Phys 506 lecture 6: Schrodinger factorization method

We know that in quantum mechanics only a handful of problems can be exactly solved. In 1940, Schrodinger described a general approach for such problems that was algebraic. It generalized the operator method for the simple harmonic oscillator to all of those other exactly solvable problems. In the next few lectures, we will explore this method and how to apply it to these different systems. It is a truly different way to solve these problems. But there is one caveat. At this stage, we do not how to generalize it to solve any problem (using a computer). I view this as an exciting new opportunity in a field where we thought we already knew everything! This comment is with regards to performing the factorization directly. There is a way to do it numerically that also employs the conventional Schrödinger differential equation.

1 Introduction to the factorization method

It is easiest to jump into the method, which will seem quite abstract at first, and then make it more concrete as we discover how to solve some problems. The approach we give now is somewhat formulaic at first. We will derive some other methodologies that will appear less so. The strategy is to write $\hat{H} = \hat{H}_0$ in a factorized form

$$\hat{H}_0 = \hat{A}_0^\dagger \hat{A}_0 + E_0.$$

Here, $\hat{A}$ and $\hat{A}^\dagger$ are operators that are Hermitian conjugates of each other. E is a number with dimensions of energy. Since $\hat{A}_0^\dagger \hat{A}_0$ is a positive semidefinite operator, we know that the ground state satisfies $\hat{A}_0 |\phi_0\rangle = 0$ and E_0 is its energy (just like what we did with the SHO). But now, we devise a set of new "auxiliary" Hamiltonians $\hat{H}_j$ and auxiliary ground states $|\phi_j\rangle$ via the following procedure

$$\hat{H}_1 = \hat{A}_1^\dagger \hat{A}_1 + E_1 \quad \cdots \quad \hat{H}_j = \hat{A}_j^\dagger \hat{A}_j + E_j$$

with

$$\hat{A}_j |\phi_j\rangle = 0 \quad \text{and} \quad \hat{H}_j |\phi_j\rangle = E_j |\phi_j\rangle$$

At this point, this seems the an exercise in futility, but we connect the auxiliary Hamiltonians via the additional requirement that

$$\hat{H}_j = \hat{A}_{j-1} \hat{A}_{j-1}^\dagger + E_{j-1}$$

So the chain is constructed as follows:

$$\hat{H} = \hat{H}_0 = \hat{A}_0^\dagger \hat{A}_0 + E_0$$
$$\hat{H}_1 = \hat{A}_0 \hat{A}_0^\dagger + E_0 \Rightarrow \hat{A}_1^\dagger \hat{A}_1 + E_1$$
$$\hat{H}_2 = \hat{A}_1 \hat{A}_1^\dagger + E_1 \Rightarrow \hat{A}_2^\dagger \hat{A}_2 + E_2$$

and so on. We also require that $E_{j+1} > E_j$. This may sound odd, but it forbids us from choosing $E_1 = E_0$ and $\hat{A}_1^\dagger = \hat{A}_0$, because that is always a choice we could make. It also tells us we must have $E_j > E_{j-1} > \cdots > E_2 > E_1$ for this method to work—the energy levels must be nondegenerate. This is a well-known consequence of the node theorem in one dimension, but arises naturally here.

Now, our situation is quite complex, for not only do we need to find a way to factorize our original $\hat{H}$, once we have $\hat{A}_0$, we next determine a new auxiliary Hamiltonian from $\hat{H}_1 = \hat{A}_0\hat{A}_0^\dagger + E_0 = \hat{H}_0 + \left[\hat{A}_0, \hat{A}_0^\dagger\right]$. Since this is usually a different potential than in $\hat{H}_0$, we need to find a way to factorize H_1 too.

This is a problem that is hard in general. But it turns out we can find a strategy to do this for all of the exactly solvable problems. It turns out all exactly solvable problems have the same form for the ladder operators—they only differ in the numerical constants in them—this allows us to do these factorizations easily. For the moment just assume we can do this. Let's investigate some consequences.

2 Consequences of the factorization method

Assume $|\psi\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue E. Hence, $\hat{H}|\psi\rangle = E|\psi\rangle$. Our first step is to work out the intertwining identity: $\hat{H}_{j+1}\hat{A}_j = \hat{A}_j\hat{H}_j$ for the auxiliary Hamiltonians.

Proof:

$$\begin{aligned}\hat{H}_{j+1}\hat{A}_j &= \left(\hat{A}_{j+1}^\dagger\hat{A}_{j+1} + E_{j+1}\right)\hat{A}_j = \left(\hat{A}_j\hat{A}_j^\dagger + E_j\right)\hat{A}_j \\ &= \hat{A}_j\hat{A}_j^\dagger\hat{A}_j + \hat{A}_jE_j = \hat{A}_j\left(\hat{A}_j^\dagger\hat{A}_j + E_j\right) = \hat{A}_j\hat{H}_j.\end{aligned}$$

Consider the set of states defined by $|\phi_{j+1}\rangle = \hat{A}_j\hat{A}_{j-1}\cdots\hat{A}_1\hat{A}_0|\psi\rangle$. We want to compute $\langle\phi_{j+1}|\,\phi_{j+1}\rangle = \langle\psi|\hat{A}_0^\dagger\hat{A}_1^\dagger\cdots\hat{A}_j^\dagger\hat{A}_j\cdots\hat{A}_1\hat{A}_0|\psi\rangle \geqslant 0$ for all j. Start with $j = 1$:

$$\begin{aligned}&\langle\phi_1|\phi_1\rangle = \langle\psi|\hat{A}_0^\dagger\hat{A}_0|\psi\rangle = \langle\psi|\left(\hat{H} - E_0\right)|\psi\rangle \\ &= E - E_0 \geq 0 \\ &\Rightarrow E = E_0 \text{ or } E > E_0. \\ &\langle\phi_2|\phi_2\rangle = \langle\psi|\hat{A}_0^\dagger\hat{A}_1^\dagger\hat{A}_1\hat{A}_0|\psi\rangle \\ &= \langle\psi|\hat{A}_0^\dagger\left(\hat{H}_1 - E_1\right)\hat{A}_0|\psi\rangle \quad \text{but } \hat{H}_1\hat{A}_0 = \hat{A}_0\hat{H}_0 \\ &= \langle\psi|\hat{A}_0^\dagger\hat{A}_0\left(\hat{H}_0 - E_1\right)|\psi\rangle \\ &= \langle\psi|\hat{A}_0^\dagger\hat{A}_0|\psi\rangle\left(E - E_1\right) = \left(E - E_1\right)\left(E - E_0\right) \geqslant 0 \\ &\Rightarrow E = E_1 \text{ or } E > E_1.\end{aligned}$$

Continuing in the same fashion, we have $E = E_j$ or $E > E_{j\,\max}$ (if the number of bound states terminates with a continuum of states above).

So, let's assume $|\psi\rangle = |\psi_j\rangle$ is a bound state and $E = E_j$. Then $\langle\phi_{j+1}|\phi_{j+1}\rangle = (E - E_j)(E - E_{j-1})\cdots(E - E_1)(E - E_0) = 0$. So $\hat{A}_j\hat{A}_{j-1}\cdots\hat{A}_1\hat{A}_0|\psi\rangle = 0$. We rewrite this as $\hat{A}_j\,|\phi_j\rangle = 0$. Now examine $\hat{H}_j\,|\phi_j\rangle = \left(\hat{A}_j^\dagger\hat{A}_j + E_j\right)|\phi_j\rangle = E_j|\phi_j\rangle$. This implies that $|\phi_j\rangle$ is an eigenstate of $\hat{H}_j$ with eigenvalue E_j. We find the eigenstate $|\psi\rangle$ via

$$|\psi_j\rangle = \frac{\hat{A}_1^\dagger \hat{A}_2^\dagger \ldots \hat{A}_{j-1}^\dagger |\phi_j\rangle}{\sqrt{(E_j - E_0)(E_j - E_1)\cdots(E_j - E_{j-1})}}$$

Now take the Hermitian conjugate of the intertwining relation:

$$\hat{A}_j \hat{H}_j = \hat{H}_{j+1}\hat{A}_j \quad \Rightarrow \quad \hat{A}_j^\dagger \hat{H}_{j+1} = \hat{H}_j \hat{A}_j^\dagger$$

so

$$\begin{aligned}
\hat{H}\,|\psi_j\rangle &= \hat{H}_0 \hat{A}_0^\dagger \hat{A}_1^\dagger \ldots \hat{A}_{j-1}^\dagger\,|\phi_j\rangle \\
&= \hat{A}_0^\dagger \hat{H}_1 \hat{A}_1^\dagger \cdots \hat{A}_{j-1}^\dagger\,|\phi_j\rangle \\
&\vdots \\
&= \hat{A}_0^\dagger \hat{A}_1^\dagger \cdots \hat{A}_{j-1}^\dagger \hat{H}_j\,|\phi_j\rangle \\
&= E_j \hat{A}_0^\dagger \hat{A}_1^\dagger \cdots \hat{A}_{j-1}^\dagger\,|\phi_j\rangle = E_j\,|\psi_j\rangle
\end{aligned}$$

Hence, it is an eigenstate as claimed!

3 Superpotential

So how do we make this work? Let's try an ansatz

$$\hat{A}_j = \frac{\hat{p}}{\sqrt{2m}} - \frac{i\hbar}{\sqrt{2m}} k_j W_j\left(k_j' \hat{x}\right)$$

where $W_j\left(k_j'\hat{x}\right)$ is called the superpotential and is a real valued function of $k_j'\hat{x}$, and we have that k_i and k_j' are real "wavevectors." Then

$$\hat{A}_j^\dagger \hat{A}_j = \frac{\hat{p}^2}{2m} + \frac{\hbar^2 k_j^2}{2m} W_j^2\left(k_j'\hat{x}\right) - \frac{i\hbar}{2m} k_j \left[\hat{p}_j, W_j\left(k_j'\hat{x}\right)\right].$$

4 Simple harmonic oscillator

So, if we can find W such that $V(\hat{x}) = \frac{\hbar^2 k_0}{2m} W_0^2\left(k_0'\hat{x}\right) - \frac{i\hbar k_0}{2m}\left[\hat{p}, W_0\left(k_0'\hat{x}\right)\right] + E_0$, then we have had our first factorization. It turns out soluble problems have the superpotentials having the same functional form, which is a property called shape invariance, and is best illustrated with an example. If there is ambiguity, we must have $kW(x) > 0$ as $x \to \infty$ and $kW(x) < 0$ as $x \to -\infty$, otherwise the wave function is not normalizable.

Let's work on an example we already know—the simple harmonic oscillator. We have $V(\hat{x}) = \frac{1}{2} m\omega_0^2 \hat{x}^2$. We find

$$\frac{1}{2} m\omega_0^2 \hat{x}^2 = \frac{\hbar^2 k_0^2}{2m} W_0^2\left(k_0'\hat{x}\right) - \frac{i\hbar k_0}{2m}\left[\hat{p}, W_0\left(k_0'\hat{x}\right)\right]$$

Now, since $[\hat{p}, \hat{x}] = -i\hbar =$ number, by inspection, we see that we should try $W_0\left(k_0'\hat{x}\right) = k_0'\hat{x}$. Then we have

$$\begin{aligned}
\frac{1}{2} m\omega_0^2 \hat{x}^2 &= \frac{\hbar^2 k_0^2 k_0'^{\,2}}{2m}\hat{x}^2 - \frac{i\hbar k_0}{2m}\left(-i\hbar k_0'\right) + E_0 \\
&= \frac{\hbar^2 k_0^2 k_0'^2}{2m}\hat{x}^2 - \frac{\hbar^2 k_0 k_0'}{2m} + E_0
\end{aligned}$$

This implies that we need $m\omega_0 = \hbar \left| k_0 k_0' \right|$ and $E_0 = \frac{\hbar^2 k_0 k_0'}{2m}$
So, we choose $k_0 k_0' = \frac{m\omega_0}{\hbar}$, in order for $W_0\left(k_0' x\right)$ to have the right sign as $|x| \to \infty$. This then implies that

$$\begin{aligned}\hat{A}_0 &= \frac{\hat{p}}{\sqrt{2m}} - \frac{i\hbar}{\sqrt{2m}} \frac{m\omega_0 \hat{x}}{\hbar} \\ &= \frac{1}{\sqrt{2m}} \left(\hat{p} - im\omega_0 \hat{x}\right) \qquad \text{the same as before!}\end{aligned}$$

Now we compute the first auxiliary Hamiltonian in the chain by reversing the order of the ladder operators

$$\begin{aligned}\hat{H}_1 &= \hat{A}_0 \hat{A}_0^\dagger + E_0 = \frac{1}{2m}\left(\hat{p} - im\omega_0 \hat{x}\right)\left(\hat{p} + im\omega_0 \hat{x}\right) + \frac{1}{2}\hbar\omega_0 \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2 \hat{x}^2 + \frac{1}{2m} im\omega_0 \underbrace{[\hat{p}, \hat{x}]}_{-i\hbar} + \frac{1}{2}\hbar\omega_0 \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2 \hat{x}^2 + \frac{3}{2}\hbar\omega_0 \\ &\Rightarrow \hat{A}_1 = \hat{A}_0 \text{ and } E_1 = \frac{3}{2}\hbar\omega_0.\end{aligned}$$

Note that this is the only example where $\hat{A}_j$ is independent of j. One can see that repeating this procedure gives the whole spectrum. The eigenstates also agree with what we did before. (Note, we can find the ground state via $\hat{A}_0 \left|\phi_0\right\rangle = 0$ and determine the wavefunction by integrating the diff eq.)

5 Particle in a box

Our next example is particle in a box, which Schrodinger called "shooting sparrows with artillery." Consider $V(\hat{x}) = 0$ inside a box from $-\frac{L}{2}$ to $\frac{L}{2}$. First recall that $[\hat{p}, f(\hat{x})] = -i\hbar f'(\hat{x})$, so $[\hat{p}, \tan\left(k'\hat{x}\right)] = -i\hbar k' \sec^2\left(k'\hat{x}\right)$. This motivates us to examine $\frac{\hbar^2 k^2}{2m} W^2\left(k'\hat{x}\right) - \frac{i\hbar k}{2m}\left[\hat{p}, W\left(k'\hat{x}\right)\right]$ for $W = \tan$. We find that it becomes

$$\frac{\hbar^2 k^2}{2m} \tan^2(k'\hat{x}) - \frac{\hbar^2 k k'}{2m} \sec^2\left(k'\hat{x}\right).$$

Now, if we choose $k = k'$, then

$$\frac{\hbar^2 (k')^2}{2m} \left(\tan^2\left(k'\hat{x}\right) - \sec^2\left(k'\hat{x}\right)\right) = -\frac{\hbar^2 k'^2}{2m} = \text{ number.}$$

Be sure to use the write trig identity to verify this.

So we choose

$$\hat{A}_0 = \frac{1}{\sqrt{2m}}\left(\hat{p} - i\hbar k' \tan\left(k'\hat{x}\right)\right)$$

and $\hat{A}_0^\dagger \hat{A}_0 = \frac{1}{2m}\hat{p}^2 - \frac{\hbar^2 k'^2}{2m} \quad \Rightarrow \quad E_0 = \frac{\hbar^2 (k')^2}{2m}$. Now we need to choose k' to have $W\left(k'x\right)$ become infinity at the boundary. Why you may ask—we will find the wavefunction vanishes when the superpotential diverges, so this is the conventional boundary condition of the wavefunction vanishing at the edges of the box. We can increase k' until

$k' = \frac{\pi}{L}$. At that point $\tan(k'\hat{x})$ will diverge at the boundary. Schrodinger argued not to increase k' further. But we will see in the homework that we can lift this restriction and still solve the problem. For now, we follow Schrodinger. Hence, we have $E_0 = \frac{\hbar^2\pi^2}{2mL^2}$. The ground state satisfies

$$\left[\hat{p} - i\hbar\frac{\pi}{L}\tan\left(\frac{\pi}{L}\hat{x}\right)\right]|\phi_0\rangle = 0\ .$$

In coordinate space, this becomes $-i\hbar\frac{d}{dx}\psi(x) = i\hbar\frac{\pi}{L}\tan\left(\frac{\pi}{L}x\right)\psi(x)$, or

$$\begin{aligned}\frac{d}{dx}\ln\psi(x) = -\frac{\pi}{L}\tan\left(\frac{\pi}{L}x\right) \Rightarrow \ln\psi(x) &= \frac{\pi}{L}\int^x \tan\left(\frac{\pi}{L}x'\right)dx' \\ &= -\ln\sec\left(\frac{\pi}{L}x\right) + c \\ \psi(x) &= c\cos\left(\frac{\pi}{L}x\right)\end{aligned}$$

which is correct. Determining the normalization gives us that $c = \sqrt{\frac{2}{L}}$.

Now we go onto the higher energy states:

$$\begin{aligned}\hat{H}_1 &= \hat{A}_0\hat{A}_0^\dagger + E_0 = \hat{H}_0 + \left[\hat{A}_0, \hat{A}_0^\dagger\right] = \frac{\hat{p}^2}{2m} + \underbrace{0}_{V(\hat{x})} + \left[\hat{A}_0, \hat{A}_0^\dagger\right] \\ &= \frac{\hat{p}^2}{2m} + \frac{i\hbar\pi}{2mL}\left[\hat{p}, \tan\left(\frac{\pi}{L}\hat{x}\right)\right]\times 2 \\ &= \frac{\hat{p}^2}{2m} + \frac{\hbar^2\pi^2}{2mL^2}\cdot 2\sec^2\left(\frac{\pi}{L}\hat{x}\right) \\ &= \frac{\hat{p}^2}{2m} + \frac{\hbar^2\pi^2}{mL^2}\left(1 + \tan^2\left(\frac{\pi}{L}x\right)\right) \\ V_1(\hat{x}) &= \frac{\hbar^2\pi^2}{mL^2}\tan^2\left(\frac{\pi}{L}\hat{x}\right) + \frac{\hbar^2\pi^2}{mL^2} = \frac{\hbar^2 k_1}{2m}W_1^2(k_1'\hat{x}) + \frac{i\hbar k_1}{2m}\left[\hat{p}, W_1(k_1'x)\right] + E_1.\end{aligned}$$

The "shape invariance" requirement suggests that we try the same form: $W_1(k_1', \hat{x}) = \tan(k_1'\hat{x})$. This gives

$$\begin{aligned}&\frac{\hbar^2 k_1^2}{2m}\tan^2(k_1'\hat{x}) + \frac{\hbar^2 k_1 k_1'}{2m}\sec^2(k_1'\hat{x}) \\ &= \frac{\hbar^2 k_1 k_1'}{2m} + \frac{\hbar^2 k_1}{2m}(k_1 + k_1')\tan^2(k_1'\hat{x}) \\ &\Rightarrow k_1' = \frac{\pi}{L} \quad k_1(k_1 + k_1') = \frac{2\pi^2}{L^2} \quad \frac{\hbar^2\pi^2}{mL^2} = \frac{\hbar^2 k_1 k_1'}{2m} + E_1 \\ &\Rightarrow k_1\left(k_1 + \frac{\pi}{L}\right) = \frac{2\pi^2}{L^2} \quad \Rightarrow \quad k_1 = \frac{\pi}{L}\text{ or } -\frac{2\pi}{L}\end{aligned}$$

$$E_1 = \frac{\hbar^2\pi^2}{mL^2} - \frac{\hbar^2 k_1\pi}{2mL} \Rightarrow \text{ pick } k_1 = -\frac{2\pi}{L} \quad \text{for } E_1 > E_0.$$

So

$$E_1 = \frac{2\hbar^2\pi^2}{mL^2} \quad \text{and} \quad \hat{A}_1 = \frac{1}{\sqrt{2m}}\left(\hat{p} - \frac{i\hbar 2\pi}{L}\tan\left(\frac{\pi\hat{x}}{L}\right)\right).$$

Let's find the wavefunction. We have

$$\hat{A}_1|\phi_1\rangle = 0 \Rightarrow \quad -i\hbar\frac{d\phi_1}{dx} = i\hbar\frac{2\pi}{L}\tan\left(\frac{\pi x}{L}\right)\phi_2$$
$$\frac{d}{dx}\ln\phi_1 = -\frac{2\pi}{L}\tan\frac{\pi x}{L}$$
$$\phi_1(x) = c'\cos^2\left(\frac{\pi x}{L}\right) = \sqrt{\frac{8}{3L}}\cos^2\left(\frac{\pi x}{L}\right)$$

and $|\psi_1\rangle = \frac{\hat{A}_0^\dagger}{\sqrt{E_1-E_0}}|\phi_1\rangle$

$$\Rightarrow \psi_1(x) = \sqrt{\frac{8}{3L}}\cdot\frac{1}{\sqrt{\frac{(4-1)\hbar^2\pi^2}{2mL^2}}}\frac{1}{\sqrt{2m}}\left(-i\hbar\frac{d}{dx}+i\hbar\frac{\pi}{L}\tan\left(\frac{\pi x}{L}\right)\right)\cos^2\left(\frac{\pi x}{L}\right)$$
$$= \sqrt{\frac{8}{3L}}\frac{L}{\sqrt{3}\pi\hbar}\cdot\hbar\left(+i\frac{\pi}{L}\cdot 2\cos\left(\frac{\pi x}{L}\right)\sin\frac{\pi x}{L}+i\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\right)$$
$$= \sqrt{\frac{2}{L}}i\sin\left(\frac{2\pi x}{L}\right) \quad \checkmark \text{ up to a phase .}$$

One can continue, but it is tedious to do so term by term. Using an "induction-like" approach, you can find that

$$k_j = -(j+1)\frac{\pi}{L}, \quad k'_j = \frac{\pi}{L}, \quad E_j = \frac{\hbar^2\,(j+1)^2\pi^2}{2mL^2}, \quad \text{and} \quad \psi_j(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{(j+1)\pi x}{L}\right)$$

just as we know from the differential equation approach.

So, why use this approach if it is harder? Two points—

- it isn't always harder—indeed it can be easier, especially for energies, because we can find energies without finding the wavefunctions;
- it provides a new perspective as we see everything really comes from $[\hat{x},\hat{p}] = i\hbar$.