

Prof. Marc Wagner NUMERISCHE METHODEN DER PHYSIK



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Exercise sheet 4

To be discussed on 25 and 28 May

Exercise 1 [The Schrödinger equation]

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 for example as discussed in the lecture for the harmonic oscillator, 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 which characterise different physical situations?
- (ii) To numerically obtain the energy eigenvalues and the wave functions of the system solving the Schrödinger equation, 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 calculating 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 setting

$$\frac{2\hbar\lambda}{m^2\omega^3} = 0.1$$
 and $\frac{2\hbar\lambda}{m^2\omega^3} = 10.0$

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

