3. Exercise for Computational Physics I

Linz, Theoretische Physik, WS 2025

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5. Show that the derivative of a function $f(x)$ can be calulated with the help of Fouriertransformation as follows:

$$f'(x) = \mathrm{FT}^{-1}[i\,q\,F(q)]$$

where FT^{-1} is the inverse Fouriertransformation.

6. *Numerical Differentiation:*

Calculate the first derivative $f'(x)$ of the Gaussian function $f(x) = e^{-x^2/(2\sigma^2)}$.

(a) Calculate $f'(x)$ using the forward or backward difference. Try different step sizes h and compare with the analytical result. Confirm that the error of the numerical differentiation scales as shown in the lecture.

(b) Calculate $f'(x)$ using the central difference. Try again different step sizes h and compare with the analytical result. Confirm again that the error of the numerical differentiation scales as shown in the lecture.

(c) Use your program from problem 4 to calculate $f'(x)$ via Fourier transformation – alternatively you can use the FFT algorithm for DFT via a library of your choice (the best known is the "FFTW" library). How does the result depend on step size and interval size? Compare the results for $f'(x)$ with those obtained in (a) and (b) (plot the error).