

CHM 673

Lecture 8: Spin operators; restricted and unrestricted wave functions

Suggested reading:

Chapter 2.5 from S&O

Chapter 3.7 from Jensen

Spin angular momentum

The algebraic theory of spin is a carbon copy theory of orbital momentum, beginning with the fundamental commutation relations:

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z; [\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x; [\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y \quad [\hat{S}^2, \hat{\vec{S}}] = 0$$

The complete set of states describing the spin of a particle should be the simultaneous eigen function of S^2 and a single component of \vec{S} , typically S_z .

Valid spin function in Dirac notation: $f_s^m \equiv |sm\rangle$

$$\hat{S}^2|sm\rangle = s(s+1)\hbar^2|sm\rangle \quad s = 0, 1/2, 1, 3/2, \dots$$

$$\hat{S}_z|sm\rangle = m\hbar|sm\rangle \quad m = -s, -s+1, \dots, s-1, s$$

(2s+1) values =
multiplicity

s – quantum number describing the total spin

m – quantum number describing z component of the spin (projection on z axis)

Spin 1/2

The electron has spin one-half. There are only two eigenstates:

$$s = 1/2$$

$$m = -s, \dots, s = -1/2, 1/2$$

In Dirac notations $|sm\rangle$:

$\left \begin{array}{c} 1 \\ 2 \end{array} \right\rangle \equiv \uparrow\rangle \equiv \alpha\rangle$	“spin up”
$\left \begin{array}{c} 1 \\ 2 \end{array} \left(-\frac{1}{2} \right) \right\rangle \equiv \downarrow\rangle \equiv \beta\rangle$	“spin down”

$|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of S^2 and S_z

$$\hat{S}^2|\alpha\rangle = \frac{3}{4}|\alpha\rangle$$

$$\hat{S}^2|\beta\rangle = \frac{3}{4}|\beta\rangle$$

$$\hat{S}_z|\alpha\rangle = \frac{1}{2}|\alpha\rangle$$

$$\hat{S}_z|\beta\rangle = -\frac{1}{2}|\beta\rangle$$

But are not eigenstates of S_x and S_y

$$\hat{S}_x|\alpha\rangle = \frac{1}{2}|\beta\rangle$$

$$\hat{S}_x|\beta\rangle = \frac{1}{2}|\alpha\rangle$$

$$\hat{S}_y|\alpha\rangle = \frac{i}{2}|\beta\rangle$$

$$\hat{S}_y|\beta\rangle = -\frac{i}{2}|\alpha\rangle$$

Ladder operators

Ladder operators (“step-up”, “step-down”) increase/decrease the value of m by one:

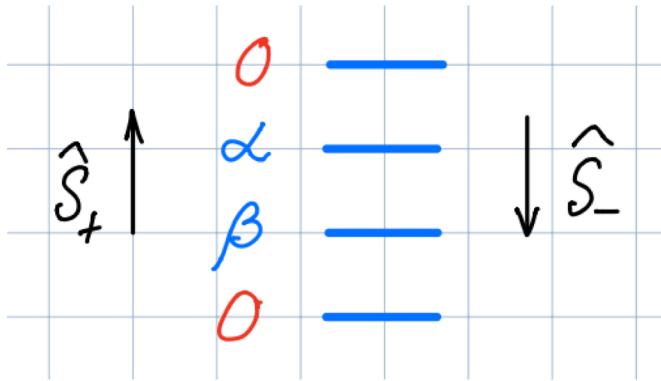
$$\hat{S}_{\pm} = \hat{S}_x \pm i\hat{S}_y$$

$$\hat{S}_+|\alpha\rangle = 0$$

$$\hat{S}_-|\alpha\rangle = \beta$$

$$\hat{S}_+|\beta\rangle = \alpha$$

$$\hat{S}_-|\beta\rangle = 0$$



Handy relations between S^2 and ladder operators:

$$\hat{S}^2 = \hat{S}_+ \hat{S}_- - \hat{S}_z + \hat{S}_z^2$$

$$\hat{S}^2 = \hat{S}_- \hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

Many-electron systems

The total spin of the many electron system is a sum of spins of each electron:

$$\hat{\vec{S}} = \sum_{i=1}^N \hat{\vec{s}}(i)$$

$$\hat{S}_z = \sum_{i=1}^N \hat{s}_z(i)$$

$$\hat{S}_{\pm} = \sum_{i=1}^N \hat{s}_{\pm}(i)$$

This is how to compute S^2 of many-electron system:

$$\hat{S}^2 = \hat{\vec{S}} \cdot \hat{\vec{S}} = \sum_{i=1}^N \sum_{j=1}^N \hat{\vec{s}}(i) \hat{\vec{s}}(j) = \hat{S}_+ \hat{S}_- - \hat{S}_z + \hat{S}_z^2 = \hat{S}_- \hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

spin quantum number S	multiplicity $2S+1$	$\langle \hat{S}^2 \rangle$	
0	1	0	singlet
1/2	2	3/4	doublet
1	3	2	triplet
3/2	4	3 3/4	quintet

Approximate solutions to Hamiltonian

Non-relativistic electronic Hamiltonian does not contain spin coordinates;

S^2 and S_z commute with H : $[\hat{H}, \hat{S}^2] = [\hat{H}, \hat{S}_z] = 0$

→ The exact eigenfunctions of the Hamiltonian are also eigenfunctions of spin-operators S^2 and S_z :

$$\hat{S}^2 |\Phi\rangle = S(S+1) |\Phi\rangle$$

$$\hat{S}_z |\Phi\rangle = M_S |\Phi\rangle$$

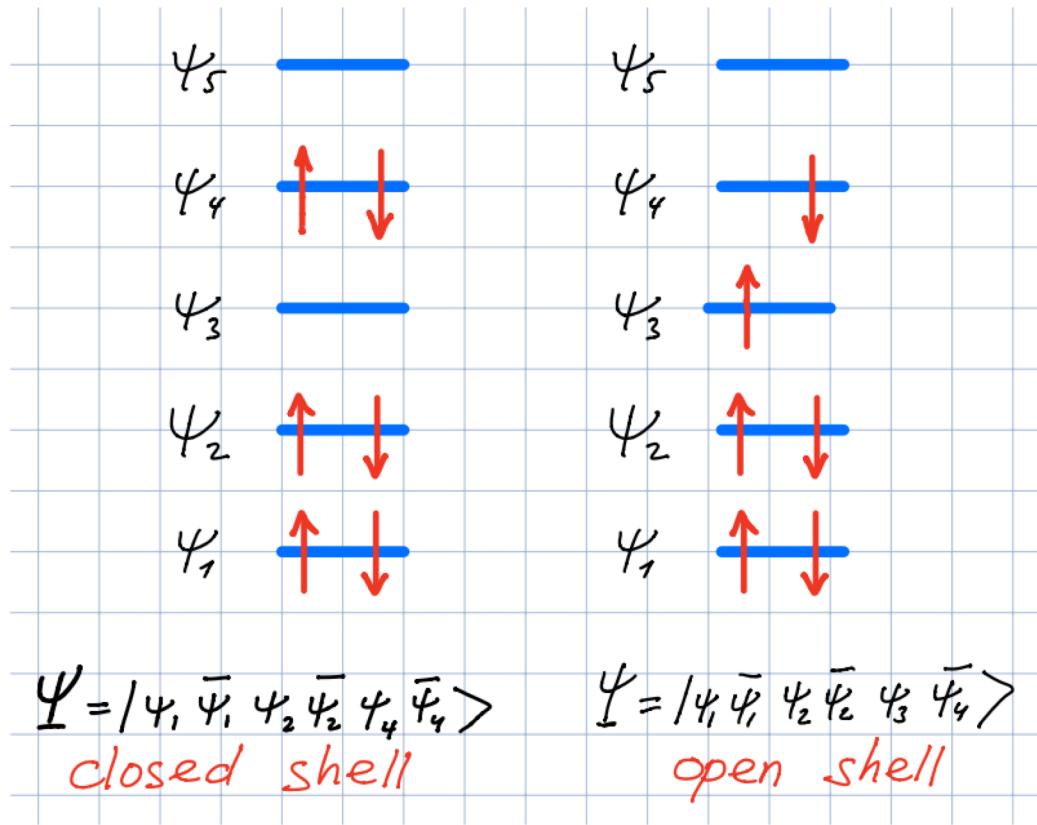
However, approximate solutions to H are not necessarily pure spin states!

Any Slater determinant is an eigenfunction of S_z :

$$\hat{S}_z |\chi_i \chi_j \dots \chi_k\rangle = \frac{1}{2}(N^\alpha - N^\beta) |\chi_i \chi_j \dots \chi_k\rangle = M_S |\chi_i \chi_j \dots \chi_k\rangle$$

But a Slater determinant is not necessarily an eigenfunction of S^2

Restricted determinants



Restricted Slater determinants (RSD) are formed by restricted spin orbitals
K spatial orbitals ψ_i , 2K spin orbitals χ_i

$$\chi_{2i-1}(x) = \psi_i(r)\alpha$$

$$\chi_{2i}(x) = \psi_i(r)\beta$$

Each spatial orbital can be occupied by 0, 1, or 2 electrons

Closed-shell determinant: all spatial orbitals are doubly-occupied

Open-shell determinant: some spatial orbitals are singly-occupied

Restricted determinants

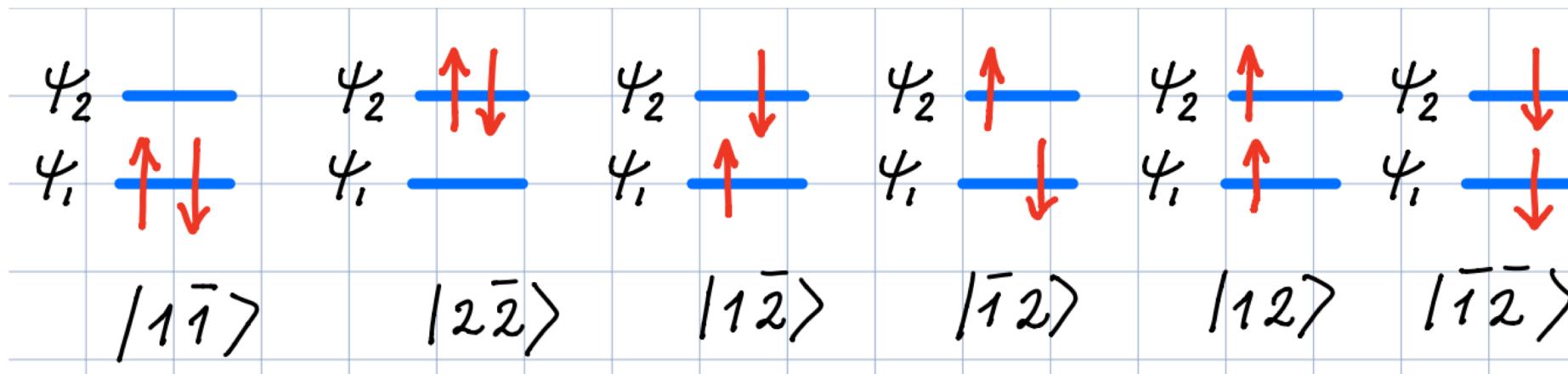
Closed-shell determinants are always pure singlets, i.e. they are eigenstates of S^2 operator:

$$\hat{S}^2 |\psi_i \bar{\psi}_i \psi_j \bar{\psi}_j \dots\rangle = 0(0+1) |\psi_i \bar{\psi}_i \psi_j \bar{\psi}_j \dots\rangle$$

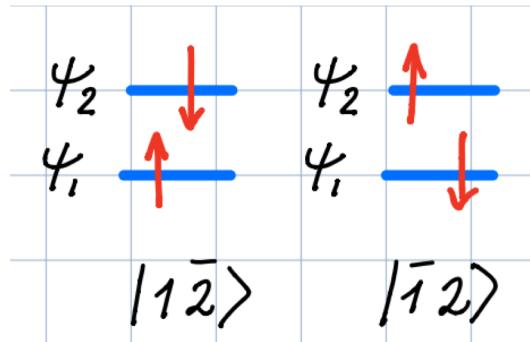
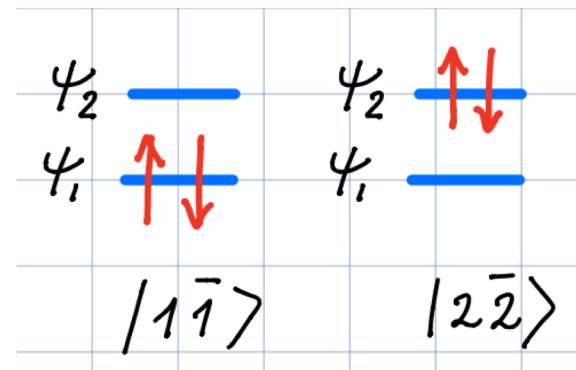
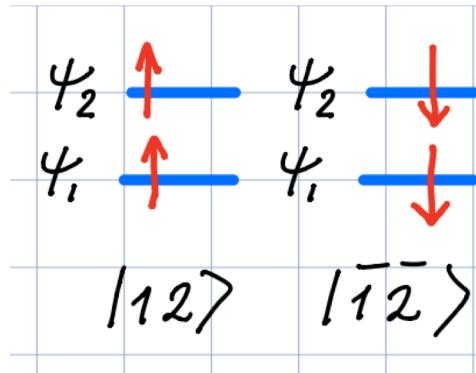
Open-shell restricted determinants are not eigenstates of S^2 operator, unless all open-shell electrons have parallel spins

Consider 2 electrons on 2 spatial orbitals

There are 6 possible SDs, two closed-shells and four open-shells



Restricted determinants: 2 by 2 case



$$|12\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\alpha(1)\psi_2(2)\alpha(2) - \psi_2(1)\alpha(1)\psi_1(2)\alpha(2)] =$$

$$\frac{1}{\sqrt{2}} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] \alpha(1)\alpha(2)$$

$$|\bar{1}\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] \beta(1)\beta(2)$$

$$|1\bar{1}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\alpha(1)\psi_1(2)\beta(2) - \psi_1(1)\beta(1)\psi_1(2)\alpha(2)] =$$

$$\frac{1}{\sqrt{2}} [\psi_1(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

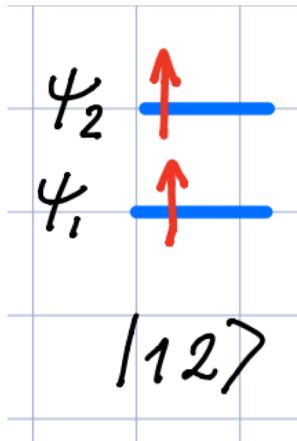
$$|2\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_2(1)\psi_2(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

$$|1\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)]$$

$$|\bar{1}2\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\beta(1)\psi_2(2)\alpha(2) - \psi_2(1)\alpha(1)\psi_1(2)\beta(2)]$$

Restricted determinants: 2 by 2 case

Let's determine $\langle S_z \rangle$ and $\langle S^2 \rangle$ of these determinants



$$|12\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] \alpha(1)\alpha(2)$$

$$\hat{S}_z |\alpha(1)\alpha(2)\rangle = (\hat{s}_z(1) + \hat{s}_z(2)) |\alpha(1)\alpha(2)\rangle = \hat{s}_z(1)|\alpha(1)\alpha(2)\rangle + \hat{s}_z(2)|\alpha(1)\alpha(2)\rangle = \frac{1}{2}|\alpha(1)\alpha(2)\rangle + \frac{1}{2}|\alpha(1)\alpha(2)\rangle = |\alpha(1)\alpha(2)\rangle$$

$M_S = 1$

$$\hat{S}^2 = \hat{S}_- \hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

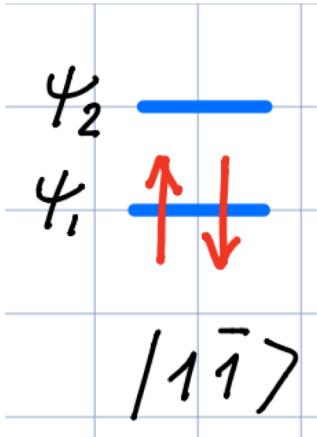
$$\hat{S}_+ |\alpha(1)\alpha(2)\rangle = (\hat{s}_+(1) + \hat{s}_+(2)) |\alpha(1)\alpha(2)\rangle = \hat{s}_+(1)|\alpha(1)\alpha(2)\rangle + \hat{s}_+(2)|\alpha(1)\alpha(2)\rangle = 0$$

$$\hat{S}^2 |\alpha(1)\alpha(2)\rangle = 0 + |\alpha(1)\alpha(2)\rangle + |\alpha(1)\alpha(2)\rangle = 2|\alpha(1)\alpha(2)\rangle$$

$S(S+1) \rightarrow S=1$ triplet state

Restricted determinants: 2 by 2 case

Let's determine $\langle S_z \rangle$ and $\langle S^2 \rangle$ of these determinants



$$|1\bar{1}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

$$\hat{S}_z |(\alpha(1)\beta(2) - \beta(1)\alpha(2))\rangle = (\hat{s}_z(1) + \hat{s}_z(2)) |(\alpha(1)\beta(2) - \beta(1)\alpha(2))\rangle =$$

$$\frac{1}{2}|\alpha(1)\beta(2)\rangle - \frac{1}{2}|\alpha(1)\beta(2)\rangle + \frac{1}{2}|\beta(1)\alpha(2)\rangle - \frac{1}{2}|\beta(1)\alpha(2)\rangle = 0$$

$$\mathbf{M}_S = 0$$

$$\hat{S}^2 = \hat{S}_- \hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

$$\hat{S}_+ |(\alpha(1)\beta(2) - \beta(1)\alpha(2))\rangle = (\hat{s}_+(1) + \hat{s}_+(2)) |(\alpha(1)\beta(2) - \beta(1)\alpha(2))\rangle = 0 - |\alpha(1)\alpha(2)\rangle + |\alpha(1)\alpha(2)\rangle - 0 = 0$$

$$\hat{S}^2 |(\alpha(1)\beta(2) - \beta(1)\alpha(2))\rangle = 0$$

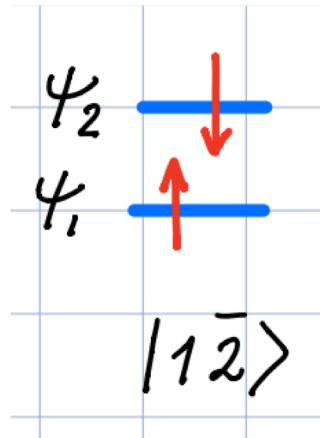


$$S(S+1) \rightarrow S=0$$

singlet state

Restricted determinants: 2 by 2 case

Let's determine $\langle S_z \rangle$ and $\langle S^2 \rangle$ of these determinants



$$|1\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)]$$

$$\hat{S}_z | (\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)) \rangle = 0 \quad \mathbf{M}_S = 0$$

$$\hat{S}^2 = \hat{S}_- \hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

$$\begin{aligned} \hat{S}_+ | (\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)) \rangle &= \\ (\hat{s}_+(1) + \hat{s}_+(2)) | (\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)) \rangle &= \\ 0 + \hat{s}_+(2) |\psi_1(1)\alpha(1)\psi_2(2)\beta(2)\rangle - \hat{s}_+(1) |\psi_2(1)\beta(1)\psi_1(2)\alpha(2)\rangle - 0 &= \\ (\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)) \alpha(1)\alpha(2) & \end{aligned}$$

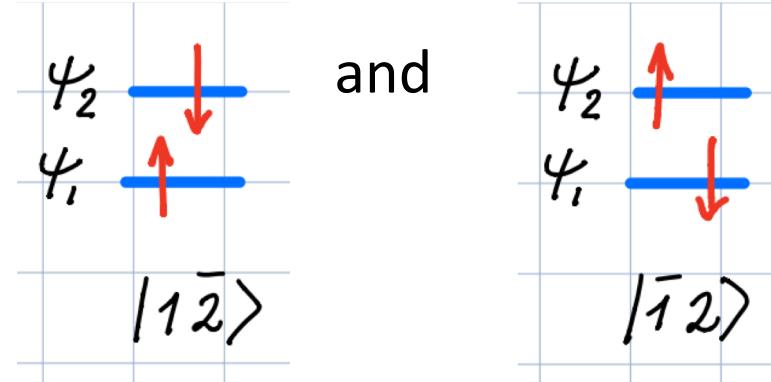
$$\begin{aligned} \hat{S}_- | (\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)) \alpha(1)\alpha(2) \rangle &= \\ (\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)) (\beta(1)\alpha(2) + \alpha(1)\beta(2)) & \end{aligned}$$

$$\begin{aligned} \hat{S}^2 |\psi_1(1)\alpha(1)\psi_2(2)\beta(2) - \psi_2(1)\beta(1)\psi_1(2)\alpha(2)\rangle &= \\ (\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)) (\beta(1)\alpha(2) + \alpha(1)\beta(2)) & \end{aligned}$$

Not the eigenstate of S^2 !

Restricted determinants: 2 by 2 case

Consider linear combinations of



$$\frac{1}{\sqrt{2}} [|1\bar{2}\rangle + |\bar{1}2\rangle] = \frac{1}{2} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] (\alpha(1)\beta(2) + \beta(1)\alpha(2)) \quad \text{triplet}$$

$$\frac{1}{\sqrt{2}} [|1\bar{2}\rangle - |\bar{1}2\rangle] = \frac{1}{2} [\psi_1(1)\psi_2(2) + \psi_2(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2)) \quad \text{singlet}$$

Generally, restricted open-shell SDs can be combined ("spin-adapted") into spin-pure states

Restricted determinants: 2 by 2 case

$$|12\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] \alpha(1)\alpha(2)$$

$$|\bar{1}\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] \beta(1)\beta(2)$$

$$\frac{1}{\sqrt{2}} [|1\bar{2}\rangle + |\bar{1}2\rangle] = \frac{1}{2} [\psi_1(1)\psi_2(2) - \psi_2(1)\psi_1(2)] (\alpha(1)\beta(2) + \beta(1)\alpha(2))$$

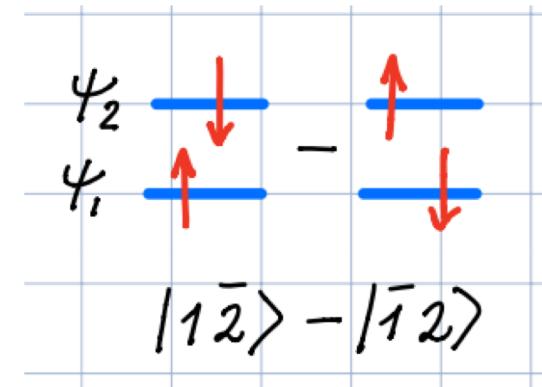
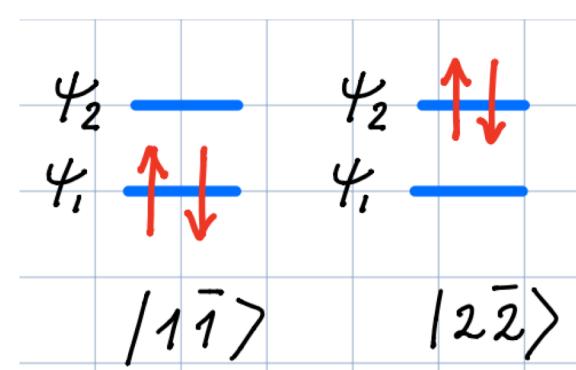
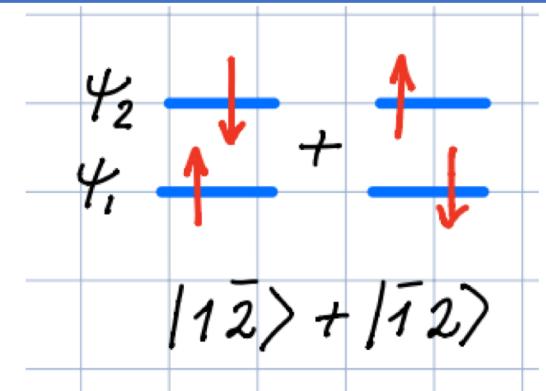
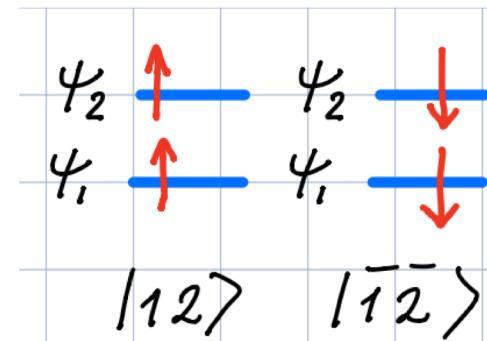
Triplets: symmetric spin-wavefunction, antisymmetric spatial wave-function

$$|1\bar{1}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

$$|2\bar{2}\rangle = \frac{1}{\sqrt{2}} [\psi_2(1)\psi_2(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

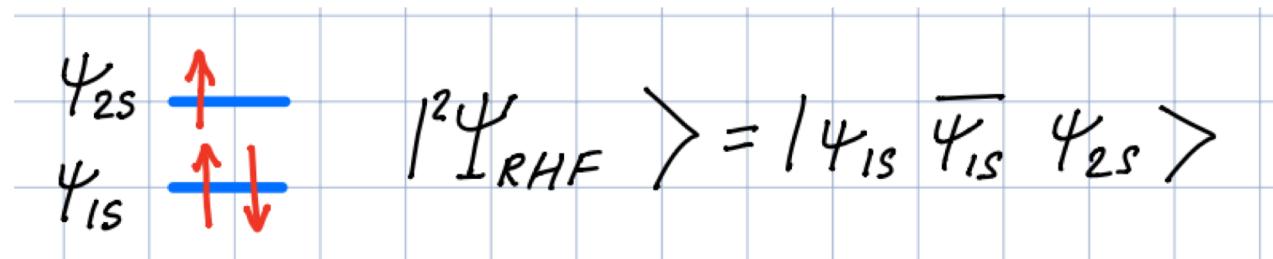
$$\frac{1}{\sqrt{2}} [|1\bar{2}\rangle - |\bar{1}2\rangle] = \frac{1}{2} [\psi_1(1)\psi_2(2) + \psi_2(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

Singlets: antisymmetric spin-wavefunction, symmetric spatial wave-function

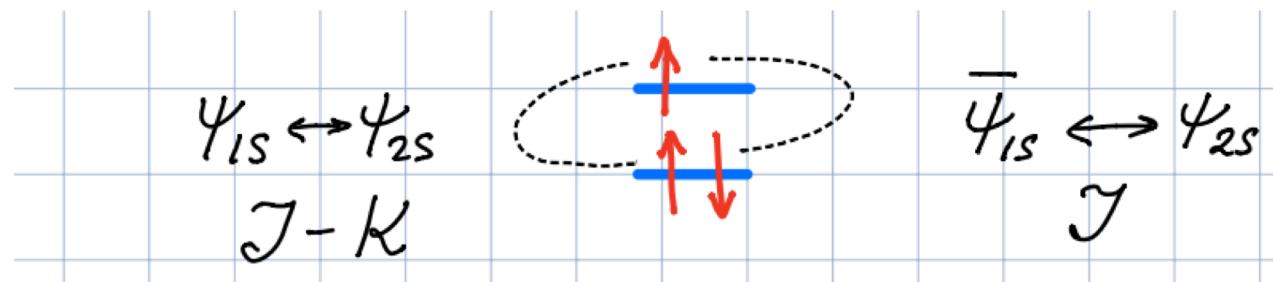


Unrestricted determinants

Consider Li atom



However, alpha electron on 2s orbital interacts differently with alpha and beta electrons on 1s

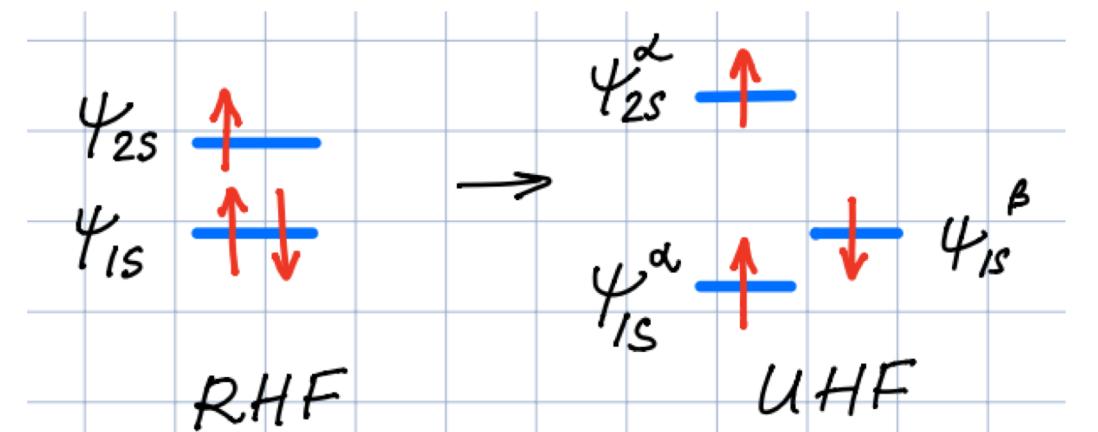


1sa and 1sb electrons experience different effective potentials due to 2sa and would prefer not to be described with the same spatial wavefunction. Thus, relaxing this constraint

$$\psi_{1s}^\alpha \neq \psi_{1s}^\beta$$

will result in lower energy

unrestricted determinant



$$|^2\Psi_{UHF} \rangle = |\psi_{1s}^\alpha \ \bar{\psi}_{1s}^\beta \ \psi_{2s}^\alpha \rangle$$

Unrestricted determinants

$$\langle \psi_i^\alpha | \psi_j^\alpha \rangle = \delta_{ij}$$

$$\langle \psi_i^\beta | \psi_j^\beta \rangle = \delta_{ij}$$

$$\langle \psi_i^\alpha | \psi_j^\beta \rangle = S_{ij}^{\alpha\beta}$$

ψ^α and ψ^β are not orthogonal, but spin-orbitals form orthonormal set

- **USDs are not eigenfunctions of S^2**
- They cannot be spin-adapted (e.g., USD for Li is not a pure doublet)
- USDs are still called singlets, doublets, triplets, etc.

Unrestricted singlets might collapse to restricted singlets (e.g., in H₂ – stay tuned!)

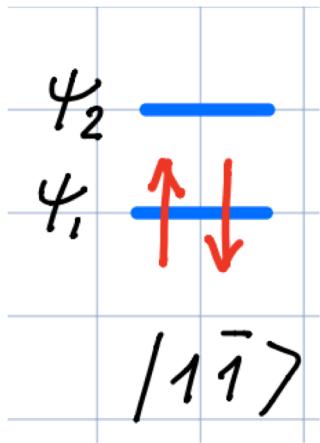
$$|^1\Psi\rangle = c_1^1|1\rangle + c_3^1|3\rangle + c_5^1|5\rangle + \dots$$

$$|^2\Psi\rangle = c_2^2|2\rangle + c_4^2|4\rangle + c_6^2|6\rangle + \dots$$

$$|^3\Psi\rangle = c_3^3|3\rangle + c_5^3|5\rangle + \dots$$

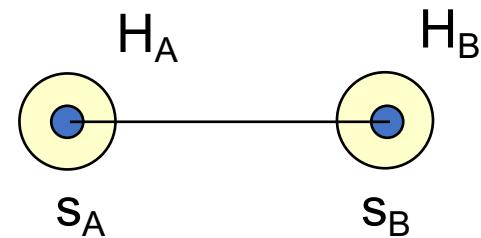
- Unrestricted states can be expanded in spin-pure states
- Unrestricted wave function is **spin-contaminated** by higher multiplicity components
- **$\langle S^2 \rangle$ is always too high**
- Unrestricted wave functions (UHF) have **lower energies** than restricted wave functions (RHF or ROHF)

H_2 in a minimal basis



Let's restrict the wave function to the correct spin symmetry (RHF). I.e., spatial part is the same for alpha and beta electrons:

$$|\Psi^{RHF}\rangle = |1\bar{1}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$



Use LCAO (linear combination of atomic orbitals) approximation:

$$|\psi\rangle = c_1|s_A\rangle + c_2|s_B\rangle$$

s_A and s_B are (normalized) atomic 1s orbitals on H_A and H_B

Spatial symmetry $C_{\infty v} \rightarrow$ inversion center $i \rightarrow g$ (gerade) and u (ungerade) irreducible representations $\rightarrow c_1 = \pm c_2$

Normalization condition: $\langle\psi|\psi\rangle = c_1^2 + c_2^2 + 2c_1c_2\langle s_A|s_B\rangle = 1$

$$c_1^2 \pm c_1^2\langle s_A|s_B\rangle = \frac{1}{2} \quad \longrightarrow \quad c_1 = \pm c_2 = \frac{1}{\sqrt{2(1 \pm S_{AB})}}$$

H_2 in a minimal basis

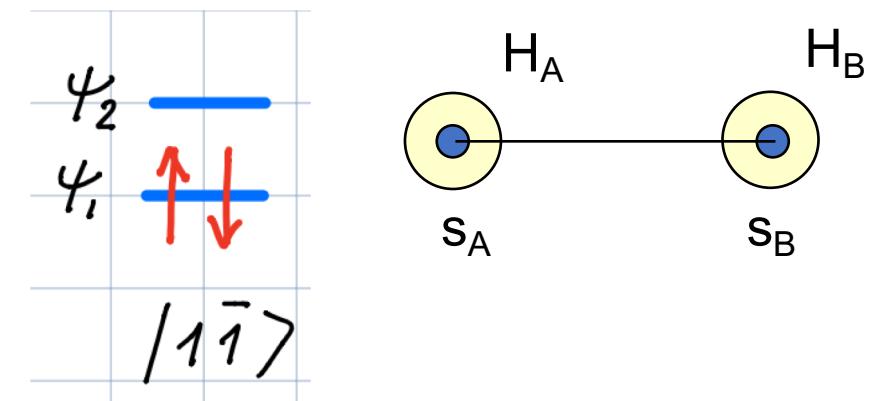
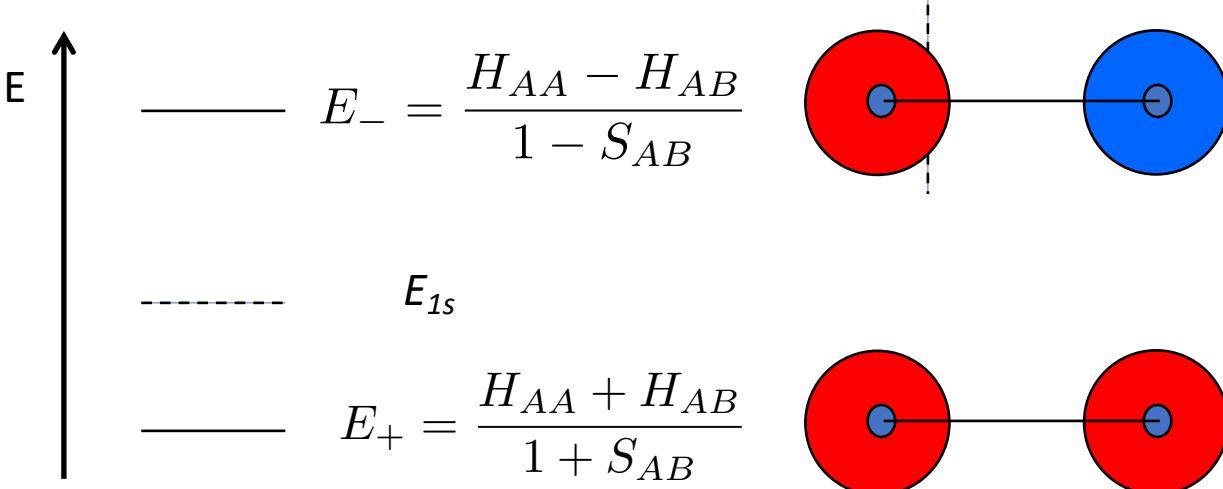
$$|\psi\rangle = c_1|s_A\rangle + c_2|s_B\rangle \quad c_1 = \pm c_2 = \frac{1}{\sqrt{2(1 \pm S_{AB})}}$$

$$|\psi_1\rangle = \sigma = \frac{1}{\sqrt{2(1 + S_{AB})}}(|s_A\rangle + |s_B\rangle) \quad \text{gerade}$$

$$|\psi_2\rangle = \sigma^* = \frac{1}{\sqrt{2(1 - S_{AB})}}(|s_A\rangle - |s_B\rangle) \quad \text{ungerade}$$

Energies of these states are

$$E_{\pm} = \frac{H_{AA} \pm H_{AB}}{1 \pm S_{AB}}$$



$H_{AA} = \langle s_A | \hat{H} | s_A \rangle = \langle s_B | \hat{H} | s_B \rangle$
-energy of s_A and s_B orbitals

$H_{AB} = \langle s_A | \hat{H} | s_B \rangle = \langle s_B | \hat{H} | s_A \rangle$
- resonance energy (coupling)

$S_{AB} = \langle s_A | s_B \rangle = \langle s_B | s_A \rangle$

- overlap integral

H_2 in a minimal basis

Let's analyze H_2 molecular orbitals

$$\begin{aligned} |\Psi^{RHF}\rangle &= |1\bar{1}\rangle = \frac{1}{\sqrt{2}} [\psi_1(1)\psi_1(2)] (\alpha(1)\beta(2) - \beta(1)\alpha(2)) \\ &\approx \sigma\sigma \approx (|s_A\rangle + |s_B\rangle)(|s_A\rangle + |s_B\rangle) = |s_As_A\rangle + |s_Bs_B\rangle + |s_As_B\rangle + |s_Bs_A\rangle = \\ &\quad \underbrace{H_A^- H_B^+ + H_A^+ H_B^-}_{\text{ionic}} + \underbrace{H_A H_B + H_A H_B}_{\text{covalent}} \end{aligned}$$

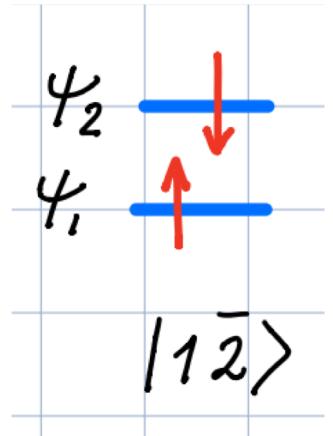
The ground state Hartree-Fock determinant is **a mixture of covalent and ionic components in a fixed proportion**: cannot vary degree of ionicity!

- It is wrong for strongly ionic or strongly covalent species
- It cannot describe both covalent and ionic dissociation of a bond

H_2 in a minimal basis: UHF

What about UHF wavefunction? At large r, spatial orbitals ψ_1 and ψ_2 became s_A and s_B , such that:

$$|\Psi^{UHF}\rangle(r \rightarrow \infty) = |s_A\alpha s_B\beta\rangle = \frac{1}{\sqrt{2}} [s_A(1)\alpha(1)s_B(2)\beta(2) - s_B(1)\beta(1)s_A(2)\alpha(2)]$$



This function describes covalent dissociation correctly!

But it is not an eigenstate of S^2

$$|\Psi_{cov}^{singlet}\rangle = [s_A(1)s_B(2) + s_B(1)s_A(2)] (\alpha(1)\beta(2) - (1)\beta(1)\alpha(2))$$

$$|\Psi_{cov}^{triplet}\rangle = [s_A(1)s_B(2) - s_B(1)s_A(2)] (\alpha(1)\beta(2) + (1)\beta(1)\alpha(2))$$

$$|\Psi^{UHF}\rangle = \frac{1}{\sqrt{2}} (|\Psi_{cov}^{singlet}\rangle + |\Psi_{cov}^{triplet}\rangle)$$

UHF wavefunction is an equal mixture of singlet and triplet determinants

For H_2 , UHF wavefunction does not have correct spatial symmetry!

H_2 in a minimal basis: Full CI

Construct FCI wavefunction: $|\Psi^{FCI}\rangle = c_0|\Psi_0\rangle + c_2|\Psi_2\rangle$

(singly-excited determinants do not mix in due to symmetry)

$$|\Psi_0\rangle = \sigma\sigma (\alpha\beta - \beta\alpha)$$

$$|\Psi_2\rangle = \sigma^*\sigma^* (\alpha\beta - \beta\alpha)$$

c_0 is large at equilibrium bond length

$c_0 = c_2$ at large separations

$$\begin{aligned} |\Psi_2\rangle &\approx \sigma^*\sigma^* \approx (|s_A\rangle - |s_B\rangle)(|s_A\rangle - |s_B\rangle) = |s_A s_A\rangle + |s_B s_B\rangle + |s_A s_B\rangle + |s_B s_A\rangle = \\ &H_A^- H_B^+ + H_A^+ H_B^- - H_A H_B - H_A H_B \end{aligned}$$

$$\begin{aligned} |\Psi_2\rangle + |\Psi_2\rangle &= H_A^- H_B^+ + H_A^+ H_B^- \\ |\Psi_2\rangle + |\Psi_2\rangle &= H_A H_B + H_A H_B \end{aligned}$$

By varying coefficients c_0 and c_2 , it is possible to describe both ionic and covalent cases

