Exe 2: Excercises for (Physical and) Theoretical Chemistry
WS 2002/03 1^{st} IGS semester Excercises No. 2
hand out: Fr. 25.10.02, return: 30.10., mail-box, AR-K6 left side wall.

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5) Show that the operator d^2/dx^2 is hermitean for the functions which vanish on the boundary.

6) Given the orthonormal basis $b_1 = sin(kx)/\sqrt{\pi}$, $b_2 = cos(kx)/\sqrt{\pi}$ (k integer) on the x-domain $[-\pi, +\pi]$. a) Represent the operators $\mathbf{Op_1} = i \cdot d/dx$ and $\mathbf{Op_2} = -d^2/dx^2$ in this basis by matrices O_1 and O_2 (determine at least one matrix element by integration). b) Calculate the product of the two matrices $O_1 * O_1$. Comment on the result. (Note: In the present case, the boundary terms are not zero individually, but still cancel each other).

7) a) According to Heisenberg's fuzziness (Unschärfe, uncertanity) relation, causality is violated in the microscopic domain. b) Therefore safe statements about atomic processes are impossible. c) An experimentalist measures property a of a molecule several times and always obtains the value a_0. He says that he now knows the wavefunction of the molecule: it is $\psi_0(x)$, obtained from $\mathbf{a} \circ \psi = \psi \cdot a$ upon inserting a_0 for a. d) His colleague says: something must be wrong with his experiment, because according to Heisenberg's principle the measurement of a cannot always give exactly the same value a_0.
What is right or wrong among a) to d), and why?

8) A small spherical bacteria, still visible in a light-microscope, has a diameter of $1\mu m$ and a density comparable to water. You determine its position with an accuracy of $0.5\mu m$ looking at it under blue light. What is the resluting velocity fuzziness ($\Delta v =?\ \mu m/h$)? What is the corresponding kinetic energy $E_{kin} = m \cdot \Delta v^2/2 = 1/2m\Delta x^2$? Compare with $E_{therm} = 3/2 \cdot kT$ at $T = 300\,\mathrm{K}$. a) give Δx in a.u.; b) mass in a.u.; c) Δv from $\Delta x \cdot m\Delta v \sim 1\hbar$; d) E_{kin} and E_{therm} in same units.