
Lecture 8

Quantum Harmonic Oscillator: Brute Force Methods

Assigned Reading:

E&R	5 _{all} , 6 _{1,2,8}
Li.	3 _{all} , 4 ₁ , 5 ₁ , 6 _{all}
Ga.	2 ₄ , 3 _{all}
Sh.	4 _{all} , 5 _{1,2}

We will now continue our journey of exploring various systems in quantum mechanics for which we have now laid down the rules.

Roughly speaking, there are two sorts of states in quantum mechanics:

1. Bound states: the particle is somewhat localized and cannot escape the potential:
2. Unbound states: the particle can escape the potential.

Note that for the same potential, whether something is a bound state or an unbound state depends on the energy considered.

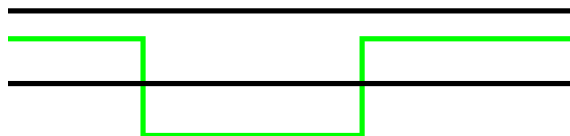


Figure 1: For the finite well, the energy represented by the lower black line is for a bound state, while the energy represented by the upper black line is for an unbound state

But note that in quantum mechanics, because of the possibility of tunneling as seen before, the definition of whether a state is bound or not differs between classical and quantum mechanics.

The point is that we need to compare E with $\lim_{x \rightarrow \pm\infty} V(x)$ to determine if a state is bound or not.

Why do we split our cases that way? Why do we study bound and unbound states separately if they obey the same equations? After all, in classical mechanics, both obey $\mathbf{F} = \dot{\mathbf{p}}$. In quantum mechanics, both obey

$$\hat{E}\psi(x, t) = i\hbar \frac{\partial \psi(x, t)}{\partial t}.$$

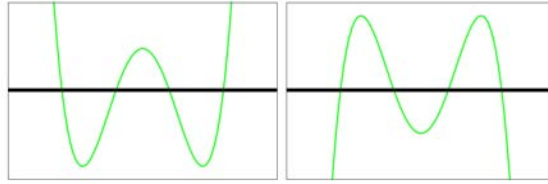


Figure 2: The same energy denoted by the black line is a bound classical and quantum state for the potential on the left, while the classical bound state is a quantum unbound state for the potential on the right

The distinction is worth making because the bound and unbound states exhibit qualitatively different behaviors:

Mechanics	Bound States	Unbound States
Classical	periodic motion	aperiodic motion
Quantum	discrete energy spectrum	continuous energy spectrum

For now, we will focus on bound states, with discussions of unbound states coming later. Let us remind ourselves of some of the properties of bound states.

1. Infinite square well:

- Ground state: no nodes
- n th excited state: n nodes (by the node theorem)
- Energy eigenfunctions chosen to be real
- Time evolution of energy eigenfunctions through complex phase $e^{-\frac{iEt}{\hbar}}$.
 - Different states evolve at different rates
 - Energy eigenstates have no time evolution in observables as $\mathbf{p}(x)$ for such states is independent of t
 - Time evolution of expectation values for observables comes only through *interference* terms between energy eigenfunctions

2. Symmetric finite square well

- Node theorem still holds
- $V(x)$ is symmetric
 - Leads to symmetry or antisymmetry of $\phi(x; E)$
 - Antisymmetric $\phi(x; E)$ are fine as $|\phi(x; E)|^2$ is symmetric
- Exponential tails in classically forbidden regions leads to discrete energy spectrum (picture of shooting for finite square well?)

3. Asymmetric finite square well

- Node theorem still holds
- Asymmetry of potential breaks (anti)symmetry of eigenfunctions
- Shallow versus deep parts of well
 - Deeper part of well \rightarrow shorter λ as $p = h\lambda^{-1}$ so particle travels faster there
 - Deeper part of well \rightarrow lesser amplitude as particle spends less time there so probability density is less there

4. Harmonic oscillator

- Node theorem still holds
- Many symmetries present
- Evenly-spaced discrete energy spectrum is very special!

So why do we study the harmonic oscillator? We do because we know how to solve it exactly, and it is a very good approximation for many, many systems. (picture of interatomic potential?)

Such problems are in general difficult. But we can expand the potential in a Taylor series about the equilibrium, and if we stay close to the equilibrium point, we can drop terms other than second-order (as the zeroth-order term is an uninteresting constant offset, the first-order term is zero at the equilibrium, and higher-than-second-order terms are negligible):

$$V(x) = \sum_{j=0}^{\infty} \frac{1}{j!} \frac{\partial^j V(x_0)}{\partial x_0^j} (x - x_0)^j \approx \frac{1}{2} \frac{\partial^2 V(x_0)}{\partial x_0^2} (x - x_0)^2 \quad (0.1)$$

where $\frac{\partial^2 V(x_0)}{\partial x_0^2}$ acts like the spring constant in a classical mechanical oscillator. Knowing how the spring constant relates to the oscillation frequency and redefining the origin for convenience, we will be studying the system

$$V(x) = \frac{1}{2} m\omega^2 x^2. \quad (0.2)$$

As a side note, can you think of systems for which this approximation is not a good one? One example might be $V(x) = \alpha x^4$ for some proportionality constant α .

The energy eigenstates of the harmonic oscillator form a family labeled by n coming from $\hat{E}\phi(x; n) = E_n\phi(x; n)$. This means that

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi(x; n)}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \phi(x; n) = E_n \phi(x; n) \quad (0.3)$$

is the energy eigenvalue equation for the harmonic oscillator. This is not an easy differential equation to solve! For now, we will solve this through brute force methods; later, this will be solved with more sophistication.

Before we dive into the brute force method, though, let us take a look at what we already know:

1. From dimensional analysis, we know that $E \propto \hbar\omega$.
2. From the uncertainty principle, we know that the ground state energy $E_0 \propto \hbar\omega$.
3. The energy operator is

$$\hat{E} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

There is a nice symmetry between \hat{x} and \hat{p} . Up to constants, our system looks the same whether we view it in position space or in momentum space. That is to say, there will be symmetries between $\phi(x; E)$ and $\tilde{\phi}(k; E)$. Do we know of a function that looks the same in both position space and momentum space? In other words, do we know of a function that is functionally similar to its Fourier transform? We do, and that is the Gaussian! We should expect to see some connection between the harmonic oscillator eigenfunctions and the Gaussian function.

4. By the node theorem, $\phi(x; n)$ should have n nodes.
5. Here is a sneak preview of what the harmonic oscillator eigenfunctions look like: (picture of harmonic oscillator eigenfunctions 0, 4, and 12?)

Our plan of attack is the following: non-dimensionalization \rightarrow asymptotic analysis \rightarrow series method \rightarrow profit! Let us tackle these one at a time.

We need to non-dimensionalize the equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi(x; E)}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \phi(x; E) = E\phi(x; E). \quad (0.4)$$

It is not good to carry around so many constants in that equation. Note that $\frac{m^2\omega^2}{\hbar^2}$ is dimensionally the same as x^{-4} . This implies that we should define the constant

$$\alpha \equiv \sqrt{\frac{\hbar}{m\omega}}$$

as our length scale. We can then define $u \equiv \frac{x}{\alpha}$ to non-dimensionalize position. Furthermore, we know that $E \propto \hbar\omega$, so non-dimensionalizing energy as $\varepsilon = \frac{E}{\hbar\omega}$ should work. This leaves the energy eigenvalue equation in fully non-dimensional form as

$$\frac{\partial^2 \phi}{\partial u^2} = (u^2 - \varepsilon)\phi. \quad (0.5)$$

This is certainly much neater, but it is not any *easier*. To make things easier, we need to develop some more mathematical techniques.

As a mathematical detour, we need to discuss *asymptotic analysis*. Let us suppose that we are solving the equation

$$\frac{\partial f(x)}{\partial x} + \left(1 + \frac{1}{x}\right) f(x) = 0. \quad (0.6)$$

In asymptotic analysis, we look at the different limits. Let us consider that

$$\lim_{x \rightarrow 0} \left(1 + \frac{1}{x}\right) \approx \frac{1}{x}.$$

This means that

$$\lim_{x \rightarrow 0} \frac{\partial f(x)}{\partial x} \approx \frac{f(x)}{x} \quad (0.7)$$

which is solved by

$$f(x) = f_0 x^{-1}.$$

But this only considers the behavior as $x \rightarrow 0$. Let us say that

$$f(x) = x^{-1} g(x)$$

where $g(x)$ is finite and well-behaved as $x \rightarrow 0$. Plugging this in yields

$$\frac{\partial g(x)}{\partial x} = -g(x),$$

which is solved by

$$g(x) = g_0 e^{-x}.$$

This means that the full solution is

$$f(x) = \frac{g_0}{x e^x} \quad (0.8)$$

which is exact! The first approximation was just to make our lives easier, and there ended up being no accuracy sacrificed anywhere. Furthermore, e^{-x} is indeed relatively constant compared to x^{-1} as $x \rightarrow 0$. To summarize, we looked at the extreme behavior of the differential equation to peel off a part of the solution. We then plugged that back in to get a simpler differential equation to solve.

But what if we did not know how to solve $\frac{\partial g(x)}{\partial x} + g(x) = 0$? How would we figure it out?

This is where the *series method* comes in. We can expand the function as a power series

$$g(x) = \sum_{j=0}^{\infty} a_j x^j \quad (0.9)$$

and perhaps figure out what the coefficients need to be. Now, we know that

$$\frac{\partial g(x)}{\partial x} = \sum_{j=0}^{\infty} j a_j x^{j-1} = \sum_{j=1}^{\infty} j a_j x^{j-1} = \sum_{s=0}^{\infty} (s+1) a_{s+1} x^s \quad (0.10)$$

first by removing the $j = 0$ term and second by redefining $s \equiv j - 1$. But s and j are just labels, so we might as well just say that

$$\frac{\partial g(x)}{\partial x} = \sum_{j=0}^{\infty} (j+1) a_{j+1} x^j. \quad (0.11)$$

This means that our differential equation is now

$$\sum_{j=0}^{\infty} ((j+1) a_{j+1} + a_j) x^j = 0. \quad (0.12)$$

The left side is a polynomial in x . If this is zero for *all* x , then the overall coefficients are identically zero:

$$(j+1) a_{j+1} + a_j = 0 \quad (0.13)$$

so

$$a_{j+1} = -\frac{a_j}{j+1} \quad (0.14)$$

implying

$$a_j = \frac{(-1)^j}{j!} a_0 \quad (0.15)$$

so

$$g(x) = \sum_{j=0}^{\infty} a_j x^j = \sum_{j=0}^{\infty} a_0 \frac{(-x)^j}{j!} = a_0 e^{-x} \quad (0.16)$$

as expected! To summarize, we just expanded the function as a power series, found the recursion relation for its coefficients, and then plugged in the initial conditions.

Let us get back into the physics of this. We want to solve the equation

$$\frac{\partial^2 \phi}{\partial u^2} = (u^2 - \varepsilon) \phi.$$

First, we apply asymptotic analysis:

$$\lim_{u \rightarrow \pm\infty} (u^2 - \varepsilon) \approx u^2 \quad (0.17)$$

so

$$\lim_{u \rightarrow \pm\infty} \frac{\partial^2 \phi}{\partial u^2} \approx u^2 \phi. \quad (0.18)$$

We can try

$$\phi(u) = \phi_0 e^{\frac{\alpha u^2}{2}}.$$

We find that

$$\frac{\partial \phi}{\partial u} = \alpha u \phi$$

and

$$\frac{\partial^2 \phi}{\partial u^2} = (\alpha + \alpha^2 u^2) \phi \approx \alpha^2 u^2 \phi$$

in the same limit. Comparing this to our differential equation, we see that we need

$$\alpha^2 = 1$$

so

$$\alpha = \pm 1.$$

We then get

$$\phi(u) = \phi_A e^{\frac{u^2}{2}} + \phi_B e^{-\frac{u^2}{2}}.$$

The first part is not normalizable, though, so we do not want that. We keep only the second part and generalize the constant to a function of u that is relatively constant and well-behaved as $u \rightarrow \pm\infty$, so we say that

$$\phi(u) = s(u) e^{-\frac{u^2}{2}}.$$

Now recall that the last step in asymptotic analysis is to plug this form into the original differential equation to yield a differential equation that can be solved for $s(u)$:

$$\frac{\partial^2 s}{\partial u^2} - 2u \frac{\partial s}{\partial u} + (\varepsilon - 1) s = 0. \quad (0.19)$$

Before we solve this, we need to figure out the behavior of $s(u)$. We know that it should grow less rapidly than $e^{+\frac{u^2}{2}}$ as $u \rightarrow \pm\infty$. Also, there should be multiple solutions corresponding to discrete bound states. Finally, the n th solution should have n nodes.

Let us try the power series expansion

$$s(u) = \sum_{j=0}^{\infty} a_j u^j \quad (0.20)$$

as our candidate solution. Plugging this into the differential equation yields

$$\sum_{j=0}^{\infty} ((j+1)(j+2)a_{j+2} - (2j+1-\varepsilon)a_j)u^j = 0. \quad (0.21)$$

Again, as this is true for *all* u , the overall coefficients must all be identically zero. This means that

$$a_{j+2} = \frac{2j+1-\varepsilon}{(j+1)(j+2)}a_j \quad (0.22)$$

is the recursion relation. This relates every *other* coefficient. This means that we need to specify both a_0 and a_1 to find all of the coefficients. Why is this the case? It is because we had a second-order differential equation. Does this meet our expectations? Let us consider large j :

$$\lim_{j \rightarrow \infty} a_{j+2} \approx \frac{2j}{j^2}a_j \approx \frac{a_j}{\frac{j}{2}} \quad (0.23)$$

so

$$a_j \approx \frac{C}{\left(\frac{j}{2}\right)!} \quad (0.24)$$

and

$$s(u) \approx C \sum_j \frac{u^j}{\left(\frac{j}{2}\right)!} = C \sum_n \frac{u^{2n}}{n!} = Ce^{u^2}. \quad (0.25)$$

Unfortunately, this is exactly what we do not want, as plugging this into $\phi(u) = s(u)e^{-\frac{u^2}{2}}$ recovers the non-normalizable solution.

Remember from before that to get a normalizable wavefunction, we had to impose a specific, discrete set of energies. If we can do that here, can we get things to work?

The only way out of this conundrum is that the series must be finite. In particular, let us suppose that there exists some n such that when $j = n$, the numerator $2j + 1 - \varepsilon = 0$. Then all of the subsequent $a_j = 0$. Imposing that condition yields that $\varepsilon = 2n + 1$. But we know that $\varepsilon \equiv 2(\hbar\omega)^{-1}E$. Therefore, the energy eigenvalues are

$$E_n = \hbar \left(n + \frac{1}{2} \right) \omega. \quad (0.26)$$

We now have our quantized energies! They are also evenly spaced as expected.

Note that imposing this condition only terminates either the odd series or the even series because the recursion relation is spaced by two. We need to separately insist that the $a_j = 0$ for the other series. This is fine because it has been shown that if the potential is symmetric, then the energy eigenfunctions can be taken to be either even or odd.

Let us construct some solutions for this. For $n = 0$, we have $\varepsilon = 1$, so $a_2 = 0$, and we can impose that $a_1 = a_3 = a_5 = \dots = 0$. This implies that $s(u) = a_0$, so

$$\phi(u; 0) = a_0 e^{-\frac{u^2}{2}}. \quad (0.27)$$

For $n = 1$, we have $\varepsilon = 3$, so finding that $a_3 = 0$ and imposing $a_0 = a_2 = a_4 = \dots = 0$ implies that $s(u) = a_1 u$, so

$$\phi(u; 1) = a_1 u e^{-\frac{u^2}{2}}. \quad (0.28)$$

Repeating this process yields

n	$\frac{2E_n}{\hbar\omega}$	$\phi(x; n)e^{+\frac{x^2}{2a^2}}$
0	1	N_0
1	3	$N_1 \cdot \left(\frac{2x}{a}\right)$
2	5	$N_2 \cdot \left(\frac{4x^2}{a^2} - 2\right)$
\vdots	\vdots	\vdots
n	$2n + 1$	$N_n \mathcal{H}_n\left(\frac{x}{a}\right)$

where $\mathcal{H}_n(u)$ is the n th Hermite polynomial, which is a special set of polynomial functions. Using the definition of these polynomials as used in mathematics yields

$$N_n = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} (2^n n!)^{-\frac{1}{2}} \quad (0.29)$$

for the normalization factors.

Let us review the properties of the harmonic oscillator:

- The energies are quantized as

$$E_n = \hbar \left(n + \frac{1}{2}\right) \omega \quad (0.30)$$

which are evenly spaced!

- There is

$$E_0 = \frac{1}{2} \hbar \omega \quad (0.31)$$

as the nonzero ground state energy. This is not arbitrary; while the bottom of the well is arbitrary, the ground state energy is $\frac{1}{2} \hbar \omega$ above that bottom.

- The eigenfunctions satisfy the node theorem as $\mathcal{H}_n(u)$ is an n th-order polynomial in u . These also satisfy even/odd parity.
- General states are given by

$$\psi(x, t) = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} \phi(x; n) = \sum_n c_n e^{-i(n+\frac{1}{2})\omega t} \phi(x; n). \quad (0.32)$$

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