UMWELTCHEMIE I

Theoretische Grundlagen der Umweltchemie II

WS 2003/04

Lösung zu Übung 2

Aufgabe 1

1.1 (a) $\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p} = \frac{h}{mv} = \dots = 3{,}7\cdot 10^{-63}\,\mathrm{m}$

(b) $\lambda = \dots = 8{,}5\cdot 10^{-36}\,\mathrm{m}$ für $m = 70\,\mathrm{kg}$, $v = 4\,\mathrm{km\,h^{-1}}$

1.2 (a) $E_{kin} = \frac{p^2}{2m_e} = \frac{1}{2m_e}\left(\frac{h}{\lambda}\right)^2 = 2{,}4\cdot 10^{-17}\,\mathrm{J}$ $= 151\,\mathrm{eV}$

(b) $E_{kin} = \frac{1}{2m_p}\left(\frac{h}{\lambda}\right)^2 = 1{,}3\cdot 10^{-20}\,\mathrm{J} = 0{,}08\,\mathrm{eV}$

1.3 $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_e E_{kin}}} = \dots = 4{,}6\,\text{Å}$

„Volumen" eines Kupferatoms:

$V = \frac{M/N}{\rho} = 1{,}2\cdot 10^{-29}\,\mathrm{m}^3$

Atomabstand: ungefähr gleich $\sqrt[3]{V} = 2{,}3\,\text{Å}$ (gleiche Größenordnung wie λ!)

Aufgabe 2

$$\Delta p \approx \frac{\hbar}{2\Delta x} = 5{,}3\cdot 10^{-26}\ \mathrm{kg\,m\,s^{-1}}$$

$$\Delta v = \frac{\Delta p}{m} \approx 5{,}3\cdot 10^{-26}\ \mathrm{m\,s^{-1}}$$

Aufgabe 3

3.1 ERRATUM: $\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}\,dx = \frac{\sqrt{\pi}}{2\alpha^{3/2}}$

$$\Delta x = \sqrt{Var[x]} = \sqrt{\int_{-\infty}^{\infty}(x-\langle x\rangle)^2|\Psi(x)|^2dx}$$

$$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\Psi(x)|^2\,dx = 0, \text{ da } |\Psi(x)| = |\Psi(-x)|$$

$$(\Delta x)^2 = \frac{1}{\sqrt{2\pi}\,\sigma_x}\int x^2 e^{-x^2/2\sigma_x^2}\,dx = \frac{1}{\sqrt{2\pi}\,\sigma_x}\cdot\frac{\sqrt{\pi}}{2\left(\frac{1}{2\sigma_x^2}\right)^{3/2}} = \dots = \sigma_x^2 \qquad \text{Q.E.D.}$$

3.2 $$a(k) = \text{const.}\int_{-\infty}^{\infty}\Psi(x)\,e^{-ikx}\,dx = \text{const.}\int_{-\infty}^{\infty}\exp\left[-\frac{1}{4\sigma_x^2}x^2 - i(k-k_0)x\right]dx$$

$$[\dots] = -\frac{1}{4\sigma_x^2}\left[x^2 - 4i\sigma_x^2(k-k_0)x\right]$$

$$= -\frac{1}{4\sigma_x^2}\Big[\underbrace{x^2 - 4i\sigma_x^2(k-k_0)x + (2i\sigma_x^2(k-k_0))^2}_{(x-2i\sigma_x(k-k_0))^2}\ \underbrace{-(2i\sigma_x^2(k-k_0))^2}_{+4\sigma_x^4(k-k_0)^2}\Big]$$

$$a(k) = \text{const.}\int_{-\infty}^{\infty} e^{-\frac{1}{4\sigma_x^2}[x-2i\sigma_x(k-k_0)]^2}\,dx \cdot e^{-(k-k_0)^2\sigma_x^2}$$

$$= \text{const.}\sqrt{\frac{\pi}{1/4\sigma_x^2}}\ e^{-(k-k_0)^2\sigma_x^2}$$

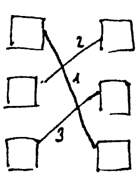
3.3 $$\phi(p) = \sqrt{\frac{2\pi}{\hbar}}\ a\left(\frac{p}{\hbar}\right) = \text{const.}\ e^{-(k-k_0)^2\sigma_x^2}$$

$$= \text{const.}\ e^{-\frac{\sigma_x^2}{\hbar^2}(p-p_0)^2}$$

$$\stackrel{!}{=} \text{const.}\ e^{-(p-p_0)^2/4\sigma_p^2}$$

$$\Rightarrow \frac{1}{4\sigma_p^2} = \frac{\sigma_x^2}{\hbar^2} \Rightarrow \sigma_x\sigma_p = \frac{\hbar}{2}$$

3.4



1) σ_x groß, σ_k klein

2) σ_x groß, σ_k klein
Farben gehen in die andere Richtung (violett-blau-grün-gelb-rot)
$\Rightarrow$ k_0 negativ

3) σ_x klein, σ_k groß