

LAB ASSIGNMENT # 07

(a)

Since, we know that the solution of the Schrodinger equation is of the form:-

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

But the problem with this solution is that the solution goes to infinity as x goes to infinity that leads to unphysical solution. But solving using $\psi(x)$ we discard that part which is going to infinity.

But numerically both the values is taken into account and that leads to instability of solution.

(b)

To remove this instability in the solution we use the Matching method. As we are solving from $x = -x_{max}$ to x_{max} but we break it into x from 0 to x_{max} and we determine the classical turning point for each state and then break our integration from 0 to x_{max} between 2 parts.

- (1) 0 to x_{cl} (classical turning point) this is called ~~backward~~ forward integration.

② x_{max} to x_{cl} this is called backward integration.

After doing these two integrations we do two important steps:

① Match the values of ψ wavefunction on x_{cl} point for both integrations using scaling technique.

② Match the derivative of the wavefunction at x_{cl} for both integrations.

After performing these matching steps, the instability in solution can be removed.

1 Discussion

1. This is the table of the Eigen values across the corresponding states for $x_{max} = 10$

	Eigen Value Numerically	Analytically
0	0.500000	0.5
1	1.500024	1.5
2	2.500085	2.5
3	3.500090	3.5
4	4.500000	4.5
5	5.500121	5.5

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Figure 1:

2. These are the waveform that we are geeting across the corresponding states for $x_{max} = 10$

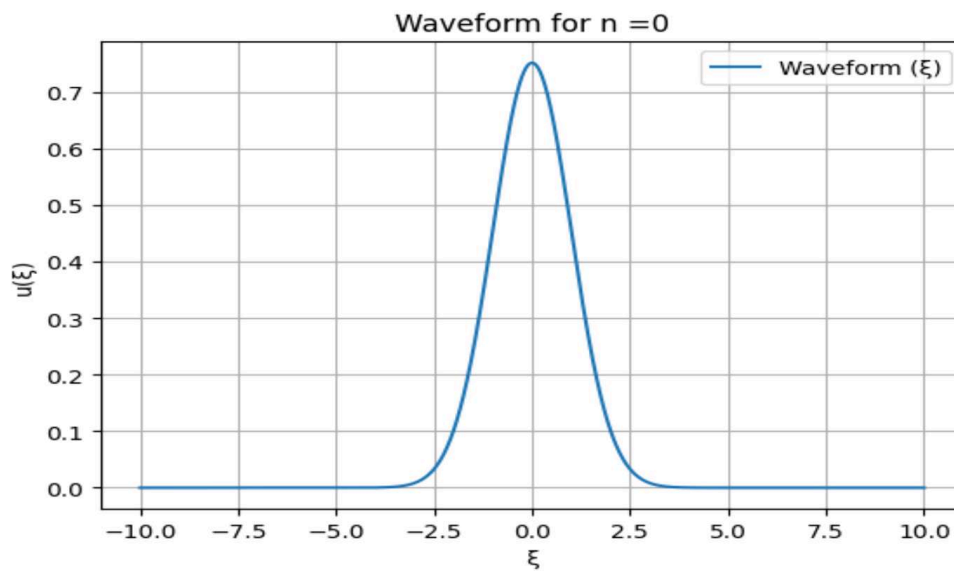


Figure 2:

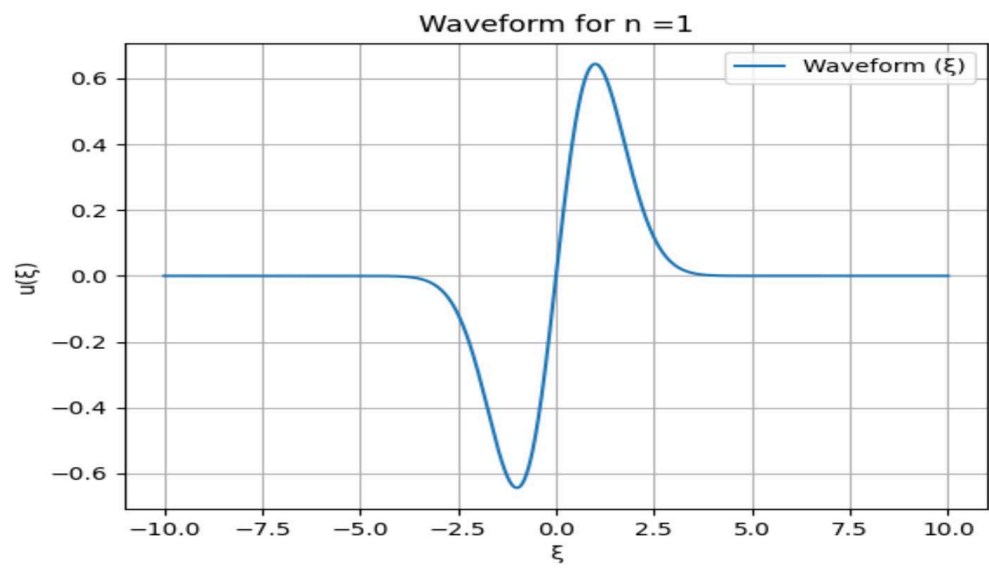


Figure 3:

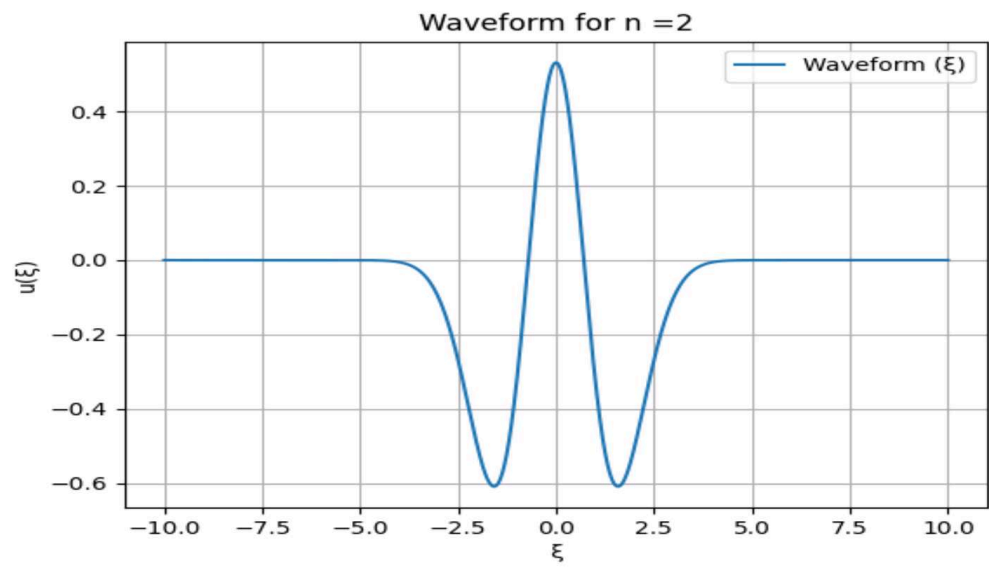


Figure 4:

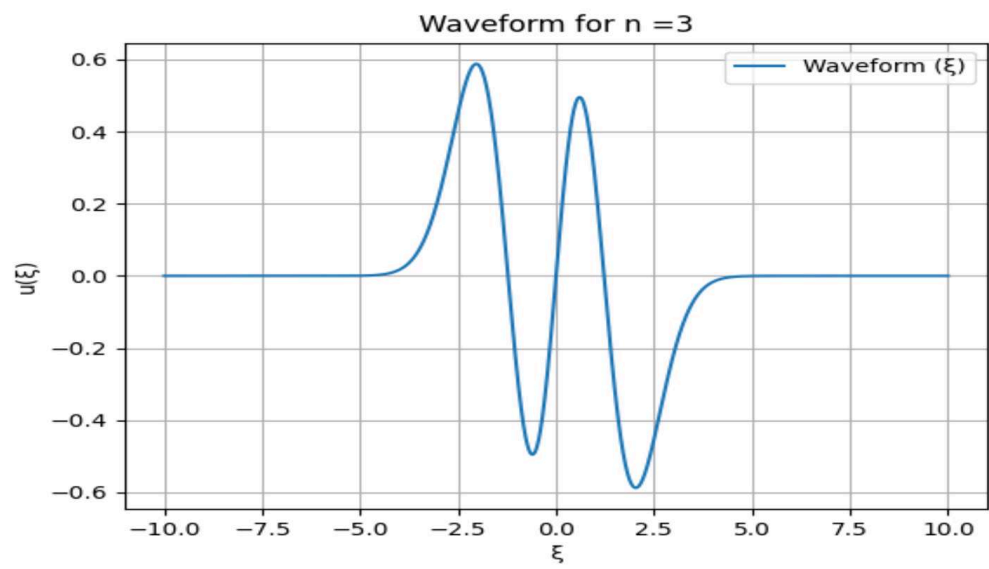


Figure 5:

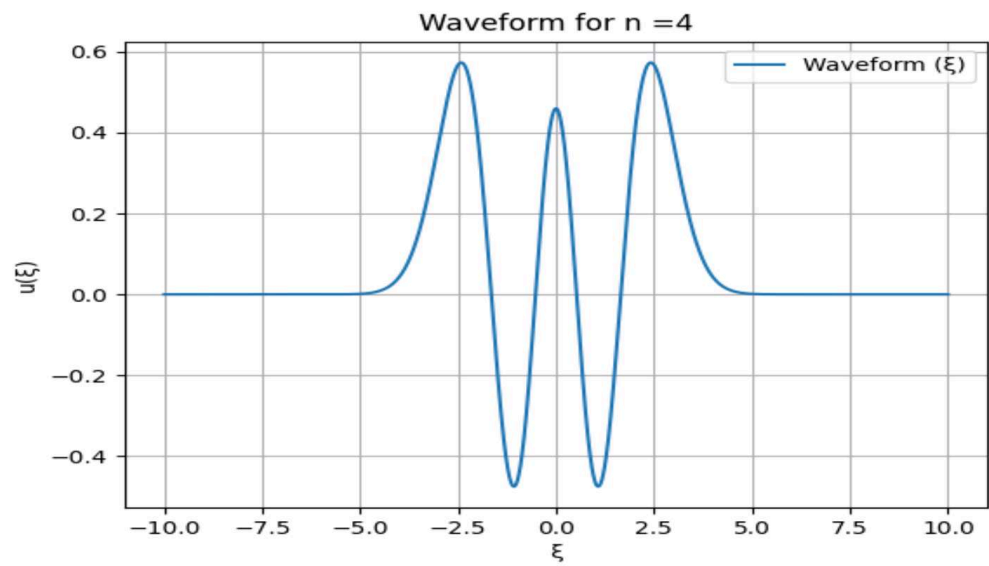


Figure 6:

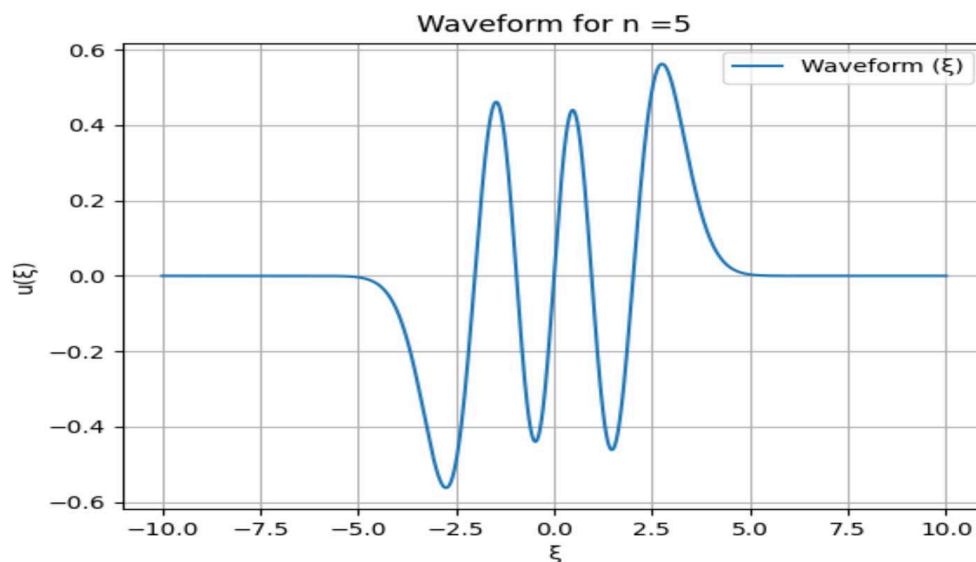


Figure 7:

3. This is the table of the Eigen values across the corresponding states for $x_{max} = 2$. Here we will get only the values for the ground and first excited state as for higher excited states with $x_{max} = 2$ we are not getting the classical turning point.

	Eigen Value Numerically	Analytically
0	0.537462	0.5
1	1.764817	1.5

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Figure 8:

1. (7 marks) **Theory**

- (a) Explain why correct asymptotic solutions are not obtained when you integrate the Schrödinger Equation from x_{min} to x_{max} .
- (b) Discuss how the instability discussed above may be controlled by matching the solution at a point in the allowed region.

2. (10 marks) **Programming**

- (a) Modify the program in assignment 6 to determine the energy eigenvalues and eigenfunctions with correct asymptotic behaviour for an electron subjected to the harmonic oscillator potential. The code should
 - i. Determine the left and right wavefunctions by integrating forward from $x = 0$ to $x = x_{cl}$ and backward from $x = x_{max}$ to $x = x_{cl}$, x_{cl} being the right classical turning point. The code should obtain the first six energy eigenvalues e_n for an electron subjected to harmonic potential.
 - ii. match the left and right wavefunctions and the derivatives
 - iii. print numerical and analytical energy eigenvalues (in units of $\hbar\omega$) in tabulated form for the ground state and first five excited states.
 - iv. Print the values of the wavefunction and its derivative at $x = x_{cl}$.
- (b) Repeat for $x_{max} = 2$ and $x_{max} = 10$.

3. (3 marks) **Discussion**

Interpret and discuss your results.