Hartree-Fock Stability

Applications to the Homogeneous Electron Gas

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Background Information

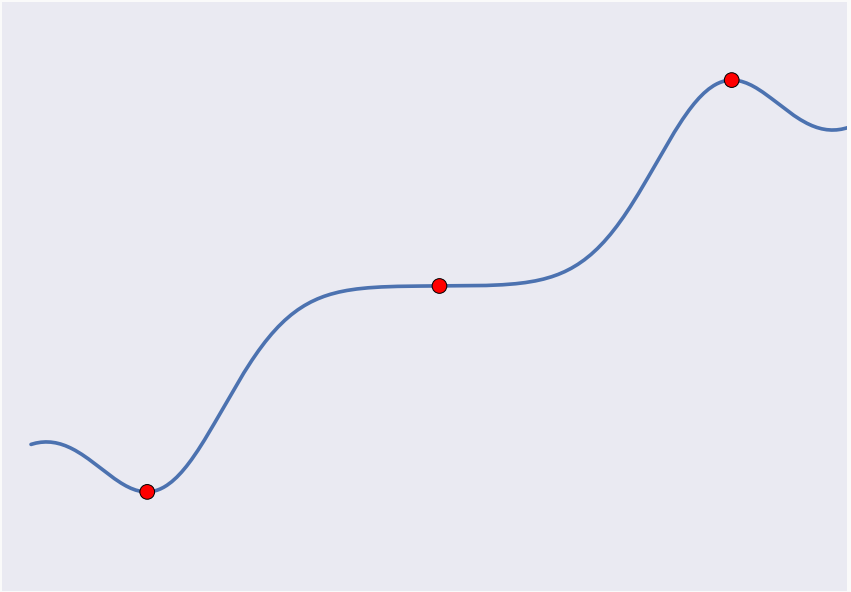
Levels of Hartree-Fock Theory

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

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

Restricted Minimization

- Hartee-Fock SCF guarantees only stationary energy w.r.t. change in orbitals
- The solution may be a maximum, minimum or saddle point



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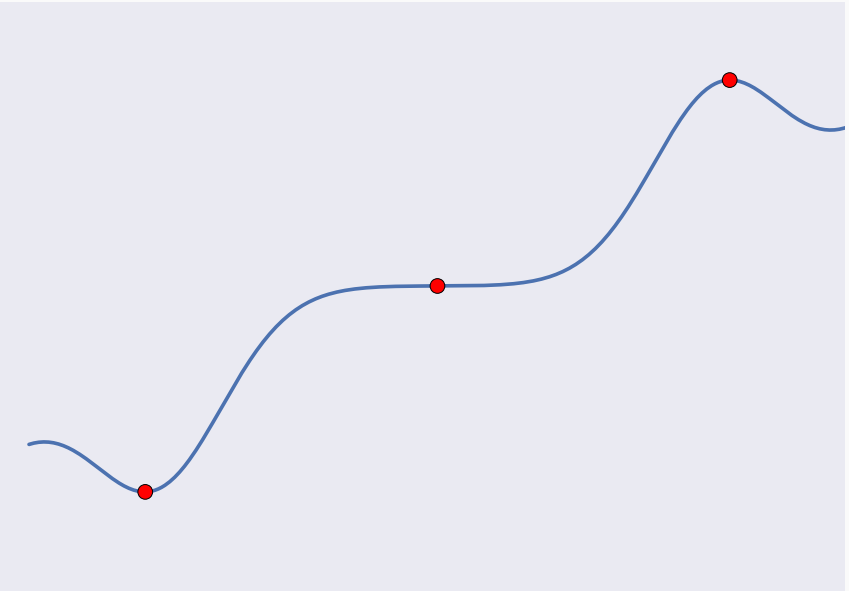
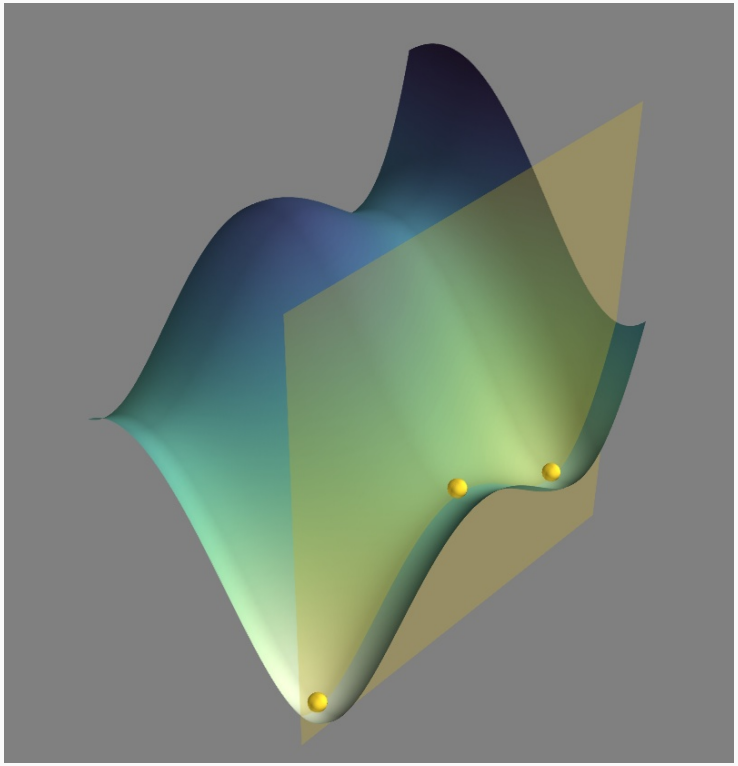
Within the Constrained Space



Restricted Minimization

- Restricted minima may correspond to minima in another dimension



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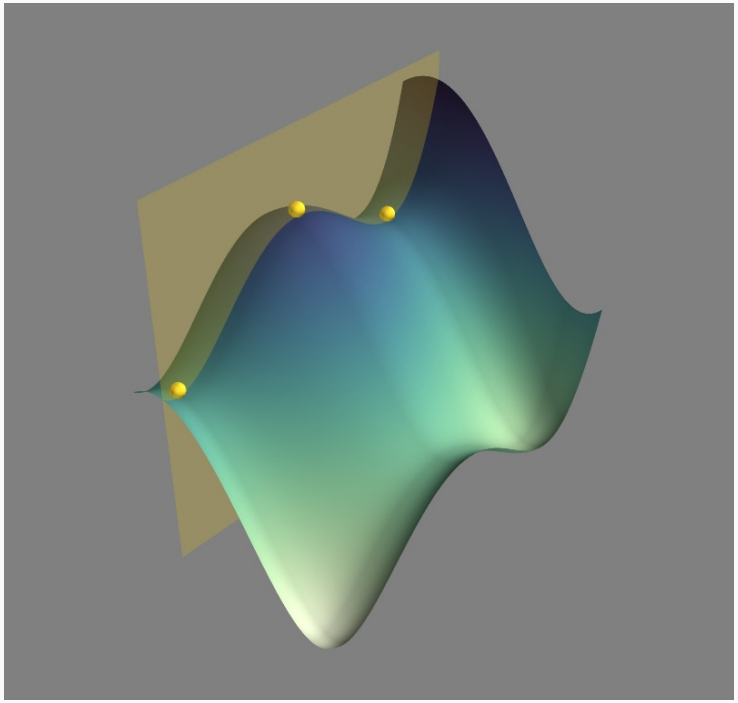

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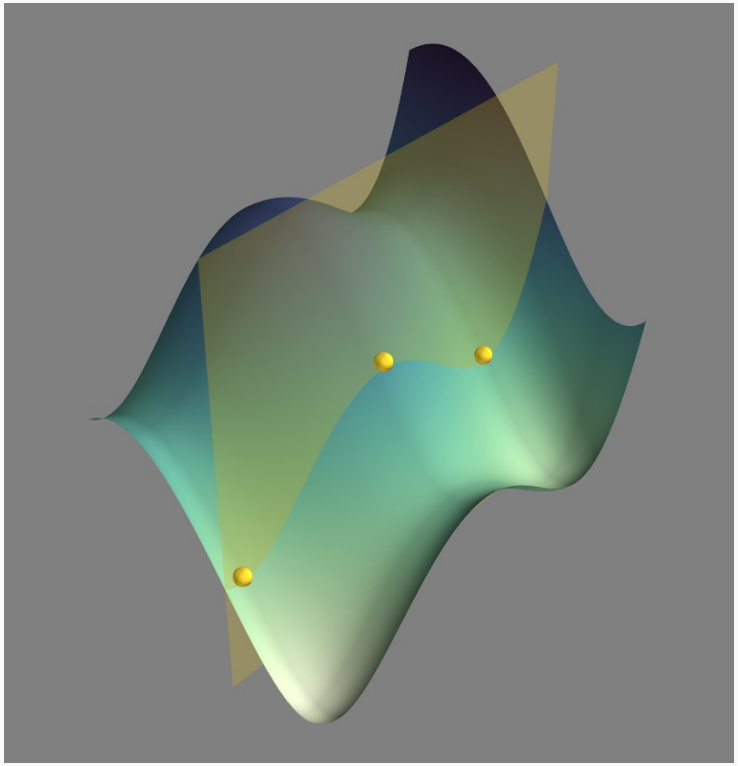
- Restricted minima may correspond to minima in another dimension
- Restricted minima may correspond to maxima in another dimension
- Restricted minima may be nonstationary



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- We can determine this if we inspect the second order variation in the energy.
- Thouless[1] showed a physically motivated derivation using Time-Dependent Hartree-Fock theory (TDHF).

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Hartree-Fock Stability Conditions

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and to first order in ρ_{ai}, the elements of the density matrix are ,

$$\rho_{ai} = C_{ai}, \quad \rho_{ia} = C^*_{ai}. \tag{4}$$

Hartree-Fock Stability Conditions

The TDHF EoM becomes,

$$
\begin{aligned}
i\hbar \frac{dC_{ai}(t)}{dt} &= (\epsilon_a - \epsilon_i) \\
&+ \sum_{i}^{occ} \sum_{b}^{vir} \left[\langle aj||ib\rangle \, C_{bj}(t) + \langle ab||ij\rangle \, C_{bj}^{*}(t) \right]. \quad (5)
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$$\begin{aligned} (\epsilon_a - \epsilon_i)\, X_{ai} + \sum_{i}^{occ}\sum_{b}^{vir}\left[\langle aj||ib\rangle\, X_{bj} + \langle ab||ij\rangle\, Y_{bj}\right] &= \hbar\omega X_{ai} \\ (\epsilon_a - \epsilon_i)\, Y_{ai} + \sum_{i}^{occ}\sum_{b}^{vir}\left[\langle aj||ib\rangle\, X_{bj} + \langle ab||ij\rangle\, Y_{bj}\right] &= -\hbar\omega Y_{ai}. \end{aligned} \quad (7)$$

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

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$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = \omega \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} \tag{8}$$

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- Where

$$\begin{aligned} A_{ia,jb} &= \left\langle {}^{a}_{i} \right| H - \langle 0|H|0\rangle \left| {}^{b}_{j} \right\rangle = (\epsilon_a - \epsilon_i)\,\delta_{ij}\delta_{ab} + \langle aj||ib\rangle \\ B_{ia,jb} &= \left\langle {}^{ab}_{ij} \right| H - \langle 0|H|0\rangle \left| 0 \right\rangle = \langle ab||ij\rangle\,. \end{aligned} \tag{9}$$

Hartree-Fock Stability Conditions

The eigenvalue equation can be factorized depending on symmetry.

TABLE I. Matrices required to have positive semidefinite character as a necessary condition for stability of self-consistent solution of type X in the space of type Y.

X \ Y	Real RHF[a]	Complex RHF	Real UHF	Complex UHF	Real GHF	Complex GHF
Real RHF[a]	$^1A' + {}^1B'$	$^1A' - {}^1B'$	$^3A' + {}^3B'$			
Complex RHF		$^1H'$		$^3H'$		
Real UHF			$A' + B'$	$A' - B'$	$A'' + B''$	
Complex UHF				H'		H''
Real GHF					$A + B$	$A - B$
Complex GHF						H

[a]Singlet closed shell case ($n_\alpha = n_\beta$) only.

Homogeneous Electron Gas

Brief Overview

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

$$V_{bg}(\mathbf{r}) = \sum_i \frac{-Ze^2}{|\mathbf{r} - \mathbf{R_i}|} \rightarrow -e^2 \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}, \tag{10}$$

- and the background and coulomb terms cancel exactly,

$$V_{ee} = e^2 \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}. \tag{11}$$

Brief Overview

- The discretized solutions are given by,

$$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \sum_{\vec{k}}^{|\vec{k}|<k_f} \langle \vec{k}, \vec{k'} | \vec{k'}, \vec{k} \rangle \tag{12}$$

- Where the two electron integral is given by

$$\langle \vec{k}, \vec{k'} | \vec{k''}, \vec{k'''} \rangle \overset{\text{2D, 3D}}{=} \begin{cases} \frac{\pi}{V} \frac{2^{D-1}}{|\vec{k}-\vec{k''}|^{D-1}} & \vec{k'''} = \vec{k} + \vec{k'} - \vec{k''} \\ 0 & \text{else} \end{cases}$$

$$\langle k, k' | k'', k''' \rangle \overset{\text{1D}}{=} \begin{cases} e^{|k-k''|^2 a^2} \text{Ei}(-|k-k''|^2 a^2) \; ; & k''' = k + k' - k'' \\ 0 \; ; & \text{else} \end{cases} \tag{13}$$

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- (Future) Can we combine this with to improve the efficacy of correlation theories (CC, MBPT)?

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Notes on Iterative Subspace Eigenvalue Methods

Subspace Methods in 1 Slide

- Sometimes the eigenvalue problem is too large to solve completely, and only a few eigenpairs are needed
- Subspace methods allow for finding some eigenpairs without full diagonalization.
- They need only a matrix-vector product (maybe diagonal elements too).
- A small subspace is constructed, then expanded slowly until the eigenpair residual norm,

$$||\mathbf{Ax} - \lambda\mathbf{x}||, \tag{14}$$

  is below some threshold.
- The Lanczos and Arnoldi methods are the most commonly used[1], while the Davidson[2] method is likely more useful in a majority of chemical applications.

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:

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- My recommendation for guess eigenvectors is

$$v_j^{(i)} = \mathit{normalize}\left(\frac{1}{|A_{ii} - A_{jj}| + 1}\right). \tag{15}$$

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Orthogonalization

- The condition number, κ, is bound from below by

$$\kappa \geq \frac{Max(\lambda_i)}{Min(\lambda_j)} \tag{16}$$

- The Gram-Schmidt procedure has numerical issues,

$$||\mathbf{I} - \mathbf{Q}^\mathbf{T}\mathbf{Q}|| \leq \frac{\alpha\kappa^2}{1 - \beta\kappa^2}. \tag{17}$$

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

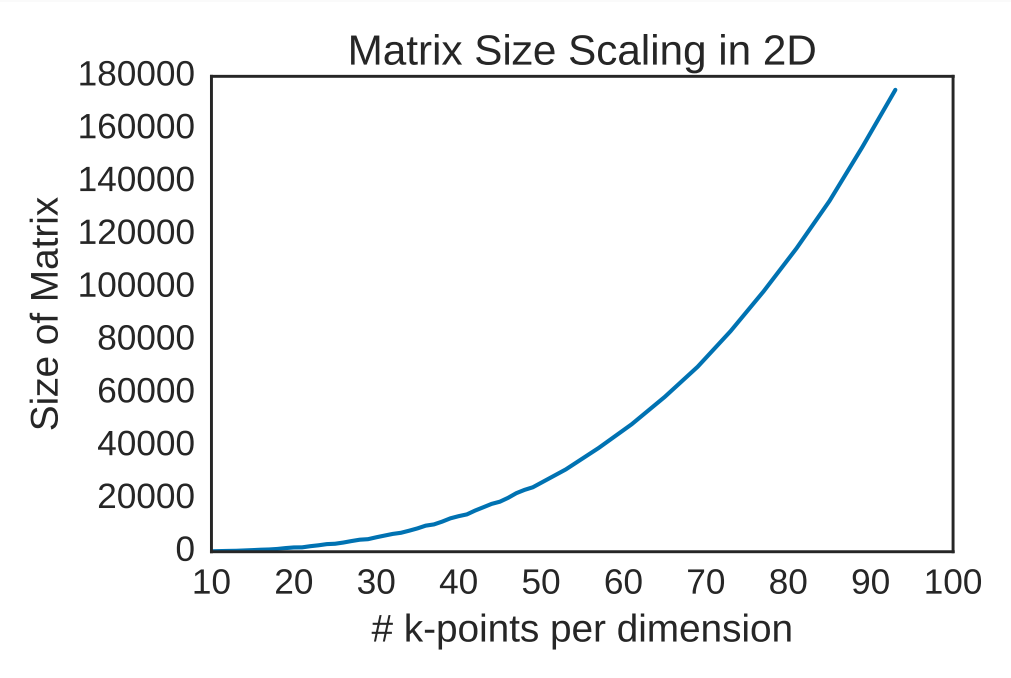
$$||\mathbf{I} - \mathbf{Q}^\mathbf{T}\mathbf{Q}|| \leq \frac{\gamma\kappa}{1 - \eta\kappa} \tag{18}$$

- May need multiple orthogonalization steps

Results

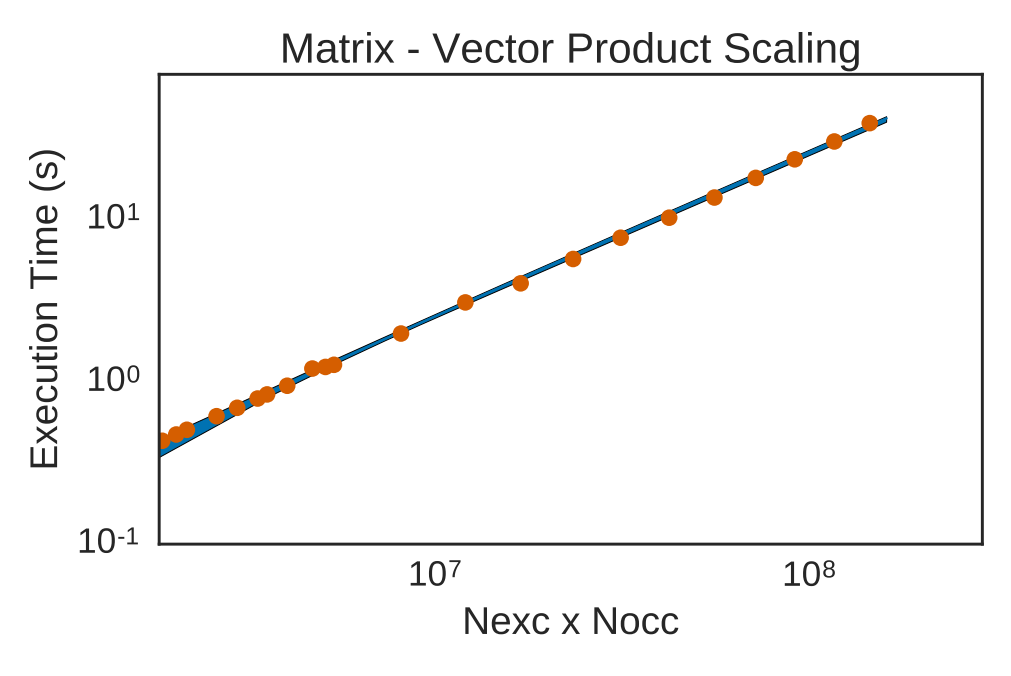
Matrix Size Scaling

- Scales as $2N_{exc}$
- N_{occ} and N_{vir} both scale with $N_{kpoints}^{D}$



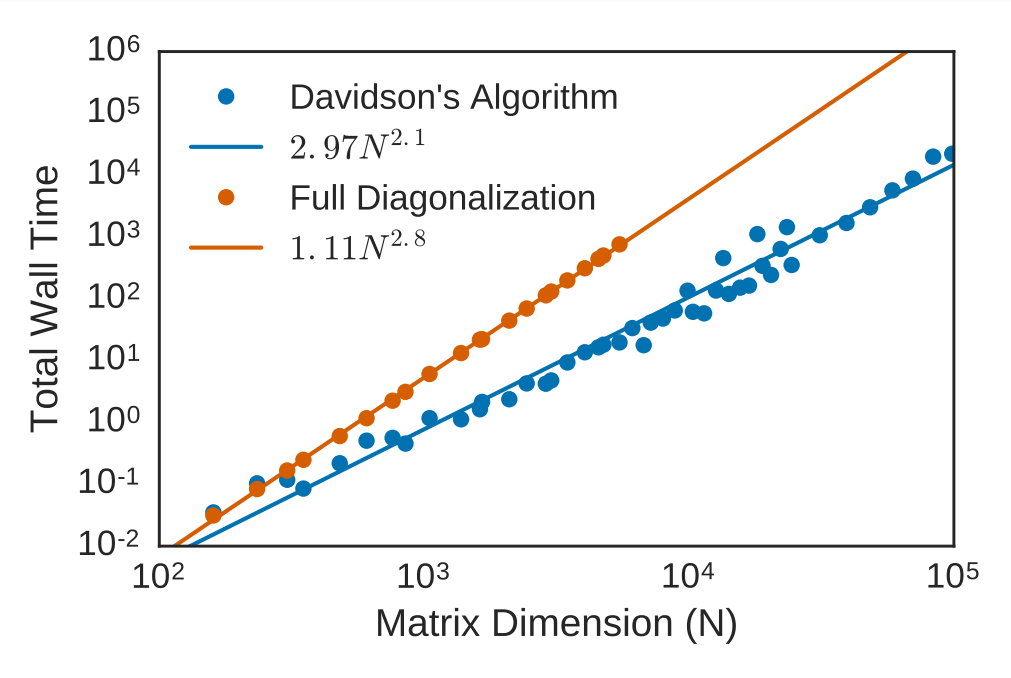
Matrix-Vector Scaling

- Scales as $N_{exc} \times N_{occ}$ due to momentum conservation



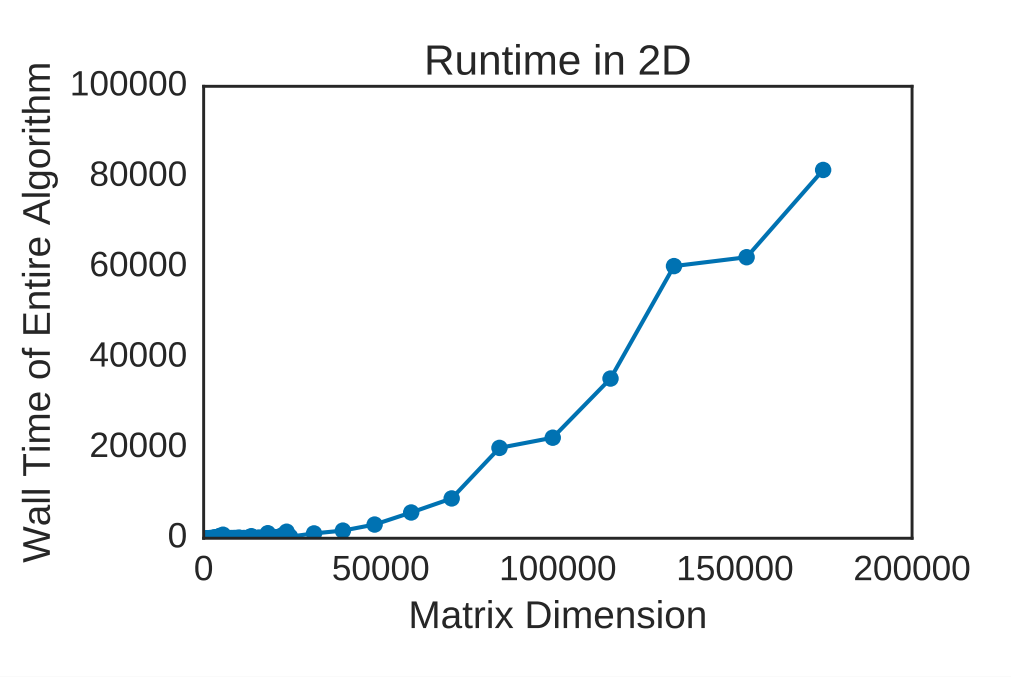
Davidson Scaling

- Davidson is Asymptotically quadratic.
- Full diagonalization is almost cubic.



Algorithm Wall time

- Roughly quadratic wrt matrix dimension.
- Outliers correspond to high condition number



Efficacy of Davidson's Algorithm

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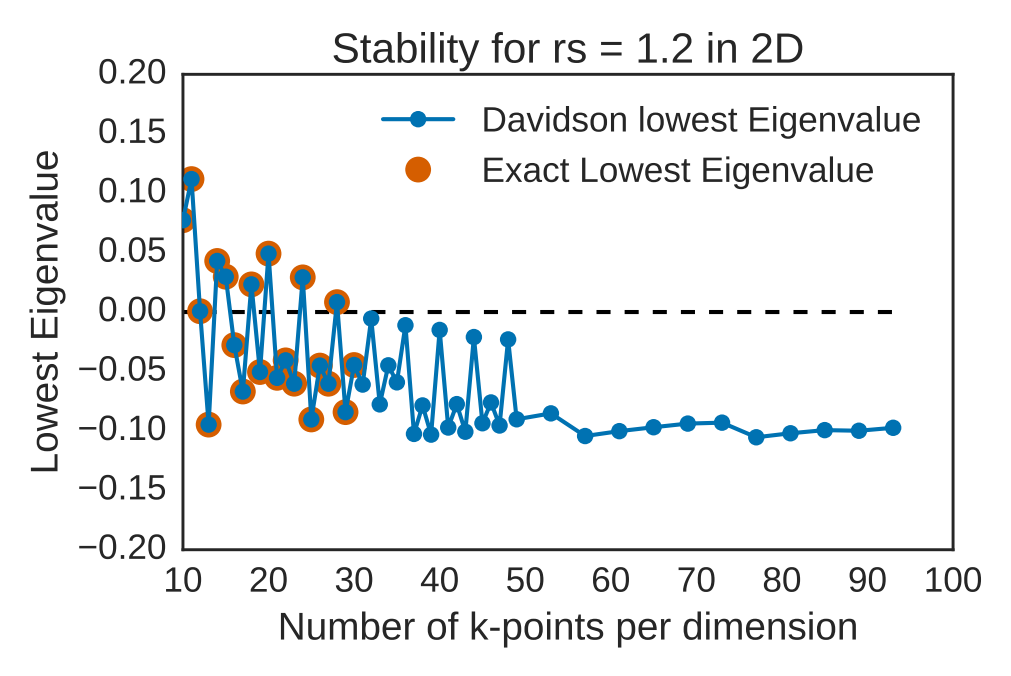
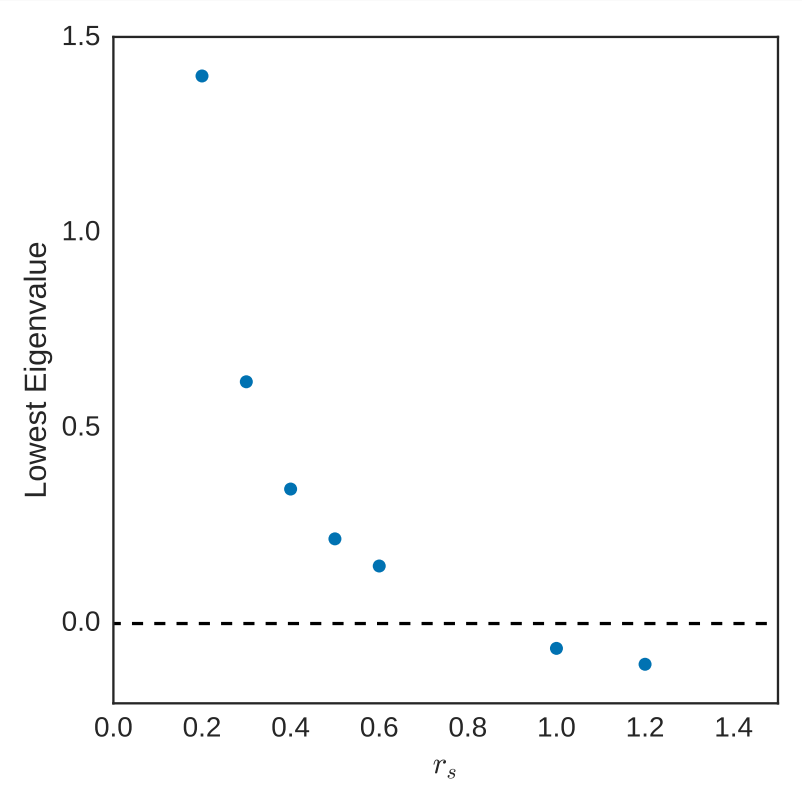
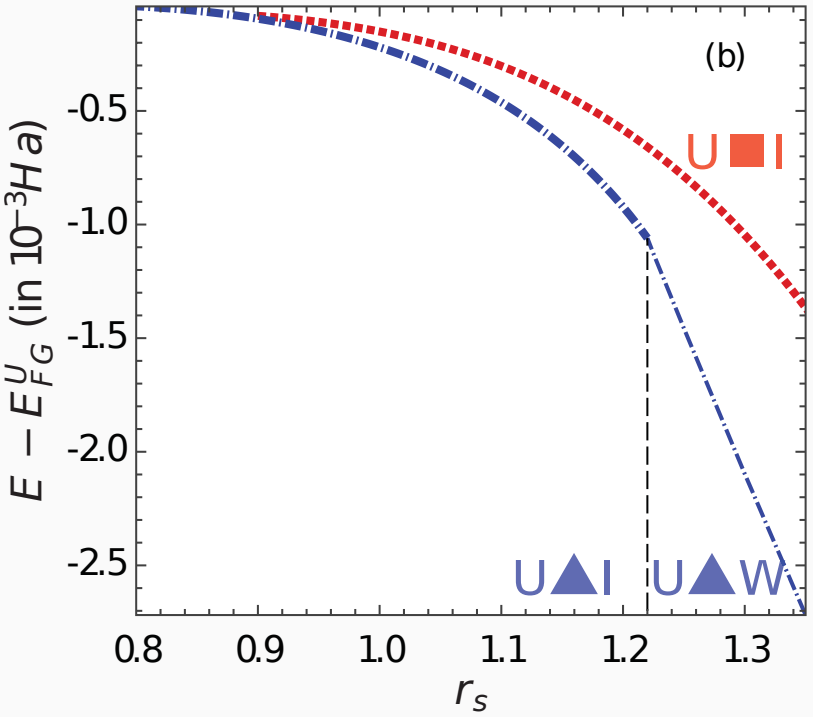


Dependence on r_s

Crossover from stable to unstable agrees with previous results.



My Result



Published Result. Red = Square Lattice, Blue = Triangular Lattice

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

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- These take time, so we want to minimize how many of these we do
- The Genetic Algorithm provides a framework for a refined global search

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Concluding Remarks

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- The Genetic Algorithm provides a framework for a refined global search
- It shines when asked to find a host of low energy solutions
- GA wrapper can be interfaced with a variety of electronic structure packages(NWChem, ORCA) and is available under the GNU Lesser General Public License at `https://github.com/adrianasupady/fafoom`

Questions?

Backup slide

Empty Backup

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