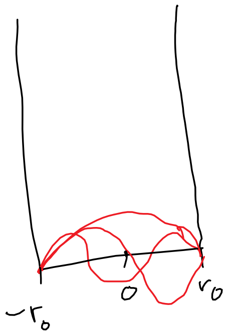
Blatt 06

Saturday, 22 May 2021 09:54

① a) identische Teilchen: $\vec{x}_1 + \vec{x}_2$, $(\vec{x}_1 - \vec{x}_2)^2$, $\vec{p}_1 \cdot \vec{p}_2$

(Observable invariant unter Vertauschung)

b)



$$\hat{H}\psi(x) = -\frac{1}{2m}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$x \in [-r_0, r_0] : \quad -\frac{1}{2m}\partial_x^2\psi(x) = E\psi(x)$$

$$\psi(x) = \sin(k(x+r_0))$$

$$\Rightarrow \frac{k^2}{2m} = E$$

Randbedingung

$$k \cdot 2r_0 = n \cdot \pi$$

$$k = \frac{n}{2r_0}\pi$$

$$\boxed{\Rightarrow E = \frac{n^2\pi^2}{8mr_0^2}}$$

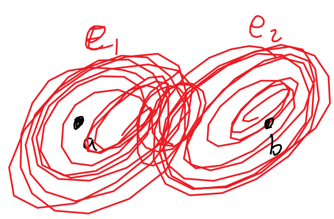
$$\psi_n(x) = \sin\left(\frac{n\pi}{2r_0}(x+r_0)\right)$$

$$\| C\psi_n(x) \| \overset{!}{=} 1 = C^2\int_{-r_0}^{r_0} \sin^2\left(\frac{n\pi}{2r_0}(x+r_0)\right) dx = C^2 \cdot r_0$$

$$\int_0^L \sin^2(\ldots) = \frac{L}{2}$$

$$\Rightarrow C = \frac{1}{\sqrt{r_0}}$$

$$\Rightarrow \boxed{\psi_n(x) = \frac{1}{\sqrt{r_0}}\sin\left(\frac{n\pi}{2r_0}(x+r_0)\right)}$$



c) $$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{\alpha}{r_{1a}} - \frac{\alpha}{r_{1b}} - \frac{\alpha}{r_{2a}} - \frac{\alpha}{r_{2b}} + \frac{\alpha}{r_{12}} + \frac{\alpha}{r_{ab}}$$

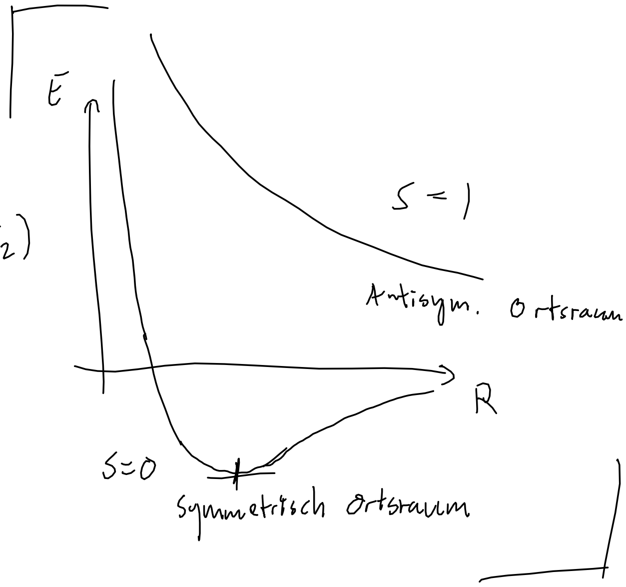
d) Molekülzustände: Symmetrisierte Atomeigenzustände

Bsp. Ein Elektron in Zustand ψ_a, 1 in Zustand ψ_b

$$\Rightarrow \quad |\psi_a \psi_b\rangle^{(\pm)} = \frac{|\psi_a^{(1)} \psi_b^{(2)}\rangle \pm |\psi_a^{(2)} \psi_b^{(1)}\rangle}{\sqrt{2}}$$

Gleicher Zustand

$$|\psi_a \psi_a\rangle = |\psi_a^{(1)} \psi_a^{(2)}\rangle$$



2. a) $$\hat{\mathcal{H}} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(r_1) + V(r_2)$$

$$\Rightarrow [\hat{\mathcal{H}}, \hat{S}] = 0 \Rightarrow \text{Simultane EZ.}$$

$$H = H_x \otimes H_s$$

Basis $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \frac{|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle}{\sqrt{2}}$

$$\frac{|\psi_{n_1} \psi_{n_2}\rangle \pm |\psi_{n_2} \psi_{n_1}\rangle}{\sqrt{2}}$$

b) Boson: Antisym. Ort und Antisym. Spin

Sym. Ort und Sym. Spin ←

Fermion: Antisym. Ort und Sym. Spin ←

Sym. Ort und Antisym. Spin

c)

				GS
Boson:	$E_n + E_m$	$\lvert\psi_m \psi_n\rangle^{(+)}$		$2E_1$
Fermion:	$E_n + E_m$	$\lvert\psi_m \psi_n\rangle^{(-)}$	(für $n \neq m$)	$E_1 + E_2$

3.

(a) $\langle g|g\rangle = \left(c_1 \langle\phi_a^{(1)}|\langle\phi_b^{(2)}| + c_2 \langle\phi_b^{(1)}|\langle\phi_a^{(2)}| \right)$

$\left(c_1 |\phi_a^{(1)}\rangle|\phi_b^{(2)}\rangle + c_2 |\phi_b^{(1)}\rangle|\phi_a^{(2)}\rangle \right)$

$$= c_1^2 \underbrace{\langle\phi_a^{(1)}|\phi_a^{(1)}\rangle}_{1} \underbrace{\langle\phi_b^{(2)}|\phi_b^{(2)}\rangle}_{1} + c_2^2$$

$$+ c_1c_2 \langle\phi_b|\phi_a\rangle\langle\phi_a|\phi_b\rangle + c_1c_2\langle\phi_a|\phi_b\rangle\langle\phi_b|\phi_a\rangle$$

$L_{ab} = \langle\phi_a|\phi_b\rangle$

$\rightsquigarrow \langle g|g\rangle = c_1^2 + c_2^2 + 2c_1c_2|L_{ab}|^2$

$\Rightarrow \langle g|\hat{H}|g\rangle$ wie VL nur allgemeiner.

4.

a) $\oplus$: $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$

$\ominus$: $|0,0\rangle$

b) $\vec{S}_1\cdot\vec{S}_2 = S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)}$

$$= \frac{1}{2}\left[S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}\right] + S_z^{(1)}S_z^{(2)}$$

$$\left(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}\right)\begin{Bmatrix}|1,0\rangle\\|0,0\rangle\\|1,-1\rangle\\|1,1\rangle\end{Bmatrix} : \begin{Bmatrix}|1,0\rangle\\-|0,0\rangle\\0\\0\end{Bmatrix}$$

$(\ |1,1\rangle \quad (\quad 0 \quad)$

$$\Rightarrow \vec{S}_1 \cdot \vec{S}_2 \, |SM\rangle = \begin{cases} \left(\frac{1}{2} - \frac{1}{4}\right) |1,0\rangle = \frac{1}{4} |1,0\rangle & \leftarrow \text{sym.} \\ \left(-\frac{1}{2} - \frac{1}{4}\right) |0,0\rangle = -\frac{3}{4} |0,0\rangle & \leftarrow \text{antisym.} \\ 0 + \frac{1}{4} \quad |1,-1\rangle = \frac{1}{4} |1,-1\rangle & \leftarrow \text{sym.} \\ 0 + \frac{1}{4} \quad |1,-1\rangle = \frac{1}{4} |1,-1\rangle & \leftarrow \text{sym.} \end{cases}$$

$$f(x) = mx + n$$

$$f(1/4) = \frac{m}{4} + n = E_-$$

$$f(-3/4) = -\frac{3m}{4} + n = E_+$$

$$\hookrightarrow \quad n = \frac{3E_- + E_+}{4}$$

$$m + 3E_- + E_+ = 4E_-$$

$$\Rightarrow m = E_- - E_+$$

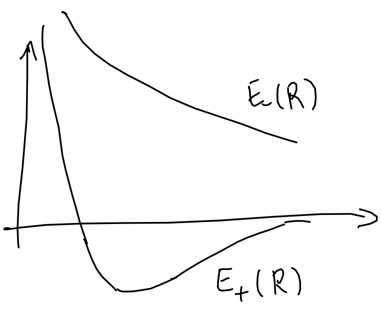
$$\boxed{\hat{\mathcal{H}} = (E_- - E_+)\, \vec{S}_1 \cdot \vec{S}_2 + \frac{3E_- + E_+}{4}}$$

$\Rightarrow$ Probe:

$$\hat{\mathcal{H}} \, |SM\rangle^{(+)} = E_- \, |SM\rangle^{(+)}$$

$$\hat{\mathcal{H}} \, |SM\rangle^{(-)} = E_+ \, |SM\rangle^{-}$$

$\rightarrow$ Lecture:



$\Rightarrow E_+ < E_- \Rightarrow |SM\rangle^{(-)}$ preferred