

Frankfurt, June 11, 2013

Exercises for Computational Methods in Solid State Theory
SS 2013

Exercise Set 5

(Due date: Monday, June 19, 2013)

Exercise 5 (Monte Carlo) (10 points)

a) **Monte Carlo integration.**

Calculate the following definite integrals a la Monte Carlo:

$$(1) \quad I_1 = \int_0^1 dx \frac{1}{\sqrt{x}},$$

$$(2) \quad I_2 = \int_0^3 dx \exp(-x^2).$$

Give the result including the standard deviation using the three-sigma rule. Show your estimates using 10^3 , 10^5 , and 10^7 samples.

b) **Monte Carlo sampling (i).**

Sample values from an exponential distribution e^{-x} between $x = 0$ and $x = 1$ using

- inverse sampling.
- the rejection-sampling algorithm.

c) **Monte Carlo sampling (ii).**

Modify the rejection-sampling algorithm to sample from tabulated data. Sample:

- polar scattering angles from the given differential cross section for elastic scattering (DCES) of electrons by atoms,
- energy losses from the given differential inelastic inverse mean free path (DIIMFP) for 500-eV electrons moving in polycrystalline Al.

Make a histogram of the sampled values and compare it with the original distributions.