Wdhlg.: Impulseigenzust.e $\{|\chi_{\vec{k}}\rangle\}$

1D → 3D

$$\boxed{\hat{\vec{p}}\,|\chi_{\vec{k}}\rangle \overset{!}{=} \hbar\vec{k}\,|\chi_{\vec{k}}\rangle}$$

Wellenfkt.

$$\boxed{\chi_{\vec{k}}(x) = e^{i\vec{k}\cdot\vec{x}}} = \langle\varphi_{\vec{x}}|\chi_{\vec{k}}\rangle$$

Orthogonalität

$$\langle\chi_{\vec{k}'}|\chi_{\vec{k}}\rangle = (2\pi)^3\delta(\vec{k}-\vec{k}')$$

Vollständigkeit

$$\mathbb{1}_{\mathcal{H}} = \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3}\,|\chi_{\vec{k}}\rangle\langle\chi_{\vec{k}}|$$

Dynamik des freien Teilchens

$$H = \frac{1}{2m}|\hat{\vec{p}}|^2$$

$$= \frac{1}{2m}\left(\hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2\right)$$

kl. Energ.-Imp. Rel

✓ $E = |\vec{p}|^2/2m$

nicht-relativistisch!

relat.:

$E^2 = m^2c^4 + c^2p^2$

⟶ Dirac-Gl.

$$i\hbar|\dot{\psi}(t)\rangle = \frac{|\hat{\vec{p}}|^2}{2m}|\psi(t)\rangle$$

d.h.

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{\hbar^2}{2m}\Delta\,\psi(\vec{x},t)}$$

$\hat{p}_\ell \longrightarrow -i\hbar \frac{\partial}{\partial x_\ell}$ $\qquad \ell = 1, 2, 3$

$\hat{\vec{p}} \longrightarrow -i\hbar \vec{\nabla}$

$|\hat{\vec{p}}|^2 \longrightarrow -\hbar^2 \Delta = -\hbar^2 \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right)$

Laplace-Op.

1D:

$$\rightarrow \boxed{i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t)} \qquad (*)$$

Lösungen?

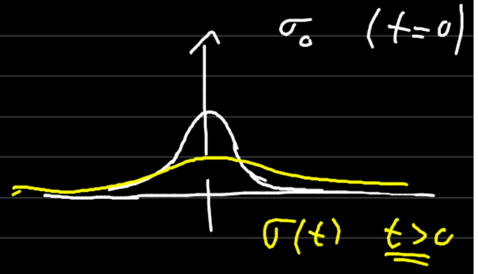
math. analog zur Wärmeleitungsgl. (1D)

$$\frac{\partial}{\partial t} T(x,t) = a \frac{\partial^2}{\partial x^2} T(x,t)$$

Temperaturleitf.

$a = \frac{\lambda}{\varrho \cdot c}$

$t \longrightarrow it$ "imag. Zeit"



$$T(x,0) \equiv T_0(x) = \alpha' \, e^{-x^2/2\sigma_0^2}$$

$$\downarrow \; F.T.,\; e^{-ak^2t},\; (F.T.)^{-1}$$

$$T(x,t) = \beta\, e^{-\frac{x^2}{2\underbrace{(\sigma_0^2+2at)}_{\sigma_t^2}}}$$

$$\sigma_t = \sigma_0 \sqrt{1+\frac{2a}{\sigma_0^2}\cdot t}$$

$\uparrow$

Wärmeleitung!

10 - S.Gl.:

$$(*) \quad \frac{\partial}{\partial t}\psi(x,t) = \boxed{\frac{\hbar}{2m}}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

$$\frac{\hbar}{2m} = a$$

$$\psi(x,0) = \psi_0(x) = \frac{1}{(\pi\sigma_0^2)^{1/4}}\, e^{-x^2/2\sigma_0^2}$$

$$\downarrow$$

$$\psi(x,t) = \beta\, e^{-\frac{x^2}{2\left(\sigma_0^2+\frac{\hbar}{m}it\right)}}$$

$$= \beta\, e^{-\frac{x^2}{2\sigma_0^2\left(1+i\frac{\hbar}{m\sigma_0^2}t\right)}}$$

- $\sigma_0^2\left(1+i\frac{\hbar}{m\sigma_0^2}t\right) = \sigma_0^2(1+it/\tau)$

  $\tau := \frac{m\sigma_0^2}{\hbar}$

- $\frac{1}{1+it/\tau} = \frac{1-it/\tau}{1+t^2/\tau^2}$

$\rightarrow \psi(x,t) = \beta\, e^{-\frac{x^2}{2\sigma_0^2(1+it/\tau)}} =$

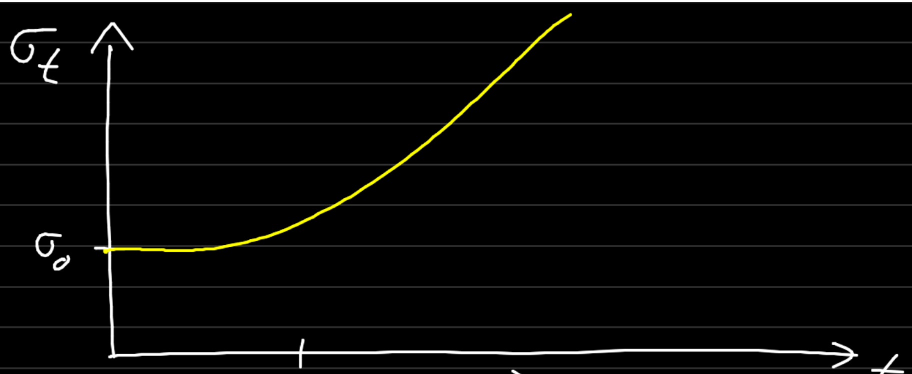
$= \beta \cdot e^{\frac{i x^2 t/\tau}{2\sigma_0^2(1+t^2/\tau^2)}} \cdot e^{-\frac{x^2}{2\sigma_0^2(1+t^2/\tau^2)}}$

$\rightarrow |\psi(x,t)|^2 = \beta^2\, e^{-\frac{x^2}{\sigma_0^2(1+t^2/\tau^2)}}$

- $\sigma_t = \sigma_0\sqrt{1+t^2/\tau^2}$

- $\tau = \frac{m\sigma_0^2}{\hbar}$

$\rightarrow |\psi(x,t)|^2 = \frac{1}{(\pi\sigma_t^2)^{1/2}}\, e^{-x^2/\sigma_t^2}$



$\tau = \frac{m\sigma_0^2}{\hbar}$

zahlen! ?

1) makrosk. Teilchen: $m = 1g = 10^{-3}\,kg$

$\sigma_0 = 1mm = 10^{-3}\,m$

$\Rightarrow \tau = \frac{10^{-3}\,10^{-6}}{10^{-34}}\,s = 10^{25}\,s = 0.3\cdot 10^{18}\,J\,!$

2) mikroskop. Teilchen:

H-Atom: $m = 10^{-27}\,kg$

$\sigma_0 = 10^{-10}\,m$

$\Rightarrow \tau = \frac{10^{-27}\cdot 10^{-20}}{10^{-34}} = 10^{-13}\,s$

$\Rightarrow \sigma(1s) = \sigma_0 \frac{1s}{\tau} = 10^{-10}\cdot 10^{13}\,m$

$= 10^{3}\,m = 1\,km\,!$

allg. Dynamik: Teilchen im Potenzial $U(\vec{x})$

- z.B. harm. Osz.: $U(\vec{x}) = \frac{1}{2}\gamma|\vec{x}|^2$
- Coulomb-Pot.: $U(\vec{x}) = \frac{q}{4\pi\varepsilon_0}\cdot\frac{1}{|\vec{x}|}$

⋮

$$\Rightarrow \boxed{\hat{H} = \frac{1}{2m}|\hat{\vec{P}}|^2 + U(\hat{\vec{X}})}$$

$[H,\hat{P}] \neq 0$ ~~Translationsinvarianz~~

S.Gl.:

$$i\hbar|\dot{\psi}(t)\rangle = \left(\frac{|\hat{\vec{P}}|^2}{2m} + U(\hat{\vec{X}})\right)|\psi(t)\rangle$$

im Ortsdarstellung:

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \left(-\frac{\hbar^2}{2m}\Delta + U(\vec{x})\right)\psi(\vec{x},t)} \quad (*)$$

(E. Schrödinger 1926)

1D

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right)\psi(x,t)$$

(*): lineare, partielle DGL 2. Ord.
im 1+3 Dim.!

Lösungen?

Standardmethode:

(I) bestimme Energieeigenzustände

$$|\phi_0\rangle, \; |\phi_1\rangle, \; |\phi_2\rangle, \; \ldots$$

zu Eigenenergien

$$E_0, \; E_1, \; E_2, \; \ldots$$

als Lösungen der Eigenwertgleichung:

$$H|\phi\rangle = E|\phi\rangle$$

$\rightsquigarrow$ in Ortsdarstellung:

$$|\phi_n\rangle \longrightarrow \phi_n(\vec{x}) = \langle \varphi_{\vec{x}} | \phi_n \rangle$$

Energieeigenzust. Energieeigenfkt.

(I'): bestimme(*) Energieeigenfkten

$$\phi_0(\vec{x}),\ \phi_1(\vec{x}),\ \ldots$$

zu Energieeigenwerten

$$E_0,\ E_1,\ \ldots$$

als Lösungen der E.W.G. in Ortsdarstellung

$$\boxed{\left(-\frac{\hbar^2}{2m}\Delta + U(\vec{x})\right)\phi(\vec{x}) = E\,\phi(\vec{x})}$$

zeitunabhängige Schrödingergl.

(*) normierbare Eigenfkten!

d.h. $\| |\phi_n\rangle \|^2 < \infty$

$$\hookrightarrow \int_{\mathbb{R}^3} d^3\vec{x}\ |\phi_n(x)|^2 < \infty\ !$$

(II): Zeitentwicklungsop. im Energiedarstellung:

$$U_t = \sum_{n=0}^{\infty} e^{-iE_n t/\hbar}\, |\phi_n\rangle\langle\phi_n|$$

$$\rightarrow \quad |\psi(t)\rangle = U_t\,|\psi_0\rangle$$

$$= \sum_{n=0}^{\infty} e^{-iE_n t/\hbar}\, |\phi_n\rangle \underbrace{\langle\phi_n|\psi_0\rangle}_{\psi_n}$$

$\langle\phi_{\vec{x}}| \cdots$

$$|\psi(t)\rangle = \sum_{n=0} e^{-iE_n t/\hbar}\, \psi_n\, |\phi_n\rangle$$

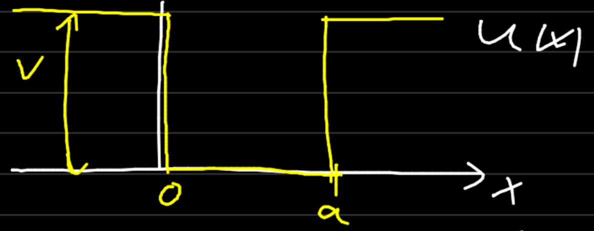
$$\psi(\vec{x},t) = \sum_{n=0}^{\infty} e^{-iE_n t/\hbar}\, \psi_n\, \phi_n(\vec{x})$$

Modellsysteme:

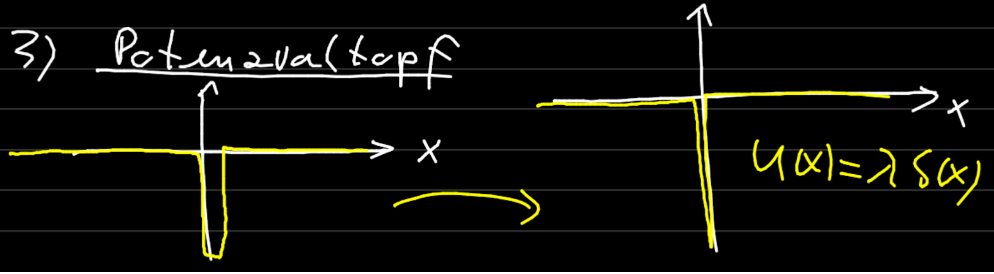
1) freies Teilchen ✓

2) "Teilchen im Kasten"

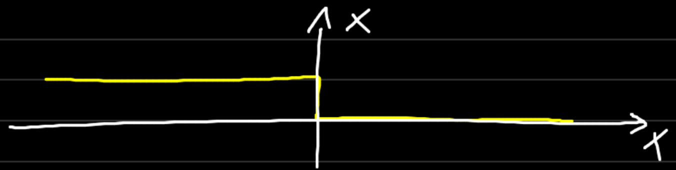
1D:

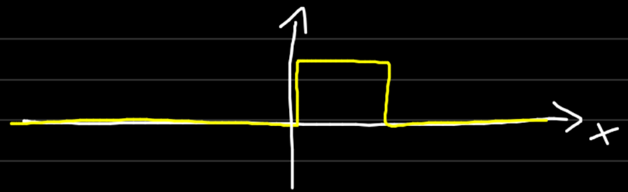


3) Potenzialtopf

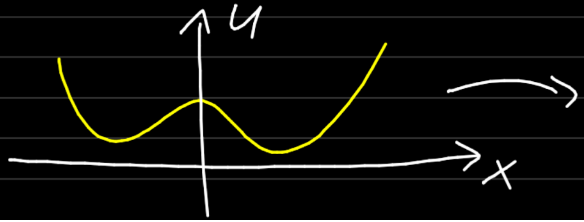


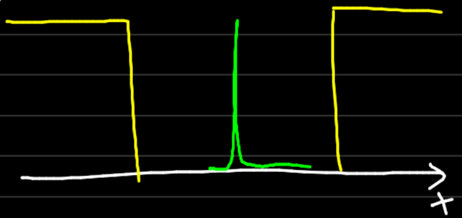
3) Potenzialstufe / -schwelle





4) Doppelmuldenpotenzial → „Doppelkasten"





5) harmonische Oszillator

1) $U(x) = \frac{1}{2}\gamma x^2$

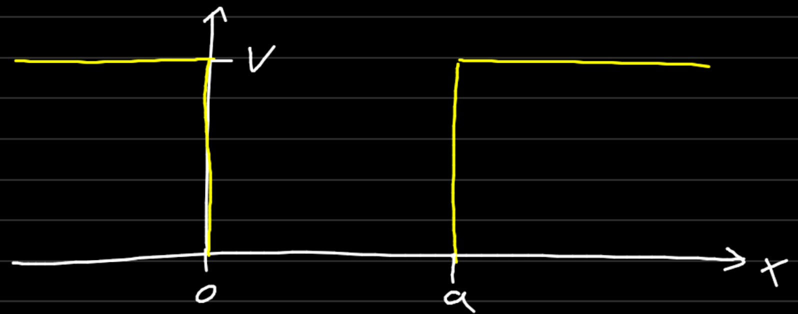
6) Teilchen im Zentralpotenzial

2) → Drehimpuls in der QM

→ H-Atom

1) "Teilchen im Kasten"

1D:
$$U(x) = \begin{cases} V : & x<0,\ x>a \\ 0 : & 0 \le x \le a \end{cases}$$



→ stat. S.G. in 1D:

$$-\frac{\hbar^2}{2m}\phi''(x) + U(x)\phi(x) = E\phi(x)$$

$$\rightarrow \phi''(x) = \frac{2m}{\hbar^2}\left(U(x) - E\right)\cdot\phi(x)$$

Annahme: $0 < E < V$

Fallunterscheidungen

1. $x < 0$: $\phi''(x) = \underbrace{\frac{2m}{\hbar^2}(V-E)}_{\varkappa^2 > 0}\phi(x)$

$$\Rightarrow \quad \phi''(x) = \varkappa^2 \phi(x)$$

$$\varkappa^2 = \frac{2m}{\hbar}(V-E).$$