Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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Exercise sheet 5

To be handed in on 15.11.2023 and discussed on 17.11.2023 and 20.11.2023.

Exercise 1 [*Finite potential well*] (0+3+3=6 pts.)

When calculating energy eigenvalues of the finite potential well in quantum mechanics, transcendental equations arise which cannot be solved analytically.

(i) Repeat the basics of this problem using a quantum mechanics textbook of your choice (e.g. F. Schwabl, "Quantenmechanik", chapter 3.4 or W. Nolting, "Grundkurs Theoretische Physik 5/1", chapter, 4.2).

(ii) The transcendental equations are

$$+q\,\tan(q) = \sqrt{\xi^2 - q^2} \quad \text{and} \quad -\,q\,\cot(q) = \sqrt{\xi^2 - q^2}\,,$$

where q is the dimensionless wave number and ξ is a dimensionless number, that characterizes the potential well. Thereby the condition $0 \leq q \leq \xi$ applies. Use $\xi = 5$ and scan both equations for all existing solutions q graphically by generating suitable plots.

(iii) Determine these solutions with the Newton-Raphson method up to a precision of four decimal places. How does the graphical solution from task (ii) help here?

Exercise 2 [*The Schrödinger equation*] (2+4+4+4=14 pts.)

Consider a quantum mechanical system with a particle of mass m moving in one dimension in the potential

$$V(x) = \frac{1}{2}\,m\,\omega^2\,x^2 + \lambda\,x^4\,,$$

where ω and λ are parameters of the system.

(i) Write down the Schrödinger equation. Introduce dimensionless quantities in order to facilitate a numerical study of the problem. Is it possible, like in the example of the harmonic oscillator discussed in the lecture, to study the system for an arbitrary set of parameters m, ω and λ with a *single* numerical simulation? If not, which are the dimensionless quantities that characterize different physical situations?

(ii) To solve the Schroedinger equation numerically and obtain the energy eigenvalues and the wave functions of the system, implement the *shooting*-algorithm discussed in the lecture. Which boundary and/or initial conditions are advantageous?

(iii) Test your code in the small-λ regime by computing the ground-state energy. Obtain analytically a good approximation of the result making use of the time-independent perturbation theory at first order and compare it with the output of your code.

(iv) Use your code to determine the first *three* energy levels for the cases

$$\frac{2\,\hbar\,\lambda}{m^2\,\omega^3} = 0.1 \qquad \text{and} \qquad \frac{2\,\hbar\,\lambda}{m^2\,\omega^3} = 10.0 \quad .$$

Interpret your results. What do you expect for very large values of λ?