Chemische binding, MOL056, opgaven week 5

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Vraag 1: H_2 in MO en VB theorie

1a.

$$\begin{aligned}
\langle\sigma|\sigma\rangle &= \langle n_+\Phi_{1s,A}+\Phi_{1s,B}|n_+\Phi_{1s,A}+\Phi_{1s,B}\rangle \\
&= n_+^2(\langle\Phi_{1s,A}|\Phi_{1s,A}\rangle+\langle\Phi_{1s,A}|\Phi_{1s,B}\rangle+\langle\Phi_{1s,B}|\Phi_{1s,A}\rangle+\langle\Phi_{1s,B}|\Phi_{1s,B}\rangle) \\
&= n_+^2(1+S+S+1)=n_+^2(2+2S)=1 \\
\text{Dus}: n_+ &= \frac{1}{\sqrt{2+2S}}.
\end{aligned}$$

$$\begin{aligned}
\langle\sigma^*|\sigma^*\rangle &= \langle n_-\Phi_{1s,A}-\Phi_{1s,B}|n_-\Phi_{1s,A}-\Phi_{1s,B}\rangle \\
&= n_-^2(\langle\Phi_{1s,A}|\Phi_{1s,A}\rangle-\langle\Phi_{1s,A}|\Phi_{1s,B}\rangle-\langle\Phi_{1s,B}|\Phi_{1s,A}\rangle+\langle\Phi_{1s,B}|\Phi_{1s,B}\rangle) \\
&= n_-^2(1-S-S+1)=n_-^2(2-2S)=1 \\
\text{Dus}: n_- &= \frac{1}{\sqrt{2-2S}}.
\end{aligned}$$

Voor N_1 werken we eerst de slater-determinant van Ψ_1 uit:

$$|\sigma\overline{\sigma}| = \begin{vmatrix}\sigma(1)\overline{\sigma(1)}\\ \sigma(2)\overline{\sigma(2)}\end{vmatrix} = \sigma(1)\overline{\sigma(2)}-\overline{\sigma(1)}\sigma(2)=\sigma\sigma(\alpha\beta-\beta\alpha)$$

Verder geldt:

$$\begin{aligned}
\langle\sigma\sigma|\sigma\sigma\rangle &= \langle\sigma|\sigma\rangle\langle\sigma|\sigma\rangle=1 \text{ want deze had je al genormeerd!} \\
\langle\alpha\beta-\beta\alpha|\alpha\beta-\beta\alpha\rangle &= \langle\alpha\beta|\alpha\beta\rangle-\langle\alpha\beta|\beta\alpha\rangle-\langle\beta\alpha|\alpha\beta\rangle+\langle\beta\alpha|\beta\alpha\rangle=1-0-0+1=2
\end{aligned}$$

Dan geldt:

$$\begin{aligned}
\langle\Psi_1^{(\mathrm{MO})}|\Psi_1^{(\mathrm{MO})}\rangle &= N_1^2\langle|\sigma\overline{\sigma}|||\sigma\overline{\sigma}|\rangle = N_1^2\langle\sigma\sigma|\sigma\sigma\rangle\langle\alpha\beta-\beta\alpha|\alpha\beta-\beta\alpha\rangle \\
&= 2N_1^2=1 \\
\text{Dus}: N_1 &= \frac{1}{\sqrt{2}}
\end{aligned}$$

Voor N_+ werken we eerst de slater-determinant van $\Psi^{(\mathrm{VB,cov})}$ uit:

$$\begin{aligned}
\Psi^{(\mathrm{VB,cov})} &= N_+\{|\Phi_{1s,A}\overline{\Phi_{1s,B}}| - |\overline{\Phi_{1s,A}}\Phi_{1s,B}|\} \\
&= N_+\left\{\begin{vmatrix}\Phi_{1s,A}(1)\overline{\Phi_{1s,B}(1)} \\ \Phi_{1s,A}(2)\overline{\Phi_{1s,B}(2)}\end{vmatrix} - \begin{vmatrix}\overline{\Phi_{1s,A}(1)}\Phi_{1s,B}(1) \\ \overline{\Phi_{1s,A}(2)}\Phi_{1s,B}(2)\end{vmatrix}\right\} \\
&= N_+\{\Phi_{1s,A}\Phi_{1s,B}\alpha\beta - \Phi_{1s,B}\Phi_{1s,A}\beta\alpha - \Phi_{1s,A}\Phi_{1s,B}\beta\alpha + \Phi_{1s,B}\Phi_{1s,A}\alpha\beta\} \\
&= N_+\{\Phi_{1s,A}\Phi_{1s,B}(\alpha\beta - \beta\alpha) + \Phi_{1s,B}\Phi_{1s,A}(\alpha\beta - \beta\alpha)\} \\
&= N_+\{(\Phi_{1s,A}\Phi_{1s,B} + \Phi_{1s,B}\Phi_{1s,A})(\alpha\beta - \beta\alpha)\}
\end{aligned}$$

Dan geldt voor het baandeel:

$$\begin{aligned}
& \langle\Phi_{1s,A}\Phi_{1s,B} + \Phi_{1s,B}\Phi_{1s,A}|\Phi_{1s,A}\Phi_{1s,B} + \Phi_{1s,B}\Phi_{1s,A}\rangle \\
= & \langle\Phi_{1s,A}\Phi_{1s,B}|\Phi_{1s,A}\Phi_{1s,B}\rangle + \langle\Phi_{1s,A}\Phi_{1s,B}|\Phi_{1s,B}\Phi_{1s,A}\rangle \\
& + \langle\Phi_{1s,B}\Phi_{1s,A}|\Phi_{1s,A}\Phi_{1s,B}\rangle + \langle\Phi_{1s,B}\Phi_{1s,A}|\Phi_{1s,B}\Phi_{1s,A}\rangle \\
= & 1 + S^2 + S^2 + 1 = 2 + 2S^2
\end{aligned}$$

Verder geldt voor het spindeel:

$$\begin{aligned}
\langle\alpha\beta - \beta\alpha|\alpha\beta - \beta\alpha\rangle &= \langle\alpha\beta|\alpha\beta\rangle - \langle\alpha\beta|\beta\alpha\rangle - \langle\beta\alpha|\alpha\beta\rangle + \langle\beta\alpha|\beta\alpha\rangle \\
&= 1 - 0 - 0 + 1 = 2
\end{aligned}$$

Dus geldt voor de hele golffunctie:

$$\begin{aligned}
\langle\Psi^{(\mathrm{VB,cov})}|\Psi^{(\mathrm{VB,cov})}\rangle &= \langle N_+\{|\Phi_{1s,A}\overline{\Phi_{1s,B}}| - |\overline{\Phi_{1s,A}}\Phi_{1s,B}|\}|N_+\{|\Phi_{1s,A}\overline{\Phi_{1s,B}}| - |\overline{\Phi_{1s,A}}\Phi_{1s,B}|\}\rangle \\
&= 2N_+^2(2 + 2S^2) = 1 \\
\text{Dus} : N_+ &= \frac{1}{\sqrt{2(2 + 2S^2}} = \frac{1}{2\sqrt{1 + S^2}}
\end{aligned}$$

$$\begin{aligned}
\langle\Phi|\Phi\rangle &= \langle N_2\Phi_{1s,A}\Phi_{1s,B}|N_2\Phi_{1s,A}\Phi_{1s,B}\rangle = N_2^2\langle\Phi_{1s,A}|\Phi_{1s,A}\rangle\langle\Phi_{1s,B}|\Phi_{1s,B}\rangle \\
&= N_2^2 = 1 \\
\text{Dus} : N_2 &= 1
\end{aligned}$$

Vraag 2: Elektronendichtheid H_2

2a. Omdat je geen rekening houdt met de interactie tussen de twee waterstofatomen, is de totale elektronendichtheid gewoon de som van de elektronendichtheden van de atomen op posities A en B.

$$\rho_{\mathrm{atoms}}(\boldsymbol{r}) = |\phi_{\mathrm{1s,A}}(\boldsymbol{r})|^2 + |\phi_{\mathrm{1s,B}}(\boldsymbol{r})|^2$$

2b. Nu gebruik je de uitdrukking voor de elektronendichtheid voor een twee-elektron golffunctie

$$\begin{aligned}
\rho_\Phi(\boldsymbol{r}) &= \int |\Phi(\boldsymbol{r},\boldsymbol{r}_2)|^2 d^3\boldsymbol{r}_2 + \int |\Phi(\boldsymbol{r}_1,\boldsymbol{r})|^2 d^3\boldsymbol{r}_1 \\
&= |\phi_{1\mathrm{s,A}}(\boldsymbol{r})|^2 \underbrace{\int |\phi_{1\mathrm{s,B}}(\boldsymbol{r}_2)|^2\, d^3\boldsymbol{r}_2}_{=1} + |\phi_{1\mathrm{s,B}}(\boldsymbol{r})|^2 \underbrace{\int |\phi_{1\mathrm{s,A}}(\boldsymbol{r}_1)|^2\, d^3\boldsymbol{r}_1}_{=1} \\
&= |\phi_{1\mathrm{s,A}}(\boldsymbol{r})|^2 + |\phi_{1\mathrm{s,B}}(\boldsymbol{r})|^2
\end{aligned}$$

Dus geldt ook

$$\rho_\Phi(\boldsymbol{r}) = \rho_{\mathrm{atoms}}(\boldsymbol{r}) \Rightarrow \rho_\Phi(\mathbf{0}) = \rho_{\mathrm{atoms}}(\mathbf{0})$$

2c. Voor de golffunctie geldt

$$\Psi_1^{(\mathrm{MO})} = \sigma(\boldsymbol{r}_1)\sigma(\boldsymbol{r}_2)\frac{\alpha(\mathbf{1})\beta(\mathbf{2}) - \beta(\mathbf{1})\alpha(\mathbf{2})}{\sqrt{2}}$$

waarbij deze opgesplitst is in een baan- en spin gedeelte. De laatste is nu genormeerd zodat je je geen zorgen hoeft te maken over integralen over de spin ruimte. De elektronendichtheid wordt dus berekend met het baandeel

$$\begin{aligned}
\rho_{\Psi_1^{(\mathrm{MO})}}(\boldsymbol{r}) &= 2|\sigma(\boldsymbol{r})|^2 \underbrace{\int |\sigma(\boldsymbol{r}_2)|^2 d^3\boldsymbol{r}_2}_{=1} \\
&= 2|\sigma(\boldsymbol{r})|^2 \\
&= 2\left|\frac{\phi_{1\mathrm{s,A}}(\boldsymbol{r}) + \phi_{1\mathrm{s,B}}(\boldsymbol{r})}{\sqrt{2+2S}}\right|^2 = \frac{1}{1+S}\{|\phi_{1\mathrm{s,A}}(\boldsymbol{r})|^2 + |\phi_{1\mathrm{s,B}}(\boldsymbol{r})|^2 + 2\phi_{1\mathrm{s,A}}(\boldsymbol{r})\phi_{1\mathrm{s,B}}(\boldsymbol{r})\}
\end{aligned}$$

Op positie $\boldsymbol{r} = \mathbf{0}$ geldt dan

$$\rho_{\Psi_1^{(\mathrm{MO})}}(\mathbf{0}) = \frac{1}{1+S}\, 4\, |\phi_{1\mathrm{s,A}}(\mathbf{0})|^2 = \frac{2}{1+S}\rho_{\mathrm{atoms}}(\mathbf{0})$$

Omdat $0 < S < 1$ is de elektronendichtheid van de MO golffunctie dus groter dan die berekend met een golffunctie die niet aan het Pauli principe voldoet, wat betekent dat er een effectieve binding is.

2d. Voor de golffunctie geldt

$$\Psi^{(\mathrm{VB,cov})} = \frac{\phi_{1\mathrm{s,A}}(\boldsymbol{r}_1)\phi_{1\mathrm{s,B}}(\boldsymbol{r}_2) + \phi_{1\mathrm{s,B}}(\boldsymbol{r}_1)\phi_{1\mathrm{s,A}}(\boldsymbol{r}_2)}{\sqrt{2+2S^2}}\frac{\alpha(\mathbf{1})\beta(\mathbf{2}) - \beta(\mathbf{1})\alpha(\mathbf{2})}{\sqrt{2}}$$

met opnieuw het spindeel genormeerd. De elektronendichtheid is

$$\begin{aligned}
\rho_{\Psi^{(\mathrm{VB})}}(\boldsymbol{r}) &= 2\int |\Psi^{(\mathrm{VB})}(\boldsymbol{r}_2)|^2 d^3\boldsymbol{r}_2 \\
&= \frac{1}{1+S^2}\int \{|\phi_{1\mathrm{s,A}}(\boldsymbol{r})|^2 \underbrace{|\phi_{1\mathrm{s,B}}(\boldsymbol{r}_2)|^2}_{=1} + |\phi_{1\mathrm{s,B}}(\boldsymbol{r})|^2 \underbrace{|\phi_{1\mathrm{s,A}}(\boldsymbol{r}_2)|^2}_{=1} \\
&\quad +2\phi_{1\mathrm{s,A}}(\boldsymbol{r})\phi_{1\mathrm{s,B}}(\boldsymbol{r}) \underbrace{\phi_{1\mathrm{s,A}}(\boldsymbol{r}_2)\phi_{1\mathrm{s,B}}(\boldsymbol{r}_2)}_{=S}\} d^3\boldsymbol{r}_2 \\
&= \frac{1}{1+S^2}\left\{|\phi_{1\mathrm{s,A}}(\boldsymbol{r})|^2 + |\phi_{1\mathrm{s,B}}(\boldsymbol{r})|^2 + 2S\phi_{1\mathrm{s,A}}(\boldsymbol{r})\phi_{1\mathrm{s,B}}(\boldsymbol{r})\right\}
\end{aligned}$$

Op positie $\boldsymbol{r} = \mathbf{0}$ geldt dan

$$\begin{aligned}
\rho_{\Psi^{(\mathrm{VB})}}(\mathbf{0}) &= \frac{1}{1+S^2}\left\{2\,|\phi_{1\mathrm{s,A}}(\mathbf{0})|^2 + 2\,S\,|\phi_{1\mathrm{s,A}}(\mathbf{0})|^2\right\} \\
&= \frac{1+S}{1+S^2}\,2\,|\phi_{1\mathrm{s,A}}(\mathbf{0})|^2 = \frac{1+S}{1+S^2}\rho_{\mathrm{atoms}}(\mathbf{0})
\end{aligned}$$

Ook nu geldt dat de elektronendichtheid toeneemt t.o.v. $\rho_{\mathrm{atoms}}(\mathbf{0})$, omdat $S > S^2$, en er dus effectief een binding is.

2e. De elektronendichtheden kunnen vergeleken worden door de op elkaar te delen

$$\frac{\rho_{\Psi^{(\mathrm{MO})}}(\boldsymbol{r})}{\rho_{\Psi^{(\mathrm{VB})}}(\boldsymbol{r})} = \frac{2}{1+S}\frac{1+S^2}{1+S}$$

En dan geldt voor $0 < S < 1$ dat

$$2 > \frac{\rho_{\Psi^{(\mathrm{MO})}}(\boldsymbol{r})}{\rho_{\Psi^{(\mathrm{VB})}}(\boldsymbol{r})} > 1$$

Kennelijk is de elektronendichtheid in de ‘binding’ groter voor de MO golffunctie dan voor de VB golffunctie. Een verklaring daarvoor is dat je in MO theorie geen elektronencorrelatie meeneemt, m.a.w. elektronen zullen elkaar niet ‘ontwijken’.

Vraag 3: Omschrijven MO en VB golffuncties voor H_2

3a.

$$\Psi^{(\mathrm{ion,A})} = \phi_{1s,A}(\boldsymbol{r}_1)\phi_{1s,A}(\boldsymbol{r}_2)\frac{\alpha\beta-\beta\alpha}{\sqrt{2}}$$

$$\Psi^{(\mathrm{ion,B})} = \phi_{1s,B}(\boldsymbol{r}_1)\phi_{1s,B}(\boldsymbol{r}_2)\frac{\alpha\beta-\beta\alpha}{\sqrt{2}}$$

3b. De Hamiltoniaan voor H_2 is

$$\begin{aligned}
\hat{H} &= \hat{H}_0(\boldsymbol{r}_1) + \hat{H}_0(\boldsymbol{r}_2) + \frac{1}{\boldsymbol{r}_{1,2}} + \frac{1}{R_{A,B}} \\
\textit{met } \hat{H}_0(\boldsymbol{r}) &= -\frac{1}{2}\nabla^2 - \frac{1}{|\boldsymbol{r} - R_A|} - \frac{1}{|\boldsymbol{r} - R_B|} \\
\hat{H}\phi_{1s,A}(\boldsymbol{r}_1)\phi_{1s,B}(\boldsymbol{r}_2) &= \left(\hat{H}_0(\boldsymbol{r}_1) + \hat{H}_0(\boldsymbol{r}_2) + \frac{1}{r_{1,2}} + \frac{1}{R_{A,B}}\right)\phi_{1s,A}(\boldsymbol{r}_1)\phi_{1s,B}(\boldsymbol{r}_2) \\
\textit{waarbij } \hat{H}_0\phi_{1s,A}(\boldsymbol{r}_1) &= \left(-\frac{1}{2}\nabla^2 - \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{R}_A|}\right)\phi_{1s,A}(\boldsymbol{r}_1) - \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{R}_B|}\phi_{1s,A}(\boldsymbol{r}_1)
\end{aligned}$$

Voor R $\to \infty$

$$\begin{aligned}
\hat{H}_0\phi_{1s,A}(\boldsymbol{r}_1) &= \epsilon_A\phi_{1s,A}(\boldsymbol{r}_1) \\
\textit{waarbij } \epsilon_A &= -\frac{1}{2}E_h \ (\textit{energie van } H - \textit{atoom}) \\
\textit{en analoog} \quad \hat{H}_0\phi_{1s,B}(\boldsymbol{r}_2) &= \epsilon_B\phi_{1s,B}(\boldsymbol{r}_2) \\
\textit{en} \quad \frac{1}{\boldsymbol{r}_{1,2}}\phi_{1s,A}(\boldsymbol{r}_1)\phi_{1s,B}(\boldsymbol{r}_2) &\to 0 \\
\textit{en} \quad \frac{1}{\boldsymbol{R}_{A,B}}\phi_{1s,A}(\boldsymbol{r}_1)\phi_{1s,B}(\boldsymbol{r}_2) &\to 0
\end{aligned}$$

Dus geldt voor $\hat{H}(\phi_{1s,A}\phi_{1s,B}) = (-1)\ \phi_{1s,A}\phi_{1s,B}$

en $\hat{H}(\phi_{1s,B}\phi_{1s,A}) = (-1)\ \phi_{1s,B}\phi_{1s,A}$

en dus $\hat{H}\Psi^{(\mathrm{VB,cov})} = (-1)\ \Psi^{(\mathrm{VB,cov})}$

3c.

$$\begin{aligned}
\Psi^{(\mathrm{MO})} &= \frac{1}{\sqrt{2}}|\sigma\ \overline{\sigma}| \\
&= \frac{1}{\sqrt{2}}\left|\left(\frac{\phi_{1s,A} + \phi_{1s,B}}{\sqrt{2}}\right)\left(\frac{\overline{\phi}_{1s,A} + \overline{\phi}_{1s,B}}{\sqrt{2}}\right)\right| \\
&= \frac{1}{2\sqrt{2}}\left(|\phi_{1s,A}\ \overline{\phi}_{1s,A}| + |\phi_{1s,B}\ \overline{\phi}_{1s,B}| + |\phi_{1s,A}\ \overline{\phi}_{1s,B}| + |\phi_{1s,B}\ \overline{\phi}_{1s,A}|\right) \\
&= \frac{1}{2\sqrt{2}}\left(|\phi_{1s,A}\ \overline{\phi}_{1s,A}| + |\phi_{1s,B}\ \overline{\phi}_{1s,B}| + |\phi_{1s,A}\ \overline{\phi}_{1s,B}| - |\overline{\phi}_{1s,A}\ \phi_{1s,B}|\right)
\end{aligned}$$

De eerste twee termen zijn geljik aan respectievelijk $\sqrt{2}\Psi^{(\mathrm{ION,A})}$ en $\sqrt{2}\Psi^{(\mathrm{ION,B})}$. De twee laatste termen zijn gelijk aan $\frac{1}{2}\Psi^{(\mathrm{VB,cov})}$.

$$|\Psi^{(\mathrm{MO})}|^2 = \frac{1}{4}\Psi^{(\mathrm{ION,A})} + \frac{1}{4}\Psi^{(\mathrm{ION,B})} + \frac{1}{2}\Psi^{(\mathrm{VB,cov})}$$

Het resultaat is dus 50% ionogeen en 50% covalent.

3d.

$$\begin{aligned} \phi_{1s,A} &= \frac{\sigma + \sigma^*}{\sqrt{2}} & \qquad \sigma &= \frac{\phi_{1s,A} + \phi_{1s,B}}{\sqrt{2}} \\ \phi_{1s,B} &= \frac{\sigma - \sigma^*}{\sqrt{2}} & \qquad \sigma^* &= \frac{\phi_{1s,A} - \phi_{1s,B}}{\sqrt{2}} \end{aligned}$$

3e.

$$\begin{aligned} \Psi^{(\mathrm{VB,cov})} &= N_+\{|\phi_{1s,A}\ \overline{\phi}_{1s,B}| - |\overline{\phi}_{1s,A}\ \phi_{1s,B}|\} \\ &= \frac{1}{2}\{|\sigma + \sigma^*\ \overline{\sigma} - \overline{\sigma}^*| - |\overline{\sigma} + \overline{\sigma}^*\ \sigma - \sigma^*|\} \\ &= \frac{1}{2}\{|\sigma\ \overline{\sigma}| - |\sigma^*\ \overline{\sigma}^*| - |\sigma\ \overline{\sigma}^*| + |\sigma^*\ \overline{\sigma}| - |\overline{\sigma}\ \sigma| + |\overline{\sigma}^*\ \sigma^*| + |\overline{\sigma}\ \sigma^*| - |\overline{\sigma}^*\ \sigma|\} \\ &= |\sigma\ \overline{\sigma}| - |\sigma^*\ \overline{\sigma}^*| \end{aligned}$$

Vraag 4: Triplet toestand voor H_2

4a. Triplet: S=1, dus het spindeel is (bijv.) $\alpha\alpha$. De functie wordt dan:

$$\Psi^{\mathrm{VB},S=1} = N|\phi_{1s,A}\phi_{1s,B}| = N\{\phi_{1s,A}\phi_{1s,B} - \phi_{1s,B}\phi_{1s,A}\}\alpha\alpha.$$

Normeren levert $N = \frac{1}{\sqrt{2-2S^2}}$.

4b.

$$\begin{aligned} \rho^{S=1}(\boldsymbol{r}) &= 2\int |\Psi^{\mathrm{VB},S=1}(\boldsymbol{r},\boldsymbol{r}_2)|^2 d^3\boldsymbol{r}_2 \\ &= \frac{2}{2-2S^2}\int |\phi_{1s,A}(\boldsymbol{r})|^2|\phi_{1s,B}(\boldsymbol{r}_2)|^2 + |\phi_{1s,B}(\boldsymbol{r})|^2|\phi_{1s,A}(\boldsymbol{r}_2)|^2 \\ &\quad - 2\phi_{1s,A}(\boldsymbol{r})\phi_{1s,B}(\boldsymbol{r})\phi_{1s,A}(\boldsymbol{r}_2)\phi_{1s,B}(\boldsymbol{r}_2)d^3\boldsymbol{r}_2 \\ &= \frac{1}{1-S^2}\{|\phi_{1s,A}(\boldsymbol{r})|^2 + |\phi_{1s,B}(\boldsymbol{r})|^2 - 2S\phi_{1s,A}(\boldsymbol{r})\phi_{1s,B}(\boldsymbol{r})\} \end{aligned}$$

$$|\phi_{1s,A}(\mathbf{0})|^2 = d$$

$$\begin{aligned} \rho^{S=1}(\mathbf{0}) &= \frac{1}{1-S^2}\{d + d - 2dS\} = \frac{1-S}{1-S^2}2d = \frac{1-S}{1-S^2}\rho_{\mathrm{atoms}}(\mathbf{0}) \\ &= \frac{1-S}{(1+S)(1-S)}\rho_{\mathrm{atoms}}(\mathbf{0}) = \frac{1}{1+S}\rho_{\mathrm{atoms}}(\mathbf{0}). \end{aligned}$$

Dus op afstanden waar de overlap $S > 0$, is de elektronendichtheid in de binding kleiner dan de som van de dichtheden van de losse atomen.

4c. Manier 1 van uitschrijven:

$$\begin{aligned}
\Psi^{\mathrm{VB},S=1} &= \frac{1}{\sqrt{2-2S^2}}\{\phi_{1s,A}\phi_{1s,B} - \phi_{1s,B}\phi_{1s,A}\}\alpha\alpha \\
&= \frac{1}{\sqrt{2-2S^2}}\left\{\frac{1}{\sqrt{2}}[\sigma(\boldsymbol{r}_1)+\sigma^*(\boldsymbol{r}_1)]\ \frac{1}{\sqrt{2}}[\sigma(\boldsymbol{r}_2)-\sigma^*(\boldsymbol{r}_2)]\right. \\
&\quad \left. -\frac{1}{\sqrt{2}}[\sigma(\boldsymbol{r}_1)-\sigma^*(\boldsymbol{r}_1)]\ \frac{1}{\sqrt{2}}[\sigma(\boldsymbol{r}_2)+\sigma^*(\boldsymbol{r}_2)]\right\}\alpha\alpha \\
&= \frac{1}{\sqrt{2-2S^2}}\{\sigma(\boldsymbol{r}_1)^*\sigma(\boldsymbol{r}_2) - \sigma(\boldsymbol{r}_1)\sigma^*(\boldsymbol{r}_2)\}\alpha\alpha.
\end{aligned}$$

Manier 2 van uitschrijven:

$$\begin{aligned}
&\Psi^{\mathrm{VB},S=1} \\
&= \frac{1}{\sqrt{2-2S^2}}|\phi_{1s,A}\phi_{1s,B}| \\
&= \frac{1}{2\sqrt{2-2S^2}}|(\sigma+\sigma^*)\ (\sigma-\sigma^*)| \\
&= \frac{1}{2\sqrt{2-2S^2}}\ \{|\sigma\ \sigma| + |\sigma^*\ \sigma| - |\sigma\sigma^*| - |\sigma^*\sigma^*|\} \\
&= \frac{1}{2\sqrt{2-2S^2}}\ \{|\sigma^*\ \sigma| - |\sigma\sigma^*|\} \\
&= \frac{1}{\sqrt{2-2S^2}}|\sigma^*\sigma|.
\end{aligned}$$