Numerical modelling of quantum harmonic oscillator

Pawel Czyz

St Hugh's College, University of Oxford,
St Margaret's Road, Oxford OX2 6LE, UK

Abstract. We present a Python module implementing various ODE solvers, enabling one to do accurate and effective numerical simulations. We investigate it's accuracy investigating a quantum harmonic oscillator in position basis.

Keywords: numerical modelling, Numerov's algorithm, quantum systems, harmonic oscillator

1 Introduction

Numerov's method [1] allows one to solve differential equations of kind:

$$y''(x) = f(x) \cdot y(x) \tag{1}$$

Examples of equation (1) include classical harmonic oscillator:

$$y''(x) = -\omega^2 \cdot y(x) \tag{2}$$

or one-dimensional, time-independent Schrodinger's equation:

$$y''(x) = \frac{2m}{\hbar^2}(E - V(x)) \cdot y(x). \tag{3}$$

Numerov's iterative metod uses an equidistant grid [1,2] $x_n = \delta n$ on which approximates y_i values via equation:

$$\left(1 - \frac{\delta^2}{12} f_{n+2}\right) y_{n+2} = \left(2 + \frac{5}{6}\delta^2 f_{n+1}\right) y_{n+1} - \left(1 - \frac{\delta^2}{12} f_n\right) y_n, \tag{4}$$

where $f_i = f(x_i)$. Equation (4) can be solved for arbitrary n knowing the values y_0 and y_1.

In practice, second-order differential equations are given Cauchy boundary conditions - $y(0) = y_0$ and $y'(0) = v_0$. Therefore, value y_1 is often approximated using Taylor polynomial:

$$y_1 = y(\delta) \approx y(0) + \sum_{n=1}^{4} \frac{\delta^n}{n!} y^{(n)}(0). \tag{5}$$

Differentiating equation (1) and substituting y'' for combinations of y and f one gets the fourth-order approximation in terms of y_0, v_0 and values of different derivatives of f, which can be evaluated symbolically or numerically:

$$y_1 \approx \frac{1}{24}\delta^4 \left(y_0 f''(0) + 2f'(0)v_0 + f_0^2 y_0\right) + \tag{6}$$

$$+\frac{1}{6}\delta^3 \left(y_0 f'(0) + f_0 v_0\right) + \frac{1}{2}\delta^2 f_0 y_0 + \delta v_0 + y_0 \tag{7}$$

2 Quantum harmonic oscillator

Schrodinger equation for quadratic potential $V(x) \propto x^2$ can be written is dimensionless form as:

$$y''(x)$$

3 Conclusions

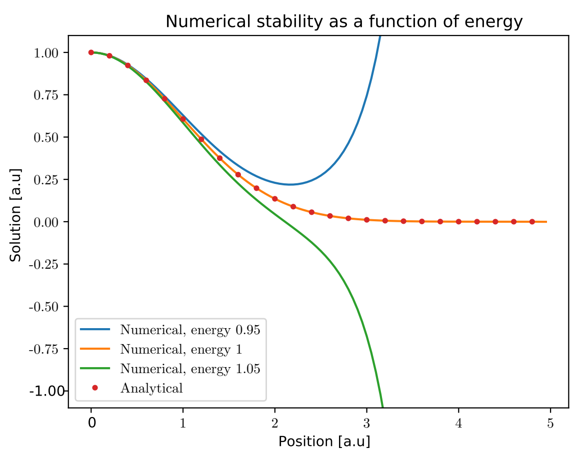
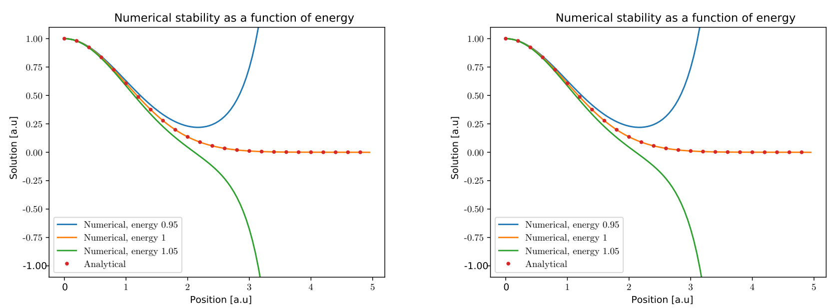


Fig. 1: Mock - just a template how to insert images.

4 References

1. C. E. Froberg, Introduction to Numerical Analysis, Addison Wesley, 1969.
2. Joint work, Solutions of Schrodinger's equation by numerical integration, University of Oxford, 2018
3. R. Schankar, Principles of Quantum Mechanics, Springer, 2008



(a) (b)

Fig. 2: Figure 2a presents response amplitude as a function of frequency. Figure 2b presents the phase-shift, dashed line denotes value $3\pi/4$ (value when the phase-shift is a quater of the whole period). Both figures show that the resonance frequency can be estimated as 136.4(1) Hz.