**Einführung in die Physikalische Chemie, Mathematische Methoden (B)**
**SS 14**

**Blatt 8**

**Aufgabe 28**

a)

Ein Operator $\hat{A}$ ist hermitesch wenn gilt: $\int_{-\infty}^{\infty} \Psi * \hat{A} \Psi \, dx = \int_{-\infty}^{\infty} \Psi \hat{A} * \Psi * dx$

Eigenwertgleichung: $\hat{A} \Psi = a \Psi$

$$\int_{-\infty}^{\infty} \Psi * \hat{A} \Psi \, dx = \int_{-\infty}^{\infty} \Psi * a \Psi \, dx = a \int_{-\infty}^{\infty} \Psi * \Psi \, dx = a$$

$$\int_{-\infty}^{\infty} \Psi \hat{A} * \Psi * dx = \int_{-\infty}^{\infty} \Psi a * \Psi * dx = a * \int_{-\infty}^{\infty} \Psi \Psi * dx = a *$$

Somit muss gelten: $a = a^*$ $\Rightarrow$ $a$ ist eine reelle Zahl.

b)

$$\int_{-\infty}^{\infty} \Psi_m^* \hat{A} \Psi_n \, dx = \int_{-\infty}^{\infty} \Psi_n \hat{A} * \Psi_m^* \, dx$$

$$\int_{-\infty}^{\infty} \Psi_m^* \hat{A} \Psi_n \, dx - \int_{-\infty}^{\infty} \Psi_n \hat{A} * \Psi_m^* \, dx \overset{!}{=} 0$$

$$\int_{-\infty}^{\infty} \Psi_m^* \underbrace{\hat{A} \Psi_n}_{a_n \Psi_n} dx - \int_{-\infty}^{\infty} \Psi_n \underbrace{\hat{A} * \Psi_m^*}_{a_m^* \Psi_m^*} dx = a_n \int_{-\infty}^{\infty} \Psi_m^* \Psi_n \, dx - a_m^* \int_{-\infty}^{\infty} \Psi_n * \Psi_m^* \, dx$$

$$= \left(a_n - a_m^*\right) \int_{-\infty}^{\infty} \Psi_m^* \Psi_n \, dx \overset{!}{=} 0$$

Ausdruck wird 0, wenn

1.) $n = m$: $\left(a_n - a_m^*\right)$, da Eigenwerte reel (laut Def. von hermiteschen Operatoren)

2.) $n \neq m$: $\left(a_n - a_m^*\right) \neq 0$ , damit muss $\int_{-\infty}^{\infty} \Psi_m^* \Psi_n \, dx = 0$ sein

c) Impulsoperator: $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

$$\int_{-\infty}^{\infty} \Psi^* \hat{p}_x \Psi \, dx \overset{!}{=} \int_{-\infty}^{\infty} \Psi \; \hat{p}_x{}^* \Psi^* \, dx$$

$$\int_{-\infty}^{\infty} \Psi^* \hat{p}_x \Psi \, dx = \int_{-\infty}^{\infty} \Psi^* (-i\hbar) \frac{d}{dx} \Psi \, dx = -i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{d}{dx} \Psi \, dx$$

part. Integration: $\int u'v \, dx = uv - \int uv' dx$

hier: $u' = \frac{d\Psi}{dx} \;\rightarrow\; u = \Psi$, $\; v = \Psi^* \rightarrow v' = \frac{d\Psi^*}{dx}$

$$-i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{d}{dx} \Psi \, dx = -i\hbar \left( \Psi\Psi^* \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \Psi \frac{d\Psi^*}{dx} dx \right) = -i\hbar \left( - \int_{-\infty}^{\infty} \Psi \frac{d\Psi^*}{dx} dx \right) = \int_{-\infty}^{\infty} \Psi \underbrace{(i\hbar) \frac{d}{dx}}_{\hat{p}_x^*} \Psi^* \, dx$$

$$\int_{-\infty}^{\infty} \Psi \underbrace{(i\hbar) \frac{d}{dx}}_{\hat{p}_x^*} \Psi^* \, dx = \int_{-\infty}^{\infty} \Psi \; \hat{p}_x{}^* \Psi^* \, dx \qquad \text{mit } \Psi(-\infty) = \Psi(\infty) = 0 \qquad \text{q.e.d.}$$

**Aufgabe 29**

a) Bestimmung der Eigenfunktionen $\psi_n$ von $\widehat{H}$ für

$n = 0$: $\quad \psi_0(y) = N_0 e^{-\frac{y^2}{2}}$

$n = 1$: $\quad \psi_1(y) = N_1 \, 2y \, e^{-\frac{y^2}{2}}$

b) Bestimmung der Eigenwerte $E_0$ und $E_1$:

$$\widehat{H}\psi_0 = \frac{\hbar\omega}{2}\left(y^2 - \frac{d^2}{dy^2}\right) N_0 e^{-\frac{y^2}{2}} = \frac{\hbar\omega}{2}(y^2 + 1 - y^2) N_0 e^{-\frac{y^2}{2}} = \frac{\hbar\omega}{2}\psi_0$$

$$\Rightarrow \quad \boxed{E_0 = \frac{\hbar\omega}{2}}$$

$$\widehat{H}\psi_1 = \frac{\hbar\omega}{2}\left(y^2 - \frac{d^2}{dy^2}\right) N_1 \, 2y \, e^{-\frac{y^2}{2}} = \frac{\hbar\omega}{2}(2y + 4y - 2y^3 + 2y^3) N_1 \, e^{-\frac{y^2}{2}}$$

$$= \frac{3\hbar\omega}{2} 2y \, N_1 \, e^{-\frac{y^2}{2}} = \frac{3\hbar\omega}{2}\psi_1$$

$$\Rightarrow \quad \boxed{E_1 = \frac{3\hbar\omega}{2}}$$

# Alle Lösungen ohne Gewähr!!!