(13) QHO, Part 1

1 Thus Far

- EESs in all kinds of piecewise flat 1D potentials

2 This Time

- Energy Eigenstates of the Quantum Harmonic Oscillator

3 The Quadratic Potential

The simple harmonic oscillator potential is given by

SHO

$$V(x) = \tfrac{1}{2}kx^2 \qquad \Rightarrow \qquad F(x) = -kx$$

The simple harmonic oscillator is a physicist's favorite toy. It is a great model for at least 2 reasons: first because any small deviation around a stable point can be represented by a SHO, and secondly because we can actually solve it.

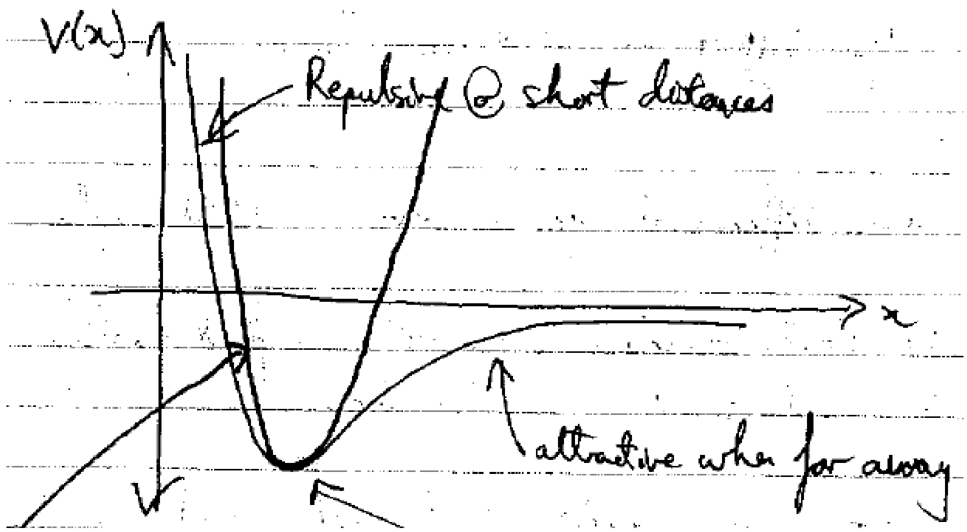
I say we can use it for any potential because any potential can be expanded as

Taylor Expansion of Any Potential at $x = x_0$

$$V(x) = V(0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots$$

We can choose our potential such that $V(x_0) = 0$, and at a stable point we know that $V'(x_0) = 0$, so the leading term is $V''(x_0)(x - x_0)^2$. For sufficiently small x, only this terms matters and we have a SHO.

Example Potential: Attraction Between Atoms



Recall that the solutions to the Classical SHO are oscillatory functions of time, which oscillate with angular frequency $\omega^2 = k/m$

Solution to Classical SHO

$$x(t) = A\sin(\omega t + \theta) \quad \text{where} \quad \omega = \sqrt{\frac{k}{m}}$$

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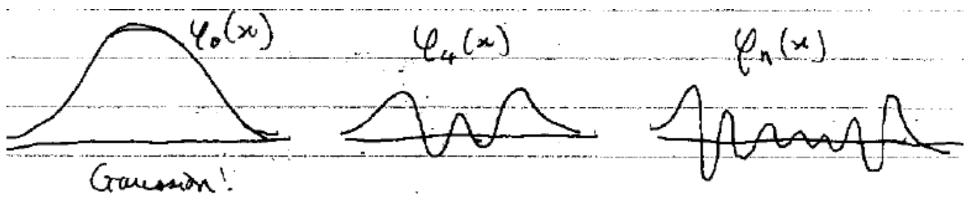
4 Qualitative Solutions to the Quadratic Potential

Before we solve the Schrödinger equation exactly to find the energy eigenstates of this potential, let's use the qualitative techniques we learned earlier to get an idea of what the solutions might look like.

Since the potential goes to infinity as $x \to \pm\infty$, we know that we are looking for a discrete set of bound states. The solutions will be real valued functions which decay to zero as $x \to \pm\infty$, and the node theorem tells us that the n^{th} bound state will have n nodes. The ground state, with $n = 0$, will have no nodes, so it is an always positive real function.

Qualitative Bound States



The solutions decay exponentially as they penetrate into the classically forbidden regions, and since the potential is growing as we go away from zero, they must decay faster than $e^{\pm\alpha x}$. The form of a the Energy operator gives us a hint as to what kind of function we are looking for

Energy Operator for SHO

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

There is symmetry between $\hat{x}$ and $\hat{p}$, which indicates that a Gaussian might appear in the solution, since Gaussian's look the same in position and momentum space.

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5 Energy Eigenstates in a Quadratic Potential: The Hard Way

Let's embark on an adventure to find the solutions of the Schrödinger equation with the SHO potential, and keep in mind along the way that the techniques used here are helpful also for other problems of this sort.

Start by writing the equation to solve.

Schrödinger Equation for SHO

$$\begin{aligned} E\phi(x) &= -\frac{\hbar^2}{2m}\partial_x^2\phi(x) + \frac{m\omega^2}{2}x^2\phi(x) \\ \Rightarrow \partial_x^2\phi(x) &= \left(\frac{m^2\omega^2}{\hbar^2}x^2 - 2\frac{m}{\hbar^2}E\right)\phi(x) \end{aligned}$$

Then define some dimensionless parameters which make the equation easier to write and think about.

Dimentionless

$$\frac{\hbar}{m\omega}\partial_x^2\phi(x) = \left(\frac{m\omega}{\hbar}x^2 - 2\frac{E}{\hbar\omega}\right)\phi(x)$$

$$\partial_u^2\phi(u) = \left(u^2 - 2\epsilon\right)\phi(u) \quad \text{for} \quad \epsilon = \frac{E}{\hbar\omega} \quad \text{and} \quad u = \sqrt{\frac{m\omega}{\hbar}}x$$

This gives us an equation which is much neater and easier to write, but not really easier to solve. We can make the solution simpler by taking the limit of large u^2, where $u^2 - 2\epsilon \simeq u^2$, which corresponds to regions deep in the classically forbidden zone. In these regions, our equation simplifies to

Approximate Solution for $u^2 \gg 2\epsilon$

$$\begin{aligned}
\partial_u^2\phi(u) &= u^2\phi(u) \qquad \text{try} \quad \phi(u) = e^{-\alpha u^2/2} \\
\Rightarrow \partial_u^2\phi(u) &= -\alpha\,\partial_u\, ue^{-\alpha u^2/2} \\
&= -\alpha\left(e^{-\alpha u^2} - \alpha u^2 e^{-\alpha u^2}\right) \\
&= (\alpha^2 u^2 - \alpha)\phi(u) \\
&\simeq \alpha^2 u^2 \phi(u) \ \Rightarrow \ \alpha = \pm 1 \\
\Rightarrow \quad & \phi(u) \simeq e^{-u^2/2} \quad \text{(Normalizable)}
\end{aligned}$$

The fact that the width of the Gaussian turned out to be 1 means that we did something right in our selection of dimensionless parameters.

Now, for the region closer to the origin. We know that we need some number of nodes for solutions above the ground state. I would like to note that an n^{th} order polynomial, with properly chosen coefficients, is a function with n nodes.

Draw some example polynomials.

So, let's try solutions which are a product of a polynomial and a Gaussian.

Solution

$$\text{try } \phi(u) = h(u)e^{-u^2/2} \text{ with } h(u) = \sum_{n=0} a_n u^n$$

$$\partial_u^2 h(u)e^{-u^2/2} = \left(u^2 - 2\epsilon\right) h(u)e^{-u^2/2}$$

$$\partial_u \left[(\partial_u h(u))e^{-u^2/2} - h(u)ue^{-u^2/2}\right] = \cdots$$

$$\left[(\partial_u^2 h(u))e^{-u^2/2} - (\partial_u h(u))ue^{-u^2/2}\right] - \cdots$$

$$\left[(\partial_u h(u))ue^{-u^2/2} + h(u)(1-u^2)e^{-u^2/2}\right] = \cdots$$

$$\Rightarrow \partial_u^2 h(u) - 2u\partial_u h(u) + (2\epsilon - 1)h(u) = 0$$

Whew! We now have a differential equation to solve for $h(u)$, and it still isn't obvious that we are winning, but I assure you we are close...

Solution, continued

$$\partial_u^2 \sum_{n=0} a_n u^n - 2u\partial_u \sum_{n=0} a_n u^n + (2\epsilon - 1)\sum_{n=0} a_n u^n = 0$$

$$\sum_{n=2} n(n-1)a_n u^{n-2} - 2u\sum_{n=1} n a_n u^{n-1} + \cdots$$

$$\sum_{n=0} (n+2)(n+1)a_{n+2}u^n - 2\sum_{n=0} n a_n u^n + \cdots$$

$$\Rightarrow \sum_{n=0} \left[(n+2)(n+1)a_{n+2} - (2n+1-2\epsilon)a_n\right] u^n = 0$$

$$\Rightarrow a_{n+2} = \tfrac{2n+1-2\epsilon}{n^2+3n+2} a_n$$

It seems that we have a solution!

To find the even a_n values, we need only specify a_0. To find the odd values, we specify a_1.

Note that this is NOT an approximate solution; it is the exact solution. (Our use of the large u approximate solution was just to help us guess the form of the exact solution.)

However, our solution has a problem: the number of terms in the polynomial is not obviously limited. And *infinitely long* polynomial can overcome our Gaussian envelope and cause convergence problems, not to mention the fact that we were looking for a solution with a fixed number of nodes to satisfy the node theorem. To avoid this trouble, we will need to choose the energy of our state such that the recursion relation for a_n terminates. This can be arranged by picking ϵ such that

Energy of Normalizable States

$$2n + 1 - 2\epsilon_n = 0 \;\Rightarrow\; a_{n+2} = 0$$
$$\Rightarrow \epsilon_n = n + \tfrac{1}{2} \quad\;\Rightarrow\; E_n = \hbar\omega(n + \tfrac{1}{2})$$

Of course, if you use this trick to terminate the series of even values of n, it will not terminate the odd series, and vice versa. We can side-step this problem by always choosing a_0 or a_1 to be zero. This means that solutions will be either even or odd, which is what we would expect from the symmetry of the potential.

The polynomials you get by running out the recursion relation appear elsewhere in math and physics and are called the Hermite polynomials. The first few of them are

Hermite Polynomials

$$\begin{aligned}
H_0(u) &= 1 \\
H_1(u) &= 2u \\
H_2(u) &= 4u^2 - 2 \\
H_3(u) &= 8u^3 - 12u \\
H_4(u) &= 16u^4 - 48u^2 + 12 \\
H_5(u) &= 32u^5 - 160u^3 + 120u \\
&\vdots
\end{aligned}$$

So, to summarize, the energy eigenstates of the simple harmonic oscillator potential are

EES of SHO potential

$$\begin{aligned} \phi_n(u) &= N_n H_n(u) e^{-u^2/2} \text{ with } \epsilon_n = n + \tfrac{1}{2} \\ \Rightarrow \phi_n(x) &= N_n \, H_n\left(x/\lambda\right) e^{-x^2/2\lambda^2} \\ \text{with} \qquad & \lambda = \sqrt{\frac{\hbar}{m\omega}} \text{ and } E_n = \hbar\omega(n + \tfrac{1}{2}) \end{aligned}$$

Where N_n is a normalization constant for each state. Some math leads to

$$N_n = \frac{1}{\sqrt{2^n n! \, \lambda \sqrt{\pi}}}$$

Note the process:

1. Rewrite the problem in dimensionless form
2. Find a solution where the equation is easy to solve (e.g., $x \to \pm\infty$)
3. Hope that a polynomial will do the rest

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6 Examples

We can try the first few of these to make sure that they work. For $n = 0$, we just have a Gaussian.

Draw it!

Ground State, $n = 0$ and $\epsilon = \frac{1}{2}$

$$\begin{aligned} \partial_u^2 \phi(u) &= (u^2 - 1)\phi(u) \quad \text{with} \quad \phi(u) = e^{-u^2/2} \\ \Rightarrow \partial_u^2 e^{-u^2/2} &= -\partial_u \, u e^{-u^2/2} \\ &= -\left(e^{-u^2/2} - u^2 e^{-u^2/2}\right) \\ &= (u^2 - 1) e^{-u^2/2} \end{aligned}$$

The first excited state is a little more challenging, but still quite doable.

Draw it!

First Excited State, $n = 1$ and $\epsilon = \frac{3}{2}$

$$\begin{aligned} \partial_u^2 \phi(u) &= (u^2 - 3)\phi(u) \quad \text{with} \quad \phi(u) = u e^{-u^2/2} \\ \Rightarrow \partial_u^2 u e^{-u^2/2} &= \partial_u \, (1 - u^2) e^{-u^2/2} \\ &= (u^2 - 3) u e^{-u^2/2} \end{aligned}$$

And from there we move on to the land of Mathematica.

Show Mathematica notebook of Hermite Gaussians.

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7 Next Time

- The Quantum Harmonic Oscillator: how to do all of this without breaking a sweat