Introduction to Quantum Computing – Assignment # 3

Marcelo Ponce

June 9, 2025

Problem Set #3 – Quantum Harmonic Oscillator, Potential Well and Tunneling

1. *Schrödinger Equation*

   (a) Let's begin by considering the 1-dim Schrödinger equation, and in particular its separation of variables. To achieve this, let's suppose that a 1-dim wave function $|\Psi(x,t)\rangle$ can be written as the product of two independent functions of position x and time t, i.e.

   $$|\Psi(x,t)\rangle = |\psi(x)\phi(t)\rangle \tag{1}$$

   By substituting this in the original Schrödinger equation and dividing the whole equation by the proposed ansatz given by Eq.(1), we can identify that each side of the equation depends only on either x or t.

   Show the aforementioned steps to reach this and the final expression of this process.

   (b) Considering what you just proved, then both the left- and right-hand sides must be independent of x and t and equal to a constant. We call this separation constant E, i.e. the total energy in the equation. Write these two differential equations depending on x and t separately.
   The equation that does not show time-dependence is known as *Time Independent Schrödinger Equation* (TISE).

   (c) Solve by direct integration the time-dependent equation.

2. *Particle in a box or the infinite well potential*
   For solving the TISE, we need to specify the particular configuration in which the system is placed, e.g. by specifying the potential energy.

   (a) Let's assume that a particle of mass m is able to move freely in only one dimension and is confined to the region defined by $0 < x < L$. In other words, we can think of the potential energy function given by,

   $$V(x) = \begin{cases} 0; & 0 < x < L \\ \infty; & x < 0, x > L \end{cases} \tag{2}$$

   Write the solution to the TISE for this potential in terms of trigonometric functions.

   (b) Impose boundary conditions, i.e. $\psi(x=0)=0, \psi(x=L)=0$, on the general solution find above; what conditions the arguments of the trigonometric functions should obey? Write the final form of the solution taking this into consideration.

(c) What important observation emerges from the solution you just found?

3. The *Harmonic Oscillator* – classical
Let's begin by considering the classical harmonic oscillator (HO), which represents a paradigm system in physics. The HO system may arise from many different scenarios, such as, a pendulum, a spring-mass system, circular motion, LC electric circuits, chemical reactions, pray-predator systems (Lotka-Volterra), etc.

   (a) Pick your favorite 1-dim harmonic oscillator system, describe it and write the *equation of motion* for it. I.e. the governing differential equation for the particular system you choose.
   (b) Find the most general solution for this system.
   (c) Plot the energy as a function of time, and a *phase-space* diagram (i.e. $x - \dot{x}$ plot).

   Hint: as a general guideline the equation of motion is represented by a second order differential equation, which should have the general form,

$$\ddot{q}(t) + \omega^2 q(t) = 0$$

4. *Quantum Harmonic Oscillator*
Now let's consider the *quantum* version of the harmonic oscillator. We will consider a one-dimensional quantum harmonic oscillator with mass m and angular frequency ω.

   (a) Let's now write the Hamiltonian for the harmonic system composed by a particle of mass m and angular frequency ω. for which consider the energetic contributions to the Hamiltonian, i.e. kinetic and potential energies in terms of operators.
   (b) You will need notice that the Hamiltonian does not explicitly depend on time, which allows us to then substitute this Hamiltonian in the corresponding TISE.

   ► On a typical physics course you would be asked to solve the differential equation obtained in the previous step. This usually involves a good amount of mathematical manipulation, which personally I consider it very useful and instructive.
   However, we will take a slight detour here and try to shortcut the process. But *do not fear!* :), if you are still interested in the full derivation process I'm happy to provide you with some guidelines in how to proceed.

   ► Similarly to the particle in the box problem, one can show that the solution to the QHO problem is **quantized**. In this case, the solution can be written as,

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{\frac{-m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \tag{3}$$

   where $n \in \mathbb{N}$ and H_n are a set of special functions known as *Hermite Polynomials* which can be defined by the following ODE,

$$H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right) \tag{4}$$

   (c) Write a Python script (or the language of your choice) to reproduce the plots shown in Fig. 1.

5. *Tunneling*

Another of the very remarkable results from quantum mechanics, is the possibility of a particle to *"tunnel"* through a potential barrier. For looking into this, let's consider a particle of mass m and total energy E that approaches a one-dimensional potential barrier defined as:

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & 0 \leq x \leq a \\ 0, & x > a \end{cases} \tag{5}$$

where $V_0 > E > 0$. Assume that the particle is incident from the left.

(a) Begin by writing down the TISE in each of the three regions defined by the potential given in Eq.(5).

(b) Provide the general form of the wave function in each of these regions. Comment on the type of solution you observe.

(c) Apply the boundary conditions at $x = 0$ and $x = a$ to relate the coefficients of the wave functions across each of the regions.

(d) Derive an expression for the transmission coefficient T, which gives the probability that the particle tunnels through the barrier.

(e) Show that for a rectangular barrier with $V_0 > E$, the transmission coefficient is approximately:

$$T \approx e^{-2\kappa a}$$

where $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$

(f) Calculate the tunneling probability for an electron ($m_e = 9.11 \times 10^{-31}$kg) encountering a barrier of height $V_0 = 5$eV, width $a = 1$nm, and energy $E = 1$eV.

(g) Provide a graphical representation of the wave functions across the different regions in the problem.

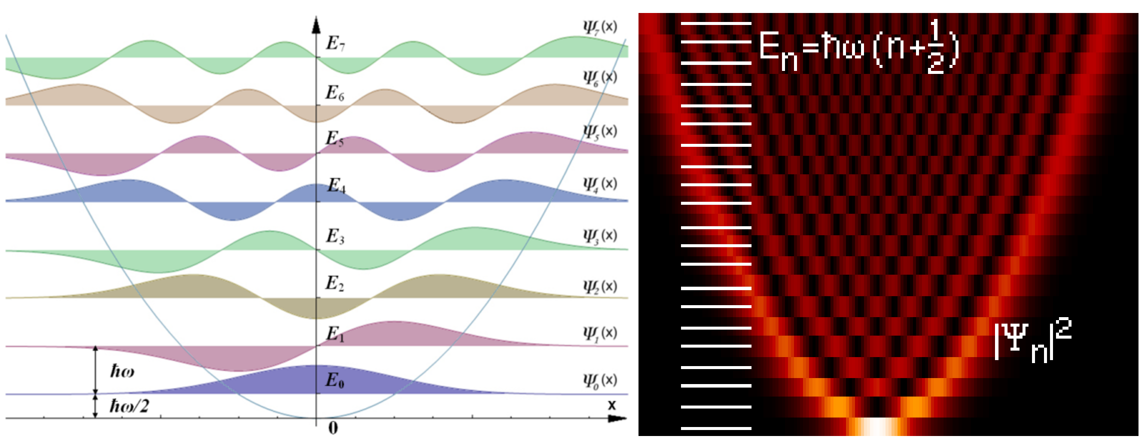

Figure 1: Representations of *wave function* (left) representations for first eight bound eigenstates, $n = 0$ to 7; *probability densities* (right) $|\psi_n(x)|^2$ for the bound eigenstates. The horizontal axis shows the position x, and brighter colors represent higher probability densities. Images sources: Wikipedia.

Why studying these phenomena?

In many quantum computing architectures, such as super-conducting qubits or trapped ions, the quantum harmonic oscillator models the quantized electromagnetic field or vibrational modes. These bosonic modes can be used to store quantum information or mediate interactions between qubits.

Harmonic oscillators, which act like quantum spring-mass systems, are used as qubits, and the tunneling effect enables these qubits to explore multiple states simultaneously, enhancing computational power.

Tunneling is a quantum phenomenon where particles can pass through a potential barrier even when their energy is less than the barrier height. In quantum computing, tunneling allows qubits to "explore" different energy states, even those separated by potential barriers. This ability to tunnel through barriers is crucial for achieving superposition and entanglement, enabling qubits to explore multiple possibilities simultaneously. Tunneling is also used in quantum algorithms and can lead to significant speedups in computation.

References:

- `https://www.nature.com/articles/s41598-021-95801-1`