Freie Universität Berlin
Fachbereich Physik
Prof. Dr. Roland Netz
http://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-netz/lehre

17.12.2018
Due date: 07.01.2019

Advanced Statistical Physics II – Problem Sheet 9

Problem 1 – Discretization
Consider the following three finite differences:

- Forward difference $\Delta_h[f](x) = f(x+h) - f(x)$
- Backward difference $\Delta_{-h}[f](x) = f(x) - f(x-h)$
- Central difference $\Delta_{h/2}[f](x) = f\left(x + \frac{1}{2}h\right) - f\left(x - \frac{1}{2}h\right)$

a) (4P) Calculate the error between the three finite differences and the first derivative $\frac{\Delta[f](x)}{h} - f'(x)$ using Taylor expansion.

b) (3P) Considering the ordinary differential equation

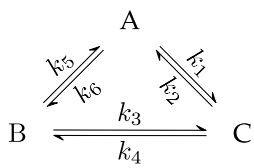
$$\frac{d^2}{dx^2}u(x) = f(x) \quad x \in [0,1] \tag{1}$$

with boundary conditions $u(0) = u(1) = 0$. Discretize the interval $[0,1]$ uniformly into n points using the central difference and rewrite (1) as a linear system:

$$A_{i,j}u_j = f_i \tag{2}$$

Find the entries of the matrix A.

Problem 2 – Reaction rate kinetics
Consider the three state model with transition rates $k_1, k_2, k_3, k_4, k_5, k_6$



of chemical substances A, B and C.

a) (3P) Write down the chemical kinetics equations for this reaction as a function of the concentrations $\phi_A(t), \phi_B(t)$ and $\phi_C(t)$.

b) (3P) Assume, that no particles can enter or leave the system, such that the sum of the masses of the substances is conserved and the transition rates $k_2 = k_3 = k_6 = 0$ and $k_5 = k_1$. Find the stationary state.

c) (2P) Which is the value of k_4 to obtain $\phi_A = \phi_B = \phi_C = 1/3$?

d) (5P) Considering the initial condition $\phi_A(0) = 1$ and $\phi_B(0) = \phi_C(0) = 0$ and the transition rates $k_2 = k_6 = k_3$, $k_1 = 0$ and $k_5 = k_4$.
$k_2 = k_6 = k_4, k_1 = 0, k_5 = k_3$
Solve the differential system for $\phi_A(t)$ and $\phi_B(t), \phi_C(t)$.

Hint: Use the Laplace transform $\hat{f}(s) = \int_0^\infty e^{-st} f(t)dt$ and the properties $\int_0^\infty dt f'(t)e^{-st} = s\hat{f}(s) - f(0)$ and $\hat{f}(s) = \frac{1}{s-a}$ for $f(t) = e^{at}$.