2. Exercise for Computational Physics I

Linz, Theoretische Physik, WS 2025

Due date: Oct. 20, 2025

3. *Proof of orthogonality:*

   In class we defined the N-dimensional vectors $\mathbf{z}^k = (z_0^k, \ldots, z_{N-1}^k)$ where $z_j = e^{i2\pi j/N}$. Show that these vectors are orthogonal, i.e. that

$$\frac{1}{N}\langle \mathbf{z}^k | \mathbf{z}^{k'} \rangle = \delta_{kk'}$$

4. We want to Fourier transform the Gaussian function $f(x) = e^{-x^2/(2\sigma^2)}$.

   (a) The Fourier transform $F(q)$ of $f(x)$ can be calculated analytically. Show that

$$F(q) = \sqrt{2\pi} s\, e^{-q^2\sigma^2/2}$$

   Let $[-a, a]$ be a sufficiently large interval such that the Gaussian "fits" well inside ($f(x)$ should be small for $x = -a$ and a). We define the grid points $x_j = -a + j\frac{2a}{N}$, $i = 0, \ldots, N-1$ and get the corresponding discretized function $f_j = f(x_j)$.

   Use the DFT to obtain the approximate Fourier transform $F(q)$ using the DFT of f_j,

$$F_k = \sum_{j=0}^{N-1} e^{-i2\pi kj/N} f_j$$

   Calculate F_k simply by "brute-force" (i.e. not the Fast-Fourier-Transform algorithm).

   (b) For a given choice of the width σ try different values for the interval bound a. How does the choice of a affect the result? Compare with the analytical result for $F(q)$. Make plots where the difference between exact and numerical result can be assessed.

   (c) Try different grid sizes N. How does the choice of N affect the result? Compare again with the analytical result for $F(q)$.

   (d) Calculate the inverse Fourier transform of $F(q)$ by using DFT^{-1}, and check if you get the correct result.