Week 4

PHY 303 Quantum Mechanics

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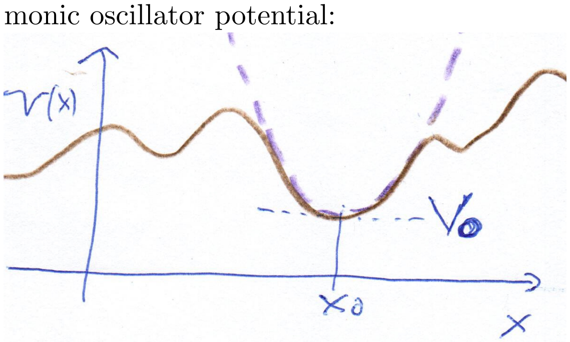
2.3 Quantum harmonic oscillator

We now finally go beyond piecewise constant potentials, to look at the harmonic oscillator potential

$$V(x) = \frac{1}{2}m\omega^2 x^2. \tag{2.41}$$

This is very important, simply because near a local minimum, any potential will look like a harmonic oscillator potential:



left: Near a local minimum at x_0, we can write $V(x) = \underbrace{V(x_0)}_{=V_0} + \frac{1}{2}V''(x)\Big|_{x=x_0}(x-x_0)^2 + \mathcal{O}(x-x_0)^3$. Defining $V''(x)\Big|_{x=x_0} = m\omega^2$, this gives us (2.41).

Because of its importance, we even provide two different methods to solve the TISE for the quantum harmonic oscillator

$$\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right]\phi_n(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right]\phi_n(x) = E_n\phi_n(x), \tag{2.42}$$

an algebraic method and the more direct solution via a power series.

2.3.1 Algebraic method

Let us define new linear combinations out of the position and momentum operators, so-called

Ladder operators

$$\hat{a}_\pm = \frac{1}{\sqrt{2m}}\left(\hat{p} \pm im\omega\hat{x}\right), \qquad = \frac{1}{\sqrt{2m}}\left(-i\hbar\frac{\partial}{\partial x} \pm im\omega\hat{x}\right). \tag{2.43}$$

where the + one is called raising operator and the one with − lowering operator.

It turns out that with these operators, we can re-write the TISE Eq. (2.42) as

$$\left[\hat{a}_+\hat{a}_- + \frac{\hbar\omega}{2}\right]\phi_n(x) = E_n\phi_n(x). \tag{2.44}$$

- Griffith discusses some motivation why we choose the form (2.43), essentially trying to bring the form $u^2 + v^2$ in the Hamiltonian into a product $(u - iv)(u + iv)$.
- However now we have to be careful since the Hamiltonian contains operators, where the ordering may be important. For example $x\frac{\partial}{\partial x}f(x) \neq \frac{\partial}{\partial x}[xf(x)]$.
- See the detailed derivation from (2.42) to (2.44) in Griffith.

In that derivation, we can use the

Commutator of ladder operators:

$$\left[\hat{a}_-, \hat{a}_+\right] \equiv \hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_- = \hbar\omega. \tag{2.45}$$

- You may remember from matrix multiplication, that usually we do not have $\underline{\underline{A}} \cdot \underline{\underline{B}} = \underline{\underline{B}} \cdot \underline{\underline{A}}$. Since operators can be viewed as infinite dimensional matrices (section 10), you should find Eq. (2.45) at least plausible.
- Proof: We must show identities involving operators by applying operators onto a testfunction $f(x)$, since e.g. having a dangling derivative as in $x\frac{\partial}{\partial x}$ that is not applied onto anything does not make sense. In this way, let us find an easier commutator first, namely

  $$\left[\hat{x}, \hat{p}\right] = (i\hbar). \tag{2.46}$$

  To see this, we write

  $$\begin{aligned}\left[\hat{x}, \hat{p}\right]f(x) &= \left(x(-i\hbar\frac{\partial}{\partial x}) - (-i\hbar\frac{\partial}{\partial x})x\right)f(x) \\ &= (-i\hbar)\left(xf'(x) - [xf(x)]'\right) = (-i\hbar)\left(xf'(x) - [1f(x) + xf'(x)]\right) = (i\hbar)f(x).\end{aligned} \tag{2.47}$$

  Since this is true for <u>any</u> testfunction $f(x)$, we have shown the operator identity (2.46).

  Using either Eq. (2.46) and the definition Eq. (2.43), or the same technique as above directly from Eq. (2.43), you can show (2.45) as an exercise.
- We will learn many additional useful rules regarding commutators in chapter 3 and discuss them much more.

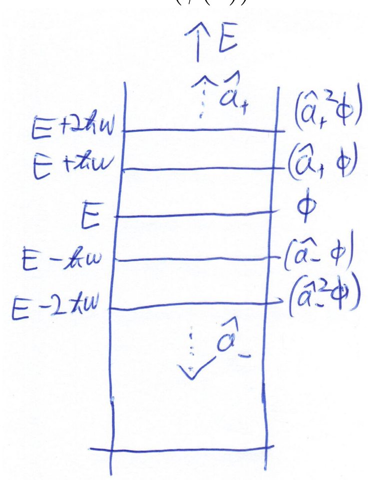
In (2.44) we just rewrote the TISE with some weird operators. Armed with the commutator (2.45), we can now attack the crucial argument why this is useful. Namely we can show that if $\phi(x)$ solves the TISE for energy E, then $\hat{a}_+\phi(x)$ solves it for energy $E+\hbar\omega$. Proof: As a first step, we see that using (2.45), we can write Eq. (2.44) also as

$$\left[\hat{a}_-\hat{a}_+ - \frac{\hbar\omega}{2}\right]\phi_n(x) = E_n\phi_n(x). \tag{2.48}$$

Then

$$\left[\hat{a}_+\hat{a}_- + \frac{\hbar\omega}{2}\right](\hat{a}_+(\phi_n(x)) = \quad \hat{a}_+ \underbrace{(\hat{a}_-\hat{a}_+)\phi_n(x)}_{\overset{Eq.\ (2.48)}{=}(E_n+\frac{\hbar\omega}{2})\phi_n} + \frac{\hbar\omega}{2}(\hat{a}_+(\phi_n(x)) = \big(E_n + \hbar\omega\big)(\hat{a}_+(\phi_n(x)). \tag{2.49}$$

which means that $\hat{a}_+(\phi_n(x))$ solves the TISE with energy $E+\hbar\omega$ as claimed. Similarly we can show that $\hat{a}_-(\phi(x))$ solves it for energy $E-\hbar\omega$.



left: This now explains why we call $\hat{a}_\pm$ ladder operators. Given ANY solution of the problem $\phi(x)$ we are raising the energy with $\hat{a}_+$, lowering it with $\hat{a}_-$, and thus can build a ladder of different energy values, see diagram on the left.

Of course to use this, we first need at least one solution $\phi(x)$, which we don't have yet. To get one, consider repeated application of $\hat{a}_-$. Since the energy is reduced everytime, at some point it would have to become negative. However it is not possible that $E < \min_x V(x)$ (see e.g. Griffith Problem 2.2). This means that at some point we require $\hat{a}_-\phi_0(x) = 0$ for some "lowest step" on the ladder ϕ_0, to terminate generating lower and lower energy solutions[9]. Writing this explicitly from (2.43) in terms of the position and momentum operator:

$$\frac{1}{\sqrt{2m}}\left(-i\hbar\frac{\partial}{\partial x} - im\omega\hat{x}\right)\phi_0 = 0. \tag{2.50}$$

This differential equation is now easy to solve, in contrast to the original one. We sort things a bit and then integrate both side':

$$\frac{d\phi_0}{dx} = -\frac{m\omega}{\hbar}x\phi_0 \Rightarrow \int\frac{d\phi_0}{\phi_0} = -\frac{m\omega}{\hbar}\int dx\, x \Rightarrow \ln\phi_0 = -\frac{m\omega}{2\hbar}x^2 + \text{const} \rightarrow \phi_0(x) = \mathcal{N}e^{-\frac{m\omega}{2\hbar}x^2}. \tag{2.51}$$

with $\sigma = \sqrt{\hbar/m/\omega}$. Since we had demanded $\hat{a}_-\phi_0(x) = 0$, we can directly see from Eq. (2.48) that the energy of this state is $E_0 = \hbar\omega/2$. With that we have now solved the TISE for the

[9] See Griffith for one other possibility, and why that does not happen.

Quantum harmonic oscillator

$$\phi_n(x) = \mathcal{N}_n(\hat{a}_+)^n e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}, \tag{2.52}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{2.53}$$

with eigenfunction ϕ_n, normalisation factor $\mathcal{N}_n$, zero point uncertainty $\sigma = \sqrt{\hbar/(m\omega)}$.

- To generate all other slutions from Eq. (2.51) we used our earlier result (2.49). For example we can generate $\phi_1(x) \sim (\hat{a}_+)^n e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}$ and then normalize it. Using Eq. (2.43), this gives us

$$\begin{aligned}\phi_1(x) &= \mathcal{N}_1 \frac{1}{\sqrt{2m}}\left(-i\hbar\frac{\partial}{\partial x} + im\omega\hat{x}\right) e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{\mathcal{N}_1}{\sqrt{2m}}\left(-i\hbar(-\frac{m\omega}{\hbar}x) + im\omega x\right) e^{-\frac{m\omega}{2\hbar}x^2} \\ &= i\mathcal{N}_1\omega\sqrt{2\hbar\omega}\left(\frac{x}{\sigma}\right) e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}. \end{aligned} \tag{2.54}$$

  We will provide drawings of this function later.

- The unknown integration constant *const* turned into $\mathcal{N}$ in (2.51) and $\mathcal{N}_n$ in (2.52) and has to be fixed for each separately by normalisation using Eq. (1.6.1).

- We will discuss the physics of the quantum SHO and detailed shape of wavefunctions shortly, first we shall see one more completely different method to arrive at the above solutions.

2.3.2 Analytical method

The solution of the preceding section is very elegant, but very tricky. I would not have thought of it myself, for sure, would you?. We can also try to solve the TISE (2.42) in a more generally applicable way. Let us first move to dimensionless units for space $\xi = x/\sigma$ and energy $K_n = 2E_n/(\hbar\omega)$. Drawing on section 2.3.1, this means that we measure space in units of the zero point uncertainty and energy in units of $\hbar\omega$. Converting the differential opertor in (2.42), we see that this tidies the equation up quite a bit, and we reach

$$\frac{d}{d\xi}\phi_n(\xi) = (\xi^2 - K_n)\phi_n(\xi). \tag{2.55}$$

We first see what happens when $\xi \to \infty$ and hence $\xi \gg K$, in that case we have $\frac{d}{d\xi}\phi_n(\xi) = \xi^2\phi_n(\xi)$. This has the approximate solution

$$\phi_n(\xi) \approx Ae^{-\xi^2/2} + Be^{-\xi^2/2}. \tag{2.56}$$

To see this take the double derivative of (2.56) wrt. ξ, and in the resultant expression use that $\xi \to \infty$ which means only the highest powers of ξ in any term need to be considered. Onlt the term $\sim A$ can be normalized, so we must chose $B = 0$. Now that we know how the function has to behave at large ξ, let us build this form into our solution attempt, by defining

$$\phi_n(\xi) \approx h(\xi) e^{-\frac{\xi^2}{2}}. \tag{2.57}$$

(Techincally we should write $h_n(\xi)$, but we shall supress that until Eq. (2.64)). We can plug (2.57) into the TISE (2.55) (see Griffith) and reach an equation for $h(\xi)$

$$\frac{d^2 h(\xi)}{d\xi^2} - 2\xi \frac{dh(\xi)}{d\xi} + (K-1)h(\xi) = 0. \tag{2.58}$$

To solve this, we express the solution in terms of a

Power series expansion:

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j. \tag{2.59}$$

We then insert (2.59) into (2.58), which gives

$$\sum_{j=0}^{\infty} \underbrace{\left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]}_{=0} \xi^j = 0. \tag{2.60}$$

Since all the different powers of ξ are linearly independent, the coefficient of all ξ^j have to vanish seperately, which gives us:

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j. \tag{2.61}$$

This is a <u>recursion formula</u>, such that if we know a_0 and a_1, it gives us all the higher a_j. One can show, that the series (2.59) with coefficients fulfilling (2.61) must terminate, i.e. possess a highest $j = n$ such that all $a_{j'} = 0$ for $j' > n$ (see e.g. Griffith). Essentially, if it did not, the resultant function would not be normalizable.

Note that Eqs. (2.59) and (2.61) effectively set up two independent power series for the even and odd part of the function

$$h_{\text{even}}(\xi) = a_0 + a_2\xi^2 + a_4\xi^4 + \cdots \qquad \text{(even)}, \tag{2.62}$$
$$h_{\text{odd}}(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots \qquad \text{(odd)} \tag{2.63}$$

We can see that the only way to terminate the series at $j = n$ is if $2n + 1 = K$. Since it only terminates one of the even or odd series, the other one must have been fully zero due to $a_0 = 0$ or $a_1 = 0$. Alternatively one can also show that an even potential $V(x) = V(-x)$ gives rise to either even or odd eigenfunctions (exercise/assignment). We can rewrite $2n+1 = K$ into $E_n = (n+1/2)\hbar\omega$, so we just re-discovered Eq. (2.53). From the discussion so far we see that $h(\xi)$ which terminates at $j = n$ is a polynamical of degree n. All up we find the

Explicit eigenfunctions of the quantum harmonic oscillator as

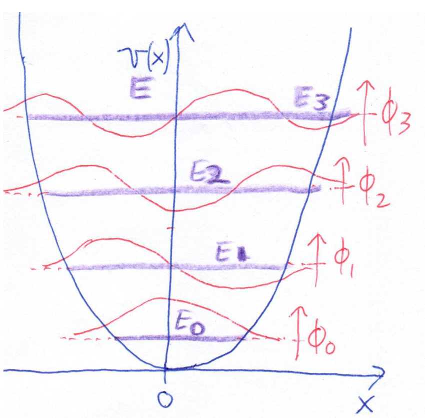
$$\phi_n(x) = \mathcal{N}_n H_n\left(\frac{x}{\sigma}\right) e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}, \tag{2.64}$$

with $\mathcal{N}_n = (\pi\sigma^2)^{-1/4}(2^n n!)^{-1/2}$ and $H_n(\xi)$ a Hermite polynomial of degree n.

- The lowest Hermite polynomials are

$$H_0 = 1, \tag{2.65}$$
$$H_1 = 2x, \tag{2.66}$$
$$H_2 = 4x^2 - 2, \tag{2.67}$$
$$H_3 = 8x^3 - 12x. \tag{2.68}$$

  Note, that with the expression for H_1, (2.64) of course agrees with the first excited state we had found in Eq. (2.54).



left: On the left we draw $V(x)$, E_n and $\phi_n(x)$ for the harmonic oscillator in the same style as for particle in the box (PIB) before (near Eq. (2.18)).

- As for the PIB, they alternate between even and odd.
- As for the finite-PIB, wavefunctions extend exponentially decaying into the classically forbidden region where $V(x) > E$.
- Unlike the PIB, the quantized energies are equidistant $E_{n+1} - E_n = \hbar\omega$.

- Again, the lowest energy is nonzero. $E = \hbar\omega/2$ is called the zero-point energy. You can calculate also the position uncertainty in the ground-state (see assignment 2, Eq. (1.35)) and you shall find $\sigma_x = \sigma$ (hence the name). This is due to what is called zero-point motion.

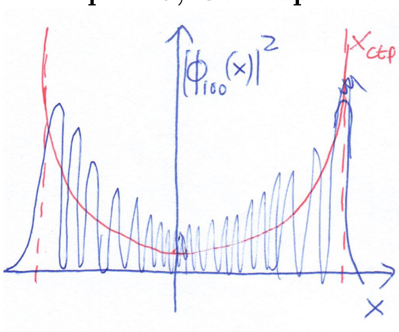
The procedure that we have used to solve the differential equation (2.55) is more generally useful:

(i) First find asymptotic solutions at large $|\xi| \to \infty$.

(ii) Build the structure of that solution into an Ansatz such as (2.57), and then solve for the detailed form with a power series such as (2.59).

On first sight, the solutions $\phi_n(x)$ seem to have little to do with what we know of the classical harmonic oscillator. However the connections are only slightly hidden. Consider the time-averaged probability distribution of the classical oscillator. We know it follows $x(t) = x_{\text{ctp}} \sin(\omega t)$. If you look at a large random ensemble of oscillators, the probability $\rho(x)$ to find in between position x and $x+dx$ must be $\rho(x) \sim dx/v(x)$. Since $v(t) = \omega x_{\text{ctp}} \cos(\omega t)$ we can write[10] $v(x) = (\omega\sqrt{x_{\text{ctp}}^2 - x^2})^{-1}$. We can now see the

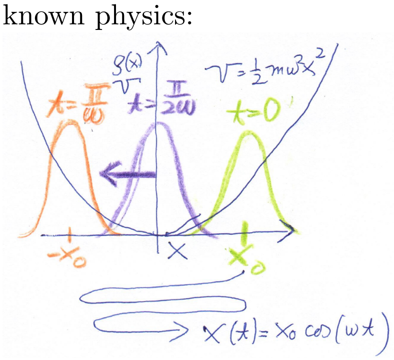
Example 15, Correspondence principle:



left: The sketch on the left shows a very high SHO state $\phi_n(x)$ (blue), and the classical probability distribution $\rho(x)$ (red). We see that the average amplitude of the quantum state precisely follows $\rho(x)$. If we now were e.g. averaging over a few adjacent SHO states, we recover the classical result.

There are more signs of the underlying classical physics: In example 13, we had seen how the PIB states can be decomposed in plane waves that correspond to a classical particle bouncing back and forth. In that case, the probability distribution $\rho(x) \sim \sin^2(p/\hbar x)$, which means the distance between zeros gave some indication of the momentum (velocity). You see in example 15 how the distance between zeros decreases in the centre and increases at the flanks. This again, reflects that we know the oscillator will move fastest around $x = 0$ and slowest near $x = x_{\text{ctp}}$ (the classical turning point).

Example 16, Making the quantum oscillator classical again: Some more hidden known physics:



left: If we e.g. solve the TDSE **??** on a computer, starting from a Gaussian wavefunction that is offset by x_0 from the centre: $\Psi(x, t = 0) = \phi_0(x - x_0)$, the probability density preserves a Gaussian shape $\rho(x) \sim e^{-(x-x(t))^2/\sigma^2}$, with $x(t) = x_0 \cos(\omega t)$. Besides retaining the zero-point uncertainty σ (independent of time), the centre of the position space distribution thus just does the classical oscillation.

You can again check this out life using this online app. *Analytical proof and discussion: Assignment 4.*

[10] Using $\cos^2 + \sin^2 = 1$.

Example 17, Quantum harmonic oscillators in science: Since every potential looks like a harmonic oscillator near local minima (and hence near stable equilibirium points), as discussed at the beginning of section 2.3, the importance of the QSHO cannot be overstated. You will encounter it again for:

- Vibrations of molecules around their equilibirum bond lengths.
- Lattice vibrations of ions in solid materials, e.g. metals.
- Ions and atoms trappe in electromagnetic fields (and otherwise vacuum), for e.g. quantum computing.

You will also see, that operators such as $\hat{a}_\pm$ and the mathematical rules induced by (2.45) can also be used to climb a ladder in terms of "particle number", instead of oscillator energy. Someof the concepts in this section thus form the basis of many-body quantum physics, quantum field theory and particle physics.