

15 Harmonic Oscillator

1. For the case of the harmonic oscillator, the potential energy is quadratic and hence the total Hamiltonian looks like:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \quad (15.1)$$

where k is the force constant for the Harmonic oscillator. (Note: the k here has nothing to do with momentum eigenvalues. It is just coincidental that we are using the same letter in the alphabet to describe these two unrelated items.) We will now look at the solution to this problem, since this forms the basis to a number of problems, for example the solution to vibrational motion in molecules and in infra-red spectroscopy. It also plays an important role in the quantum theory of solids.

2. The classical harmonic oscillator comprises a single mass attached to the end of a spring. When the spring is stretch the particle undergoes a simple harmonic motion. This is characterized by the particle moving from one end to the other and back and when there is no external disturbance this motion is perpetual. Furthermore all values of energy are possible, since the particle can vibrate about its equilibrium position with any amount of energy. (The energy determines how much the spring stretches.) It is possible for the particle to have zero energy (no motion). *There is no zero point energy in classical mechanics.* The simple pendulum is another example of the classical harmonic oscillator.
3. The quantum mechanical treatment of the harmonic oscillator

leads to a different set of results. The particle can have zero point energy. The energy will be discrete. All this, as we can guess, will be enforced by the boundary conditions as we have seen before for PIB.

4. Plus, the zero point energy is something that reflects the Heisenberg uncertainty principle. Classically you can have the particle stationary at a given point. *But this amounts to knowing its position as well as velocity (or momentum), which is clearly in violation of the uncertainty principle.*

5. The harmonic oscillator energy eigenvalue problem (or the time-independent Schrödinger Equation) is:

$$\begin{aligned}
 H\psi &= E\psi \\
 \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right] \psi &= E\psi \\
 \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} kx^2 \right] \psi &= 0 \\
 \frac{d^2\psi}{dx^2} + [\lambda - \alpha^2 x^2] \psi &= 0 \tag{15.2}
 \end{aligned}$$

where we have substituted $\lambda = \frac{2mE}{\hbar^2}$ and $\alpha^2 = \frac{mk}{\hbar^2}$.

6. We will use an asymptotic analysis to solve this problem. [We will do something similar for the hydrogen atom later in the semester.]
7. As $x \rightarrow \infty$, $\alpha^2 x^2 \gg \lambda$ and this leads to:

$$\frac{d^2\psi}{dx^2} = \alpha^2 x^2 \psi \tag{15.3}$$

For large x the solution to this equation is

$$\psi(x) = \exp \left[\pm \frac{\alpha}{2} x^2 \right]. \tag{15.4}$$

This is true because:

$$\frac{d^2}{dx^2} \exp \left[\pm \frac{\alpha}{2} x^2 \right] = [\alpha^2 x^2 \pm \alpha] \exp \left[\pm \frac{\alpha}{2} x^2 \right] \tag{15.5}$$

and for large x the second term in the bracket is small as compared to the first term which helps us recover Eq. (15.3). Furthermore, as $x \rightarrow \infty$ only $\exp \left[-\frac{\alpha}{2} x^2 \right]$ remains finite and $\exp \left[+\frac{\alpha}{2} x^2 \right]$ becomes infinitely large. Hence, only $\exp \left[-\frac{\alpha}{2} x^2 \right]$ is an acceptable solution.

8. We propose the following solution to the Harmonic oscillator problem:

$$\psi(x) = \exp\left[-\frac{\alpha}{2}x^2\right] f(x). \quad (15.6)$$

We want to approximate $f(x)$ as a power series.

9. And when substitute this into the differential equation we can get an equation that involves the coefficients of the power series used to approximate the function $f(x)$. And we can equate like powers of x^i for all values i . We end up with another *special function* as a solution to this equation. And this function is known as the Hermite polynomials!! I am gonna solve this on the board so you guys have an idea how one would solve such an equation.

10. The $n = 0$ state is a Gaussian (proportional to $\exp [-(\alpha/2) x^2]$) and the wavefunction and the probability density look as follows:

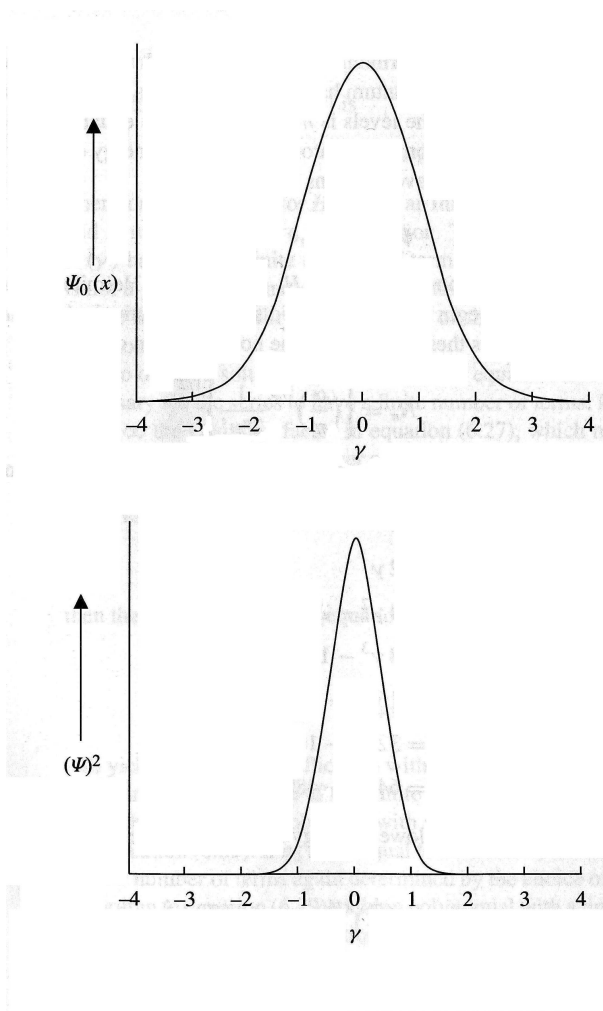


Figure 16: $n = 0$ wavefunction and probability for the harmonic oscillator. The x-axis is γ .

11. Consider the point where the total energy is equal to the potential energy:

$$\frac{1}{2}h\nu = \frac{1}{2}kx^2 = \frac{1}{2}h\nu\gamma^2 \quad (15.7)$$

Note now that what this expression means is the total energy is equal to the potential energy. This could only happen at the “turning point” of the *classical* oscillator. Hence the classical turning point for the ground state oscillator is at $\gamma = \pm 1$. But from the above figure we see that the ground state wavefunction of the quantum harmonic oscillator is *not* zero at this point. Hence there is substantial tunneling!! In fact 0.16 of the probability exists beyond the classical turning point.

12. Another striking feature from Fig. 16 is that the probability is a maximum at $\gamma = 0$. We should compare this with the classical harmonic oscillator. In the classical case the velocity is maximum at $\gamma = 0$. And in fact the velocity is zero at the edges, which is why it turns back towards the equilibrium point. Since the classical harmonic oscillator moves very fast at the equilibrium point and very slow at the classical turning point, we would conclude that the classical harmonic oscillator spends the least bit of time at the equilibrium point and the maximum at the turning point. Hence the likelihood of finding the classical particle is maximum at the edges (or the turning point) and is minimum at the equilibrium point. This is exactly contradictory to what we have for the quantum harmonic oscillator ground state as seen in Fig. 16.

13. In Fig. 17 a few higher harmonic oscillator wavefunctions are presented and in Fig. 18 the probability density for the $n = 10$ state is presented.

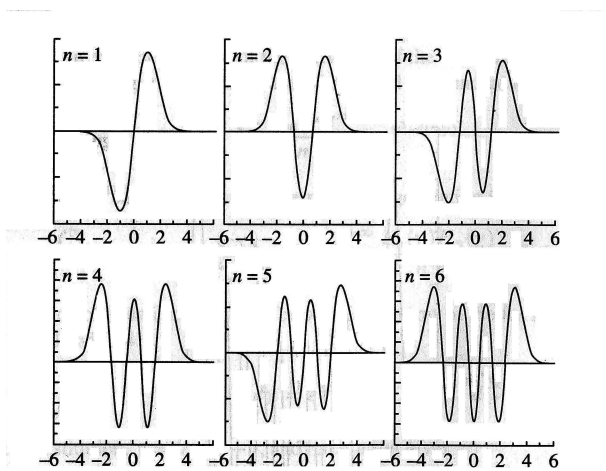
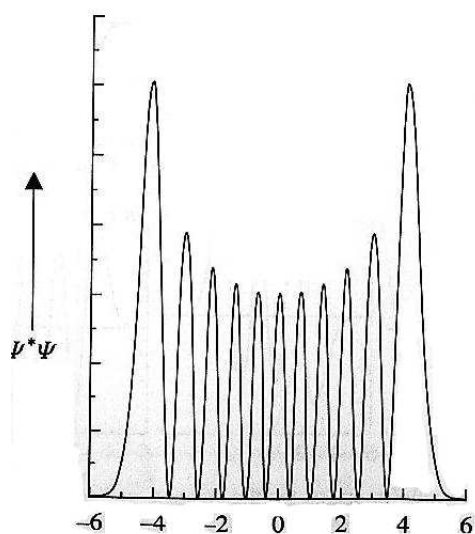


Figure 17: The harmonic $n = 1$ through $n = 6$ states. Note each state has $n - 1$ nodes. The x-axis is γ .

14. From both of these figures the probability along the edges increases and the state becomes more and more “classical-like” for large n . But is this really true?

Figure 18: Probability of the $n = 10$ state.

15. In fact the quantum description of a macroscopic harmonic oscillator is exactly equivalent to a classical description. Let's see if this makes sense. Consider a 1 gram mass connected to a spring that is initially displaced an amount equal to 1 cm. Let the frequency of oscillation be 1 Hz. This implies the force constant, $k = 4\pi^2 g/s^2$. At the classical turning point, $x = 1\text{ cm}$ and the total energy is equal to the potential energy $\frac{1}{2}kx^2 = 2\pi^2 g\text{ cm}^2/s^2$. Now if we were to treat the exact same system quantum mechanically then we would have $(n + \frac{1}{2}) h\nu = \frac{1}{2}kx^2 = 2\pi^2 g\text{ cm}^2/s^2$, which gives approximately $n = 10^{27}$!! This means the classical system corresponds to the quantum system at this very large quantum number. But the quantum system has $(10^{27} - 1)$ nodes with an average separation of 10^{-27} cm very much smaller than what we can measure. Hence the quantum density also looks smooth and is indistinguishable from the classical density!!

16. This last argument very nicely demonstrates the Bohr correspondence for the harmonic oscillator.

16 Inverted Harmonic potential

1. We derived the harmonic oscillator eigenstates and the eigenvalues. The eigenstates turned out to Hermite polynomials multiplied by Gaussian functions.
2. We saw the shapes of these eigenfunctions and noted that while the ground state of the Harmonic oscillator displays a maximum probability of being found at the minimum of the potential (which is totally non-classical), the higher energy states seem to tend towards a more classical description with maximum probabilities closer to the edges. In fact, we found that for extremely high energy states are identical to the classical description. This lends some more support to the Bohr correspondence rule that we saw earlier for the PIB.
3. Also when you make k negative the potential becomes an inverted harmonic oscillator and starts resembling the top of a reaction barrier.
4. Since our mathematical description of the Harmonic oscillator is independent of the sign on k , we are able to write the solution of the inverted Harmonic oscillator as well.
5. Homework: Write down the eigenvalues of the eigenfunctions for inverted Harmonic oscillator directly using what we did last time for standard Harmonic oscillator. Explain the imaginary eigenvalues. How does this affect the time-dependence of these states and what does it physically mean? Note also that the indices on the Hermite polynomials now become complex!