Zusammenfassung Quantenmechanik

1 Operatoren

Ortsdarstellung:

$$\begin{aligned} \hat{x} &= x \\ \hat{p} &= -i\hbar \overset{x}{\nabla} \end{aligned}$$

Impulsdarstellung:

$$\begin{aligned} \hat{x} &= i\hbar \overset{p}{\nabla} \\ \hat{p} &= p \end{aligned}$$

1.1 Hamiltonoperatoren

freies Teilchen: $\hat{H} = \frac{\hat{p}^2}{2m}$

stationär: $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

harmonischer Oszillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

starrer Rotator: $\hat{H} = \frac{1}{2\Theta}\hat{L}^2$

1.2 weitere Operatoren

$\hat{E} = i\hbar\frac{\partial}{\partial t}$ $\qquad$ $\hat{U}(t) = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t}$

$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$ $\qquad$ $\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$

$\hat{S}_i = \frac{\hbar}{2}\sigma_i$ $\qquad$ $\hat{L} = \hat{x} \times \hat{p}$ $\qquad$ $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$

1.2.1 Anwendung der Operatoren auf jeweilige Eigenzustände

$\hat{a}\left|n\right\rangle = \sqrt{n}\cdot\left|n-1\right\rangle$ $\qquad$ $\hat{a}^\dagger\left|n\right\rangle = \sqrt{n+1}\cdot\left|n+1\right\rangle$

$\hat{L}^2\left|lm\right\rangle = \hbar^2 l(l+)\left|lm\right\rangle$ $\qquad$ $\hat{L}_3\left|lm\right\rangle = \hbar m\left|lm\right\rangle$

$\hat{L}_\pm\left|lm\right\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\left|l\,m\pm 1\right\rangle$

2 Kontinuitätsgleichung

$$\frac{\partial}{\partial t}\rho(\vec{x},t) + \vec{\nabla}\cdot\vec{j}(\vec{x},t) = 0$$

mit:

$$\begin{aligned} \rho(\vec{x},t) &= \Psi^*\Psi \\ \vec{j}(\vec{x},t) &= -\frac{\hbar i}{2m}\left[\Psi^*\left(\vec{\nabla}\Psi\right) - \left(\vec{\nabla}\Psi^*\right)\Psi\right] \end{aligned}$$

3 Schrödingergleichung

$$\hat{H}\Psi = \hat{E}\Psi \quad \Longleftrightarrow \quad \left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

3.1 stationäre Schrödingergleichung

$$\hat{H}\,\Phi(\vec{x}) = E\,\Phi(\vec{x}) \qquad \text{mit } \Psi(\vec{x},t) = \Phi(\vec{x})\ \mathrm{e}^{-\frac{i}{\hbar}E\cdot t} \text{ stationäre Zustände}$$

4 Kommutatoren

$$[A,B] := AB - BA$$

4.1 wichtige Relationen

$$[A, B + C] = [A,B] + [A,C]$$

$$[A, B\ C] = B\,[A,C] + [A,B]\,C$$

$$\big[A,[B,C]\big] + \big[B,[C,A]\big] + \big[C,[A,B]\big] = 0$$

4.2 wichtige Kommutatoren

$$[\hat{x},\hat{p}] = i\hbar \qquad [f(\hat{x}),\hat{p}] = i\hbar\, f'(\hat{x}) \qquad [\hat{x}, f(\hat{p})] = i\hbar\, f'(\hat{p})$$

$$\left[\hat{a}^\dagger,\hat{a}\right] = 1$$

$$\left[\hat{L}_i,\hat{L}_j\right] = i\hbar\,\varepsilon_{ijk}\,\hat{L}_k \qquad \left[\hat{L}_i,\hat{x}_j\right] = i\hbar\,\varepsilon_{ijk}\,\hat{x}_k \qquad \left[\hat{L}_i,\hat{p}_j\right] = i\hbar\,\varepsilon_{ijk}\,\hat{p}_k$$

$$\left[\hat{L}^2,\hat{L}_z\right] = 0 \qquad \left[\hat{L}_+,\hat{L}_-\right] = -2i\left[\hat{L}_x,\hat{L}_y\right] = 2\hbar\hat{L}_z$$

$$\left[\hat{L}^2,\hat{L}_\pm\right] = 0 \qquad \left[\hat{L}_\pm,\hat{L}_z\right] = -i\hbar\,\hat{L}_y \pm i\left(i\hbar\,\hat{L}_x\right) = \pm\hbar\,\hat{L}_\pm$$

5 Pauli-Matrizen

$$\sigma_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

5.1 Eigenschaften

- $\mathrm{Tr}\ \sigma_i = 0$
- $\sigma_i \cdot \sigma_j = \delta_{ij}\mathbb{1} + i\,\varepsilon_{ijk}\,\sigma_k$
- $[\sigma_i,\sigma_j] = 2i\,\varepsilon_{ijk}\,\sigma_k$

6 Dirac-Notation

$$\langle a \mid b \rangle^* = \langle b \mid a \rangle \qquad \left\langle a \middle| \hat{O} \middle| b \right\rangle^* = \left\langle b \middle| \hat{O}^\dagger \middle| a \right\rangle$$

$$\Psi(x) = \langle x \mid \Psi \rangle \qquad \widetilde{\Psi}(p) = \langle p \mid \Psi \rangle$$

$$\hat{x}\,|x\rangle = x\,|x\rangle \qquad \hat{p}\,|p\rangle = p\,|p\rangle$$

$$\int\limits_{-\infty}^{\infty} \mathrm{d}^3x\,|x\rangle\,\langle x| = \mathbb{1} \qquad \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}^3p}{(2\pi\hbar)^3}\,|x\rangle\,\langle x| = \mathbb{1} \qquad \text{(Vollständigkeit)}$$

$$\langle x \mid x' \rangle = \delta(x - x') \qquad \langle p \mid p' \rangle = (2\pi\hbar)^3\,\delta(p - p') \qquad \text{(Orthogonalität)}$$

$$\langle x \mid p \rangle = \mathrm{e}^{i\frac{x\cdot p}{\hbar}} \qquad \langle p \mid x \rangle = \mathrm{e}^{-i\frac{p\cdot x}{\hbar}}$$

7 Störungstheorie

7.1 zeitunabhängig

Hamiltonoperator $\hat{H} = \hat{H}_0 + \hat{V}$ mit $\hat{V}$: Störpotential

bekannt: $\hat{H}_0\left|n^{(0)}\right\rangle = \hat{E}_n^{(0)}\left|n^{(0)}\right\rangle$

Energiekorrektur: $E_n^{(1)} = \langle n^{(0)}|\hat{V}|n^{(0)}\rangle$ $\qquad E_n^{(2)} = \sum\limits_{m\neq n} \dfrac{\left|\langle m^{(0)}|\hat{V}|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}$

Korrektur zur Wellenfunktion: $|n^{(1)}\rangle = \sum\limits_{m\neq n} |m^{(0)}\rangle\,\dfrac{\langle m^{(0)}|\hat{V}|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$