Applications and Toy Models in Quantum Mechanics

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Lecture II: Quantum Foundations

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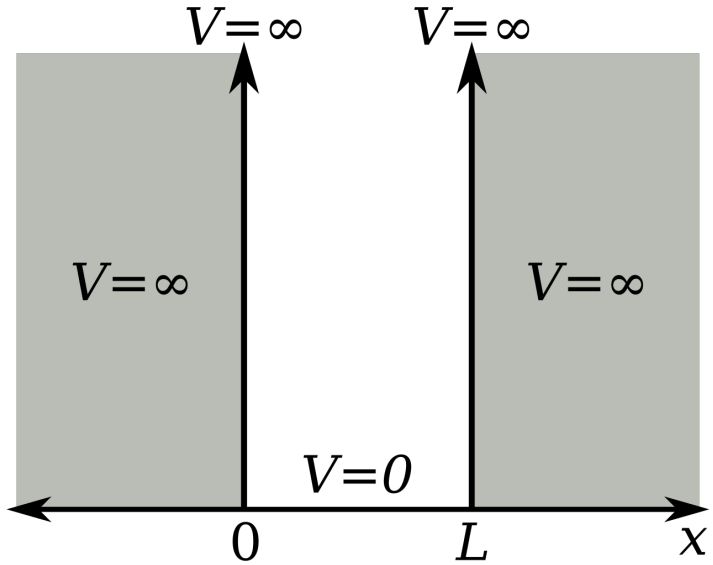
Abstract

In this talk, we will explore the fundamental applications of Quantum mechanics that we have learnt so far, and begin to appreciate how the mathematical tools and intuition predict observable phenomena, and our road forward to further evolve our understanding of quantum mechanics, including Supersymmetry, and its scope in revolutionizing quantum physics (and more).

First Problem for all Quantum Physicists: The Infinte Square Well

Establishing the Problem- the first step for solving all problems in QM(and physics)

The premise



Setting up the Schrodinger's Equation

We know that the Schrodinger equation is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{1}$$

And so,

$$\frac{d^2\psi}{dx^2} = k^2\psi \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{2}$$

Equation (2) is simply the simple harmonic oscillator equation, whose general solution is,

$$\psi(x) = A\sin kx + B\cos kx \tag{3}$$

Using Boundary Conditons for solutions

Continuity of $\psi(x)$ requires that,

$$\psi(0) = \psi(a) = 0$$

This is called the boundary conditions for our problem at hand. Now imposing this on A and B,

$$\psi(0) = A\sin 0 + B\cos 0 = B \tag{4}$$

So $B = 0$, and hence,

$$\psi(x) = A\sin kx \tag{5}$$

Then, $\psi(a) = A\sin ka$, so $\sin ka = 0$, which means that,

$$ka = 0,\ \pm\pi,\ \pm 2\pi,\ \pm 3\pi... \tag{6}$$

The solutions: Eigenvalues

Eigenvalues of energy

Negative solutions are insignificant, so the distinct solutions are,

$$k_n = \frac{n\pi}{a}, \text{ with } n = 1, 2, 3, ... \tag{7}$$

And so the possible values (eigenvalues) of E are,

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{8}$$

The solutions: Eigenfunction

The Eigenfunction of $\psi(x)$

Finding A using by normalisation,

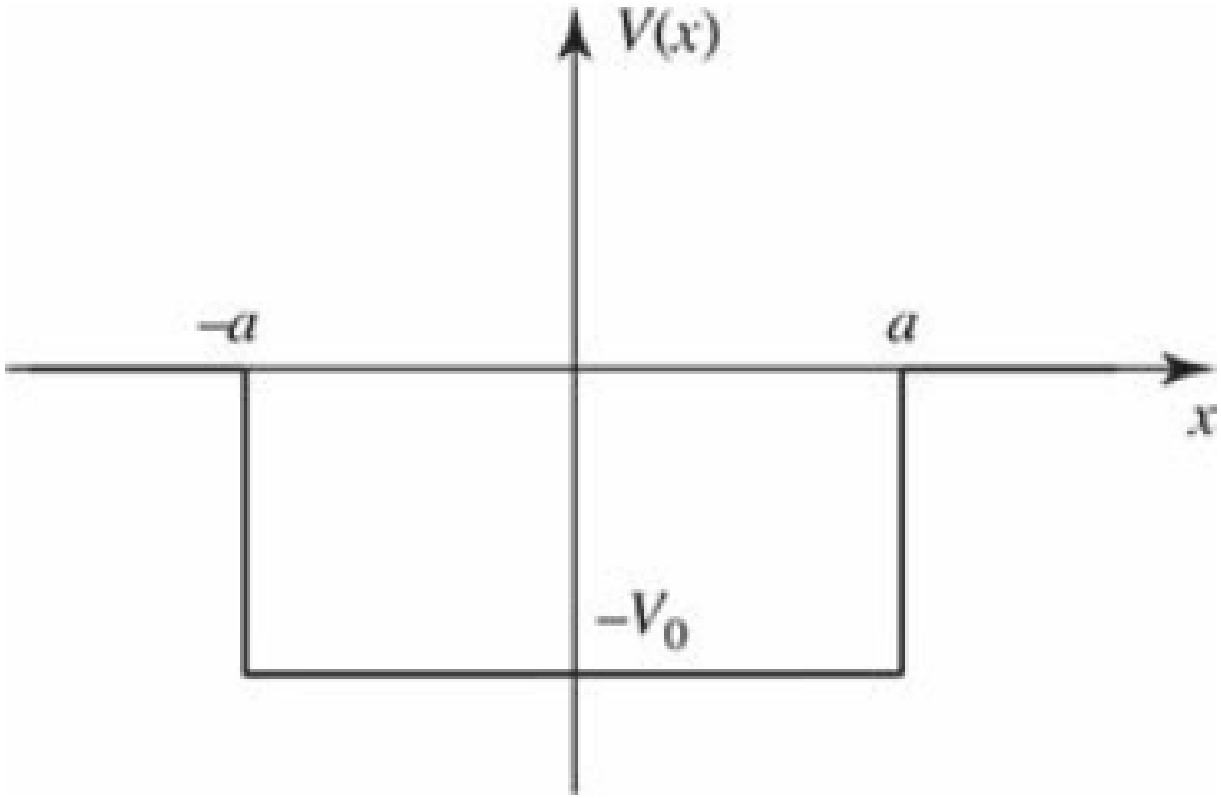
$$\int_0^a |A|^2 \sin^2(kx)dx = |A|^2 \frac{a}{2} = 1 \text{ so } |A|^2 = \frac{2}{a} \tag{9}$$

Now the eigenfunction is,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \tag{10}$$

The Finite Square Well: A slightly complicated Infinte Square Well

The Problem



Setting up the equation for $x < -a$

For the region $x < -a$, the potential is zero, so the Schrodinger equation reads,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \text{ or } \frac{d^2\psi}{dx^2} = \kappa^2\psi \tag{11}$$

Where,

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$$

is real and positive. The general solution is $\psi(x) = A\exp(\kappa x) + B\exp(\kappa x)$, but the first term blows up, so the physically admissible solution is,

$$\psi(x) = Be^{\kappa x} \tag{12}$$

Setting equations for $-a < x < a$

In the region $-a < x < a$, the potential $V(x) = -V_0$, and the Schrodinger equation reads,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \text{ or } \frac{d^2\psi}{dx^2} = -l^2\psi \tag{13}$$

where,

$$l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{14}$$

Now, the general solution is,

$$\psi(x) = C\sin(lx) + D\cos(lx) \tag{15}$$

where C and D are arbitrary constants.

The final set of equations

Now, for the region $x > a$, the solution is similar as $x < -a$, but with a different constant,

$$\psi(x) = Fe^{-\kappa x} \tag{16}$$

The equations we are trying to solve are,

$$\psi(x) = \begin{cases} Fe^{-\kappa x} \\ D\cos(lx) \\ \psi(-x) \end{cases} \tag{17}$$

Imposing boundary conditions

The continuity of $\psi(x)$ at $x = a$ says,

$$Fe^{\kappa a} = D\cos(la) \tag{18}$$

And the continuity of $d\psi/dx$ says,

$$-\kappa F^{-\kappa a} = -lD\sin(la) \tag{19}$$

Dividing the two equations,

$$\kappa = l\tan(la) \tag{20}$$

This is the formula for allowed energies. Using better notation,

$$z \equiv la \text{ and } z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0} \tag{21}$$

Solving for energy eigenvalues

Now, we can rewrite Equation (20) as,

$$tanz = \sqrt{(z_0/z)^2 - 1} \tag{22}$$

Wide, deep well

For a wide deep well, z_0 is vary large, and hence the eigenvalues become similar to the infinite square well,

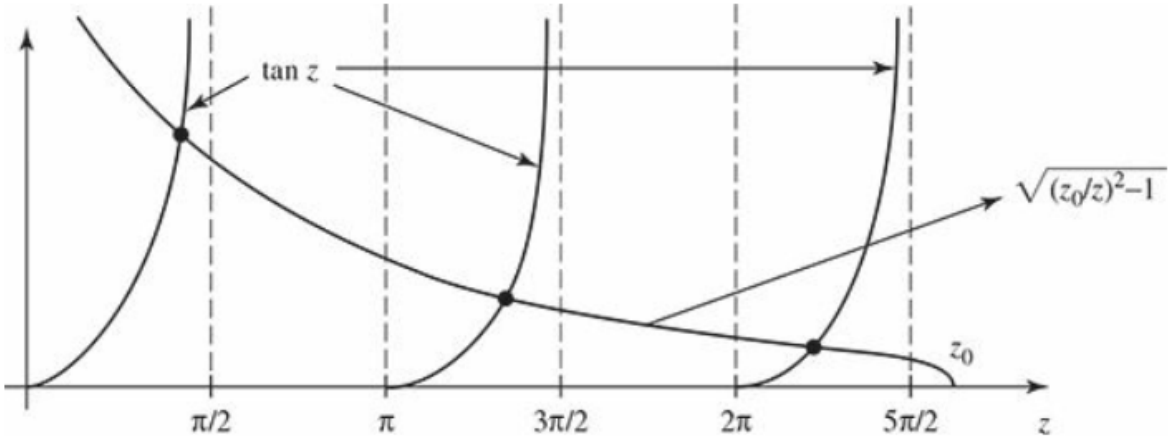
$$E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{23}$$

But for any finite V_0, there are only a finite number of bound states.

Solving for energy eigenvalues

Shallow, narrow well

As z_0 decreases, there are fewer and fewer bound states, until $z_0 < \pi/2$, only one remains. However, not that no matter how weak the well is, there will always be one bound state.



The scattering states

For $E > 0$, you have the scattering states. To the left,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{24}$$

Inside the well,

$$\psi(x) = C\sin(lx) + D\cos(lx) \tag{25}$$

To the right, assuming there are no incoming waves,

$$\psi(x) = Fe^{ikx} \tag{26}$$

Here, A is the incident amplitude, B is the reflected amplitude and F is the transmitted amplitude.

Boundary conditions for scattering states

There are 4 boundary conditions. Continuity of $\psi(x)$ at $-a$,

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \tag{27}$$

Continuity of $d\psi/dx$ at -a gives,

$$ik[Ae^{-ika} - Be^{ika}] = l[C\cos(la) + D\sin(la)] \tag{28}$$

Continuity of $\psi(x)$ at $+$a yields,

$$C\sin(la) + D\cos(la) = Fe^{ika} \tag{29}$$

and continuity of $d\psi/dx$ at $+$a requires,

$$l[C\cos(la) - D\sin(la)] = ikFe^{ika} \tag{30}$$

Solving the equations for scattering states

Using these to eliminate C and D, and solving for B and F,

$$B = i\frac{sin(2la)}{2kl}(l^2 - k^2)F \tag{31}$$

$$F = \frac{e^{2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}sin(2la)} \tag{32}$$

And writing the transmission coefficient ($T = |F|^2/|A|^2$), in terms of the original variables,

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right) \tag{33}$$

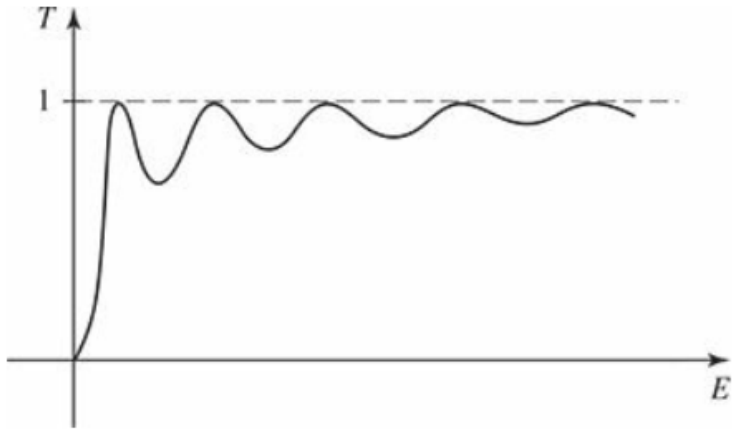
The final result

Notice that $T = 1$ whenever sine is zero, hence,

$$\frac{2a}{\hbar}\sqrt{2m(E + V_0)} = n\pi \tag{34}$$

where n is any integer. The energies for perfect transmission, then are given by,

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{35}$$



The Harmonic Oscillator: The power of operators in QM

Setting up the problem

For a harmonic oscillator, we try to solve the Schrodinger equation with the potential,

$$V(x)\frac{1}{2}m\omega^2x^2 \tag{36}$$

And so,

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \tag{37}$$

Writing this more neatly,

$$\frac{1}{2m}[\hat{p}^2+(m\omega x)^2]\psi=E\psi \tag{38}$$

where $\hat{p}\equiv -i\hbar d/dx$ is the momentum operator. Here, we are simply trying to factor out the Hamiltonian,

Setting up the ladder operators

The Hamiltonian can be said to be,

$$\hat{H} = \frac{1}{2m}[\hat{p}^2 + (m\omega x)^2] \tag{39}$$

But we cannot factor out the Hamiltonian that easily, since the quanitites are operators and they do not commute. So we introduce a new quantity

$$\hat{a}\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x) \tag{40}$$

Now,

$$\hat{a_-}\hat{a_+} = \frac{1}{2\hbar m\omega}(i\hat{p} + m\omega x)(-i\hat{p} + m\omega x) \tag{41}$$

$$= \frac{1}{2\hbar m\omega}[\hat{p} + (m\omega x)^2 - im\omega(x\hat{p} - \hat{p}x)] \tag{42}$$

Using the ladder operators

Now, writing this using commutator brackets,

$$\hat{a_-}\hat{a_+} = \frac{1}{2\hbar m\omega}[\hat{p}^2 + (m\omega x)^2] - \frac{i}{2\hbar}[x, \hat{p}] \tag{43}$$

Using the canonical commutation relation,

$$[x, \hat{p}] = i\hbar$$

$$\hat{a_-}\hat{a_+} = \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2} \tag{44}$$

Rearranging

$$\hat{H} = \hbar\omega\left(\hat{a_-}\hat{a_+} - \frac{1}{2}\right) \tag{45}$$

Schrodinger Equation in terms of operators

Now doing the same for the other case,

$$\hat{H} = \hbar\omega\left(\hat{a_+}\hat{a_-} + \frac{1}{2}\right) \tag{46}$$

The Schrodinger equation can be written as,

$$\hbar\omega\left(\hat{a^{\pm}}\hat{a^{\mp}} \pm \frac{1}{2}\right)\psi = E\psi \tag{47}$$

Now, we make the claim,

$$\hat{H}\psi = E\psi$$
$$\hat{H}(\hat{a_+}\psi) = (E + \hbar\omega)(\hat{a_+}\psi)$$

Obtaining the eigenfunction

Applying the lowering operator to the ground state wavefunction,

$$\hat{a_-}\psi_0 = 0 \tag{48}$$

Now $\psi_0(x)$,

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi(0) = 0 \tag{49}$$

or,

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}\psi_0 \tag{50}$$

Solving this differential equation,

$$\int \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}\int x dx = \ln(\psi_0) = -\frac{m\omega}{2h}x^2 + C \tag{51}$$

Obtaining the eigenvalues

From Equation (51),

$$\psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2} \tag{52}$$

From normalisation we have,

$$A^2 = \sqrt{m\omega/\pi\hbar} \tag{53}$$

And now,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \tag{54}$$

Now our ground state energy is given by,

$$E_0 = \frac{1}{2}\hbar\omega \tag{55}$$

The final results

From here, we can just apply the raising operators from the ground state to obtain our excited state eigenfunctions and energies,

$$\psi_n(x) = A_n(\hat{a_+})^n \psi_0(x) \tag{56}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{57}$$

The Hydrogen Atom

The Hydrogen atom

Defining Potential

Hydrogen atom system consists of one proton and its orbiting electron.
The wavefunction of the orbiting electron needs to be determined.
The potential energy of the electron is given by,

$$V(r) = -\frac{e^2}{r} \tag{58}$$

Recollecting the Radial Wave equation

We can recollect that the radial wave equation is,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] u = Eu \tag{59}$$

The Hydrogen atom

Allowed Energy Eigenvalues

The only allowed energy values for obtaining a normalisable solutions are,

$$E_n = -\frac{me^2}{2\hbar^2 n^2} = -\alpha^2 mc^2 \left(\frac{1}{2n^2}\right) = -13.6eV/n^2 \tag{60}$$

Where $n = 1, 2, 3...$ and,

$$\alpha \equiv \frac{e^2}{\hbar c} = \frac{1}{137.06}$$

is called the fine structure constant.

The Hydrogen atom

The Normalised Wavefunction

From Equation (59) and (60), we can obtain its corresponding normalised wavefunction to be,

$$\psi_{n,l,m_l}(r,\theta\phi) = \left\{ \left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} e^{r}/na \left(\frac{2r}{na}\right)^{l} L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right) Y_l^{m_l}(\theta,\phi) \quad (61)$$

Where,

$$a \equiv \frac{\hbar^2}{me^2} = 0.529 \times 10^{-8} cm$$

is the Bohr Radius.

The Hydrogen atom

The Laguerre Polynomials - Interlude

The associated Laguerre Polynomial, $L^p_{q-p}(z)$ is given by,

$$L^p_{q-p}(z) \equiv (-1)^p \left(\frac{d}{dz}\right)^p \left[e^z \left(\frac{d}{dz}\right)^q (e^{-z} z^q)\right] \tag{62}$$

Where it is a solution for the second order linear differential equation of the form

$$xy^n + (1-x)y' + ny = 0 \tag{63}$$

SUSY: A new way to solve problems and more!

What is supersymmetry?

Defining SUSY

Supersymmetry (often abbreviated SUSY) is a mathematical concept which arose from theoretical arguments and led to an extension of the Standard Model (SM) as an attempt to unify the forces of nature. It is a symmetry which relates fermions (half integer spin) and bosons (integer spin) by transforming fundamental particles into superpartners with the same mass and a difference of $\frac{1}{2}$spin.

SUSY in Quantum Mechanics

Physicists tried to find out how this symmetry could be broken, since it has not been observed in nature. This search of spontaneous symmetry breaking lead us to SUSY in QM. Essentially, the use of Factorised Hamiltonians and partner potentials provided a much more accurate approximation techniques than the existing ones, such as WKB approximations.
Again, it all starts with our general Hamiltonian,

$$H_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_1(x) \tag{64}$$

Next, we will try to factorise this equation, so that we can reduce the second order derivative to a derivative of first order.

Factorising the Hamiltonian

Assuming ψ_0 to be nodeless (vanishes at $x = \pm\infty$), we can write the Schrodinger equation for ψ_0 as,

$$0 = \frac{\hbar^2}{2m}\psi_0\frac{d^2}{dx^2} + V_1(x)\psi_0 \tag{65}$$

Because the ground state is nodeless, we can solve the Schrodinger equation for the potential

$$V_1(x) = \frac{\hbar^2}{2m}\frac{\psi_0''(x)}{\psi_0(x)} \tag{66}$$

The Superpotential

We factorise the Hamiltonian as follows,

$$H = A^\dagger A \tag{67}$$

Where,

$$A = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} W(x)$$

$$A^\dagger = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} W(x)$$

Where $W(x)$ is referred to as the superpotential

The Riccati Equation

The relation between the regular potential and the superpotential can be found by inserting the factors into the Hamiltonian,

$$H\psi(x) = \left(-\frac{\hbar}{\sqrt{2m}}\frac{d}{dx}W(x)\right)\left(\frac{\hbar}{\sqrt{2m}}\frac{d}{dx}W(x)\right)\psi(x) \tag{68}$$

Simplifying this gives us,

$$V(x) = W^2 - \frac{\hbar}{\sqrt{2m}}W'(x) \tag{69}$$

This is called the Riccati Equation. Now solving for the superpotential $W(x)$,

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{\psi_0'(x)}{\psi_0(x)} \tag{70}$$

The partner potential

Now, using factorisation, we create a new Hamiltonian, called the partner Hamiltonian,

$$H_2 = AA^\dagger \tag{71}$$

Using the same calculations,

$$V_2(x) = W^2 + \frac{\hbar}{\sqrt{2m}} W'(x) \tag{72}$$

This is called the supersymmetric partner potential.

Setting up the Radial Equation

The Coulomb force is with the potential,

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} \tag{73}$$

Plugging this into the radial equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] u(r) = E_0 u(r) \tag{74}$$

Now the shifted radial potential reads,

$$\tilde{V}(r) = \left[-\frac{1}{4}\frac{e^2}{4\pi\epsilon_0}\right]\frac{1}{r} + \left[\frac{\hbar^2 l(1+1)}{2m}\right]\frac{1}{r^2} - E_0 \tag{75}$$

Finding the superpotential

Now we begin to find the corresponding superpotential,

$$\tilde{V}(r) = W(r)^2 - \frac{\hbar}{\sqrt{2m}} W'(r) \tag{76}$$

Making the ansatz,

$$W(r) = C - \frac{D}{r} \tag{77}$$

Substituting and simplifying gives,

$$W(r) = \frac{\sqrt{2m}}{\hbar} \frac{e^2}{2 \cdot 4\pi\epsilon_0 (l+1)} - \frac{\left(\frac{\hbar}{2m}(l+1)\right)}{r} \tag{78}$$

Deriving the partner potential

We can also see that the ground state energy of the radial Hamiltonian is,

$$E_0 = -C^2 = -\frac{e^4}{4 \cdot 16\pi^2\epsilon_0^2(l+1)^2}\frac{2m}{\hbar^2} = -2.18 \cdot 10^{-18} \approx -13.6eV \quad (79)$$

Now we can find the partner potential from Equation (72)

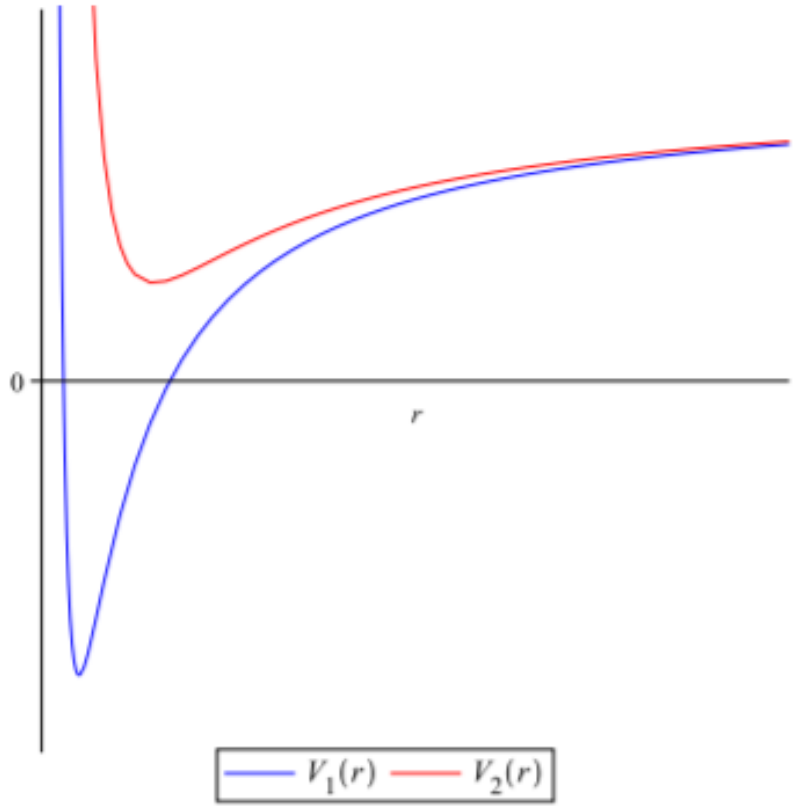
$$V_2(r) = \left[-\frac{1}{4}\frac{e^2}{\pi\epsilon_0}\right]\frac{1}{r} + \left[\frac{\hbar^2(l+1)(l+2)}{2m}\right]\frac{1}{r^2} + \left[\frac{e^4 m}{32\pi^2\hbar^2\epsilon_0^2(l+1)^2}\right] \quad (80)$$

The potential shape invariance is satisfied, when we compare this potential to the first potential, and it obeys the condition,

$$V_2(x; a_1) = V_1(x; a_2) + R(a_1) \quad (81)$$

Brief overlook of the Shape invariant potentials (SIPs)

If we look at the graph of the first two hydrogen partner potentials,



The remainder R(l)

We see that the relation between the parameters,

$$a_2 = f(a_1) \Rightarrow f(l) = l + 1 \tag{82}$$

And so the remainder here is,

$$R(l) = \frac{e^4 m(2l+3)}{32\pi^2\hbar^2\epsilon_0^2(l+1)^2(l+2)^2} \tag{83}$$

And this remainder is equal to the energy gap between zero energy and the first excited state,

$$E_{\Delta 0 \rightarrowtail 1} = \frac{e^4 m(2l+3)}{32\pi^2\hbar^2\epsilon_0^2(l+1)^2(l+2)^2} \tag{84}$$

The final results

Shifting the energy down by the previous shift E_0 (since ground energy is non-zero),

$$E_1 = \frac{e^4 m}{32\pi^2\hbar^2\epsilon_0^2(l+1)^2} + \frac{e^4 m(2l+3)}{32\pi^2\hbar^2\epsilon_0^2(l+1)^2(l+2)^2} \tag{85}$$

Generalising this to n^{th} energy level E_n,

$$E_n = E_0 + \sum_{i=1}^{n} \frac{e^4 m((2l+n-1)+3)}{32\pi^2\hbar^2\epsilon_0^2(l+n)^2(l+n+1)^2} \tag{86}$$

For $l = 0$,

$$E_n = \frac{e^4 m}{32\pi^2\hbar^2\epsilon_0^2(n+1)^2} \tag{87}$$

Which is the known formula for energy levels of the Hydrogen atom.

Reflections