RWTH Aachen — Institute for Theoretical Solid State Physics

Computational Physics (SS 2020)

Prof. Dr. Riccardo Mazzarello

Sheet 1 (20 points)
Submission: 16 April, 2020, 10:00 a.m.

Important remarks

- Please hand in your solutions in teams of two students.
- Provide a *single* PDF-file containing the written solutions of all exercises, i. e. analytical derivations, numeric results, their interpretation, etc. If it contains a scan, please make sure it is well readable. Plots can either be embedded into this file or, alternatively, given separately (e. g. as PNG-files) and referred to in the PDF.
- Use a current version of Python 3 for your implementations.
- Write readable and *commented* code with self-explanatory variable names.
- Please hand in your solutions (PDF-file with answers, source code files, and, if not embedded in the PDF, PNG-files of plots) as a **single** ZIP-file named

  Surname1-MatNum1-Surname2-MatNum2-SheetX.zip,

  where MatNum is your matriculation number, by uploading it to RWTH Gigamove (`https://gigamove.rz.rwth-aachen.de`). Please send the download link using your RWTH address to

  manconi@physik.rwth-aachen.de

  and write in the object of the email

  CP SheetX - Surname1-MatNum1-Surname2-MatNum2.

1. **Derivative Formula** (3 points)

   Prove the following 5-point formula for the second derivative, paying attention to correctly handling the error terms:

$$f''(x) = \frac{-\frac{1}{12}f(x+2h) + \frac{4}{3}f(x+h) - \frac{5}{2}f(x) + \frac{4}{3}f(x-h) - \frac{1}{12}f(x-2h)}{h^2} + \mathcal{O}(h^4)$$

2. **Simpson Rule** (4 points)

   - Implement the Simpson rule for the numerical integration of a function $f(x)$ on a finite interval $x \in [a, b]$ using N points of function evaluation, where N is allowed to be even or odd.

- Test your code by integrating $f(x) = \sin(x)$ on the interval $[0, \pi/2]$ for different values of h. Plot the deviation from the analytical result together with the theoretical discretization error against h in a log–log plot. Explain the behavior of the deviations for values of h around and below 10^{-4}.

3. **Romberg Integration** (13 points)

- Show that the second column of the Neville scheme (i.e. the R_{n1}) in the Romberg integration method corresponds to the Simpson rule. (5 points)
- Implement the Romberg integration scheme and calculate the following integrals. For each test function, calculate and plot logarithmically the deviation of the R_{ii} in the Neville scheme from the analytical result against increasing i. Interpret your results. (8 points)

$$(i) \int_0^1 e^x \,\mathrm{d}x \qquad (ii) \int_0^{2\pi} \sin^4(8x)\,\mathrm{d}x \qquad (iii) \int_0^1 \sqrt{x}\,\mathrm{d}x$$