THE QUANTUM WORLD 2021 - 2022

COURSEWORK SET 1

This coursework forms **5%** of your assessment for The Quantum World module.

DEADLINE FOR SUBMISSION: 15:00 on Wednesday Nov 10

Contact: Philip Moriarty or Moustafa Gharamti

The Hamiltonian, $\hat{H}$, for a simple harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k_{\text{eff}}x^2,$$

where k_{eff} is an effective spring constant (that could, for example, be associated with the "stiffness" of a chemical bond between two atoms[1].) The natural frequency, ω_0, is given by $\omega_0 = \sqrt{k_{\text{eff}}/m}$. By a judicious choice of units ($\frac{\hbar^2}{m} = m\omega_0^2 = 1$), we can rewrite the Hamiltonian as:

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

(a) By making use of the standard integral given at the bottom of the following page, calculate the normalisation constants, C_0 and C_1 for the first and second eigenstates of the Hamiltonian, $\hat{H}$ $\{\mathbf{2}\}$:

$$u_0(x) = C_0 e^{-x^2/2}, \qquad u_1(x) = C_1 x e^{-x^2/2}$$

(b) Write a Python program to plot $u_0(x)$ for the range $|x| <= 4$. Initially set $C_0 = 1$ (for which $u_0(x)$ will not be correctly normalised). Use 1000 data points. Plot $V(x) = \frac{1}{2}x^2$, on the same axes. $\{\mathbf{3}\}$ Extend your Python code so that it normalises the wavefunction $u_0(x)$. $\{\mathbf{2}\}$

(c) The eigenstates of $\hat{H}$, i.e. $u_n(x)$, are a set of functions involving the product of a particular type of polynomial (known as a Hermite polynomial) with a Gaussian (see Fig.1.) $u_0(x)$ and $u_1(x)$ are of the form given above. The third (normalised) eigenstate, $u_2(x)$, is

$$u_2(x) = \frac{1}{(\sqrt{8})\pi^{1/4}}(4x^2 - 2)e^{-x^2/2}$$

Confirm that $u_2(x)$ is an eigenfunction of $\hat{H}$. $\{\mathbf{3}\}$ What is the value of the associated energy eigenvalue, E_2?$\{\mathbf{1}\}$

(d) Extend your Python code so that it calculates and plots the modulus squared of the Fourier transform of $u_0(x)$, i.e. $|u_0(k)|^2$. $\{\mathbf{3}\}$.On the basis of this plot, what is the expectation value for momentum? $\{\mathbf{1}\}$.

[1] See Video SP10 Part 2 from the Year 1 *From Newton To Einstein* module.

(e) Use the *shooting method* algorithm outlined below (see also Video #14), to numerically calculate the second eigenstate, $u_1(x)$, of the Hamiltonian. $\{\mathbf{10}\}$

1 We first rewrite the TISE in terms of finite differences rather than derivatives:

$$u_1(x+\Delta x) \approx 2u_1(x) - [2\Delta x^2 u_1(x)(E - V(x))] - u_1(x - \Delta x) \tag{1}$$

2 Eqn. 1 provides the next value of u_1, i.e. $u_1(x+\Delta x)$, on the basis of the preceding two values, $u_1(x)$ and $u_1(x-\Delta x)$. We thus need two values of the eigenfunction u_1 to start. Choose these to be $u_1(x-\Delta x) = 0$ and $u_1(x) = 1\times 10^{-6}$. Start with a value of -4 for $(x-\Delta x)$.

3 Now choose a value of E that is initially $\sim 20\%$ less than the expected eigenvalue. Use that value of E in Eqn 1 to calculate the wavefunction for 1000 values of x equally spaced between $x = \pm 4$ (i.e. $\Delta x = 0.008$.)

4 Unless we have chosen the correct energy eigenvalue associated with the eigenstate the wavefunction will diverge at the other edge (i.e. at $x = 4$).

5 Therefore, after using Eqn 1 to calculate the 1000 values of the wavefunction for a given E, check if the last value of $u_1(x)$ is close to zero by using this criterion: $|u_1(x)| < 0.001$. (Note that $u_1(x)$ is a real function.) If this condition is met, great, you're finished. If not, increment E by a small amount (say 0.001) and go back to Step 4. Keep repeating until the overshoot is negligible. What value of E does your code produce at this point? Why?

6 Normalise the wavefunction found by the shooting method.

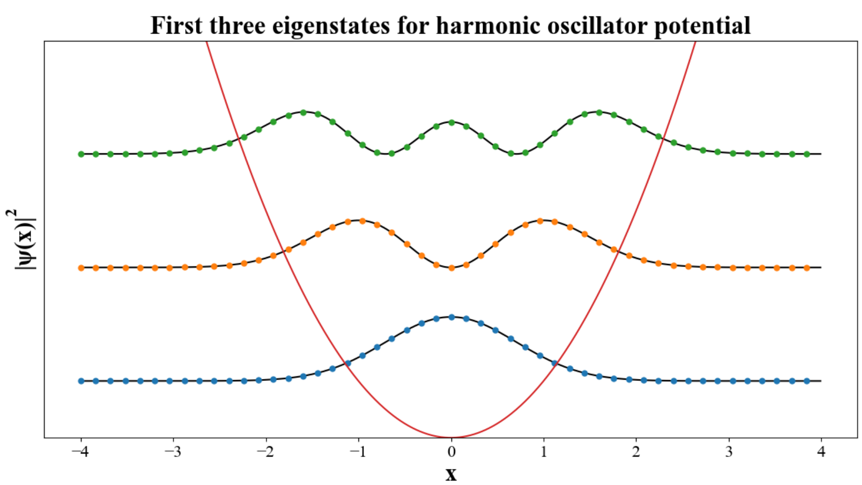

Figure 1: The probability density for the first three eigenstates of $\hat{H}$. The dots represent the output of the shooting method algorithm described in part (f), whereas the solid lines are the analytical functions given in parts (a) and (c). Only every 20th data point of the calculated wavefunction is shown, for clarity.

You will need to make use of the following standard integral: $\int_{-\infty}^{+\infty} x^n e^{-x^2} dx = \begin{cases} 0, & \text{if n is odd} \\ \dfrac{n!\sqrt{\pi}}{2^n (n/2)!}, & \text{if n is even} \end{cases}$