Bsp. 1)

a) i) NEIN; ii) NEIN; iii) JA; iv) NEIN; (v) JA; (vi) NEIN

b) plötzlicher Zerfall $\Rightarrow$ SUDDEN Approx. !

$$|\psi(t)\rangle = \sum_{nlm} \langle \psi_{nlm}^{He^+} | \psi_{100}^{Tritium} \rangle \, | \psi_{nlm}^{He^+} \rangle$$

Übergänge: 100 Tritium nach

- 100 von He^+ (1s von He^+) : $\langle \psi_{100}^{He^+} | \psi_{100}^{Tritium} \rangle = \int d\hat{\Omega} |Y_0^0|^2 \int_0^{+\infty} dr\, r^2 R_{10}^{Z=2}(r) R_{10}^{Z=1}(r)$

$\neq 0$ Ja, möglich

- 200 (2s) von He^+ : $\langle \psi_{200}^{He^+} | \psi_{100}^{Tritium} \rangle = \int d\hat{\Omega} |Y_0^0|^2 \int_0^{+\infty} dr\, r^2 R_{20}^{Z=2}(r) R_{10}^{Z=1}(r)$

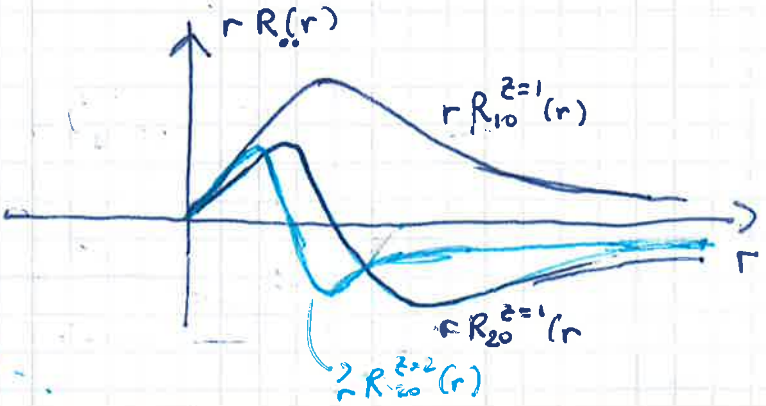
$\neq 0$ Ja, möglich (*)

- 21$\begin{pmatrix}1\\0\\-1\end{pmatrix}$ von He^+ [2p Orbitale] : $\langle \psi_{21m}^{He^+} | \psi_{100}^{Tritium} \rangle = \int d\hat{\Omega}\, Y_1^m Y_0^0 \int dr\, r^2 R_{21}^{Z=2}(r) R_{10}^{Z=1}(r)$

$\emptyset$ NEIN, nicht möglich !

(*) $\int_0^{+\infty} dr\, r^2 R_{20}^{Z=2}(r) R_{10}^{Z=1}(r) \neq 0$ da $R_{20}^{Z=2}(r)$ und $R_{10}^{Z=1}(r)$ sind radiale Funktionen von Atomen mit unterschiedlichen Z !

z.B. ganz grob



der exakte Ausgleich, der die Orthogonalität zwischen R_{20} und R_{10} mit dem selben Z garantiert ist nicht mehr gültig

1c) $\rho_1 = \mathrm{Spur}_2 \; |\psi\rangle\langle\psi| = \langle D|_2 \; |\psi\rangle\langle\psi| \; |D\rangle_2 + \langle E|_2 \; |\psi\rangle\langle\psi| \; |E\rangle_2$

$$= \frac{1}{3}\left(|a\rangle_1 + i|b\rangle_1\right)\left(\langle a|_1 - i\langle b|_1\right) + \frac{1}{3}|c\rangle_1 \langle c|_1$$

Als Matrix

$$\underline{\rho_1} = \begin{array}{c} \\ \frac{1}{3} \end{array} \begin{array}{c} \begin{matrix} |a\rangle & |b\rangle & |c\rangle \end{matrix} \\ \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{array}$$

$\langle b | \rho_1 | a \rangle$

$$\rho_1^2 = \frac{1}{9}\begin{pmatrix} 2 & ? & 0 \\ ? & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathrm{Spur}\,\rho_1^2 = \frac{5}{9} < 1$$

$\Rightarrow$ Kein reiner Zustand

Bsp. 2) mit $\psi(0) = \psi(L) \equiv 0$

a) $H_0 \psi_n(x) = \varepsilon_n \psi_n(x) \Rightarrow \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\cancel{\sqrt{\frac{2}{L}}} \sin\left(\frac{n\pi x}{L}\right) = \varepsilon_n \cancel{\sqrt{\frac{2}{L}}} \sin\left(\frac{n\pi x}{L}\right)$

$\Rightarrow \left(\frac{\pi^2\hbar^2}{2mL^2} n^2\right) \cancel{\sin\left(\frac{n\pi x}{L}\right)} = \varepsilon_n \cancel{\sin\left(\frac{n\pi x}{L}\right)} \Rightarrow \varepsilon_n = \frac{\pi^2\hbar^2}{2mL^2} n^2$

b) $n=1$ Grundzustand ; $n>1$ angeregte Zustände

$$a_{m1}^{(1)}(t) = \frac{1}{i\hbar}\int_0^t dt' \langle \psi_m | V_S^I(t') | \psi_1 \rangle = \frac{1}{i\hbar}\int_0^t dt' e^{\frac{i(\varepsilon_n - \varepsilon_1)t'}{\hbar}} \langle \psi_n | V_S(t') | \psi_1 \rangle$$

$$= \frac{A}{i\hbar}\left[\int_0^t dt' e^{i\omega_{m1}t'} \sin(\omega t')\right]\left[\frac{2}{L}\int_0^L dx \sin\left(\frac{m\pi}{L}x\right)\left(x \cancel{-\frac{L}{2}}\right)\sin\left(\frac{\pi x}{L}\right)\right]$$

$$= \frac{A}{i\hbar}\frac{2}{L}\left[\int_0^t dt' e^{i\omega_{m1}t'} \sin(\omega t')\right]\left[\underbrace{\int_0^L dx\; x \sin\left(\frac{m\pi}{L}x\right)\sin\left(\frac{\pi x}{L}\right)}_{J_{m1}}\right]$$

$$P_{m\leftarrow 1}^{(1)}(t) = \frac{|A|^2}{\hbar^2}\frac{4}{L^2}\left|\int_0^t dt' e^{i\omega_{m1}t'} \sin(\omega t')\right|^2 \underbrace{\left|\int_0^L dx\; x \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi}{L}x\right)\right|^2}_{|J_{m1}|^2}$$

c) Übergang G.Z. $(n=1)$ nach 1. Angeregten Zustand $(n=2)$ $(1 \to 2)$

$$\omega_{21} = \frac{\varepsilon_2 - \varepsilon_1}{\hbar} = \frac{\pi^2\hbar}{2mL^2}(4-1) = \frac{3}{2}\frac{\pi^2\hbar}{mL^2}$$

Zeitintegral in: $a_{21}^{(1)}(t)$: $\int_0^t dt' e^{i\omega_{21}t'} \sin(\omega t') =$

$$= \int_0^t dt' e^{i\omega_{21}t'}\left[\frac{e^{i\omega t'} - e^{-i\omega t'}}{2i}\right] = \frac{1}{2i}\int_0^t dt' \left[e^{i(\omega_{21}+\omega)t'} - e^{i(\omega_{21}-\omega)t'}\right]$$

$$= \frac{1}{2i}\left[\frac{e^{i(\omega_{21}+\omega)t} - 1}{i(\omega_{21}+\omega)} - \frac{e^{i(\omega_{21}-\omega)t} - 1}{i(\omega_{21}-\omega)}\right]$$

oder auch:

$$\frac{1}{i}\left[\frac{e^{i\frac{(\omega_{21}+\omega)t}{2}}}{\omega_{21}+\omega}\left(\frac{e^{\frac{i(\omega_{21}+\omega)t}{2}}-e^{\frac{-i(\omega_{21}+\omega)t}{2}}}{2i}\right)-\frac{e^{i\frac{(\omega_{21}-\omega)t}{2}}}{\omega_{21}-\omega}\left(\frac{e^{\frac{i(\omega_{21}-\omega)t}{2}}-e^{\frac{-i(\omega_{21}-\omega)t}{2}}}{2i}\right)\right]$$

$$=\frac{1}{i}\left[e^{i\frac{(\omega_{21}+\omega)t}{2}}\frac{\sin\left(\frac{\omega_{21}+\omega}{2}t\right)}{\omega_{21}+\omega}-e^{i\frac{(\omega_{21}-\omega)t}{2}}\frac{\sin\left(\frac{\omega_{21}-\omega}{2}t\right)}{\omega_{21}-\omega}\right]$$

$$=F(\omega_{21}+\omega)-F(\omega_{21}-\omega)$$

In $P^{(1)}_{2\leftarrow 1}(t)$ hätte man: $|F(\omega_{21}+\omega)-F(\omega_{21}-\omega)|^2$

$$\Rightarrow\quad |F(\omega_{21}+\omega)|^2+|F(\omega_{21}-\omega)|^2+\text{Gemischtes Produkt}$$

zu Vernachlässigen (laut Angabe)

$$=\frac{\sin^2\left(\frac{\omega_{21}+\omega}{2}t\right)}{(\omega_{21}+\omega)^2}+\frac{\sin^2\left(\frac{\omega_{21}-\omega}{2}t\right)}{(\omega_{21}-\omega)^2}$$

d*) $J_{21} = \int dx\, x \sin\left(\frac{2\pi}{L}x\right)\sin\left(\frac{\pi}{L}x\right) = \left(\frac{L}{\pi}\right)^2 \int_0^{\pi} dy\, y \sin(2y)\sin(y)$

$y = \frac{\pi}{L}x$

$= 2\left(\frac{L}{\pi}\right)^2 \int_0^{\pi} dy\, \underbrace{y}_{u} \underbrace{\sin^2 y \cos y}_{v'}$ mit $v = \int \underbrace{dy \cos y}_{d\sin y} \sin^2 y = \frac{\sin^3 y}{3}$

$= 2\left(\frac{L}{\pi}\right)^2 \left[\cancel{y \frac{\sin^3 y}{3}}\Big|_0^{\pi} - \frac{1}{3}\int_0^{\pi} \sin^3 y\, dy \right] = -\frac{2}{3}\left(\frac{L}{\pi}\right)^2 \int_0^{\pi} dy \sin^3 y$

0

$= -\frac{2}{3}\left(\frac{L}{\pi}\right)^2 \left[\frac{\cos^3 y}{3} - \cos y\right]_0^{\pi} = -\frac{2}{3}\left(\frac{L}{\pi}\right)^2\left[\frac{2}{3} + \frac{2}{3}\right] = -\frac{8}{9}\left(\frac{L}{\pi}\right)^2$

Vollständiger expliziter Ausdruck von

$$a_{21}^{(1)}(t) = \frac{A}{\hbar}\left(\frac{2}{L}\right)\frac{8}{9}\left(\frac{L}{\pi}\right)^2 \left[e^{i\frac{(\omega_{21}+\omega)t}{2}} \frac{\sin\left(\frac{\omega_{21}+\omega}{2}t\right)}{\omega_{21}+\omega} - e^{i\frac{(\omega_{21}-\omega)t}{2}} \frac{\sin\left(\frac{\omega_{21}-\omega}{2}t\right)}{\omega_{21}-\omega} \right]$$

$$P_{2\leftarrow 1}(t) = \frac{A^2}{\hbar^2}\frac{L^2}{\pi^4}\left(\frac{8}{9}\right)^2 \left[\frac{\sin^2\left(\frac{\omega_{21}+\omega}{2}t\right)}{\left(\frac{\omega_{21}+\omega}{2}\right)^2} + \frac{\sin^2\left(\frac{\omega_{21}-\omega}{2}t\right)}{\left(\frac{\omega_{21}-\omega}{2}\right)^2} + \cancel{\text{Gemischter Beitrag}} \right]$$

zu Vernachlässigen laut Angabe

c) Adiabatische Näherung: das System bleibt im G.Z. von $\hat{H}(t)$ $\Rightarrow$ für $\bar{t} = \frac{\pi}{\omega}$ $\sin(\omega \bar{t}) = \sin\pi = \emptyset \Rightarrow \hat{H}(\bar{t}) = \hat{H}_0$

$\Rightarrow \psi(x,\bar{t}) = \text{G.Z. von } H_0 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)$ mit $E_1(\bar{t}) = \varepsilon_1 = \frac{\hbar^2\pi^2}{2mL^2}$

Bedingung: $\tau_S \sim \frac{1}{\omega} \gg \tau_{H_0} \sim \frac{\hbar}{|\varepsilon_2 - \varepsilon_1|} = \frac{2mL^2}{3\hbar\pi^2}$

Test A: $aV_i = v_i$
Test B $V_2 \to -V_2$

Aufgabe 3

$$V(r) = a \sum_i V_i\, \delta(r - R_i) \qquad j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho}$$

a)

$$f_s = -\frac{2ma}{\hbar^2}\int dr' \cancel{r'^2} \sum_i V_i\, \delta(r - R_i) \left(\frac{\sin(kr')}{k\cancel{r'}}\right)^2$$

$$= -\frac{2ma}{\hbar^2 k^2} \sum_i V_i \sin^2(kR_i)$$

$$f_p = -\frac{2ma}{\hbar^2} \sum_i V_i R_i^2 \left(\frac{\sin(kR_i)}{(kR_i)^2} - \frac{\cos(kR_i)}{kR_i}\right)^2$$

$$= -\frac{2ma}{\hbar^2 k^2} \sum_i V_i \left(\frac{\sin(kR_i)}{kR_i} - \cos(kR_i)\right)^2$$

$$f(\theta) = f_s + \underset{(2\ell+1)\, P_\ell(\cos\theta)}{3\cos\theta}\, f_p$$

b) Taylor expansion of f_p in k:

$$f_p = -\frac{2ma}{\hbar^2 k^2} \sum_i \frac{V_i}{9} \cdot (kR_i)^4 \overset{!}{=} 0 \iff \frac{V_1}{V_2} = -\left(\frac{R_2}{R_1}\right)^4$$

c) standard formalism

$$f(\theta) = -\frac{2m}{\hbar^2}\int dr\, V(r)\, r \sin(qr)/q \qquad q = 2k\sin\left(\frac{\theta}{2}\right)$$

$$= -\frac{2ma}{\hbar^2} \sum_i V_i R_i \sin(qR_i)/q$$

$$\overset{|k| \ll 1}{=} -\frac{2ma}{\hbar^2} \sum_i V_i R_i \cdot \left(R_i - \cancel{\frac{2}{3}k^2 \sin^2\left(\frac{\theta}{2}\right) R_i^3}\right)$$

$$= -\frac{2ma}{\hbar^2} \sum_i V_i R_i^2$$

same

$$f_s \overset{|k| \ll 1}{=} -\frac{2ma}{\hbar^2 k^2} \sum_i V_i \left(k^2 R_i^2 + \cancel{O(k^4)}\right) = -\frac{2ma}{\hbar^2} \sum_i V_i R_i^2$$

4 a) Da $S_1^+ |\uparrow\rangle_i = 0$ und $S_i^- |\downarrow\rangle_i = 0$

folgt, dass $H |\uparrow\rangle_1 |\uparrow\rangle_2 = H |\downarrow\rangle_2 |\downarrow\rangle_2 = 0 \Rightarrow$ EFen EWe

Weitere Zustände

$$H |\uparrow\rangle_1 |\downarrow\rangle_2 = 2J \, |\downarrow\rangle_1 |\uparrow\rangle_2$$

$$H |\downarrow\rangle_1 |\uparrow\rangle_2 = 2J \, |\uparrow\rangle_1 |\downarrow\rangle_2 \qquad (*)$$

bzw. als Matrix

$$\underline{\underline{H}} = \begin{array}{c} \\ 2J \; {\color{red}-2g} \end{array} \begin{array}{c} \begin{array}{cccc} \uparrow\uparrow & \downarrow\downarrow & \uparrow\downarrow & \downarrow\uparrow \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array}$$

$$\Rightarrow \text{EF} \quad \frac{|\downarrow\rangle_1 |\uparrow\rangle_2 \pm |\uparrow\rangle_1 |\downarrow\rangle_2}{\sqrt{2}}$$

haben EW $\pm 2J$ wegen *

$$J>0 \Rightarrow \text{Grundzustand} \quad \frac{|\downarrow\rangle_1 |\uparrow\rangle_2 - |\uparrow\rangle_1 |\downarrow\rangle_2}{\sqrt{2}} = |\Psi_0\rangle$$

b) Reduzierte Dichtematrix 1. Qu. punkt

$$\rho_1 = \text{Spur}_2 \, |\Psi\rangle\langle\Psi| \overset{S.1c)}{=} \tfrac{1}{2} |\downarrow\rangle_1 \langle\downarrow| + \tfrac{1}{2} |\uparrow\rangle_1 \langle\uparrow|_1$$

Dichtematrix gesamtsystem

$$\rho = |\Psi_0\rangle\langle\Psi_0| = \tfrac{1}{2}\Big(|\downarrow\rangle_1 |\uparrow\rangle_2 \, {}_2\langle\downarrow| \, {}_1\langle\uparrow| + |\uparrow\rangle_1 |\downarrow\rangle_2 \, {}_2\langle\uparrow| \, {}_1\langle\downarrow|$$
$$- |\downarrow\rangle_1 |\uparrow\rangle_2 \, {}_1\langle\uparrow| \, {}_2\langle\downarrow| - |\uparrow\rangle_1 |\downarrow\rangle_2 \, {}_2\langle\downarrow| \, {}_1\langle\uparrow| \Big)$$

bzw. als Matrix

$$\rho = \frac{1}{2}\begin{array}{c} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \\ \begin{array}{cccc} \uparrow\uparrow & \downarrow\downarrow & \uparrow\downarrow & \downarrow\uparrow \end{array} \end{array}$$

c)

$S_{1+2} = 0$ reiner Zustand $\quad S_1 = S_2$ Symmetrie

$$S_1 = -k_B \operatorname{Spur} \rho \ln \rho = -k_B \left(\tfrac{1}{2} \ln \tfrac{1}{2} + \tfrac{1}{2} \ln \tfrac{1}{2} \right)$$

$$= -k_B \ln \underbrace{\tfrac{1}{2}}_{<1} > 0$$

$\Rightarrow \quad S_{1+2} \leq S_1 + S_2 \quad$ qed.