

# Multireference calculations

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In this chapter we will begin by

## I. BASICS

In quantum mechanics we are often interested in solving the time-independent Schrödinger equation to obtain the ground and excited state energies and wavefunctions of a system. The Schrödinger equation is an eigenvalue equations of the type

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \quad (1)$$

where  $\hat{H}$  is the electronic Hamiltonian,  $E$  and  $|\Psi\rangle$  are respectively the eigenenergies and eigenfunction (the desired wavefunction) of the system. Under the Born-Oppenheimer approximation the electronic Hamiltonian in atomic units is given by

$$\hat{H} = \sum_i -\frac{\nabla_i^2}{2} - \sum_{iI} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{r_{ij}}, \quad (2)$$

where the first term is the kinetic energy of all electron, the second term is the coulomb interaction between the electron  $i$  and nucleus  $I$  with charge  $Z_I$  and the last term is the electron interaction between the electron  $i$  and  $j$  ( $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ ). The solution of the Schrödinger equation using the Hamiltonian in Equation 2 will give the electronic energy  $E(\mathbf{R})$  which is a function of the nuclear coordinates (also known as the potential energy surface) and the electronic wavefunction  $|\Psi\rangle = \Psi(\mathbf{r}; \mathbf{R})$  which is a function of the electronic coordinates and parametrically depends on the nuclear coordinates. The line under  $\mathbf{r}$  and  $\mathbf{R}$  denotes that it is now a vector containing coordinates of all the electrons and nuclei respectively.

What is not apparent from the electronic Schrödinger equation is that the electronic coordinate is defined not just by their spatial coordinate  $\mathbf{r}_i$  but also by their spin  $\sigma_i$  which can take two values  $\alpha$  or  $\beta$ . The combined coordinates of an electron will be specified by  $\mathbf{x}_i \triangleq \{\mathbf{r}_i, \sigma_i\}$ . Another important property of the electronic wavefunction is that it is anti-symmetric under exchange of electrons, i.e.

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots) = -\Psi(\mathbf{r}_1, \dots, \mathbf{r}_j, \dots, \mathbf{r}_i, \dots). \quad (3)$$

Can you see how the anti-symmetry of the wavefunction leads to the Pauli exclusion principle?

So far we have represented the wavefunction in the real space coordinates which is used in several quantum Monte Carlo approaches and methods based on adaptive mesh generation. However, for a large majority of quantum chemistry techniques the wavefunction is represented as linear combination of many body states constructed out of single-electron states ( $\{\psi_i(\mathbf{r})\}$ ) which are also known as orbitals. These orbitals are often written as a linear combination of a single electron basis set which in practice is a gaussian or a plane wave function ( $\{\phi_\mu(\mathbf{r})\}$ )

$$\psi_i(\mathbf{r}) = \sum_{\mu} C_{\mu i} \phi_{\mu}(\mathbf{r}). \quad (4)$$

Note, that basis states are often not orthogonal, i.e.

$$\int \phi_{\mu}^*(\mathbf{r}) \phi_{\nu}(\mathbf{r}) d\mathbf{r} = S_{\mu, \nu}, \quad (5)$$

where  $S_{\mu, \nu} \neq \delta_{\mu, \nu}$  ( $\delta_{\mu, \nu}$  is the Kronecker delta function), however in most cases one requires that the orbitals are orthogonal, i.e.

$$\int \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) d\mathbf{r} = \delta_{i, j}. \quad (6)$$

Although, the concept of orbitals is very general and any set of orthogonal functions can be used, in practice one often uses the orbitals obtained from a Hartree Fock, or multiconfiguration self consistent field calculation. As we go along we will see several ways of generating a useful set of orbitals.

- Can you show that  $C^\dagger SC = I$ , where  $S$  is the overlap matrix in Equation 5 and  $C$  is the orbital coefficient matrix in Equation 4?

The number of “spatial” orbitals is equal to the number of basis functions, we will denote this number as  $k$ . As mentioned earlier an electron carries another degree of freedom, namely the spin, which gives rise to the concept of a “spin” orbital. The number of spin orbitals is merely equal  $2k$ , twice the number of spatial orbitals because spin of an electron can be either  $\alpha$  or  $\beta$ . In what follows we will denote  $\psi_i$  as an orbital with an electron with  $\alpha$  spin and  $\bar{\psi}_i$  as an orbital with an electron with  $\beta$  spin. It is easy to imagine that one could construct many body states by taking product of orbitals for each electron coordinate

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots) = \psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\dots, \quad (7)$$

however, the serious difficulty with this state is that it is not antisymmetric with respect to electron coordinates and thus Pauli principle is not satisfied. One can instead use the antisymmetric product of the orbitals given as

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots) = \hat{\mathcal{A}}\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\dots. \quad (8)$$

$\hat{\mathcal{A}}$  is the antisymmetrizer (its a projection operator) and is defined as

$$\hat{\mathcal{A}} = \frac{1}{N!} \sum_{P \in S_N} (-1)^\pi \hat{P}, \quad (9)$$

where the summation is over all the  $N!$  elements  $\hat{P}$  of the symmetric group  $S_N$  and  $\pi$  is the parity associated with the operator  $\hat{P}$ . Parity  $\pi$  of a permutation operator  $\hat{P}$  is equal to the number of transposition operators that can be used to construct it. Operator  $\hat{\mathcal{A}}$  has the nice property that when it acts on a state, it either gives 0 or an anti-symmetric component of the state. Operator  $\hat{\mathcal{A}}$  is also idempotent, i.e.  $\hat{\mathcal{A}}^2 = \hat{\mathcal{A}}$ , which implies that once the operator  $\hat{\mathcal{A}}$  has been applied to a state, another application of  $\hat{\mathcal{A}}$  does not change it. Two other useful properties of antisymmetrizer are  $\hat{\mathcal{A}}^\dagger = \hat{\mathcal{A}}$  and  $[\hat{\mathcal{A}}, \hat{H}] = 0$ .

- Can you use the group property of  $\hat{P}$  to show that  $\hat{\mathcal{A}}^2 = \hat{\mathcal{A}}$ ?
- Can you show that the Slater determinant  $\frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_i(1) & \psi_j(1) & \psi_k(1) \\ \psi_i(2) & \psi_j(2) & \psi_k(2) \\ \psi_i(3) & \psi_j(3) & \psi_k(3) \end{vmatrix}$  is an anti-symmetric function of three electron in three orbitals  $\psi_i, \psi_j, \psi_k$  which is equal to  $\sqrt{N!}\hat{\mathcal{A}}(\psi_i(1)\psi_j(2)\psi_k(3))$ .
- Show that the Slater determinant is normalized as long as the orbitals used to construct it are orthogonal.

Thus we can construct a set of anti-symmetric states by simply applying the anti-symmetrizer to all the possible product states. Notice that if there are repeated orbitals then the antisymmetrizer will give 0. Also note that if the set of orbitals only differ from each other by their order then the anti-symmetrizer will merely give the same anti-symmetrized state with an overall change of sign.

As a matter of definition the Slater determinant  $\sqrt{N!}\hat{\mathcal{A}}(\psi_i(1)\psi_j(2)\dots)$  is also written as  $|\psi_i\psi_j\dots\rangle$ , note that the electron labels have been removed from the symbol. Can you show that the number of unique many-body anti-symmetric states that can be obtained by acting the anti-symmetrizer on a product of states is  ${}^{2k}C_n$ , where  $n$  is the number of electrons and here is assumed to be less than  $2k$ .

We will not go into detail here, but by using the properties of the anti-symmetrizer we can derive the Slater-Condon rules which are shown in Table I. These rules give us the recipe for calculating the transition matrix element of an operator  $\hat{O}$  between two Slater determinants  $|L\rangle$  and  $|K\rangle$ , i.e.  $\langle K|\hat{O}|L\rangle$ .

$$\langle i|h|j\rangle = \int \psi_i^*(\mathbf{r})h(\mathbf{r})\psi_j(\mathbf{r})d\mathbf{r} \quad (10)$$

$$\langle ij|kl\rangle = \int \psi_i^*(\mathbf{r}_1)\psi_j^*(\mathbf{r}_2)\frac{1}{r_{ij}}\psi_k(\mathbf{r}_1)\psi_l(\mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2 \quad (11)$$

TABLE I: Slater Codon rules. See the test for the definition of the integrals in the last column.

Type	$ K\rangle,  L\rangle$	Operator ( $\hat{O}$ )	$\langle K \hat{O} L\rangle$
Same states	$ K\rangle =  \psi_1\psi_2\cdots\rangle$	$\sum_i \hat{h}(i)$	$\sum_i \langle i h i\rangle$
	$ L\rangle =  \psi_1\psi_2\cdots\rangle$	$\frac{1}{2} \sum_{i \neq j} \hat{V}(i, j)$	$\frac{1}{2} \sum_{ij} (\langle ij ij\rangle - \langle ij ji\rangle)$
Differ by one orbital	$ K\rangle =  \psi_1\psi_2\cdots\psi_m\cdots\rangle$	$\sum_i \hat{h}(i)$	$\langle m h n\rangle$
	$ L\rangle =  \psi_1\psi_2\cdots\psi_n\cdots\rangle$	$\frac{1}{2} \sum_{i \neq j} \hat{V}(i, j)$	$\sum_i (\langle mi ni\rangle - \langle mi in\rangle)$
Differ by two orbitals	$ K\rangle =  \psi_1\psi_2\cdots\psi_m\psi_n\cdots\rangle$	$\sum_i \hat{h}(i)$	0
	$ L\rangle =  \psi_1\psi_2\cdots\psi_o\psi_p\cdots\rangle$	$\frac{1}{2} \sum_{i \neq j} \hat{V}(i, j)$	$(\langle mn op\rangle - \langle mn po\rangle)$

## II. SECOND QUANTIZATION

The antisymmetry of the wavefunction is an essential property of the wavefunction and this is why we expand the wavefunction as a linear combination of Slater determinants. Working with Slater determinants is quite a bit more complicated than just with product states. Although Slater-Condon rules tend to simplify things substantially we will later come across theories that benefit greatly from the introduction of a new language, that of second quantization. In this language the requirement of antisymmetry is entirely absorbed into the operators and not the states. Further this language allows us to work in the Fock space which does not have a fixed number of particles but instead is a union of the Hilbert spaces containing any number of particles.

The first change of notation is the use of occupation representation to denote the states. **Write about the occupation number notation.**

The Slater-Condon rules tell us that although the many-body Hamiltonian is a large matrix containing  $2^k C_n$  rows and columns, all the matrix elements can be calculated using just the  $(2k)^4$  integrals given in Equation 11 (there are symmetry properties of integrals which allows one to reduce to storage cost to  $k^4/8$ ). The language of second quantization explicitly

## III. VARIATIONAL METHOD AND NUMERICAL TECHNIQUES

## IV. SELF-CONSISTENT FIELD THEORY

## V. MULTICONFIGURATION SELF-CONSISTENT FIELD THEORY

Occupation number!

$$|P\rangle = |p_1 p_2 \cdots p_{2k}\rangle$$

$$p_i = \begin{cases} 0 & \text{unoccupied} \\ 1 & \text{occupied} \end{cases}$$

$$|q\rangle = |q_1 q_2 \cdots q_{2k}\rangle$$

$$\langle P|q\rangle = \prod_i \delta_{p_i q_i}$$

We have the vacuum state  
 $|vac\rangle = |000\dots\rangle$   
 $\langle vac|vac\rangle = 1$

$$|\phi_1 \phi_2 \cdots \phi_n\rangle \longleftrightarrow |1 0 1 \cdots 1 \cdots\rangle$$

$$|\Psi\rangle = \sum_P C_P |P\rangle$$

## Creation and Annihilation :-

$$\hat{a}_i^+ |p_1 p_2 \dots 0_i \dots\rangle = \Gamma(p, i) |p_1 p_2 \dots 1_i \dots\rangle$$

increase in the number of electrons.

$$\hat{a}_i^+ |p_1 p_2 \dots 1_i \dots\rangle = |vac\rangle$$

$$\Gamma(p, i) = (-1)^{\sum_{k=i-1} p_k}$$

Can you now show that -

$$a_i^+ a_j^+ + a_j^+ a_i^+ = 0$$

$$\text{if } a_i^+ a_j^+ |p_1 \dots 0_i \dots 0_j \dots\rangle$$

$$= a_i^+ \Gamma(p, j) |p_1 \dots 0_i \dots 1_j \dots\rangle$$

$$= \Gamma(p, i) \Gamma(p, j) |p_1 \dots 1_i \dots 1_j \dots\rangle$$

$$a_j^+ a_i^+ |p_1 \dots 0_i \dots 0_j \dots\rangle$$

$$= a_j^+ \Gamma(p, i) |p_1 \dots 1_i \dots 0_j \dots\rangle$$

$$= -\Gamma(p, j) \Gamma(p, i) |p_1 \dots 1_i \dots 1_j \dots\rangle$$

$$\therefore \boxed{a_i^+ a_j^+ = -a_j^+ a_i^+} \Rightarrow \boxed{a_i^+ a_j^+ + a_j^+ a_i^+ = 0}$$

Can you show that

$$\boxed{a_i^+ a_i + a_i a_i^+ = 1}$$

$$[a_i^+, a_j]_+ = \delta_{ij}$$

$$[a_i^+, a_j^+]_+ = 0$$

$$[a_i, a_j]_+ = 0$$

The number operator

$\hat{N}_i = a_i^+ a_i$  will act on any occupation number vector and return the same state multiplied by the number of electrons in orbital  $i$ .

$$\hat{N} |p\rangle = \left( \sum_i p_i \right) |p\rangle$$

$$\hat{N} = \sum_i a_i^+ a_i$$

Quantum mechanical operators in second Quantization:

$$\sum_i h(i) \implies \sum_{pq} \langle p|h|q\rangle a_p^+ a_q$$

$$\sum_{i \neq j} \frac{1}{r_{ij}} \implies \sum_{pqrs} \langle pq|rs\rangle a_p^+ a_q^+ a_s a_r$$

↑ notice ↑  
{some of endless pairs}

Exact operator

projected into a basis set

Exercise:

Show that

$$\begin{aligned} [a_i^+ a_j, [a_k^+ a_l, a_m^+ a_n]] &= \delta_{lm} \delta_{jn} a_i^+ a_n \\ &\quad - \delta_{lm} \delta_{in} a_k^+ a_j \\ &\quad - \delta_{kn} \delta_{jm} a_i^+ a_l \\ &\quad + \delta_{kn} \delta_{il} a_m^+ a_j \end{aligned}$$

$$\begin{aligned} [a_k^+ a_l, a_m^+ a_n] &= a_k^+ a_l a_m^+ a_n - a_m^+ a_n a_k^+ a_l \\ &= a_k^+ a_n - a_k^+ a_m^+ a_l a_n - a_m^+ a_l + a_m^+ a_k^+ a_n a_l \\ &= \delta_{lm} a_k^+ a_n - a_m^+ a_k^+ a_n a_l - a_m^+ a_l + a_m^+ a_k^+ a_n a_l \\ &= \delta_{lm} a_k^+ a_n - a_m^+ a_l \delta_{kn} \end{aligned}$$

$$\begin{aligned} [a_i^+ a_j, \delta_{lm} a_k^+ a_n - \delta_{kn} a_m^+ a_l] \\ &= \delta_{lm} a_i^+ a_j a_k^+ a_n - \delta_{kn} a_i^+ a_j a_m^+ a_l \\ &\quad - \delta_{lm} a_k^+ a_n a_i^+ a_j + \delta_{kn} a_m^+ a_l a_i^+ a_j \\ &= \delta_{lm} \delta_{kj} a_i^+ a_n - \delta_{lm} a_i^+ a_k^+ a_j a_n - \delta_{kn} \delta_{jm} a_i^+ a_l \end{aligned}$$

→

$$\begin{aligned}
 & + \delta_{kn} a_i^+ a_m^+ a_j a_e \\
 & - \delta_{em} a_{ic}^+ a_j + \delta_{em} a_{ic}^+ a_i^+ a_n a_j - \delta_{kn} a_{ie}^+ a_m^+ a_j \\
 & + \delta_{kn} a_m^+ a_i^+ a_e a_j
 \end{aligned}$$

Another:

$$\begin{aligned}
 [\hat{A}, \hat{B}_1 \hat{B}_2] &= \hat{A} \hat{B}_1 \hat{B}_2 - \hat{B}_1 \hat{B}_2 \hat{A} \\
 &= \hat{A} \hat{B}_1 \hat{B}_2 - \hat{B}_1 \hat{A} \hat{B}_2 - \hat{B}_1 \hat{B}_2 \hat{A} \\
 &\quad + \hat{B}_1 \hat{A} \hat{B}_2 \\
 &= [\hat{A}, \hat{B}_1] \hat{B}_2 - \hat{B}_1 [\hat{B}_2, \hat{A}]
 \end{aligned}$$

Excitation operator! - [Note that  $\langle i_k | h | i_j \rangle = \langle i_\beta | h | i_\alpha \rangle$  so we introduce spin free operators]

$a_i^+ a_j \rightarrow$  takes an electron from  $j$  to  $i$

spin free excitation operator

$$E_j^i = a_{i\alpha}^+ a_{j\alpha} + a_{i\beta}^+ a_{j\beta}$$

$$E_j^i |\psi(S, m)\rangle = |\phi(S, m)\rangle \quad \left\{ \begin{array}{l} \text{the spin and} \\ \text{z-component of} \\ \text{spin does not} \\ \text{change.} \end{array} \right.$$

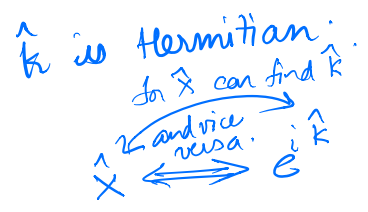
$$[E_j^i, E_n^m] = E_n^i \delta_{mj} - E_j^m \delta_{in}$$

Rotations:

$$\hat{\phi}_i = \sum_a X_{ai} \phi_a$$

the matrix  $X$  is unitary if  $X^\dagger X = I$

$\exp(i\hat{k})$  is unitary if  $i\hat{k}$  is anti-Hermitian -  
 $\hat{X} = (e^{i\hat{k}})$



Hermitian matrix:

$$k_{ij} = k_{ji}^*$$

if  $\hat{\phi}_0$  is real and  $\phi$  is also real then  $X$  are called orthogonal i.e.  $X^T X = I$

for orthogonal matrices  $X = \exp(\hat{k})$ .  
 $\rightarrow \hat{k}$  is a real antisymmetric matrix.

$|\psi\rangle = \exp(-\hat{k}) |\phi_0\rangle$   
 $\downarrow$   
 optimize  $k_{ij}$  to minimize Energy -  
 { Hartree Fock  
 MC-SCF.



$$\min_{\underline{x}} f(\underline{x}) = 0 \quad \text{e.g. } \min_{c, i} \langle \psi(c) | H | \psi(c) \rangle$$

if  $x^*$  is the minimum; but we start with some  $x$ .  
and generate a model for the function; then we minimize this model.

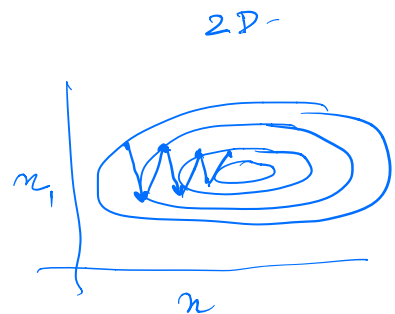
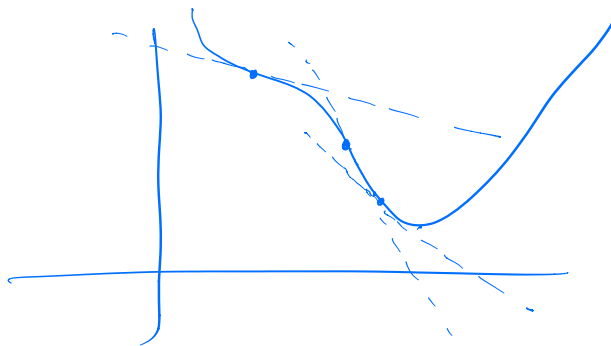
$$f(x) = f(x_c) + \underline{g}(x_c)^T (x - x_c) + \frac{1}{2} (x - x_c)^T \underline{H}(x_c) (x - x_c)$$

$$\underline{g}(x_c) = \nabla f(x_c) \quad \underline{H}(x_c) = \nabla^2 f(x_c)$$

### Linear model or steepest descent

you are unable to calculate or store  $\underline{H}(x^*)$  because its too large, then

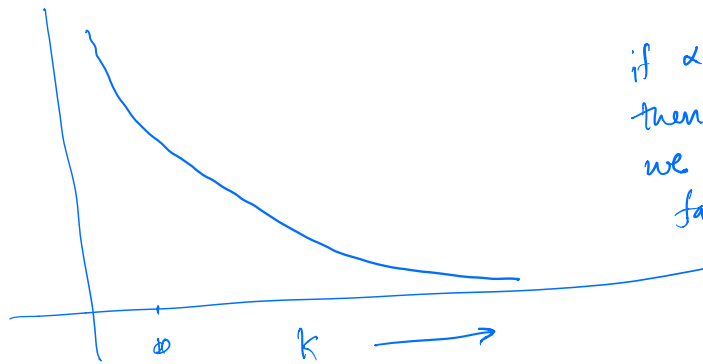
you take a step  $s \rightarrow$  in the direction  $-\alpha \underline{g}(x_c)$   
 $\downarrow$   
 step  
 [line search]



the convergence is linear: i.e.

$$\lim_{k \rightarrow \infty} \frac{|e_{k+1}|}{|e_k|} = \underline{\alpha} \quad e_k = x_k - x^*$$

$\downarrow$   
 $1/k \rightarrow$  condition number of the Hessian  $\Rightarrow 10^{12} - 10^{14}$



if  $\alpha = 10$ .  
 then at each iteration  
 we reduce the error by  
 factor of  $\alpha$ .

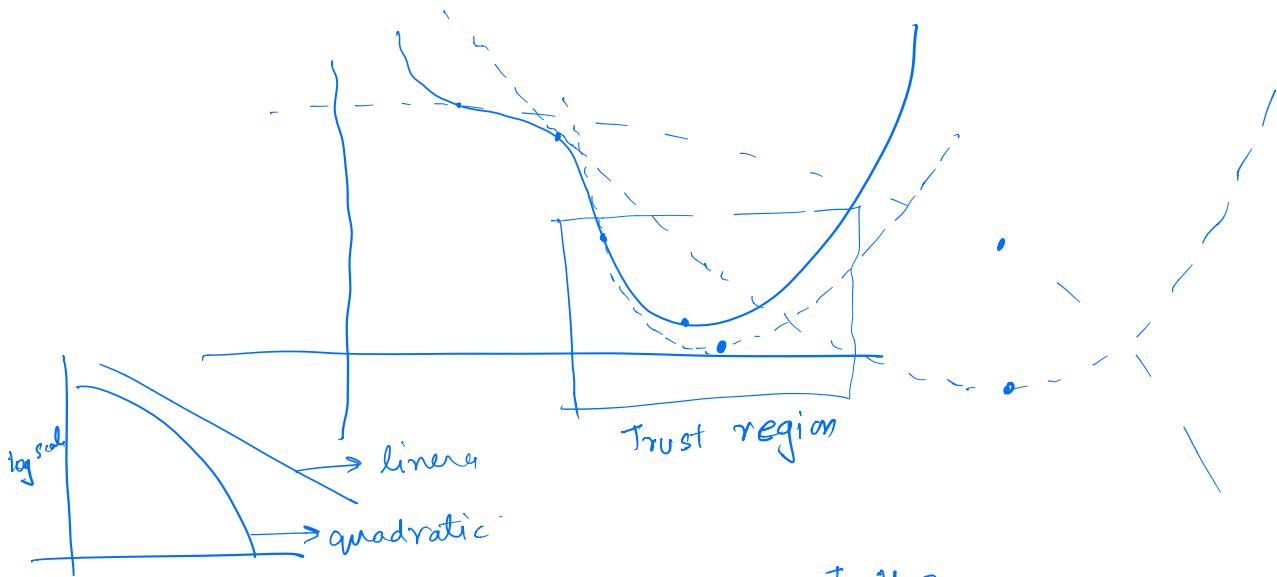
Newton and Quasi-newton method:

$$f(x) = f(x_0) + g^T s + \frac{1}{2} s^T H s.$$

$$\frac{\partial f}{\partial x} = 0.$$

$$g^T + Hs = 0 \Rightarrow Hs = -g^T$$

$$s = -H^{-1} g^T$$



$$f_{AH}(x) = f(x_0) +$$

$$\frac{g^T s + \frac{1}{2} s^T H s}{1 + s^T A s}$$

$\underbrace{s^T A s}_{\text{metric symmetric matrix}}$

\*

macro iterations!

$$k \rightarrow x^k$$

Can you derive it?

$$\begin{pmatrix} 0 & g^T \\ g & H \end{pmatrix} \begin{pmatrix} 1 \\ s \end{pmatrix} = E \begin{pmatrix} 1 \\ s \end{pmatrix}$$

$$H^k s^k = g^k$$

→ microiteration

$$s^k = H^{-1} g^k$$

} Linear equation with symmetric matrices

$$k+1 \rightarrow x^{k+1}$$

$$H^{k+1} s^{k+1} = g^{k+1}$$

microiterations

$$s^{k+1} = H^{-1} g^{k+1}$$

↓  
conjugate gradient method

A slightly different problem:

$$\min f(x) \quad \text{subject to constraint} \\ c(x) = 0$$

$$L(x, \lambda) = f(x) + \lambda c(x)$$

$$\frac{\partial L}{\partial x} = 0 \quad \text{and} \quad \frac{\partial L}{\partial \lambda} = 0$$

$$g^T + \lambda c^T = 0 \quad \text{and} \quad c = 0$$

in many cases.

$$f(x) = \frac{1}{2} H^T x$$
$$c(x) = \frac{1}{2} S^T x$$

one obtains.

$$\underline{H} \underline{x} + \lambda \underline{S} \underline{x} = 0 \quad \left\{ \begin{array}{l} \text{generalized} \\ \text{Eigen value} \\ \text{equation} \\ \text{or secular equation} \end{array} \right.$$

if  $S=I$  then  $\underline{H} \underline{x} - \lambda \underline{x} = 0$

Eigenvalue problem:-

if  $A \quad |\lambda_1| > |\lambda_2| > |\lambda_3| \dots$   
 $\quad \quad \quad v_1 \quad v_2 \quad v_3 \dots$

power method

$$c_1 = \frac{H c_0}{\|H c_0\|}$$

$$c_2 = \frac{H c_1}{\|H c_1\|}$$

$\vdots$

$$c_n \rightarrow v_1$$

$$\text{and } c_n^T H c_n \rightarrow \lambda_1$$

converges slowly.

Krylov space:-

$$c = a_0 c_0 + a_1 c_1 + a_2 c_2 + \dots$$

$\{a_i\} \rightarrow$  determined by projecting  $H$  on to the space  $\{c_i\}$ . ~~and~~ to get  $\bar{H}$  and diagonalizing  $H$ .

Davidson!

instead of taking  $c_i = H c_{i-1}$

we use  $c'_i = \frac{1}{H_0 - E_0} (H - E_0) c_{i-1}$ .

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Ankit - Make a python code for DMRG on <sup>1D</sup> hubbard model.

James :- Make a document showing how to select active space for.

benzene, tetracene and Fe-porphyrin.

Xubo ↓  
Bastien :- Do a molpro calculation on  $I_2$  [minimal active space] and an SHCI calculation and with Bagel [states] [compare with expt].

Bastien :- Make a document showing how the CCSD equations can be derived using SQA.

Ilyja :- Implement exact second order MCSCF solver for a hubbard model with 10 sites and 4 active orbitals



$$\frac{g^+ s + \frac{1}{2} s^+ G s}{1 + s^+ S s}$$

$$s = \begin{bmatrix} s \\ 1 \end{bmatrix}$$

$$s^+ = \begin{bmatrix} s^+ & 1 \end{bmatrix}$$

$$= \frac{1}{2} \frac{\begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} G & g \\ g^+ & 0 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}{\begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} S & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}} =$$

$$= \frac{\frac{1}{2} \begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} Gs + g \\ g^+ s \end{bmatrix}}{\frac{1}{2} \begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} Ss \\ 1 \end{bmatrix}} = \frac{1}{2} \frac{s^+ Gs + s^+ g + g^+ s}{s^+ Ss + 1}$$

diff  
s.

$$\frac{1}{2} \frac{\begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} G & g \\ g^+ & 0 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}{\begin{bmatrix} s^+ & 1 \end{bmatrix} \begin{bmatrix} S & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}$$

$$= \frac{\frac{1}{2} \cdot 2 \frac{\begin{bmatrix} G & g \\ g^+ & 0 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}{D^2} - \frac{\cancel{2} \cdot \cancel{N} \cdot \begin{bmatrix} S & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}{D^2}}$$

$$= \frac{\begin{bmatrix} G & g \\ g^+ & 0 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}{\begin{bmatrix} S & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} s \\ 1 \end{bmatrix}}$$