Numerical Methods HW2 - Notes and Plots

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1 Quantum Mechanics on a Computer

The time-independent Schrödinger equation for a single particle in one spatial dimension:

$$-\frac{1}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

We may rewrite this as a system of two first order ODEs as follows, letting:

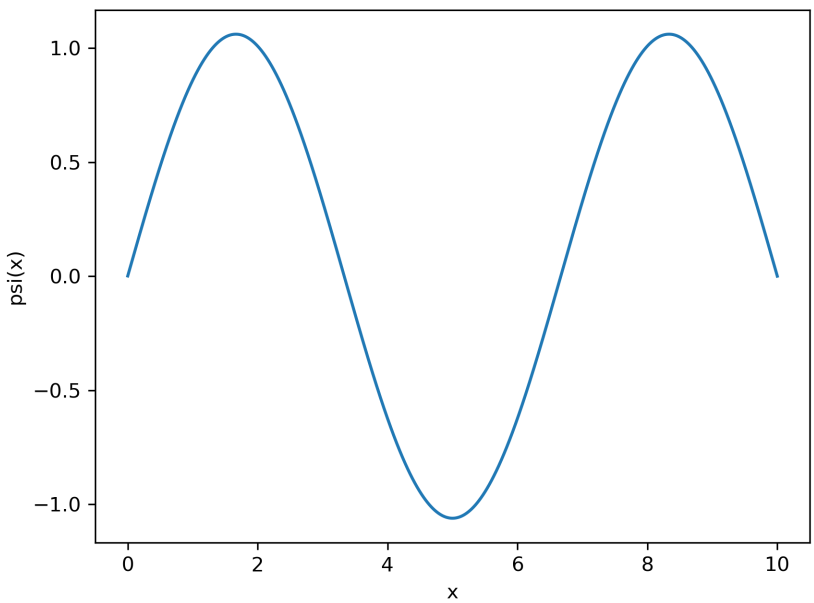
$$z = \frac{d\psi}{dx}$$

$$\dot{z} = \frac{d^2\psi}{dx^2} = -2m[E - V(x)]\psi$$

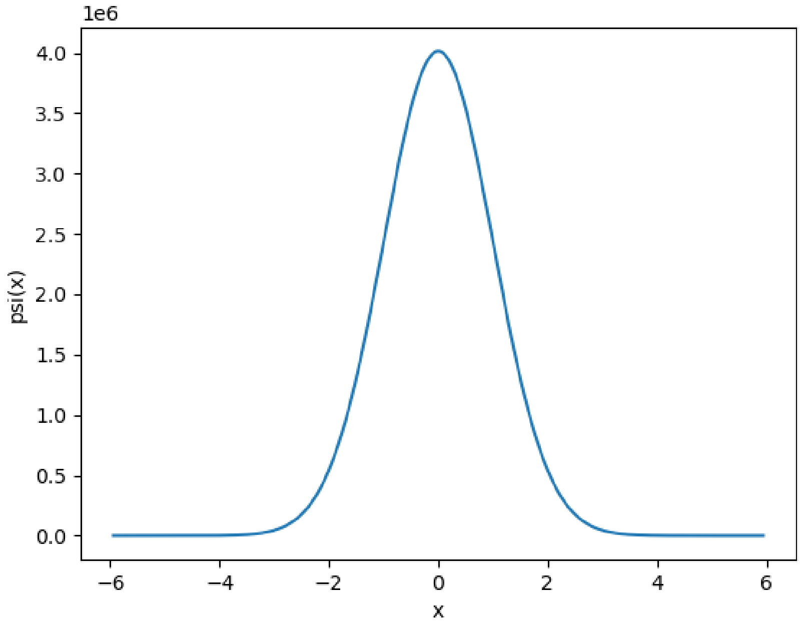
In matrix notation, we can express this as:

$$\frac{d}{dx}\begin{pmatrix}\psi \\ z\end{pmatrix} = \begin{pmatrix}0 & 1 \\ 2m[V(x) - E] & 0\end{pmatrix}\begin{pmatrix}\psi \\ z\end{pmatrix}$$

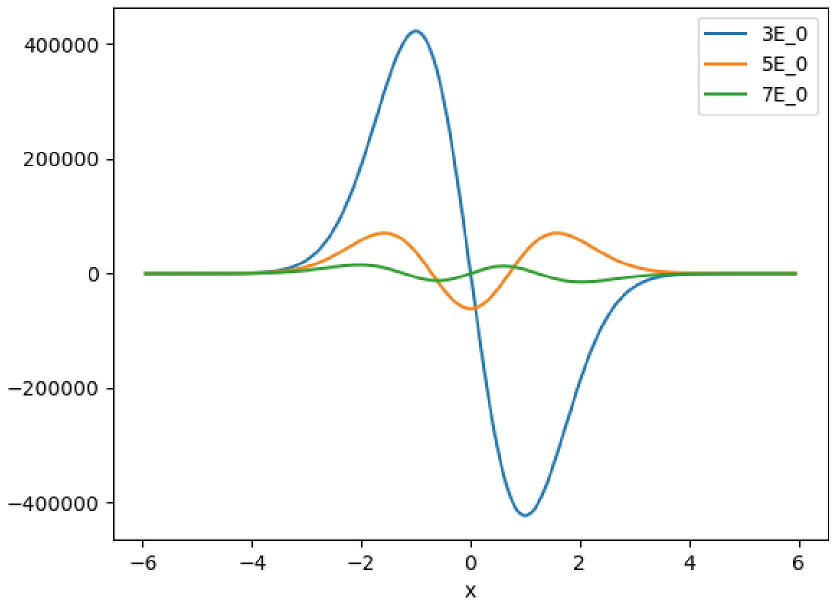
We are asked to solve this using RK4. In the first case we use $V(x) = 0$ on $[0, 10]$ with $N = 10000$ steps and initial conditions $\psi(0) = 0$ and $d\psi/dx(0) = 1$, and I also set $m = 1$ Using the bisection method to find an energy such that $\psi(10) \approx 0$, I found a value of $E = 0.44412841796874997$ at which $\psi(10) = 4.255607252376587e - 05$. The plotted solution for ψ using this energy value is:



Now we are asked to solve ψ for a harmonic potential. Specifically, we have to find a such that using the initial data $\psi(-a) = 0$ and $d\psi/dx(-a) = 1$ and solving over the interval $x = [-a, a]$ reproduces the ground state. I once again use the bisection method to find values for a such that these initial conditions in terms of a lead to $\psi(a) \approx 0$. Using a tolerance of 10^{-4} I find this value to be $a = 5.944244384765625$. The plotted solution is, where I use $E = \omega/2$ and set $\omega = 1$:



What happens to the wavefunction as we change the energy in odd multiples of the ground state energy $E_0 = \omega/2$. Some results are plotted below:

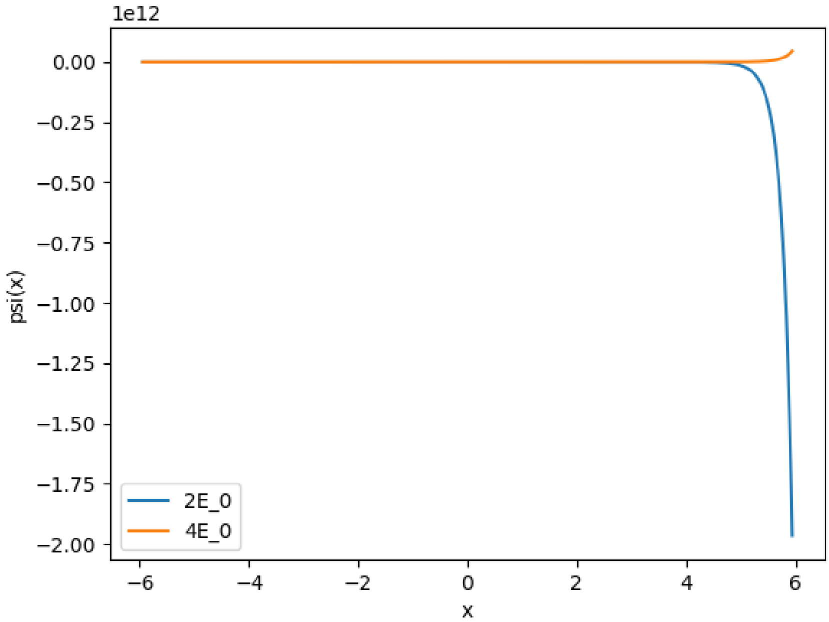


These solutions at these energies that are odd integer multiples of the ground state energy still satisfy $\psi(a) \approx 0$. These correspond to the known quantum harmonic oscillator energy levels:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

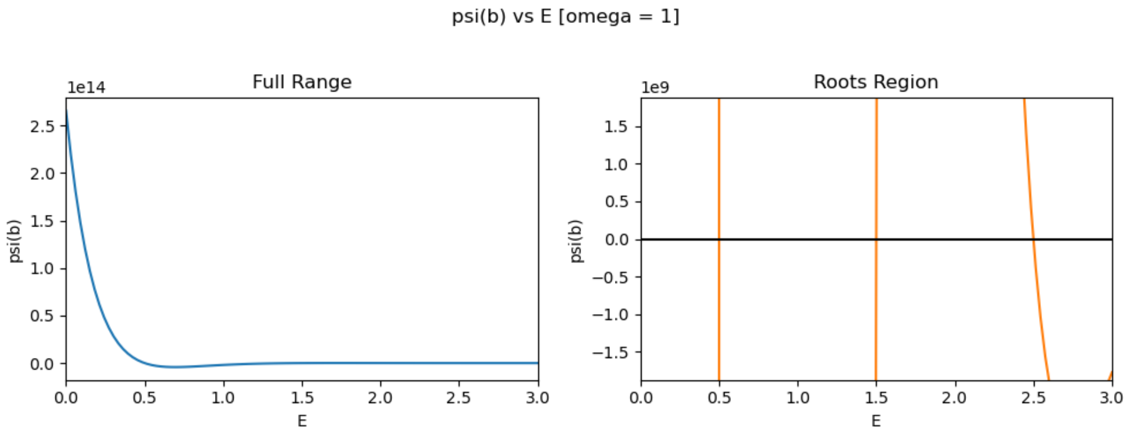
$3E_0$ corresponds to $n = 1$ and has one node at which the wavefunction equals 0, $5E_0$ corresponds to $n = 2$ and has two nodes, $7E_0$ corresponds to $n = 3$ and has 3 nodes, etc. So generally, these $E = \omega/2, 3\omega/2, etc.$ energies correspond to the quantized energy levels of the quantum harmonic oscillator.

If I increase the energy but not in quantitates that satisfy the E_n expression, we no longer get wavepacket solutions that satisfy $\psi(a) \approx 0$.



2 The Shooting Method

We now use the shooting method.
a) In part a, we solve the schrodinger equation for a given E over $[a, b]$, constructing a function that returns $\psi(b) := \psi(b; E)$. We set $\psi(a) = 0$ and $d\psi/dx(a) = 1$.



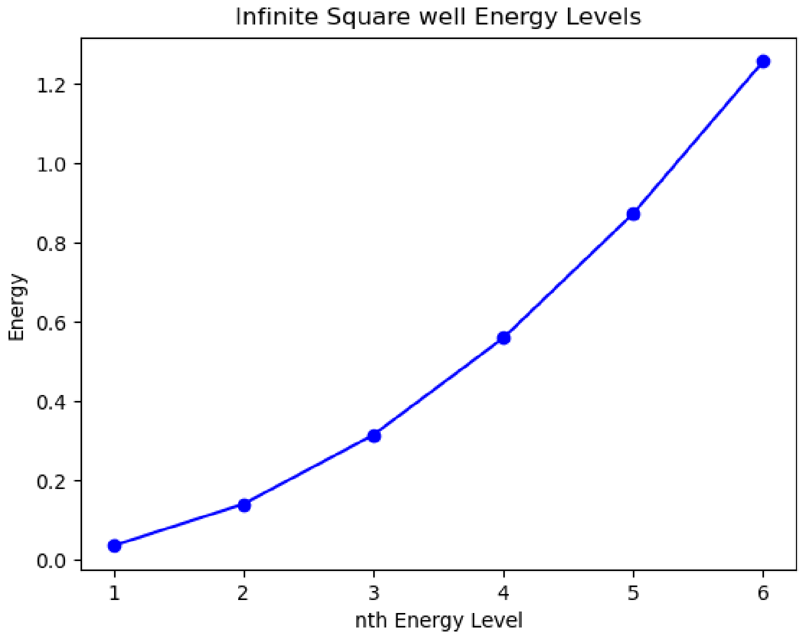
b) Here we are asked to write a function that uses the bisection method to find the roots of $g(E) = \psi(b; E)$, and testing it on $U(x) = 0$ first. I found the first 6 energy levels:
Comparing with the known result for the energy levels of an infinite well, given by:

$$E_n = \frac{n^2\pi^2\hbar}{2mL^2} \tag{2}$$

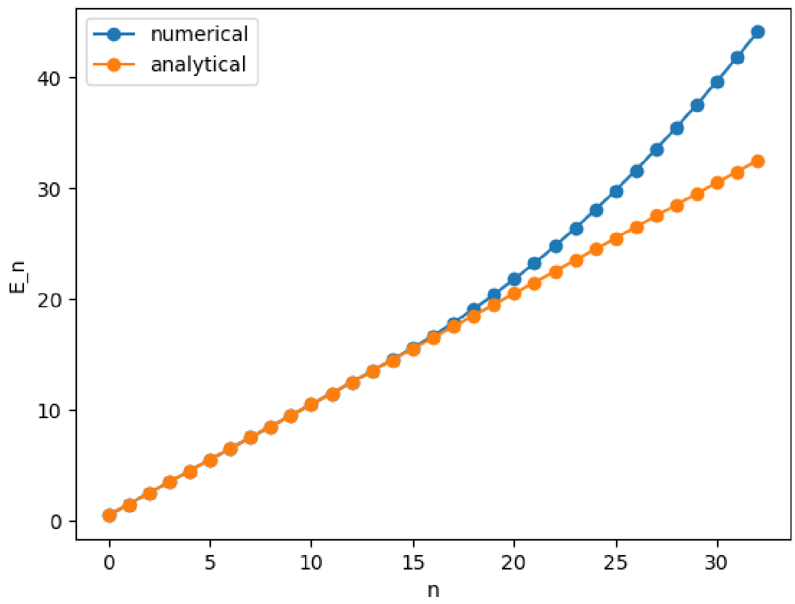
We then expect a quadratic relationship between E_n and n. This was found as expected:

n	Analytical	Numerical
1	0.03491535371	0.034918224886059765
2	0.1396614148	0.13967289932072158
3	0.3142381834	0.31426402337849146
4	0.5586456593	0.558691597208381
5	0.8728838427	0.8729556206613783
6	1.256952733	1.257056093737484

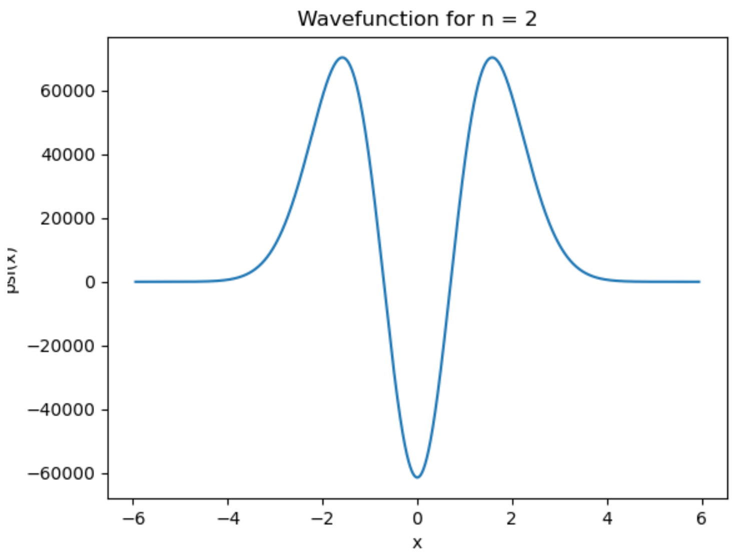
Table 1: Analytical vs Numerical energy values for infinite well potential.

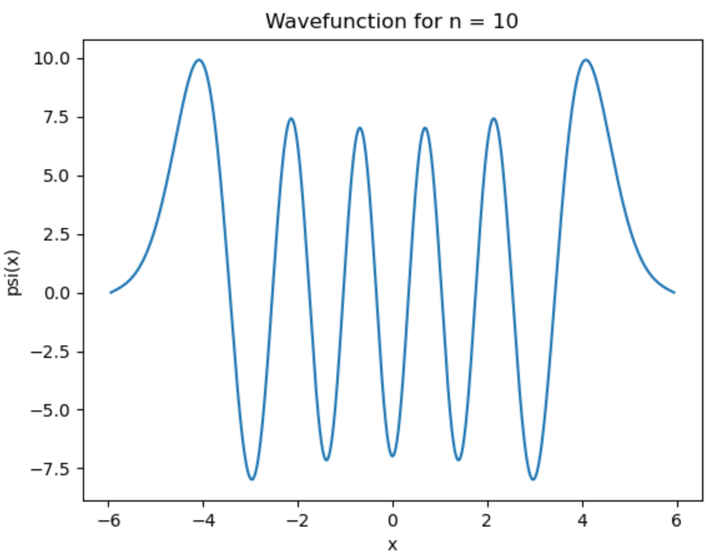


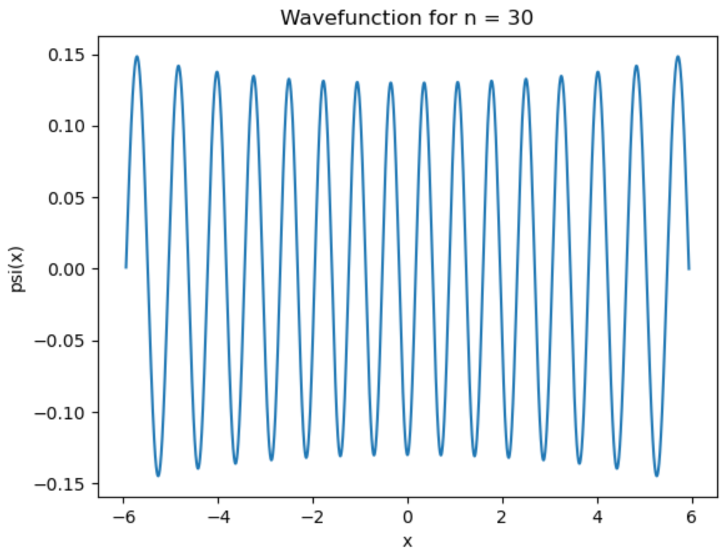
For my specific parameters, I expect to get the following values, which I compare to my numerically obtained solutions:
c) Here we are asked to implement the shooting method for the harmonic oscillator potential. We see that for the first few energy levels, results are as expected $1/2, 3/2, 5/2...$ where I have set $\omega = 1$. As the energy level is increased, we see they begin to diverge from the expected harmonic oscillator behaviour of half integer multiples of ω, and begins to look somewhat quadratic as would be expected for the infinite well.



I'd say divergence from the expected value begins to be significant at $n = 20$.
We are asked to plot the eigenstates for some energy levels above and below this region of divergence:







As n and therefore the energy is increased, we begin to see the effects of the infinite well that we have confined the harmonic potential in, and so the energy eigenstates begin to look sinusoidal (although in the n=30 case the amplitude is not completely uniform yet), as would be expected for the infinite well.