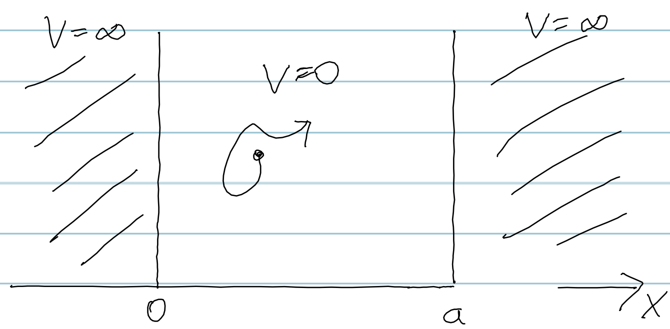
To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

Vorlesung 21.11.2013

2.4 Beispiele

b) Teilchen in einem 1-dim. Kasten

Anwendung: π-e^- in konjug. Systemen



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

außerh. des Kastens: $V=\infty$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \infty\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \infty\psi = 0$$

↳ nur triviale Lsg: $\psi = 0 \to \psi^2 = 0$

↳ Teilchen ist innerhalb des Kastens!

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

innerhalb des Kastens $V=0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+0\,\psi=E\psi$$

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

$$\boxed{\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi}$$

Lösungsansatz: $\psi=A\cdot\sin\alpha x$

$\psi'=\alpha A\cdot\cos\alpha x$

$\psi''=-\alpha^2\underbrace{A\sin\alpha x}_{\psi}$

$$\psi''=-\alpha^2\psi$$

$$\Leftrightarrow \boxed{\alpha^2=\frac{2mE}{\hbar^2}}$$

jede Energie ist möglich!

Randbed.: $\psi(0)=\psi(a)=0$

$$\psi(0)=A\sin\alpha\cdot 0=0$$

$$\psi(a)=A\sin\alpha\cdot a=0$$

$$\alpha\cdot a=n\pi \qquad n=1,2,3,\ldots$$

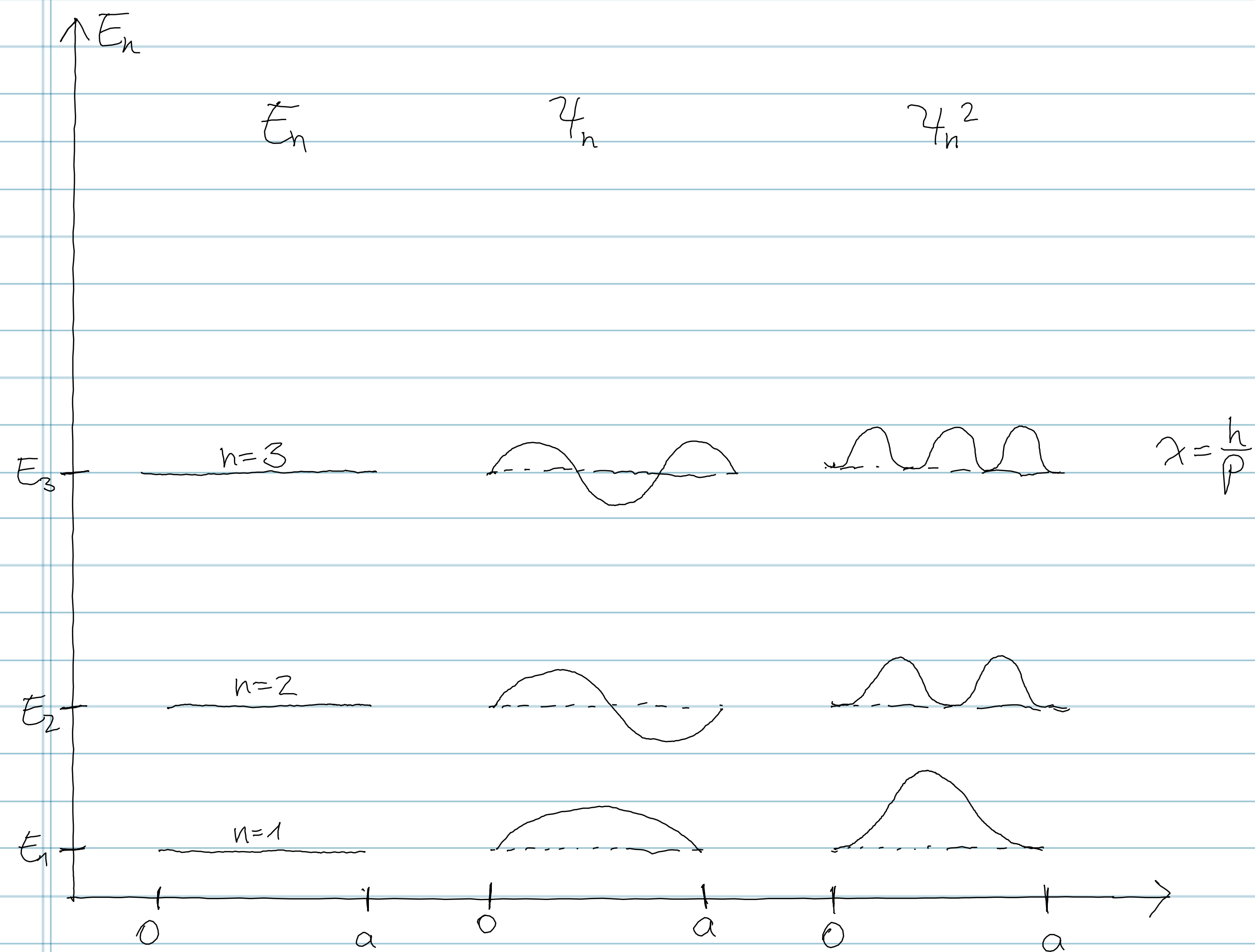
$$\to \alpha=\frac{n\pi}{a}$$

$$\Leftrightarrow \alpha^2=\frac{n^2\pi^2}{a^2}$$

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

↳ Energieeigenwerte $\boxed{E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}}$

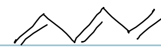
↳ Eigenfunktionen $\boxed{\psi_n = A \sin \frac{n\pi}{a} \cdot x}$



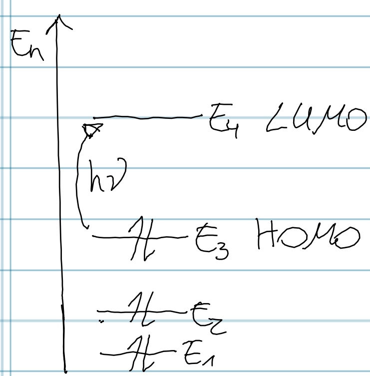
Masse m u. Länge a groß → Energieniveaus dicht (Kontinuum)

" " klein → Quantelung

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

Bsp: π-e^- in Hexatrien 

$6\pi e^-$



$$\Delta E = \frac{h^2}{8m_e a^2}\underbrace{\left(n_{LUMO}^2 - n_{HOMO}^2\right)}_{7}$$

$$a = 3 \times 135\,pm + 2 \times 154\,pm = 713\,pm$$

$$\Delta E = h\nu = h\frac{c}{\lambda}$$

$$\rightarrow \lambda = \frac{hc}{\Delta E} = 240\,nm \quad (exp.\ 268\,nm)$$

Eigenschaften der Wellenfunktion

$$\psi_n(x) = A \cdot \sin\frac{n\pi}{a}\cdot x$$

Normierung: $\int_0^a \psi_n^2\,dx = 1$

$$A^2\int_0^a \sin^2 \underbrace{\frac{n\pi}{a}x}_{\varphi}\,dx$$

Subst: $\varphi = \frac{n\pi}{a}x \qquad \frac{d\varphi}{dx} = \frac{n\pi}{a}$

$$\frac{a}{n\pi}A^2\int_0^{n\pi}\sin^2\varphi\,d\varphi = \frac{a}{\cancel{n\pi}}A^2\left(\frac{\cancel{n\pi}}{2}\right) = 1$$

$$\frac{a}{2}A^2 = 1 \rightarrow A = \sqrt{\frac{2}{a}}$$

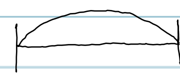
$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x} \qquad n = 1, 2, 3, \ldots$$

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

Orthogonalität: ψ_1, ψ_2

$$\int_0^a \psi_1 \psi_2 \, dx = 0 = \langle \psi_1 | \psi_2 \rangle$$

$\psi_1 = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$



ψ_1

$\psi_2 = \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$

ψ_2

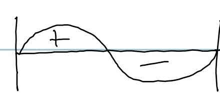
$$\langle \psi_1 | \psi_2 \rangle = \frac{2}{a} \int_0^a \sin \frac{\pi x}{a} \cdot \sin \frac{2\pi x}{a} \, dx$$

$$\sin 2\varphi = 2 \sin\varphi \cos\varphi$$

$$\langle \psi_1 | \psi_2 \rangle = \frac{2 \cdot 2}{a} \int_0^a \sin^2 \frac{\pi x}{a} \cos \frac{\pi x}{a} \, dx$$

$$= \frac{4}{a} \left(\frac{a}{3\pi} \sin^3 \frac{\pi}{a} \cdot x \right) \Big|_0^a = 0$$

$\langle \psi_1 | \psi_2 \rangle = 0$



$\psi_1 \cdot \psi_2$

$\langle \psi_1 | \psi_3 \rangle = 0$ $\quad$ $\langle \psi_1 | \psi_1 \rangle = 1$

$\langle \psi_2 | \psi_3 \rangle = 0$ $\quad$ $\langle \psi_2 | \psi_2 \rangle = 1$

$\vdots$ $\quad$ $\vdots$

allg.:

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

↑ Kronecker-Symbol

$$\delta_{ij} \begin{cases} = 1 & \text{für } i = j \\ = 0 & \text{für } i \neq j \end{cases}$$

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

Orthonormalsystem

1) Wellenfkt sind normiert

2) Wellenfkt ψ_n, ψ_m sind paarweise orthogonal

Impuls

x-Komp. Impuls, ψ_1

$$\hat{p}_{x,1}\psi_1 = -i\hbar \frac{d}{dx}\left(\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}\right) = -i\hbar \sqrt{\frac{2}{a}} \cdot \frac{\pi}{a} \cos \frac{\pi x}{a}$$

$\Rightarrow$ ψ_1 ist <u>keine</u> Eigenfkt von $\hat{p}_{x,1}$

Mittelwertbildung

$$\bar{p}_{x,1} = \int_0^a \psi_1 \hat{p}_{x,1} \psi_1 \, dx \Big/ \underbrace{\int_0^a \psi_1^2 dx}_{1}$$

$$\bar{p}_{x,1} = \int_0^a \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} (-i\hbar) \sqrt{\frac{2}{a}} \frac{\pi}{a} \cos \frac{\pi x}{a} \, dx$$

$$\bar{p}_{x,1} = \frac{2}{a}(-i\hbar)\frac{\pi}{a}\int_0^a \sin \frac{\pi x}{a} \cdot \cos \frac{\pi x}{a} \, dx$$

$$\bar{p}_{x,1} = -i\hbar \frac{2\pi}{a^2}\left(\frac{1}{2}\sin^2 \frac{\pi x}{a}\right)\Big|_0^a = \underline{0}$$

Quadrat x-Komp. Impuls, Zustand ψ_1

$$\hat{p}_{x,1}^2 \psi_1 = -\hbar^2 \frac{d^2}{dx^2}\left(\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}\right) = +\hbar^2 \frac{\pi^2}{a^2} \underbrace{\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}}_{\psi_1}$$

$\hat{p}_{x,1}^2 \psi_1 = p_{x,1}^2 \psi_1$ $\Rightarrow$ ψ_1 ist eine Eigenfkt. von $\hat{p}_{x,1}^2$

To hear and view this Pencast PDF on your computer,
click here to get the latest version of Adobe® Reader®

$$p_{x,1}^2 = \frac{\hbar^2 \pi^2}{a^2} = 2mE_1 \qquad E_{kin} = \frac{p^2}{2m}$$

$$p_{x,1} = \pm\sqrt{2mE_1}$$

Genauigkeit: $2\sqrt{2mE_1}$