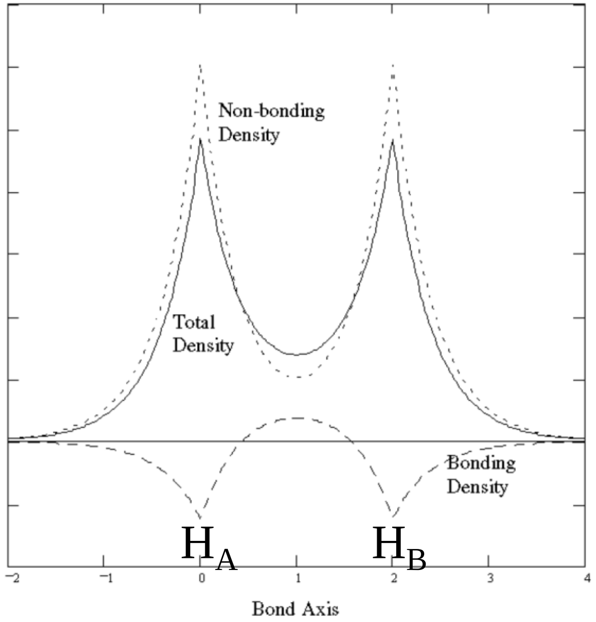
Using 2p_z Orbitals Hand waving

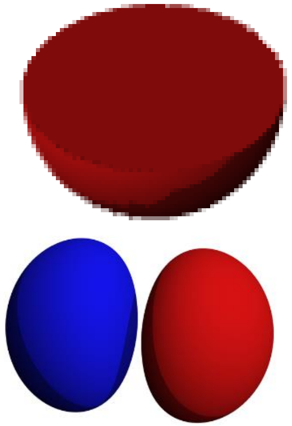
$1s(\zeta = 1.000)$	$-0.564\,83$	2.49
$1s(\zeta = 1.238)$	$-0.586\,51$	2.00
$1s(\zeta$ $)$	$-0.565\,91$	2.00

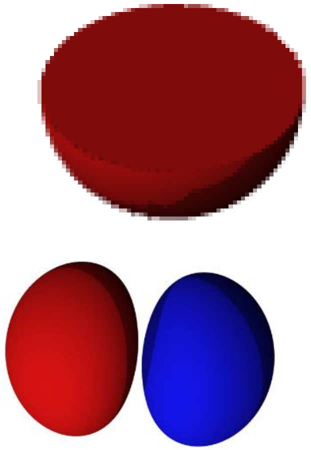


Bonding Orbital

The bonding orbital has asymmetric distribution around nuclei

Better described by a 2p_z orbital





Polarization orbital!

Expectation values of Slater Determinant

Born-Oppenheimer Approximation

Solve for the electron at a fixed nuclear geometry

$$\hat{H}^0(\mathbf{r};\mathbf{R})\Psi_n^{el}(\mathbf{r};\mathbf{R}) = \left[-\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2 + V(\mathbf{r},\mathbf{R})\right]\Psi_n^{el}(\mathbf{r};\mathbf{R}) = E_n(\mathbf{R})\Psi_n^{el}(\mathbf{r};\mathbf{R})$$

Calculate many nuclear geometries to obtain the potential energy surface

$$\hat{H}_{NU}(\mathbf{R})\chi_{n,v_n}^{NU}(\mathbf{R}) = E_{el,NU}\,\chi_{n,v_n}^{NU}(\mathbf{R})$$

$$\hat{H}_{NU}(\mathbf{R}) = \left(-\frac{1}{2}\sum_{I=1}^{N}\frac{1}{M_I}\nabla_I^2 + V(\mathbf{R})\right)$$

Problem To Solve

$$\hat{H}^0(\mathbf{r};\mathbf{R})\Psi_n^{el}(\mathbf{r};\mathbf{R})$$
$$=\left[-\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2+\sum_{I=1}^{N}\sum_{J\neq I}^{N}\frac{Z_I Z_J}{\left|\mathbf{R}_I-\mathbf{R}_J\right|}-\sum_{I=1}^{N}\sum_{i=1}^{n}\frac{Z_I}{\left|\mathbf{R}_I-\mathbf{r}_i\right|}+\sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{1}{\left|\mathbf{r}_i-\mathbf{r}_j\right|}\right]\Psi_n^{el}(\mathbf{r};\mathbf{R})$$
$$=E_n(\mathbf{R})\Psi_n^{el}(\mathbf{r};\mathbf{R})$$

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots\mathbf{x}_n)=\frac{1}{\sqrt{n!}}\begin{vmatrix}\psi_i(\mathbf{x}_1) & \psi_j(\mathbf{x}_1) & \cdots\cdots & \psi_k(\mathbf{x}_1)\\ \psi_i(\mathbf{x}_2) & \psi_j(\mathbf{x}_2) & \cdots\cdots & \psi_k(\mathbf{x}_2)\\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots\\ \psi_i(\mathbf{x}_n) & \psi_j(\mathbf{x}_n) & \cdots\cdots & \psi_k(\mathbf{x}_n)\end{vmatrix}$$

Operators and Matrix Elements

Hamiltonian is a sum of one and two electron operators

For example hydrogen molecule

$$\left[-\frac{1}{2}\nabla_1^2-\frac{1}{|\mathbf{r}_{1A}|}-\frac{1}{|\mathbf{r}_{1B}|}-\frac{1}{2}\nabla_2^2-\frac{1}{|\mathbf{r}_{2A}|}-\frac{1}{|\mathbf{r}_{2B}|}+\left[\frac{1}{|\mathbf{R}|}+\frac{1}{|\mathbf{r}_{12}|}\right]\right]$$

$$=\left[h_1+h_2+\frac{1}{|\mathbf{R}|}+\frac{1}{|\mathbf{r}_{12}|}\right]$$

$$h_1 = h(r_1) = -\frac{1}{2}\nabla_1^2 - \frac{1}{|r_{1A}|} - \frac{1}{|r_{1B}|}$$

h_1, h_2 : one electron operator

Electron kinetic energy

Electron nuclear attraction

$\frac{1}{|\mathbf{r}_{12}|}$: two electron operator

Electron electron repultion

$$\Psi_0(\mathbf{x}_1,\mathbf{x}_2)=\frac{1}{\sqrt{2}}\left(\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)-\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\right)$$

One Electron Operator Matrix Element

$$\langle 0|h_1|0\rangle = 2^{-1}\iint d\mathbf{x}_1 d\mathbf{x}_2 \left(\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)-\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\right)^*$$

$$\times h(\mathbf{r}_1)\left(\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)-\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\right)$$

$$= 2^{-1}\iint d\mathbf{x}_1 d\mathbf{x}_2 \left[\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\right.$$

$$+\psi_j^*(\mathbf{x}_1)\psi_i^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)$$

$$-\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)$$

$$\left.-\psi_j^*(\mathbf{x}_1)\psi_i^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\right]$$

Due to orthonormality of the spin orbitals last two are zero with integration with respect to $\mathbf{x}_2$

One Electron Operator 2

$$\langle 0|h_1|0\rangle = 2^{-1}\iint d\mathbf{x}_1 d\mathbf{x}_2 \left[\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\right.$$

$$\left. + \psi_j^*(\mathbf{x}_1)\psi_i^*(\mathbf{x}_2)h(\mathbf{r}_1)\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\right]$$

$$= 2^{-1}\int \psi_i^*(\mathbf{x}_1)h(\mathbf{r}_1)\psi_i(\mathbf{x}_1)d\mathbf{x}_1 + 2^{-1}\int \psi_j^*(\mathbf{x}_1)h(\mathbf{r}_1)\psi_j(\mathbf{x}_1)d\mathbf{x}_1$$

$$= 2^{-1}\left(\langle \psi_i|h|\psi_i\rangle + \langle \psi_j|h|\psi_j\rangle\right)$$

$$\langle 0|h_2|0\rangle = 2^{-1}\left(\langle \psi_i|h|\psi_i\rangle + \langle \psi_j|h|\psi_j\rangle\right)$$

$$\langle 0|h_2|0\rangle = \langle 0|h(r_2)|0\rangle \text{ so same as the case for } \langle 0|h_1|0\rangle$$

$$= 2^{-1}\left(\langle \psi_i|h|\psi_i\rangle + \langle \psi_j|h|\psi_j\rangle\right)$$

Two Electron Operator Matrix Element

$$\begin{aligned}
\left\langle 0 \left| |\mathbf{r}_{12}|^{-1} \right| 0 \right\rangle &= 2^{-1} \iint d\mathbf{x}_1 d\mathbf{x}_2 \left(\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2) - \psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2) \right)^* \\
&\quad \times |\mathbf{r}_{12}|^{-1} \left(\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2) - \psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2) \right) \\
&= 2^{-1} \iint d\mathbf{x}_1 d\mathbf{x}_2 \Big[\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2) |\mathbf{r}_{12}|^{-1} \psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2) \\
&\quad + \psi_j^*(\mathbf{x}_1)\psi_i^*(\mathbf{x}_2) |\mathbf{r}_{12}|^{-1} \psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2) \\
&\quad - \psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2) |\mathbf{r}_{12}|^{-1} \psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2) \\
&\quad - \psi_j^*(\mathbf{x}_1)\psi_i^*(\mathbf{x}_2) |\mathbf{r}_{12}|^{-1} \psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2) \Big]
\end{aligned}$$

Since $|\mathbf{r}_{12}|$ is equal to $|\mathbf{r}_{21}|$ perform interchange of electron 1 and electron 2 and first and second are the same and third and fourth are the same

Two Electron Operator 2

$$\langle 0 | |\mathbf{r}_{12}|^{-1} | 0 \rangle = \iint d\mathbf{x}_1 d\mathbf{x}_2 \Big[\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)|\mathbf{r}_{12}|^{-1}\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)$$

$$-\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)|\mathbf{r}_{12}|^{-1}\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\Big]$$

$$= \langle ij | ij \rangle - \langle ij | ji \rangle$$

$$\langle ij | kl \rangle = \langle ji | lk \rangle = \langle kl | ij \rangle^* = \langle lk | ji \rangle^*$$

Symbols physics people use: $\langle ij \| kl \rangle = \langle ij | kl \rangle - \langle ij | lk \rangle$

Symbols chemistry people use:

$$[ij | kl] = \langle ik | jl \rangle = \iint d\mathbf{x}_1 d\mathbf{x}_2 \big[\psi_i^*(\mathbf{x}_1)\psi_j(\mathbf{x}_1)|\mathbf{r}_{12}|^{-1}\psi_k^*(\mathbf{x}_2)\psi_l(\mathbf{x}_2)$$

So the expectation value of the hamiltonian with the Slater determinant for two electron system is

$$\langle 0|H|0\rangle = \langle \psi_i|h|\psi_i\rangle + \langle \psi_j|h|\psi_j\rangle + \langle ij | ij \rangle - \langle ij | ji \rangle$$

Expectation Value of Slater Det

$$|\psi_1\psi_2\ldots\psi_n\rangle = \frac{1}{\sqrt{n!}}\begin{vmatrix} \psi_i(\mathbf{x}_1) & \psi_j(\mathbf{x}_1) & \ldots\ldots\ldots\ldots\ldots\ldots & \psi_n(\mathbf{x}_1) \\ \psi_i(\mathbf{x}_2) & \psi_j(\mathbf{x}_2) & \ldots\ldots\ldots\ldots\ldots\ldots & \psi_n(\mathbf{x}_2) \\ \ldots\ldots\ldots & \ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots \\ \psi_i(\mathbf{x}_n) & \psi_j(\mathbf{x}_n) & \ldots\ldots\ldots\ldots\ldots\ldots & \psi_n(\mathbf{x}_n) \end{vmatrix}$$

For one electron operators we consider the sum of each electron, for two electron operators the sum of pairs of electrons

two electron system Hamiltonian was $\left[h_1 + h_2 + \frac{1}{|\mathbf{R}|} + \frac{1}{|\mathbf{r}_{12}|}\right]$

one electron operators for n electron system $\sum_{i=1}^{n} h_i$

two electron operator for n electron system $\sum_{i=1}^{n}\sum_{j>i}^{n} |\mathbf{r}_{ij}|^{-1}$

Expectation of One Electron Operator of Slater Det

$$\left\langle \psi_1\psi_2\ldots\psi_n \middle| \sum_{i=1}^{n} h_i \middle| \psi_1\psi_2\ldots\psi_n \right\rangle = \langle \psi_1\psi_2\ldots\psi_n | h_1 + h_2 + \ldots h_n | \psi_1\psi_2\ldots\psi_n \rangle$$

Since electron in slater determinant is indistinguishable we consider for just electron 1 and multiply by the number of electrons

$$\left\langle \psi_1\psi_2\ldots\psi_n \middle| \sum_{i=1}^{n} h_i \middle| \psi_1\psi_2\ldots\psi_n \right\rangle = n\langle \psi_1\psi_2\ldots\psi_n | h_1 | \psi_1\psi_2\ldots\psi_n \rangle$$

$$= \sum_{i=1}^{n} \langle \psi_i | h_1 | \psi_i \rangle$$

Summation of orbital contributions

Expectation Value of a Two electron Operator for Slater Det

$$\left\langle \psi_1\psi_2\ldots\psi_n \left| \sum_{i=1}^{n}\sum_{j>i}^{n} \left|\mathbf{r}_{ij}\right|^{-1} \right| \psi_1\psi_2\ldots\psi_n \right\rangle$$

$$= \left\langle \psi_1\psi_2\ldots\psi_n \left| \left|\mathbf{r}_{12}\right|^{-1} + \left|\mathbf{r}_{13}\right|^{-1} + \ldots \left|\mathbf{r}_{n-1n}\right|^{-1} \right| \psi_1\psi_2\ldots\psi_n \right\rangle$$

Since electron in slater determinant is indistinguishable we solve for electron 1 and 2 and multiply by the number of pairs

$$\left\langle \psi_1\psi_2\ldots\psi_n \left| \sum_{i=1}^{n}\sum_{j>i}^{n} \left|\mathbf{r}_{ij}\right|^{-1} \right| \psi_1\psi_2\ldots\psi_n \right\rangle$$

$$= \frac{n(n-1)}{2} \left\langle \psi_1\psi_2\ldots\psi_n \left| \left|\mathbf{r}_{12}\right|^{-1} \right| \psi_1\psi_2\ldots\psi_n \right\rangle$$

$$= \frac{1}{2}\sum_{i=1}^{n}\sum_{j\neq i}^{n}\left(\langle ij \mid ij\rangle - \langle ij \mid ji\rangle\right) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle ij \mid ij\rangle - \langle ij \mid ji\rangle\right)$$

Why the summation is not j≠i

Hartree-Fock Roothaan Equation
Electronic Structure

Kaito Takahashi

Hartree Fock Approximation 1

$$\hat{H}^0(\mathbf{r};\mathbf{R}) = \sum_{i=1}^{n} h_i + \sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{1}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}$$

$$\left|\psi_1\psi_2\ldots\psi_n\right\rangle = \frac{1}{\sqrt{n!}}\begin{vmatrix} \psi_i(\mathbf{x}_1) & \psi_j(\mathbf{x}_1) & \cdots\cdots & \psi_n(\mathbf{x}_1) \\ \psi_i(\mathbf{x}_2) & \psi_j(\mathbf{x}_2) & \cdots\cdots & \psi_n(\mathbf{x}_2) \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \psi_i(\mathbf{x}_n) & \psi_j(\mathbf{x}_n) & \cdots\cdots & \psi_n(\mathbf{x}_n) \end{vmatrix}$$

$$\left\langle \psi_1\psi_2\ldots\psi_n \middle| \hat{H}^0 \middle| \psi_1\psi_2\ldots\psi_n \right\rangle = \sum_{i=1}^{n}\left\langle \psi_i \middle| h_1 \middle| \psi_i \right\rangle + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle ij \mid ij\rangle - \langle ij \mid ji\rangle\right)$$

$$\left\langle \psi_i \mid \psi_j \right\rangle = \delta_{ij}$$

How do you find the best answer for the spin orbitals?

Hartree Fock Approximation 2

Variational theory functional minimization with constraint

$$\Im(\{\psi_i\}) = \left\langle \psi_1\psi_2\ldots\psi_n \middle| \hat{H}^0 \middle| \psi_1\psi_2\ldots\psi_n \right\rangle - \sum_{i=1}^{n}\sum_{j=1}^{n} \varepsilon_{ji}\left(\left\langle \psi_i | \psi_j \right\rangle - \delta_{ij}\right) \rightarrow \min$$

Functional derivative with respect to change of spin orbital

$\psi_i \rightarrow \psi_i + \delta\psi_i$ should be zero

$$\Im(\{\psi_i + \delta\psi_i\}) - \Im(\{\psi_i\}) = \delta\Im(\{\psi_i\}) = 0$$

$$\delta\Im(\{\psi_i\}) = \delta\left\langle \psi_1\psi_2\ldots\psi_n \middle| \hat{H}^0 \middle| \psi_1\psi_2\ldots\psi_n \right\rangle - \sum_{i=1}^{n}\sum_{j=1}^{n} \varepsilon_{ji}\left(\delta\left\langle \psi_i | \psi_j \right\rangle\right) = 0$$

$$\delta\left\langle \psi_i | \psi_j \right\rangle = \left\langle \delta\psi_i | \psi_j \right\rangle + \left\langle \psi_i | \delta\psi_j \right\rangle$$

Hartree Fock Approximation 3

$$\delta\left\langle \psi_1\psi_2\ldots\psi_n\middle|\hat{H}^0\middle|\psi_1\psi_2\ldots\psi_n\right\rangle = \sum_{i=1}^{n}\left\langle \delta\psi_i\middle|h_1\middle|\psi_i\right\rangle + \sum_{i=1}^{n}\left\langle \psi_i\middle|h_1\middle|\delta\psi_i\right\rangle$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle \delta ij \mid ij\rangle - \langle \delta ij \mid ji\rangle\right) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle i\delta j \mid ij\rangle - \langle i\delta j \mid ji\rangle\right)$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle ij \mid \delta ij\rangle - \langle ij \mid \delta j i\rangle\right) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle ij \mid i\delta j\rangle - \langle ij \mid j\delta i\rangle\right)$$

Remember the exchange relationship of two electron integral

$$\langle ij \mid kl\rangle = \langle ji \mid lk\rangle = \langle kl \mid ij\rangle^* = \langle lk \mid ji\rangle^*$$

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle i\delta j \mid ij\rangle - \langle i\delta j \mid ji\rangle\right) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle \delta j i \mid ji\rangle - \langle \delta j i \mid ij\rangle\right)$$

$$= \frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n}\left(\langle \delta ij \mid ij\rangle - \langle \delta ij \mid ji\rangle\right)$$

Hartree Fock Approximation 4

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle ij\,|\,\delta i j\rangle-\langle ij\,|\,\delta j\, i\rangle\Big)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle \delta i j\,|\,ij\rangle *-\langle \delta j\, i\,|\,ij\rangle *\Big)$$

$$=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle \delta i j\,|\,ij\rangle *-\langle \delta i j\,|\,j i\rangle *\Big)$$

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle ij\,|\,i\delta j\rangle-\langle ij\,|\,j\delta i\rangle\Big)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle i\delta j\,|\,ij\rangle *-\langle j\delta i\,|\,ij\rangle *\Big)$$

$$=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle \delta j\, i\,|\,j i\rangle *-\langle \delta i j\,|\,j i\rangle *\Big)$$

$$=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\langle \delta i j\,|\,ij\rangle *-\langle \delta i j\,|\,j i\rangle *\Big)$$

Hartree Fock Approximation 5

$$\delta\Im(\{\psi_i\}) = \delta\left\langle \psi_1\psi_2\ldots\psi_n \middle| \hat{H}^0 \middle| \psi_1\psi_2\ldots\psi_n \right\rangle - \sum_{i=1}^{n}\sum_{j=1}^{n}\varepsilon_{ji}\left(\delta\langle\psi_i \mid \psi_j\rangle\right) = 0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\varepsilon_{ji}\left(\langle\delta\psi_i \mid \psi_j\rangle + \langle\psi_i \mid \delta\psi_j\rangle\right) = \sum_{i=1}^{n}\sum_{j=1}^{n}\varepsilon_{ji}\left(\langle\delta\psi_i \mid \psi_j\rangle\right) + cc$$

Complex conjugate

$$\delta\left\langle \psi_1\psi_2\ldots\psi_n \middle| \hat{H}^0 \middle| \psi_1\psi_2\ldots\psi_n \right\rangle = \sum_{i=1}^{n}\langle\delta\psi_i | h_1 | \psi_i\rangle + \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle\delta ij \mid ij\rangle - \langle\delta ij \mid ji\rangle\right) + cc$$

$$\sum_{i=1}^{n}\langle\delta\psi_i | h_1 | \psi_i\rangle + \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\langle\delta ij \mid ij\rangle - \langle\delta ij \mid ji\rangle - \varepsilon_{ji}\langle\delta\psi_i \mid \psi_j\rangle\right) + cc = 0$$

$$\sum_{i=1}^{n}\int \delta\psi_i^*(\mathbf{x}_1)h(\mathbf{r}_1)\psi_i(\mathbf{x}_1)d\mathbf{x}_1 + \sum_{i=1}^{n}\sum_{j=1}^{n}\iint d\mathbf{x}_1 d\mathbf{x}_2\left(\delta\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)|\mathbf{r}_{12}|^{-1}\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2)\right)$$

$$-\sum_{i=1}^{n}\sum_{j=1}^{n}\iint d\mathbf{x}_1 d\mathbf{x}_2\left(\delta\psi_i^*(\mathbf{x}_1)\psi_j^*(\mathbf{x}_2)|\mathbf{r}_{12}|^{-1}\psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2)\right) - \sum_{i=1}^{n}\sum_{j=1}^{n}\varepsilon_{ji}\iint \delta\psi_i^*(\mathbf{x}_1)\psi_j(\mathbf{x}_1)d\mathbf{x}_1$$