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— Computational Quantum Physics —

2 July 2018
Sommersemester

Exercise 5

Task 1: Harmonic oscillator I (6 points)

a) Write down the explicit wavefunctions $\psi_n(x)$ for the harmonic oscillator for $n = 0, 1, 2$ and plot the corresponding probability densities for the case $\hbar = \omega = m = 1$.

Consider a particle of mass m in the potential of a harmonic oscillator with angular frequency ω. At the time $t = 0$, the particle is described by the (normalized) wavefunction

$$\phi(x, 0) = C \cdot \left[2 \left(\sqrt{\frac{m\omega}{\hbar}}\, x - 1 \right)^2 - 3 \right] \cdot \exp\left(-\frac{m\omega}{2\hbar} x^2 \right), \qquad C = \frac{1}{\sqrt{10}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4}.$$

b) Find the time evolution $\phi(x, t)$ of the particle for $t \geq 0$.

c) What is the probability of finding the particle at the time $t \geq 0$ in the n-th energy level? What is the expectation value of the energy at $t \geq 0$?

Task 2: Harmonic oscillator II (6 points)

Solve the one-dimensional Schrödinger equation for the harmonic oscillator ($\hbar = \omega = m = 1$) numerically by applying a 2nd-order finite-difference scheme.

a) Compute and plot the lowest few eigenstates.

b) Plot the lowest eigenvalues. Compare to the exact values and explain the differences.

c) Repeat the last task for a 4th-order finite-difference scheme.

Task 3: Dispersion relation for a free particle (6 points)

Solve the free Schrödinger equation ($\hbar = m = 1$) by applying a 2nd-order finite-difference scheme.

a) Plot the lowest few eigenstates and obtain an expression for the wavenumber $k_n = \frac{2\pi}{\lambda_n}$ associated with the n-th eigenstate.

b) Plot the energy as a function of the wavenumber and compare the numerical results to the exact dispersion relation $E = \frac{k^2}{2}$.

c) The exact solution of the free Schrödinger equation is $\Psi_i = \exp(ikx_i)$, $k = p/\hbar$. Substitute this exact solution into the into the discretized Schrödinger equation in order to explain the difference between the numerical and exact results.

d) Repeat a) and b) with a 4th-order finite-difference scheme.