Computer course

Winter semester 13/14

4. Exercise

Main focus: Distribution Functions
Normalisation
Expectation values
Partial differential equations
Standard deviation

1. Normalise the following probability densities:

   (a) Gauss function

   $$w_G(x) = exp(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}) \tag{1}$$

   (b) Cauchy-Lorentz function

   $$w_L(x) = \frac{\sigma}{x^2+\sigma^2} \tag{2}$$

   Calculate for Gauss and Lorentz distribution functions of random variable x, the expectation values and the standard deviations.

2. The Maxwell-Boltzmann distribution $w(v)$ for the speed of particles of mass m in gases at Temperature T is a statistic distribution in classical physics.

   $$w(v) = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{3/2} exp\left(-\frac{mv^2}{2kT}\right) \tag{3}$$

   (k is Boltzmann's constant). Verify that the distribution is normalized! Determine the average speed $< v >$ and kinetic energy $< e_{kin} >$ of a molecule.

3. An electron is confined in a molecule of length $L = 1$ nm. Calculate its ground state energy and the first excitation energy in the approximation of an infinitely strong binding potential. What is the probability P to find the electron in the range between $x = 0$ and $x = 0.2$ nm in the ground state?