① $$\hat{H}_0 = \sum_{b\{L,V\}} \sum_{k} \varepsilon_{kb}\, a^{+}_{kb} a_{kb}$$

$$\hat{V} = \sum_{k} \left(t_k\, a^{+}_{kV} a_{kL} + t_k^{*}\, a^{+}_{kL} a_{kV} \right)$$

$$E^{(0)}_{kb} = \langle kb | \hat{H}_0 | kb \rangle$$

$$= \langle kb | \sum_{k'b'} \varepsilon_{k'b'} \underbrace{\hat{n}_{k'b'}}_{\delta_{kk'}\delta_{bb'}} | kb \rangle = \varepsilon_{kb}$$

$$E^{(1)}_{kL} = \langle kL | \hat{V} | kL \rangle$$

$$= \langle kL | \sum_{k'} (t_{k'}\, a^{+}_{k'V} a_{k'L} + t^{*}_{k'}\, a^{+}_{k'L} a_{k'V} | kL \rangle$$

$$= t_k \langle kL | kV \rangle = 0$$

$$E^{(1)}_{kV} = 0 \qquad \text{analog}$$

$$E^{(2)}_{kL} = \sum_{\{k'b\} \neq \{kL\}} \frac{|\langle k'b | \hat{V} | kL \rangle|^2}{E^{(0)}_{kL} - E^{(0)}_{k'b}} .$$

$$= \sum_{\{k'b\} \neq \{kL\}} \frac{|t_k \langle k'b | kV \rangle|^2}{E^{(0)}_{kL} - E^{(0)}_{k'b}} = \frac{|t_k|^2}{\varepsilon_{kL} - \varepsilon_{kV}}$$

$$E^{(2)}_{kV} = \frac{|t_k|^2}{\varepsilon_{kV} - \varepsilon_{kL}}$$

Version mit reinen Vielteilchenzuständen

(war nicht Pflicht)

$$|\psi\rangle = |\{k_1 b_1, k_2 b_2, \ldots\ldots, k_N b_N\}\rangle$$

$$a_{kb}|\psi\rangle = \begin{cases} 0 & \text{falls } kb \notin \psi \\ |\psi \setminus \{kb\}\rangle & \text{falls } kb \in \psi \end{cases}$$

$$= n^{kb}_{|\psi\rangle} \, |\psi \setminus \{kb\}\rangle$$

$$a^{+}_{kb}|\psi\rangle = (1 - n^{kb}_{|\psi\rangle}) \, |\psi \cup \{kb\}\rangle$$

$$E^{(0)}_{|\psi\rangle} = \langle \psi | \hat{H}_0 | \psi \rangle = \sum_{kb} n^{kb}_{|\psi\rangle} \varepsilon_{kb}$$

$$E^{(1)}_{|\psi\rangle} = \langle \psi | \hat{V} | \psi \rangle$$

$$= \sum_k \left(t_k \langle \psi | a^{+}_{kV} a_{kL} | \psi \rangle + t^{*}_k \langle \psi | a^{+}_{kL} a_{kV} | \psi \rangle \right)$$

$$= \sum_k t_k \, n^{kL}_{|\psi\rangle} (1 - n^{kV}_{|\psi\rangle}) \underbrace{\langle \psi | \psi \setminus \{kL\} \cup \{kV\} \rangle}_{0} + 0 = 0$$

$$E^{(2)}_{|\psi\rangle} = \sum_{|\psi'\rangle \neq |\psi\rangle} \frac{|\langle \psi' | \hat{V} | \psi \rangle|^2}{E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi'\rangle}}$$

$$= \sum_{|\psi'\rangle \neq |\psi\rangle} \frac{|\langle \psi' | \sum_k (t_k a^\dagger_{kV} a_{kL} + t^*_k a^\dagger_{kL} a_{kV}) |\psi\rangle|^2}{E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi'\rangle}}$$

$$= \sum_{|\psi'\rangle \neq |\psi\rangle} \frac{1}{E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi'\rangle}} \Big\{$$

$$\sum_k t_k \, n^{kL}_{|\psi\rangle} (1 - n^{kV}_{|\psi\rangle}) \langle \psi' | \psi \setminus \{kV\} \cup \{kL\} \rangle$$

$$+ \sum_k t^*_k \, n^{kV}_{|\psi\rangle} (1 - n^{kL}_{|\psi\rangle}) \langle \psi' | \psi \setminus \{kL\} \cup \{kV\} \rangle$$

$$= \sum_k \frac{|t_k \, n^{kL}_{|\psi\rangle} (1 - n^{kV}_{|\psi\rangle})|^2}{E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi \setminus \{kV\} \cup \{kL\}\rangle}}$$

$$+ \sum_k \frac{|t^*_k \, n^{kV}_{|\psi\rangle} (1 - n^{kL}_{|\psi\rangle})|^2}{E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi \setminus \{kL\} \cup \{kV\}\rangle}}$$

$$E^{(0)}_{|\psi\rangle} - E^{(0)}_{|\psi \setminus \{kV\} \cup \{kL\}\rangle}$$

$$= \sum_{k' \neq k} \sum_{b} \left(\cancel{n^{k'b}_{|\psi\rangle}} \varepsilon_{k'b} - \cancel{n^{k'b}_{|\psi\rangle}} \varepsilon_{k'b} \right) + \varepsilon_{kL} n^{kL}_{|\psi\rangle} + \varepsilon_{kV} \left(n^{kV}_{|\psi\rangle} - 1 \right)$$

$$= -\sum_{k} \frac{|t_k|^2 \, n^{kL}_{|\psi\rangle} \left(1 - n^{kV}_{|\psi\rangle}\right)}{\varepsilon_{kL} n^{kL}_{|\psi\rangle} - \varepsilon_{kV}\left(1 - n^{kV}_{|\psi\rangle}\right)} + \sum_{k} \frac{|t_k|^2 \, n^{kV}_{|\psi\rangle} \left(1 - n^{kL}_{|\psi\rangle}\right)}{\varepsilon_{kV} n^{kV}_{|\psi\rangle} - \varepsilon_{kL}\left(1 - n^{kL}_{|\psi\rangle}\right)}$$

2

$$\frac{df}{dt} = \frac{1}{i\hbar} \underline{\mu} \cdot \underline{\mathcal{E}}(t) \left[p^*(t) - p(t) \right]$$

$$\frac{dp}{dt} = \frac{1}{i} \omega_p \, p(t) + \frac{1}{i\hbar} \underline{\mu} \cdot \underline{\mathcal{E}}(t) \left[1 - f_e(t) - f_h(t) \right]$$

$$\underline{\mathcal{E}}(t) = \frac{1}{2} \left[\underline{\tilde{\mathcal{E}}}(t) e^{-i\Omega t} + \underline{\tilde{\mathcal{E}}}^*(t) e^{+i\Omega t} \right]$$

$$p = \tilde{p} e^{-i\Omega t}$$

$$\Rightarrow \frac{df}{dt} = \frac{1}{i\hbar} \underline{\mu} \cdot \frac{1}{2} \left[\underline{\tilde{\mathcal{E}}}(t) e^{-i\Omega t} + \underline{\tilde{\mathcal{E}}}^*(t) e^{+i\Omega t} \right] \cdot \left[\tilde{p}^* e^{+i\Omega t} - \tilde{p} e^{-i\Omega t} \right]$$

$$= \frac{1}{2i\hbar}\, \underline{\mu} \cdot \left[\underline{\tilde{\mathcal{E}}}(t)\, \tilde{p}^* - \cancel{\underline{\tilde{\mathcal{E}}}(t)\, \tilde{p}\, e^{-2i\Omega t}} \right.$$

$$\left. + \cancel{\underline{\tilde{\mathcal{E}}}^* \tilde{p}^*\, e^{+2i\Omega t}} - \underline{\tilde{\mathcal{E}}}^* \tilde{p} \right]$$

$$= \frac{1}{\hbar}\, \mathrm{Im}\left[\underline{\mu} \cdot \underline{\tilde{\mathcal{E}}}(t)\, \tilde{p}^* \right]$$

$$\frac{d\tilde{p}}{dt} = e^{+i\Omega t} \frac{dp}{dt} + i\Omega\, \tilde{p}$$

$$= \frac{\Delta}{i}\, \tilde{p}(t) + \frac{1}{i\hbar} e^{+i\Omega t}\, \underline{\mu} \cdot \underline{\mathcal{E}}(t) \left[1 - f_e(t) - f_h(t) \right]$$

$\omega_p - \Omega$

$$\underline{\mathcal{E}}(t) = \frac{1}{2}\left[\underline{\tilde{\mathcal{E}}}(t)\, e^{-i\Omega t} + \underline{\tilde{\mathcal{E}}}^*(t)\, e^{+i\Omega t} \right]$$

$$= \frac{\Delta}{i}\, \tilde{p}(t) + \frac{1}{2i\hbar}\, \underline{\mu}\, \underline{\tilde{\mathcal{E}}}(t) \left[1 - f_e(t) - f_h(t) \right]$$

b) $\tilde{p}(t) = \frac{i}{2} \sin\Theta(t)$, $\Theta(t) = \frac{1}{\hbar} \int_{-\infty}^{t} \underline{\mu} \cdot \underline{\tilde{\mathcal{E}}}(t')\, dt'$

$$F'(x) = f(x)$$

$$\int_{-\infty}^{x} f(x')\, dx' = F(x) - F(-\infty)$$

$$\frac{d}{dx} \int_{-\infty}^{x} f(x')\, dx' = \frac{d}{dx} F(x) = f(x)$$

$$\frac{d\tilde{p}}{dt} = \frac{i}{2} \cos\Theta(t)\, \frac{1}{\hbar}\, \underline{\mu}\, \underline{\tilde{\mathcal{E}}}(t)$$

$$\stackrel{!}{=} \frac{\mu \cdot \tilde{\mathcal{E}}(t)}{2i\hbar}\left[1 - f_e(t) - f_h(t)\right]$$

$$\Rightarrow 1 - f_e(t) - f_h(t) = -\cos\theta(t)$$

$$\frac{df}{dt} = \frac{1}{2}\frac{d}{dt}\cos\theta(t)$$

$$= -\frac{1}{2}\sin\theta(t)\frac{1}{\hbar}\mu\cdot\tilde{\mathcal{E}}(t)$$

$$= \frac{i}{\hbar}\mu\cdot\tilde{\mathcal{E}}(t)\underbrace{\tilde{p}(t)}_{\in i\mathbb{R}}$$

$$-i\,\mathrm{Im}\left[\tilde{p}^*(t)\right]$$

$$= \frac{1}{\hbar}\mu\cdot\tilde{\mathcal{E}}(t)\,\mathrm{Im}\left[\tilde{p}^*(t)\right]$$

passt!

3 Wasserstoffatom

$x_0 = 0$

- Potential: $V(x) = -\frac{e^2}{4\pi\varepsilon_0}\delta(x - x_0)$

- Schrödinger-Gl:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{e^2}{4\pi\varepsilon_0}\delta(x)\right]\psi(x) = E\psi(x)$$

- **Ansatz** $\psi_1(x) = A_1 e^{\lambda x} + \cancel{A_2 e^{-\lambda x}}$, $x < 0$

$$\psi_2(x) = \cancel{B_1 e^{\lambda x}} + B_2 e^{-\lambda x}, \quad x \geq 0$$

- Normierungsbedingung: $A_2 = B_1 = 0$
- Stetigkeit: $\psi_1(0) \overset{!}{=} \psi_2(0)$

$$A_1 e^{\lambda 0} = B_2 e^{-\lambda 0}$$

$$A_1 = B_2 := A$$

allg. Lsg: $\psi(x) = A \begin{cases} e^{\lambda x}, & x < 0 \\ e^{-\lambda x}, & x \geq 0 \end{cases}$

- Betrachte $\psi'(x)$: Ableitung hat Sprung bei $x = 0$

$$\lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \psi(x)\, dx = 0$$

$$\overset{SG}{\Leftrightarrow} \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \frac{1}{\varepsilon} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - \frac{e^2}{4\pi\varepsilon_0} \delta(x)\, \psi(x) \right) = 0$$

$$\Leftrightarrow \lim_{\varepsilon \to 0} \; -\frac{\hbar^2}{2m} \left[\psi'(0) - \psi'(-0) \right] - \frac{e^2}{4\pi\varepsilon_0} \psi(0) = 0$$

$$-A\lambda e^{-\lambda 0} - A\lambda e^{\lambda 0} = -\frac{2me^2}{4\pi\varepsilon_0 \hbar^2} A e^{\lambda 0}$$

$$-2\lambda = -\frac{2me^2}{4\pi\varepsilon_0 \hbar^2}$$

$$\lambda = \frac{me^2}{4\pi\varepsilon_0\hbar^2} = \frac{1}{a_B}$$ – Bohr'scher Radius

· <u>Bestimmung von A aus Normierung</u>

$$\langle\psi|\psi\rangle = \int_{-\infty}^{0} dx\, A^2 e^{2\lambda x} + \int_{0}^{\infty} dx\, A^2 e^{-2\lambda x}$$

$$= A^2\left[\frac{1}{2\lambda}\left(e^0 - \cancel{e^{-\infty}}\right) - \frac{1}{2\lambda}\left(e^{-\infty} - e^0\right)\right]$$

$$= \frac{A^2}{2\lambda}\cdot 2 = \frac{A^2}{\lambda} \stackrel{!}{=} 1$$

$$\Rightarrow A = \sqrt{\lambda} = \frac{1}{\sqrt{a_B}}$$

$$\psi(x) = \frac{1}{\sqrt{a_B}}\begin{cases} e^{x/a_B}, & x < 0 \\ e^{x/a_B}, & x \geq 0 \end{cases}$$

b) Energie E $(x \neq 0)$

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)$$

$x < 0$: $$E\frac{1}{\sqrt{a_B}}e^{x/a_B} = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{a_B}}\cdot\frac{1}{a_B^2}e^{x/a_B}$$

$$E = -\frac{\hbar^2}{2m}\cdot\frac{1}{a_B{}^2}$$

(4) $$V(x) = \frac{m\omega^2 x^2}{2} - eEx$$

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2x^2}{2} - eEx$$

Leiteroperatoren: $$b = \frac{1}{\sqrt{2m\hbar\omega}}\hat{p} - i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}$$

$$b^+ = \frac{1}{\sqrt{2m\hbar\omega}}\hat{p} + i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}$$

- $$\hat{x} = \frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\,(b^+ - b)$$

- $$\hat{p} = \sqrt{\frac{m\hbar\omega}{2}}\,(b^+ + b)$$

$$H = \frac{1}{2\cancel{m}}\,\frac{\cancel{m}\hbar\omega}{2}(b^+ + b)^2 + \frac{\cancel{m}\omega^{\cancel{2}}}{2}\,\frac{\hbar}{2\cancel{m}\cancel{\omega}}\cdot\underbrace{\frac{1}{i^2}}_{-1}(b^+ - b)^2$$

$$-eE\,\frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\,(b^+ - b)$$

$$= \frac{\hbar\omega}{4}\left(\cancel{b^{+2}} + b^+b + bb^+ \cancel{+b^2} \cancel{-b^{+2}} + b^+b + bb^+ \cancel{-b^2}\right)$$

$$-eE\,\frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\,(b^+ - b)$$

$$= \frac{\hbar\omega}{2}\left(b^+b + bb^+\right) - eE\frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}\left(b^+ - b\right)$$

$$[b, b^+] = 1 \Rightarrow bb^+ = b^+b + 1$$

$$\Rightarrow$$

$$H = \frac{\hbar\omega}{2}\left(b^+b + b^+b + 1\right) - eE\frac{1}{i}\cdots$$

$$H = \hbar\omega\left(b^+b + \frac{1}{2}\right) + ieE\sqrt{\frac{\hbar}{2m\omega}}\left(b^+ - b\right)$$

b)
$$\dot{F} = \frac{\partial F}{\partial t} + \frac{i}{\hbar}[H, F]$$

$$\dot{b} = + \frac{i}{\hbar}\left[\hbar\omega\left(b^+b + \frac{1}{2}\right) + ieE\sqrt{\frac{\hbar}{2m\omega}}\left(b^+ - b\right), b\right]$$

$$[b^+b, b] = b^+bb - bb^+b = b^+bb - (b^+b + 1)b$$
$$= -b$$

$$\dot{b} = -i\omega b - \frac{eE}{\sqrt{2m\hbar\omega}}$$

(c)
$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$\langle\alpha|\alpha\rangle \overset{!}{=} 1$$

$$= \sum_m \sum_n e^{-|\alpha|^2} \langle n| \frac{\alpha^{*n}}{\sqrt{n!}} \cdot \frac{\alpha^m}{\sqrt{m!}} |m\rangle$$

$\langle n|m\rangle = \delta_{nm}$ $$= \sum_n e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!}$$

$$= e^{-|\alpha|^2} e^{|\alpha|^2} = 1$$

(d) $$\bar{E}(\alpha, \alpha^*) = \frac{\langle\alpha|\hat{H}|\alpha\rangle}{\underbrace{\langle\alpha|\alpha\rangle}_{1}}$$

$$= \langle\alpha|\hat{H}|\alpha\rangle$$

$$= \langle\alpha| \hbar\omega(b^+b + \tfrac{1}{2}) + iC(b^+ - b)|\alpha\rangle$$

$$\boxed{\begin{array}{l} b|\alpha\rangle = \alpha|\alpha\rangle \\ \langle\alpha|b^+ = \langle\alpha|\alpha^* \end{array}} = \hbar\omega(|\alpha|^2 + \tfrac{1}{2}) + iC(\alpha^* - \alpha)$$

$$\frac{\partial\bar{E}}{\partial\alpha} \overset{!}{=} 0$$

$$\Rightarrow \hbar\omega\alpha^* - iC = 0$$

$$\Rightarrow \alpha^* = \frac{iC}{\hbar\omega} \qquad \alpha = -\frac{iC}{\hbar\omega}$$

$$E_0 = \tilde{E}(\zeta^*, \zeta)$$

$$= \hbar\omega\left(\frac{c^2}{(\hbar\omega)^2} + \frac{1}{2}\right) + ic\left(\frac{ic}{\hbar\omega} + \frac{ic}{\hbar\omega}\right)$$

$$= \frac{\hbar\omega}{2} + \frac{c^2}{\hbar\omega}(1-2) - \frac{\hbar\omega}{2} - \frac{c^2}{\hbar\omega}$$

$$= \frac{\hbar\omega}{2} - \frac{(eE)^2}{2m\omega^2}$$