# Schrödinger factorization method

We know that in quantum mechanics only a handful of problems can be exactly solved. In 1940, Schrödinger described a general approach for such problems that was algebraic. It generalized the operator method for the simple harmonic oscillator to all of these 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!

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 devise some other methodologies that will appear less so.

The strategy is to write $\hat{H} = \hat{H}_0$ in a factorized form

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

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

At this point, this seems like 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 goes as follows: (2)

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

and so on.

We also require that $E_{j+1} > E_j$.

This may sound odd, but it forbids us from choosing $E_1 = E_0$, $\hat{A}_1^+ = \hat{A}_0$.
Because that is always a choice, it also tells us we must have $E_j > E_{j-1} > \cdots > E_2 > E_1$ for this method to work.

Now, our situation is quite complex, for not only do we need to find a way to factrize our original $\hat{H}$. Once we have $\hat{A}_0$, we can determine a new auxiliary Hamiltonian from $\hat{H}_1 = \hat{A}_0\hat{A}_0^+ + E_0 = \hat{H}_0 + [\hat{A}_0, \hat{A}_0^+]$
At this point we need to find a way to factrize $\hat{H}_1$.
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. For the moment just assume we can do this. Let's investigate some consequences.

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:
$$\hat{H}_{j+1}\hat{A}_j = \left(\hat{A}_{j+1}^+ \hat{A}_{j+1} + E_{j+1}\right)\hat{A}_j = \left(\hat{A}_j\hat{A}_j^+ + E_j\right)\hat{A}_j$$
$$= \hat{A}_j\hat{A}_j^+\hat{A}_j + \hat{A}_j E_j = \hat{A}_j\left(\hat{A}_j^+\hat{A}_j + E_j\right) = \hat{A}_j\hat{H}_j$$

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 $\langle \phi_{j+1} | \phi_{j+1}\rangle = \langle \psi | \hat{A}_0^+ \hat{A}_1^+ \cdots \hat{A}_j^+ \hat{A}_j \cdots \hat{A}_1 \hat{A}_0 |\psi\rangle \geq 0$
for all $j$. Start with $j=1$:

$$\langle \phi_1|\phi_1\rangle = \langle\psi|\hat{A}_0^+\hat{A}_0|\psi\rangle = \langle\psi|(\hat{H} - E_0)|\psi\rangle$$
$$= E - E_0 \geq 0$$

$\Rightarrow$ $E = E_0$ or $E > E_0$.

$$\langle\phi_2|\phi_2\rangle = \langle\psi|\hat{A}_0^+\hat{A}_1^+\hat{A}_1\hat{A}_0|\psi\rangle$$
$$= \langle\psi|\hat{A}_0^+(\hat{H}_1 - E_1)\hat{A}_0|\psi\rangle$$

but $\hat{H}_1\hat{A}_0 = \hat{A}_0\hat{H}_0$ by intertwining

$$= \langle\psi|\hat{A}_0^+\hat{A}_0(\hat{H}_0 - E_1)|\psi\rangle$$
$$= \langle\psi|\hat{A}_0^+\hat{A}_0|\psi\rangle(E - E_1) = (E-E_1)(E-E_0) \geq 0$$

$\Rightarrow$ $E = E_1$ or $E > E_1$.

Continuing in the same fashion, we have

$$E = E_j \quad \text{or} \quad E > E_{j\,max} \quad \text{(if the number of}$$

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 $\hat{H}_j |\phi_j\rangle = (\hat{A}^+_j \hat{A}_j + E_j)|\phi_j\rangle = E_j |\phi_j\rangle$

$\Rightarrow |\phi_j\rangle$ is an eigenstate of $\hat{H}_j$ with eigenvalue $E_j$.

We find the normalized eigenstate $|\psi\rangle$ via

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

Now take the hermitian conjugate of the intertwining relation

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

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

So, it is an eigenstate as claimed!

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

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

where $W_j(k'_j \hat{x})$ is called the superpotential and is a real valued function of $k'_j \hat{x}$, $k_j$ and $k'_j$ are real "wave vectors".

Then

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

So, if we can find $W$ such that $V(\hat{x}) = \frac{\hbar^2 k_j}{2m} W_j^2(k'_j \hat{x}) - \frac{i\hbar k_j}{2m}[\hat{p}_j, W_j(k'_j \hat{x})] + E_1$

then, we have had our first factorization. It turns out solvable problems have the superpotentials having the same functional form, which is a property called shape invariance, and 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 SHO.

Here $V(\hat{x}) = \frac{1}{2} m \omega_0^2 \hat{x}^2$

We find

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

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

$$\tfrac{1}{2} m\omega_0^2 \hat{x}^2 = \frac{\hbar^2 k_0^2 k_0'^2}{2m}\hat{x}^2 - \frac{i\hbar k_0}{2m}(-i\hbar k_0') + E_0$$

$$= \frac{\hbar^2 k_0^2 k_0'^2}{2m}\hat{x}^2 - \frac{\hbar^2 k_0 k_0'}{2m} + E_0$$

$\Rightarrow$ need $m\omega_0 = \hbar|k_0 k_0'|$ $\quad E_0 = +\frac{\hbar^2 k_0 k_0'}{2m}$

so, we choose $k_0 k_0' = \frac{m\omega_0}{\hbar}$ in order for $W_0(k_0'x)$ to have the right sign as $|x|\to\infty$

$$\Rightarrow \quad \hat{A}_1 = \frac{\hat{p}}{\sqrt{2m}} - \frac{i\hbar}{\sqrt{2m}}\frac{m\omega_0}{\hbar}\hat{x}$$

$$= \frac{1}{\sqrt{2m}}(\hat{p} - im\omega_0\hat{x}) \qquad \text{same as before}$$

Now we compute

$$\hat{H}_1 = \hat{A}_0\hat{A}_0^\dagger + E_0 = \frac{1}{2m}(\hat{p} - im\omega_0\hat{x})(\hat{p} + im\omega_0\hat{x}) + \tfrac{1}{2}\hbar\omega_0$$

$$= \frac{\hat{p}^2}{2m} + \tfrac{1}{2}m\omega_0^2\hat{x}^2 + \frac{1}{2m} i m\omega_0 \underbrace{[\hat{p},\hat{x}]}_{= -i\hbar} + \tfrac{1}{2}\hbar\omega_0$$

$$= \frac{\hat{p}^2}{2m} + \tfrac{1}{2}m\omega_0^2\hat{x}^2 + \tfrac{3}{2}\hbar\omega_0$$

$\Rightarrow$ $\hat{A}_1 = \hat{A}_0$ and $E_1 = \tfrac{3}{2}\hbar\omega_0$.

Note that this is the <u>only</u> 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 GS via $\hat{A}_0|\phi_0\rangle = 0$ and get the wavefunction by integrating the diff eq).

Our next example is particle in a box, which Schrödinger 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 $[\hat{p}, \tan(k'\hat{x})] = -i\hbar k' \sec^2(k'\hat{x})$

So examine $\frac{\hbar^2 k^2}{2m} W^2(k'\hat{x}) - \frac{i\hbar k}{2m}[\hat{p}, W(k'\hat{x})]$ for $W = \tan$

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

If we choose $k=k'$, then

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

So we choose

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

and $\hat{A}_0^\dagger \hat{A}_0 = \frac{1}{2m}\hat{p}^2 - \frac{\hbar^2 k'^2}{2m} \Rightarrow E_0 = \frac{\hbar^2 k'^2}{2m}$

Now we need to choose $k'$ have $W(k'x)$ become infinity at the boundary, which has $\psi \to 0$. We can increase $k'$ until $k' = \frac{\pi}{L}$. At that point $\tan(k'\hat{x})$ will diverge at the boundary. Schrödinger 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 schroedinger.

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 $\frac{d}{dx}\ln\psi(x) = -\frac{\pi}{L}\tan\left(\frac{\pi}{L}x\right) \Rightarrow \ln\psi(x) = \frac{\pi}{L}\int^x \tan\left(\frac{\pi}{L}x'\right)dx'$

$$= -\ln\sec\left(\frac{\pi}{L}x\right) + C$$

$$\psi(x) = c\cos\left(\frac{\pi}{L}x\right)$$

which is correct. normalization $\Rightarrow c = \sqrt{\frac{2}{L}}$

Now the higher energy states:

$$\hat{H}_1 = \hat{A}_0\hat{A}_0^\dagger + E_0 = \hat{H}_0 + [\hat{A}_0, \hat{A}_0^\dagger] = \frac{\hat{p}^2}{2m} + \underset{V(\hat{x})}{0} + [\hat{A}_0, \hat{A}_0^\dagger]$$

$$= \frac{\hat{p}^2}{2m} + \frac{i\hbar\pi}{2mL}\left[\hat{p}, \tan\left(\frac{\pi}{L}\hat{x}\right)\right]\times 2$$

$$= \frac{\hat{p}^2}{2m} + \frac{\hbar^2\pi^2}{2mL^2}\cdot 2\sec^2\left(\frac{\pi}{L}\hat{x}\right)$$

$$= \frac{\hat{p}^2}{2m} + \frac{\hbar^2\pi^2}{mL^2}\left(1+\tan^2\left(\frac{\pi}{L}\hat{x}\right)\right)$$

$$V_1(\hat{x}) = \frac{\hbar^2\pi^2}{mL^2}\tan^2\left(\frac{\pi}{L}\hat{x}\right) + \frac{\hbar^2\pi^2}{mL^2} = \frac{\hbar^2 k_1}{2m}W_1^2(k_1'\hat{x}) + \frac{i\hbar k_1}{2m}[\hat{p}, W_1(k_1'\hat{x})] + E_1$$

The "shape invariance" requirement suggest we try the same form: $W_1(k_1'\hat{x}) = \tan(k_1'\hat{x})$

This gives

$$\frac{\hbar^2 k_1'^2}{2m} \tan^2(k_1'\hat{x}) + \frac{\hbar^2 k_1 k_1'}{2m} \sec^2(k_1'\hat{x})$$

$$= \frac{\hbar^2 k_1 k_1'}{2m} + \frac{\hbar^2 k_1}{2m}(k_1 + k_1')\tan^2(k_1'\hat{x})$$

$$\Rightarrow k_1' = \frac{\pi}{L} \qquad k_1(k_1+k_1') = \frac{2\pi^2}{L^2} \qquad \frac{\hbar^2\pi^2}{mL^2} = \frac{\hbar^2 k_1 k_1'}{2m} + E_1$$

$$\Rightarrow k_1\left(k_1 + \frac{\pi}{L}\right) = \frac{2\pi^2}{L^2} \quad \Rightarrow \quad k_1 = \frac{\pi}{L} \text{ or } -\frac{2\pi}{L}$$

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

so $E_1 = \dfrac{2\hbar^2\pi^2}{mL^2}$ $\qquad \hat{A}_1 = \dfrac{1}{\sqrt{2m}}\left(\hat{p} - \dfrac{i\hbar 2\pi}{L}\tan\left(\dfrac{\pi\hat{x}}{L}\right)\right)$

let's find the wave function.

$$\hat{A}_1|\phi_1\rangle = 0 \Rightarrow -i\hbar\frac{d\phi_1}{dx} = i\hbar\frac{2\pi}{L}\tan\left(\frac{\pi x}{L}\right)\phi_2$$

$$\frac{d}{dx}\ln\phi_1 = -\frac{2\pi}{L}\tan\frac{\pi x}{L}$$

$$\phi_1(x) = c'\cos^2\left(\frac{\pi x}{L}\right) = \sqrt{\frac{8}{3L}}\cos^2\left(\frac{\pi x}{L}\right)$$

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

$$\Rightarrow \psi_1(x) = \sqrt{\frac{8}{3L}} \cdot \frac{1}{\sqrt{\frac{(4-1)\hbar^2\pi^2}{2mL^2}}} \frac{1}{\sqrt{2m}}\left(-i\hbar\frac{d}{dx} + i\hbar\frac{\pi}{L}\tan\left(\frac{\pi x}{L}\right)\right)\cos^2\left(\frac{\pi x}{L}\right)$$

$$= \sqrt{\frac{8}{3L}}\frac{L}{\sqrt{3}\pi\hbar}\cdot\hbar\left(+i\frac{\pi}{L}\cdot 2\cos\left(\frac{\pi x}{L}\right)\sin\frac{\pi x}{L} + \frac{i\pi}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\right)$$

$$= \sqrt{\frac{2}{L}}\, i \sin\left(\frac{2\pi x}{L}\right) \quad \checkmark \text{ up to a phase}$$

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

$$k_j = -(j+1)\frac{\pi}{L} \qquad k_j' = \frac{\pi}{L} \qquad E_j = \frac{\hbar^2(j+1)^2\pi^2}{2mL^2}$$

and $\psi_j(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{(j+1)\pi x}{L}\right)$

just as we know from the dif. eq approach.

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

- it isn't always harder – indeed it can be easier, esp. for energies
- it provides a new perspective as we see everything really comes just from $[\hat{x},\hat{p}] = i\hbar$.