**Exe 3: Excercises for (Physical and) Theoretical Chemistry**

WS 2002/03 $1^{st}$ IGS semester Excercises No. 3

*hand out: Mo, 28.10.02, return: Wed, 6. Nov., mail-box, AR-K6 left side wall.*

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**9)** Stationary States: Given the simple state function $\phi(x,t) = \psi(x) \cdot e^{i\omega t}$ . Evaluate the probablity destribution $W(x,t) = \phi^* \cdot \phi$ . What is $dW/dt$ ?

**10)** Heisenberg uncertainty: A particle of mass $M$ is "moving forth and back" with momentum $\pm p$ in a linear box of length $L$. The positional smearing of the stationary quantum state is $\Delta x^2 = L^{-1} \cdot \int_0^L dx(x - L/2)^2$. The kinetic energy of the quantum state of quantum number $n$ is $T = p^2/2M = n^2\pi^2\hbar^2/2ML^2$. The momentum smearing for $\pm p$ is $\Delta p^2 = Ave[(0 \pm p)^2] = p^2$. Evaluate the "fuzziness product" $\Delta x \cdot \Delta p$ .

**11)** Order of magnitude of atoms: In an atom with nuclear charge $+Ze$ the electrons are distributed in x-direction between $-R, +R$, $\Delta x \sim R \sim$ atomic radius. The nuclear-electron attraction energy is $V \sim Ze \cdot -e/R$. Similarly, the momenta in $x$-direction are distributed between $-P$ and $+P$, $\Delta p \sim P$ and the kinetic energy is $T = P^2/2m$. Assume $\Delta x \cdot \Delta p \sim n \cdot \hbar$. Search for the smallest energy. Give $P, R, T, V, E$. What are the ratios of $T : V : E$ ?

**12)** Heavy Atoms: Choose $n = 1$. What is the electron's velocity $v$ for nuclear charge $Z$? It's relativistic effective mass is not 1 but $1/\sqrt{1 - (v/c)^2}$. How does $R$ change due to relativity? How many % for Hg ($Z = 80$)?