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Project part III

1 Overview

See section 4 of the lecture notes "Bestimmung quantenmechanischer Energieniveaus durch numerisches Lösen der Schrödinger-Gleichung".

2 Assignment

Consider the 1-dimensional Schrödinger equation with potential

$$V(x) = \begin{cases} m\omega^2 x^2 & \text{if} \quad -L/2 \leq x \leq +L/2\,, \\ 0 & \text{otherwise,} \end{cases} \tag{1}$$

i.e. a harmonic potential with hard walls at $x = \pm L/2$. It is convenient to define the dimensionless quantities

$$\hat{x} = \frac{x}{L}\,, \qquad \hat{E} = \frac{2mL^2 E}{\hbar^2}\,, \qquad \hat{\omega} = \frac{m\omega L}{\hbar}\,. \tag{2}$$

The Schrödinger equation expressed exclusively in dimensionless quantities together with the hard wall boundary conditions is then

$$\frac{\mathrm{d}^2}{\mathrm{d}\hat{x}^2}\psi(\hat{x}) = \left(\hat{\omega}^2\hat{x}^2 - \hat{E}\right)\psi(\hat{x})\,, \qquad \psi(\hat{x} = \pm 1/2) = 0\,. \tag{3}$$

Consider in the following $\hat{\omega} = 70$ unless explicitly stated otherwise.

(i) Compute the lowest three energy levels $\hat{E}_n$, $n = 0, 1, 2$. They should be close to the ordinary quantum mechanical harmonic oscillator $\hat{E}_n^{\mathrm{HO}} = \omega(2n+1)$, because $\hat{E}_n \approx \hat{E}_n^{\mathrm{HO}} \ll \hat{\omega}^2/4$ is fulfilled $(70, 210, 350 \ll 1225)$. Compare your numerical results to this crude analytical expectation and compute the relative difference $(\hat{E}_n - \hat{E}_n^{\mathrm{HO}})/\hat{E}_n$.

(ii) Now consider energy levels with $\hat{E}_m \gg \hat{\omega}^2/4$, which should be close to those of the infinite well. For example one might expect energy levels close to $\hat{E}_n^{\mathrm{IW}} = \pi^2(n+1)^2$ with $n = 17, 18, 19$, because $\pi^2 \cdot 18^2, \pi^2 \cdot 19^2, \pi^2 \cdot 20^2 \approx 3198, 3563, 3948 \gg 1125$. Compute these energy levels using $3198, 3563, 3948$ as starting values for $\hat{E}$ for the shooting method and compare your results to the crude analytical expectation. As before, provide the relative difference, i.e. $(\hat{E}_m - \hat{E}_n^{\mathrm{IW}})/\hat{E}_m$.

(iii) Determine all energy levels in between those computed in task (i) and task (ii) and count them. What is the index of the energy level $\hat{E}_m$ found in task (ii), which is close to $\hat{E}_{19}^{\mathrm{IW}}$?

Hint: Even though one might naively expect $m = n = 19$, you should find $m \neq n = 19$.

(iv) Investigate your (possibly) surprising result from task (iii) in more detail. To this end, compute all energy levels $\hat{E}_n$ with $\hat{E}_n < 5000$ as functions of $\hat{\omega}$ in the range $0 \leq \hat{\omega} \leq 70$ (it is sufficient to sample this $\hat{\omega}$ range by the values $\hat{\omega} = 0, 10, 20, 30, 40, 50, 60, 70$).
Plot all $\hat{E}_n(\hat{\omega})$ in a single plot (horizontal axis $\hat{\omega}$ [range $0 \ldots 70$], vertical axis $\hat{E}$ [range $0 \ldots 1000$]). Show in the same plot the analytically known energy levels of the ordinary HO as functions of $\hat{\omega}$ (the ten lowest energy levels of the ordinary HO are sufficient). Discuss the plot, in particular the region of large $\hat{\omega}$ and small $\hat{E}$.

Plot all $\hat{E}_n(\hat{\omega})$ in a single plot (horizontal axis $\hat{\omega}$ [range $0 \ldots 70$], vertical axis $\hat{E}$ [range $0 \ldots 5000$]). Show in the same plot the analytically known energy levels of the infinite well up to $\hat{E} = 5000$ (since they do not depend on $\hat{\omega}$, these are just horizontal lines). Discuss the plot. Start with the region of small $\hat{\omega}$. Then continue your discussion with larger values of $\hat{\omega}$ with particular focus on the three energy levels computed in task (ii). Try to understand and explain the reason for the difference between the indices m and n observed in task (iii).

(v) Focus again on $\hat{\omega} = 70$ and compute the difference of neighboring energy levels, i.e. $\hat{E}_n - \hat{E}_{n-1}$ for energies $\hat{E}_n < 5000$. Compare to the corresponding differences for the analytically known energy levels of the infinite potential well, i.e. $\hat{E}^{\mathrm{IW}}_n - \hat{E}^{\mathrm{IW}}_{n-1}$. What do you observe?

(vi) Formulate conclusions based on your investigations and findings from tasks (i) to (v), i.e. try to summarize, how $\hat{\omega}$ changes the energy levels, and in which parameter regions (i.e. small/large values of $\hat{\omega}$ and $\hat{E}$) the numerically computed energy levels exhibit similarities to those of the ordinary HO and to those of the infinite well.

3 Code design

In this final part of the programming project there is not much new to implement. The focus is on using your implemented methods from part I and part II and to carry out an extensive numerical analysis for a problem from 1-dimensional quantum mechanics.

It is, in principle, sufficient to take your code from part II of the programming project and just change the potential (i.e. modify a single line). We recommend, however, to add a few more lines to your code, which will most likely save you some time, in particular when generating the large set of data points for the plots in task (v).

Here are our suggestions:

- Task (i) and (ii): Replace the potential and proceed with your existing code as in part II of the programming project.
- Task (iii): To count the energy levels, we recommend that you use your function `energy_scan` at sufficiently high resolution. It might be convenient to plot the violation of the boundary condition $\mathrm{vbc}(E)$ on a logarithmic scale. A simple possibility is to plot the quantity $\log(|\mathrm{vbc}(E)| + 1)$.
- Task (iv): For the plots $\mathcal{O}(2000)$ energy levels have to be computed. Manually providing a starting value each time and running your program is tedious and not professional. You should automatically loop over the values for $\hat{\omega}$ and the indices n of the resulting energy levels $\hat{E}_n$. At first glance, it might be difficult to automatically provide a good starting value for $\hat{E}$ (i.e. close to the energy level $\hat{E}_n$ you are interested in), when calling the shooting method. This, however, can be achieved in a simple way by minimally extending your function `energy_scan`. Add a few lines of code, such that it does not just print $\mathrm{vbc}(E)$, but checks, whether there was a change in the sign compared to the previous $\mathrm{vbc}(E)$ data point. If this is the case (and the energy resolution you use is sufficiently fine), you can interpolate the two data points by a straight line and take the intersection with 0 (do not do this numerically; it is a simple formula, which you can derive analytically). In this way you obtain an excellent starting value for the shooting method.