Übungsaufgaben X, von 14.1.2002

Musterlösungen

1.

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\psi_{(x,y,z)} = \cos(ax)\cdot\cos(by)\cdot\cos(cz)$$

$$\frac{\partial^2}{\partial x^2}\psi_{(x,y,z)} = -a^2\psi_{(x,y,z)}$$

$$\frac{\partial^2}{\partial y^2}\psi_{(x,y,z)} = -b^2\psi_{(x,y,z)}$$

$$\frac{\partial^2}{\partial z^2}\psi_{(x,y,z)} = -c^2\psi_{(x,y,z)}$$

$$\nabla^2\psi_{(x,y,z)} = -(a^2 + b^2 + c^2)\psi_{(x,y,z)}$$

$\Rightarrow$ $\psi_{(x,y,z)}$ ist Eigenfunktion mit Eigenwert $-(a^2 + b^2 + c^2)$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{(x,y,z)} = \underbrace{\frac{\hbar^2}{2m}(a^2 + b^2 + c^2)}_{E}\psi_{(x,y,z)}$$

2.

$\hat{H}\psi = E\psi$ wobei $\hat{H} = \hat{E}_{kin.} + \hat{E}_{pot.} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$

$$\hat{H}? = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\psi + \frac{1}{2}kx^2\psi$$

Für $\psi_0 = N.e^{-x^2/2\alpha^2}$ mit $N = \frac{1}{\sqrt{\alpha\sqrt{\pi}}}$

$$\hat{H}\psi_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_0 + \frac{1}{2}kx^2\psi_0$$

$$\frac{d}{dx}\psi_0 = -\frac{2x}{2\alpha^2}Ne^{-x^2/2\alpha^2} = -\frac{x}{\alpha^2}Ne^{-x^2/2\alpha^2} = -\frac{x}{\alpha^2}\psi_0$$

$$\frac{d^2}{dx^2}\psi_0 = -\frac{1}{\alpha^2}Ne^{-x^2/2\alpha^2} + (-\frac{x}{\alpha^2}).(-\frac{x}{\alpha^2})Ne^{-x^2/2\alpha^2} = \left(\frac{x^2}{\alpha^4} - \frac{1}{\alpha^2}\right)Ne^{-x^2/2\alpha^2}e^{-ax^2} = \left(\frac{x^2}{\alpha^4} - \frac{1}{\alpha^2}\right)\psi_0$$

$$\Rightarrow \hat{H}\psi_0 = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\psi_0 + \frac{1}{2}kx^2\psi_0 = -\frac{\hbar^2}{2\mu}\left(\frac{x^2}{\alpha^4} - \frac{1}{\alpha^2}\right)\psi_0 + \frac{1}{2}kx^2\psi_0 =$$

$$= -\frac{\hbar^2}{2\mu}\left(\frac{x^2\mu k}{\hbar^2} - \frac{1}{\hbar}\sqrt{\mu k}\right)\psi_0 + \frac{1}{2}kx^2\psi_0 = -\frac{\hbar^2}{2\mu}\cdot\frac{x^2\mu k}{\hbar^2}\psi_0 + \frac{\hbar^2}{2\mu}\frac{\sqrt{\mu k}}{\hbar}\psi_0 + \frac{1}{2}kx^2\psi_0 =$$

$$= \left(-\frac{x^2k}{2} + \frac{\hbar\sqrt{\mu k}}{2\mu} + \frac{x^2k}{2}\right)\psi_0 = \frac{\hbar\sqrt{\mu k}}{2\mu}\psi_0 = \frac{\hbar}{2}\cdot\sqrt{\frac{k}{\mu}}\psi_0 = E_0\psi_0$$

wobei $E_0 = \frac{\hbar}{2} \cdot \sqrt{\frac{k}{\mu}}$

Für $\psi_1 = 2\frac{x}{\alpha} N.e^{-x^2/2\alpha^2}$ mit $N = \frac{1}{\sqrt{2\alpha\sqrt{\pi}}}$

$$\hat{H}\psi_1 = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\psi_1 + \frac{1}{2}kx^2\psi_1$$

$$\frac{d}{dx}\psi_1 = \frac{2}{\alpha}Ne^{-x^2/2\alpha^2} - \frac{2x}{2\alpha^2}\cdot 2\frac{x}{\alpha}Ne^{-x^2/2\alpha^2} = \frac{2}{\alpha}Ne^{-x^2/2\alpha^2} - \frac{2x^2}{\alpha^3}Ne^{-x^2/2\alpha^2}$$

$$\frac{d^2\psi_1}{dx^2} = -\frac{2x}{2\alpha^2}\cdot\frac{2N}{\alpha}e^{-x^2/2\alpha^2} - \frac{2N\cdot 2x}{\alpha^3}e^{-x^2/2\alpha^2} - \frac{2Nx^2}{\alpha^3}\cdot -\frac{2x}{2\alpha^2}e^{-x^2/2\alpha^2} =$$

$$= \frac{2Nx^3}{\alpha^5}e^{-x^2/2\alpha^2} - \frac{2Nx}{\alpha^3}e^{-x^2/2\alpha^2} - \frac{4Nx}{\alpha^3}e^{-x^2/2\alpha^2} =$$

$$= \left(\frac{x^2}{\alpha^4} - \frac{1}{\alpha^2} - \frac{2}{\alpha^2}\right)\psi_1 = \left(\frac{x^2}{\alpha^4} - \frac{3}{\alpha^2}\right)\psi_1$$

$$\Rightarrow \hat{H}\psi_1 = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\psi_1 + \frac{1}{2}kx^2\psi_1 = -\frac{\hbar^2}{2\mu}\left(\frac{x^2}{\alpha^4} - \frac{3}{\alpha^2}\right)\psi_1 + \frac{1}{2}kx^2\psi_1 =$$

$$= \left(-\frac{\hbar^2}{2\mu}\cdot\frac{x^2\mu k}{\hbar^2} - \frac{\hbar^2}{2\mu}\cdot -\frac{3\sqrt{\mu k}}{\hbar}\right)\psi_1 + \frac{1}{2}kx^2\psi_1 = \left(-\frac{kx^2}{2} + \frac{3\hbar\sqrt{\mu k}}{2\mu} + \frac{kx^2}{2}\right)\psi_1 =$$

$$= \frac{3\hbar\sqrt{\mu k}}{2\mu}\psi_1 = \frac{3\hbar}{2}\sqrt{\frac{k}{\mu}}\psi_1 = E_1\psi_1$$

wobei $E_1 = \frac{3\hbar}{2}\sqrt{\frac{k}{\mu}}$

3

Absorption wenn $\Delta E = E_{n+1} - E_n = h\nu = h\frac{c}{\lambda}$

$$\Delta E = E_{n+1} - E_n = \left[\left(n+1+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{\mu}}\right] - \left[\left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{\mu}}\right] = \hbar\sqrt{\frac{k}{\mu}}$$

$$\Rightarrow \hbar\sqrt{\frac{k}{\mu}} = h\frac{c}{\lambda}$$

$$\hbar^2\frac{k}{\mu} = \left(h\frac{c}{\lambda}\right)^2$$

$$\Rightarrow k = \frac{\mu h^2 c^2}{\lambda^2\hbar^2} = \frac{\mu 4\pi^2\hbar^2 c^2}{\lambda^2\hbar^2} = \frac{4\pi^2 c^2}{\lambda^2}\mu$$

$$\mu = \frac{m_H.m_{Cl}}{(m_H + m_{Cl})} = \left(\frac{(1.0078)\cdot(34.969)}{(1.0078)+(34.969)}\right)\cdot 1.6605\cdot 10^{-27}\,kg = 1.6266\cdot 10^{-27}\,kg$$

$$\Rightarrow k = \frac{(39.44).(2.998\cdot 10^8\,ms^{-1})^2}{(3.344\cdot 10^{-6}\,m)^2}\cdot 1.6266\cdot 10^{-27}\,kg = 516\,Nm^{-1}$$

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4. $\int \psi^* \psi d\tau = 1$

a) $\psi = N\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}$

$$\int \psi^* \psi d\tau = N^2 \int_0^\infty \left(2 - \frac{r}{a_0}\right)^2 e^{-r/a_0} \underbrace{d\tau}_{r^2 \sin\theta dr d\theta d\phi} = N^2 \int_0^\infty r^2 \left(2 - \frac{r}{a_0}\right)^2 e^{-r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi =$$

$$= N^2 \int_0^\infty r^2 \left(4 - \frac{4r}{a_0} + \frac{r^2}{a_0^2}\right) e^{-r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = N^2 \int_0^\infty \left(4r^2 - \frac{4r^3}{a_0} + \frac{r^4}{a_0^2}\right) e^{-r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi =$$

$$= N^2 \cdot \left(4 \cdot 2a_0^3 - \frac{4}{a_0} \cdot 6a_0^4 + \frac{1}{a_0^2} \cdot 24a_0^5\right) \cdot (2) \cdot (2\pi) = N^2 \cdot 8a_0^3 \cdot 4\pi = 32\pi a_0^3 N^2 = 1$$

für $N = \sqrt{\frac{1}{32\pi a_0^3}}$

$$!\left(\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}\right)!$$

b) $\psi = N \cdot r \cdot \sin\theta \cdot \cos\phi \cdot e^{-r/2a_0}$

$$\int \psi^* \psi d\tau = N^2 \int_0^\infty r^2 \sin^2\theta \cos^2\phi e^{-r/a_0} \underbrace{d\tau}_{r^2 \sin\theta dr d\theta d\phi} = N^2 \int_0^\infty r^2 \cdot r^2 e^{-r/a_0} dr \int_0^\pi \sin^2\theta \sin\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi =$$

$$= N^2 \int_0^\infty r^4 e^{-r/a_0} dr \int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi = N^2 \cdot ((4!) \cdot a_0^5) \cdot \int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi$$

$$\int_0^\pi \sin^3\theta d\theta = \left(-\cos\theta + \frac{1}{3}\cos^3\theta\right)\Big|_0^\pi = \left(\frac{2}{3} + \frac{2}{3}\right) = \frac{4}{3}$$

$$\int_0^{2\pi} \cos^2\phi d\phi = \left(\frac{1}{2}\phi + \frac{1}{4}\sin 2\phi\right)\Big|_0^{2\pi} = \left(\pi + \underbrace{\frac{1}{4}\sin 4\pi}_{0} - 0\right) = \pi$$

$$\Rightarrow N^2 \cdot ((4!) \cdot a_0^5) \cdot \int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi = N^2 \cdot 24a_0^5 \cdot \frac{4}{3} \cdot \pi = 32\pi a_0^5 N^2 = 1$$

für $N = \sqrt{\frac{1}{32\pi a_0^5}}$

$$!\left(\int \sin^3 x dx = -\cos x + \frac{1}{3}\cos^3 x\right)!$$

$$!\left(\int \cos^2 x dx = \frac{1}{2}x + \frac{1}{4}\sin 2x\right)!$$