
	Real RHF	Complex RHF	Real UHF	Complex UHF	Real GHF	Complex GHF
Real RHF	${}^1\mathbf{A}' + {}^1\mathbf{B}'$	${}^1\mathbf{A}' - {}^1\mathbf{B}'$	${}^3\mathbf{A}' + {}^3\mathbf{B}'$	${}^3\mathbf{A}' - {}^3\mathbf{B}'$	${}^3\mathbf{A}' + {}^3\mathbf{B}'$	${}^3\mathbf{A}' - {}^3\mathbf{B}'$
Complex RHF	-	${}^1\mathbf{H}'$	-	${}^3\mathbf{H}'$	-	${}^3\mathbf{H}'$
Real UHF	-	-	$\mathbf{A}' + \mathbf{B}'$	$\mathbf{A}' - \mathbf{B}'$	$\mathbf{A}'' + \mathbf{B}''$	$\mathbf{A}'' - \mathbf{B}''$
Complex UHF	-	-	-	$\mathbf{H}'$	-	$\mathbf{H}'$
Real GHF	-	-	-	-	$\mathbf{A} - \mathbf{B}$	$\mathbf{A} - \mathbf{B}$
Complex GHF	-	-	-	-	-	$\mathbf{H}$

Table reproduced from Seeger & Pople<sup>1</sup>

1) Seeger, R.; Pople, J. A. J. Chem. Phys. 1977, 66 (7), 3045.

# Homogeneous Electron Gas

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# Brief Overview of HEG

- Homogeneous Electron Gas (HEG) model, also known as Uniform Electron Gas or Jellium Model.
- Characterized by  $r_s$ , inversely proportional to density
- Electrons in a box with "smeared" nuclei  $\rightarrow$  uniform positive background charge
- The total charge is constrained to be neutral,

$$V_{bg}(\mathbf{r}) = \sum_i \frac{-Ze^2}{|\mathbf{r} - \mathbf{R}_i|} \rightarrow -e^2 \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}, \quad (3)$$

- and the background and coulomb terms cancel exactly,

$$V_{ee} = e^2 \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}. \quad (4)$$

# Brief Overview of HEG

- The discretized solutions are given by,

$$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \sum_{\vec{k}'}^{|\vec{k}'| < k_f} \langle \vec{k}, \vec{k}' | \vec{k}', \vec{k} \rangle \quad (5)$$

- Where the 2D and 3D two electron integral is given by

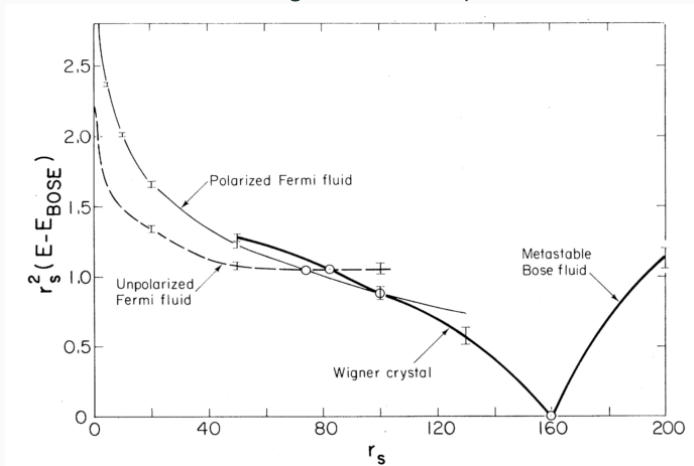
$$\langle \vec{k}, \vec{k}' | \vec{k}'', \vec{k}''' \rangle = \begin{cases} \frac{\pi}{V} \frac{2^{D-1}}{|\vec{k} - \vec{k}''|^{D-1}} & \vec{k}''' = \vec{k} + \vec{k}' - \vec{k}'' \\ 0 & \text{else} \end{cases}$$

- In 1D, if  $V(r_{12}) = V_0 \delta(r_{12})$ ,

$$\langle k, k' | k'', k''' \rangle = \begin{cases} V_0 ; & k''' = k + k' - k'' \\ 0 ; & \text{else} \end{cases} \quad (6)$$

# Energies of Some Phases are Known Exactly

QMC Energies for various phases



# Project Questions

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- It is known that the GHF solution persists at all densities for the HEG<sup>1</sup>.

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# Project Questions

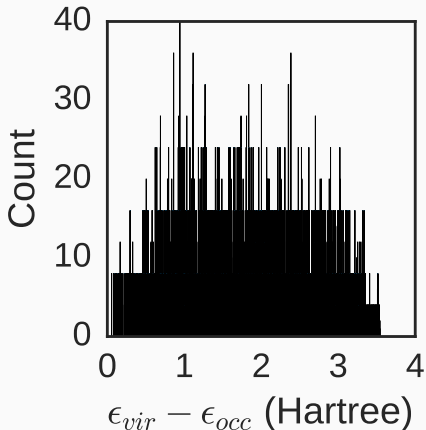
- Can we use the HF-Stability analysis to determine where the HEG is unstable?
- Will this predict the known tendency of crystallization at low density?
- It is known that the GHF solution persists at all densities for the HEG<sup>1</sup>.
- Can we show this numerically?
- (Future) Can we find a lower energy GHF solution to reduce “correlation energy”?

## Results

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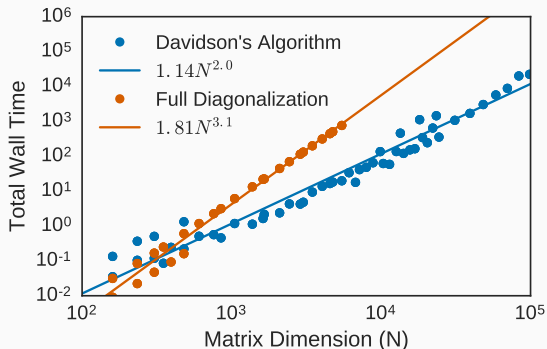
# Implementation Problems

- **H** Too big to construct or diagonalize
- Spectrum is dense, leading to numerical issues



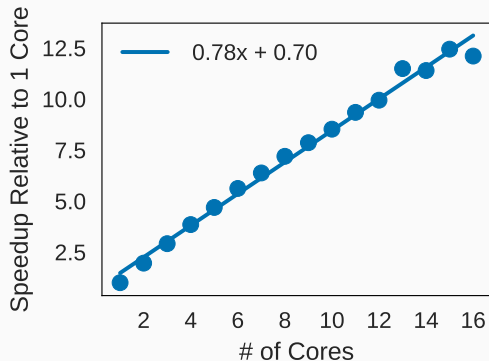
# Implementation Solutions 1: Davidson's Algorithm

- Davidson requires no explicit matrix storage
- Davidson is Asymptotically quadratic
- Full diagonalization is cubic

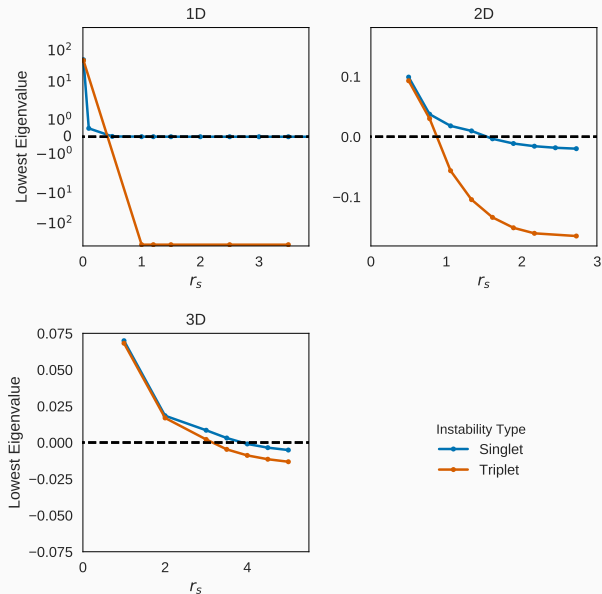


## Implementation Solutions 2: Parallelization

- Access to Blue Waters
- Depending on # of cores, 400-1000 fold speedup compared to serial



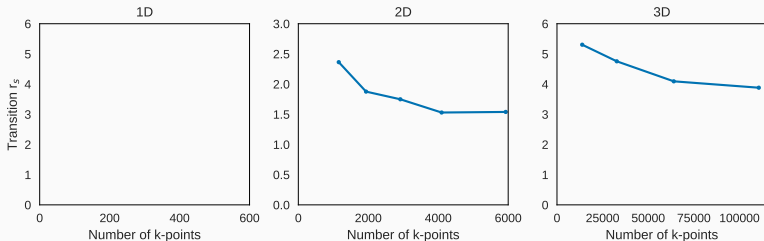
# Stability Curves Show Clear Transition





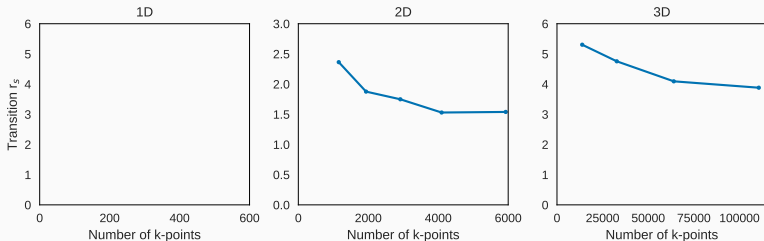
# Stability Onset Converges With k-points

## Singlet Instabilities

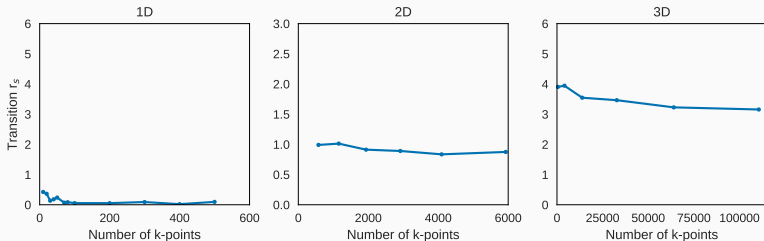


# Stability Onset Converges With k-points

## Singlet Instabilities



## Triplet Instabilities



# Transitions are Consistent with Others

# Dimensions	Instability $r_s$ (Me)	Phase Boundary $r_s$ (Literature)
1	0.09	$0^1$
2	0.87	$0.8^2$
3	3.15	$3.0^3$

(1) Overhauser, A. W. Phys. Rev. 1962, 128 (3), 14371452.

(2) Bernu, B.; Delyon, F.; Holzmann, M.; Baguet, L. Phys. Rev. B 2011, 84 (11), 115115.

(3) Baguet, L.; Delyon, F.; Bernu, B.; Holzmann, M. Phys. Rev. B 2014, 90 (16), 165131.

## **Future Directions**

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- Find the lowest energy GHF solution

(1) Ohno, K. Chem. Rec. 2016, 16 (5), 21982218.

(2) Supady, A.; Blum, V.; Baldauf, C. J. Chem. Inf. Model. 2015, 55 (11), 23382348.

# Brute Force GHF

- Find the lowest energy GHF solution
- Use algorithms inspired by similar problems (atomic configuration)

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- Global Reaction Route Mapping (GRRM) / Anharmonic Downard Distortion (ADD)<sup>1</sup>

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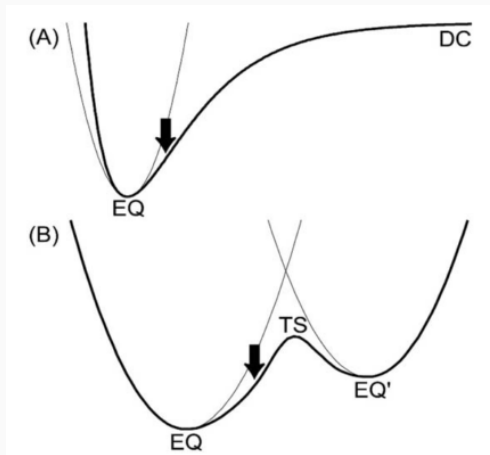
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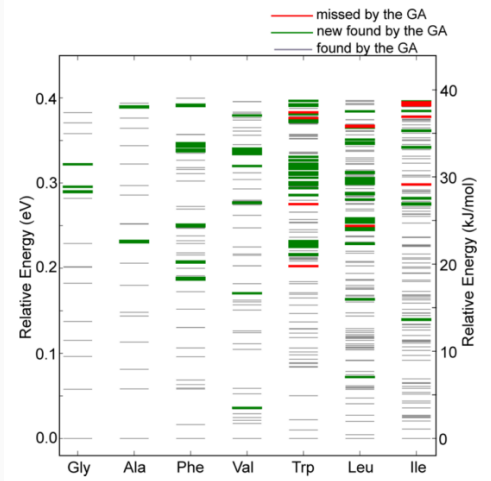
# Anharmonic Downward Distortion



Replace atomic coordinates with MO coefficients and vibrational information with MO eigenvalues/vectors

# Genetic Algorithm

Genetic Algorithm promising in finding many low energy solutions



# Proposal: Genetic Algorithm

- Use as the gene the density matrix / MO coefficients
- Less human input
- Less dependence on underlying PES structure
- How the HF solution gets found is irrelevant

# Concluding Remarks

- Paramagnetic HEG instabilities are successfully reproduced by the MO hessian approach
- HF Stability analysis can show when restrictions should be lifted
- It is feasible that even stable HF are not global minimum
- Other approaches should be used to find even lower energy HF solutions
- Inspiration from similar problems could help; GRRM or Genetic Algorithms

**Questions?**

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and to first order in  $\rho_{ai}$ , the elements of the density matrix are ,

$$\rho_{ai} = C_{ai}, \quad \rho_{ia} = C_{ai}^*. \quad (10)$$

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The TDHF EoM becomes,

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whose amplitudes,  $X_{ai}$  and  $Y_{ai}$  satisfy,

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These are the equations of the Random Phase Approximation (RPA)

# Matrix Factorizations

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \mathbf{d}^* \end{bmatrix} = 2E_2 \begin{bmatrix} \mathbf{d} \\ \mathbf{d}^* \end{bmatrix}$$

We can now apply the similarity transform defined by the Unitary matrix

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{I} & -\mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix}$$

after which the transformed eigenvalue problem has the form

$$\begin{aligned} \frac{1}{2} \begin{bmatrix} \mathbf{A} + \mathbf{B} + \mathbf{A}^* + \mathbf{B}^* & -\mathbf{A} + \mathbf{A}^* + \mathbf{B} - \mathbf{B}^* \\ -\mathbf{A} + \mathbf{A}^* - \mathbf{B} + \mathbf{B}^* & \mathbf{A}^* + \mathbf{A} - \mathbf{B} - \mathbf{B}^* \end{bmatrix} \begin{bmatrix} \mathbf{d} + \mathbf{d}^* \\ \mathbf{d} - \mathbf{d}^* \end{bmatrix} &= 2E_2 \begin{bmatrix} \mathbf{d} + \mathbf{d}^* \\ -\mathbf{d} + \mathbf{d}^* \end{bmatrix} \\ &= 2E_2 \begin{bmatrix} \text{Re}(\mathbf{d}) \\ \text{Im}(\mathbf{d}) \end{bmatrix} \end{aligned}$$

If  $\mathbf{A}$  and  $\mathbf{B}$  are both real,  $\mathbf{A} = \mathbf{A}^*$  and  $\mathbf{B} = \mathbf{B}^*$  and the above simplifies to

$$\begin{bmatrix} \mathbf{A} + \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} - \mathbf{B} \end{bmatrix} \begin{bmatrix} \text{Re}(\mathbf{d}) \\ \text{Im}(\mathbf{d}) \end{bmatrix} = 2E_2 \begin{bmatrix} \text{Re}(\mathbf{d}) \\ \text{Im}(\mathbf{d}) \end{bmatrix}$$

# Correlation Energy Increases at Small Gap

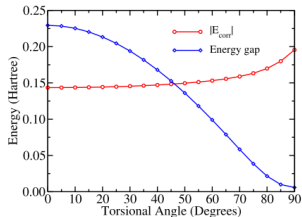


FIG. 6: Correlation energy and energy gap for the twisted ethylene  $C_2H_4$  as a function of the torsion angle around the  $C=C$  double bond.

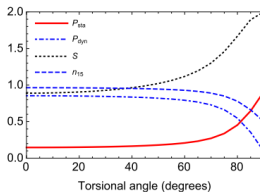


FIG. 7: Correlation curves for ethylene.  $P_{sta}$  and  $P_{dyn}$  as well as the occupancy of the highest occupied natural spin-orbital and the von Neumann entropy  $S$  are plotted as functions of the torsion angle around the  $C=C$  double bond.

# Physicist's Strong Correlation

*However, because all repulsive short-range interactions renormalize towards the Fermi surface, their presence does not destroy the underlying free-particle picture of a Fermi Liquid. That is, the interactions can be integrated out, leaving behind renormalized electron or quasi-particle states. Hence, in a Fermi liquid there is a simple principle that can be invoked to lay plain that free electrons are the propagating degrees of freedom. Without the assumption of a Fermi surface, no principle exists that allows us to smooth away the interactions. We refer to such problems as being strongly correlated, namely those in which no obvious principle, ... exists that governs the renormalization of the electron-electron interactions.*



# Iterative Subspace Eigenvalue Methods

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# Davidson's Algorithm

$$\mathbf{Ax} = \lambda \mathbf{x}$$

Eigenvalue Problem

$$\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_M]$$

Guess vectors

$$\tilde{\mathbf{A}} = \mathbf{V}^\dagger \mathbf{A} \mathbf{V}$$

Transform into subspace

$$\tilde{\mathbf{A}} \tilde{\mathbf{x}} = \tilde{\lambda} \tilde{\mathbf{x}}$$

Solve the subspace problem

$$\mathbf{x}_i \approx \mathbf{x}_i^R = \mathbf{V} \tilde{\mathbf{x}}_i$$

Approximate eigenvectors

$$\lambda_i \approx \lambda_i^R = \tilde{\lambda}_i$$

Approximate eigenvalues

$$\mathbf{r}_i = (\mathbf{A} - \lambda_i \mathbf{I}) \mathbf{x}_i^R$$

Calculate the residue

$$\delta_i = c_i \mathbf{r}_i$$

Correction vectors

$$c_i = \frac{1}{\lambda_i \mathbf{I} - \mathbf{D}}$$

Diagonal Precondition

$$\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_M, \delta_1, \delta_2, \dots, \delta_I]$$

Append to guess and restart

$$\mathbf{V} = \textit{orthonormalized}(\mathbf{V})$$

Ensure orthonormal projection

1. Saad, Y. Numerical Methods for Large Eigenvalue Problems; SIAM, 2011.

2. Davidson, E. R. J. Comput. Phys. 1975, 17 (1), 8794.

# Convergence Properties

- The convergence of these subspace algorithms depends on:

1. Saad, Y. Numerical Methods for Large Eigenvalue Problems; SIAM, 2011.
2. Li, R.-C.; Zhang, L.-H. Convergence of Block Lanczos Method for Eigenvalue Clusters; 2013.

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  - The density of the eigenvalue spectrum
  - The initial guess eigenvectors
  - The preconditioner (Davidson only)
- They can have convergence issues if:

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- My recommendation for guess eigenvectors is

$$v_j^{(i)} = \text{normalize} \left( \frac{1}{|A_{ii} - A_{jj}| + 1} \right). \quad (14)$$

# Orthogonalization

- The condition number,  $\kappa$ , is bound from below by

$$\kappa \geq \frac{\text{Max}(A_{ii})}{\text{Min}(A_{jj})} \quad (15)$$

- The Gram-Schmidt procedure has numerical issues,

$$\|\mathbf{I} - \mathbf{Q}^T \mathbf{Q}\| \leq \frac{\alpha \kappa^2}{1 - \beta \kappa^2}. \quad (16)$$

- Modified Gram-Schmidt is better, but not perfect,

$$\|\mathbf{I} - \mathbf{Q}^T \mathbf{Q}\| \leq \frac{\gamma \kappa}{1 - \eta \kappa} \quad (17)$$

- May need multiple orthogonalization steps