6. Tutorium - Quantentheorie I - 07.12.2012 - Lösung

1

$$V(x) = \frac{1}{2}K\Big(x - x_0\Big)^2$$

wobei:
x ... Abstand der Atome
x_0 ... Gleichgewichtsposition

$$\text{reduzierte Masse: } m = \frac{m_1 \cdot m_2}{m_1 + m_2}$$

$$\text{harmonischer Oszillator} \quad \ddot{x} + \omega_0^2 x = 0$$

$$F = m \cdot a = -kx \longrightarrow \ddot{x} + \omega_0^2 x = 0 \qquad \omega_0 = \sqrt{\frac{k}{m}} = 2\pi f$$

allg. (konservatives) Kraftfeld: $\vec{F} = -\vec{\nabla} V$

Taylorreihe:

$$V(x) = V(x_0) + \frac{\partial V}{\partial x}(x_0)(x - x_0) + \frac{1}{2}\frac{\partial^2 V}{\partial x^2}(x_0)(x - x_0)^2 + \dots$$

$\longrightarrow x \dots min = \frac{\partial V}{\partial x} = 0$

$$\longrightarrow V(x) \sim \frac{1}{2}\underbrace{\frac{\partial^2 V}{\partial x^2}}_{K}(x - x_0)^2 = \frac{1}{2}K(x - x_0)^2$$

b)

$$\longrightarrow E_n = \hbar\omega\Big(n + \frac{1}{2}\Big) \qquad n = 0, 1, 2, \dots$$

$$E_0 = \frac{\hbar\omega}{2} \qquad \omega = \sqrt{\frac{k}{\mu}} \qquad \mu = 320\ \Big[\frac{N}{m}\Big]$$

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \xrightarrow{m_1 = m_2 = m} \frac{m^2}{2m} = \frac{m}{2}$$

$$Cl_{17} - Cl_{17}$$

$$1 \times Cl_{17} \longrightarrow 35.45 \longrightarrow 1u = 1.66 \cdot 10^{-27}\ kg \longrightarrow \mu = \frac{1.66}{2} \cdot 10^{-27}\ kg$$

$$E_0 = \frac{\hbar\omega}{2} = \frac{\hbar}{2} \cdot \sqrt{\frac{k}{\mu}} = 2.049 \cdot 10^{-19}\ J = 1.28\ eV$$

c)

$$E_1 = \hbar\omega\Big(1 + \frac{1}{2}\Big) = \frac{3\hbar\omega}{2} \qquad\qquad \omega = \sqrt{\frac{k}{\mu}} = 6.2 \cdot 10^{14}\ \frac{1}{s}$$

$$\Delta E = E_1 - E_0 = \underbrace{\frac{3\hbar\omega}{2}}_{=E_1} - \frac{\hbar\omega}{2} = \frac{3\hbar\omega - \hbar\omega}{2} = \hbar\omega = 2.5\ eV$$

$$\Delta E = \hbar\omega \ \longrightarrow\ \underbrace{\omega}_{=2\pi f} = \frac{\Delta E}{\hbar}$$

$$f = \frac{2\pi\Delta E}{\hbar} = \underbrace{3.8 \cdot 10^{15}\ \frac{1}{s}}_{\text{UV}}$$

d)

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

$$E = V(x) = \frac{1}{2}m\omega^2 x^2 \ \longrightarrow\ x_{1,2} = \pm\sqrt{\frac{2E}{m\omega^2}}$$

$$\Big|W(x)\Big|^2 = \int \psi^\dagger \psi\ dx$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$$

$$\longrightarrow W(x)_{verboten} = 1 - \int_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}} \psi_0^\dagger\ \psi_0\ dx = 1 - \int_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{\hbar}x^2}\ dx$$

mit

$\mu = \frac{1.66}{2} \cdot 10^{-27}\ kg$ $\qquad$ $k = 320\ \left[\frac{N}{m}\right]$

$\hbar = 6.6 \cdot 10^{-34}\ Js$ $\qquad$ $x_{1,2} = \sqrt{\frac{2E}{m\omega^2}} = \pm 3.54 \cdot 10^{-11}$

$\sqrt{\frac{m\omega}{\hbar\pi}} = 1.58 \cdot 10^{10}$ $\qquad$ $\frac{m\omega}{\hbar} = 7.79 \cdot 10^{20}$

$$\longrightarrow\ \Big|W(x)\Big|_{verboten} = 1 - \underbrace{\int_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{\hbar}x^2}\ dx}_{\text{erlaubter Bereich}} =$$

$$= 1 - \int_{-3.54\cdot 10^{-11}}^{3.54\cdot 10^{-11}} 1.58 \cdot 10^{10} \cdot e^{-7.79\cdot 10^{20}x^2}\ dx = 0.1595$$

Wolframalpha-Code für die numerische Integration:

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1-NIntegrate[1.58*10^10*Exp[-7.79*10^20*x^2],
{x, -3.54*10^-11, 3.54*10^-11}]
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