

Supersymmetric Treatment of the Hydrogen Atom

The hydrogen atom, whose radial wavefunctions are determined by the radial Schrödinger equation

$$H_l = -\frac{\hbar^2}{2m} d_r^2 - \frac{e^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \quad (1)$$

can be solved by tedious power series methods. However, there is an elegant and instructive operator method that is well within the abilities of advanced undergraduates to understand and use. There are various versions of this method, beginning with famous papers by Schrödinger and Schwinger, but a particularly appealing version has been developed within the context of supersymmetric quantum mechanics.

Missing from undergraduate textbooks is this remarkable fact: given the energies E_{0k} and eigenstates ψ_{0k} , $k = 0, 1, 2, \dots$, for a particle moving in a potential V_0 , a supersymmetric partner potential V_1 can be constructed whose energies are $E_{1k} = E_{0k+1}$. The energy levels of the two potentials are identical, save the supersymmetric partner lacking the level corresponding to the ground state ψ_{00} .

In what follows, we assume that an appropriate scaling has been chosen so that the Schrödinger equation is written in dimensionless units as

$$-\frac{1}{2} d_s^2 \psi + U(s) \psi = \epsilon \psi \quad (2)$$

To do this, a length scale a_0 has been chosen so that $r = a_0 s$, $V = \frac{\hbar^2}{ma_0^2} U$, $E = \frac{\hbar^2}{ma_0^2} \epsilon$

1 Supersymmetry in Quantum Mechanics

We assume, to begin with, that we know the energies ϵ_{0n} and eigenfunctions ψ_{0n} of the Schrödinger equation with $U = U_0$. We begin by focusing on the ground state ψ_{00} , and writing it as

$$\psi_{00} = e^{-\int W_0(s) ds} \quad (3)$$

Taking the second derivative and using the Schrödinger equation, we get

$$\frac{1}{\psi_{00}} d_s^2 \psi_{00} = (W_0^2 - W_0') = 2(U_0 - \epsilon_{00}) \quad (4)$$

where $W_0' = d_s W_0$. The "superpotential" W_0 is linked to U_0 by the first-order differential equation (4).

EXERCISE 1: Find the superpotential for a particle in a box.

Now let us define the operator

$$A_0 = d_s + W_0 \quad (5)$$

and its Hermitian conjugate

$$A_0^\dagger = -d_s + W_0 \quad (6)$$

The Hamiltonian can be rewritten in terms of these operators as

$$H_0 = \frac{1}{2} A_0^\dagger A_0 + \epsilon_{00} \quad (7)$$

$$= \frac{1}{2} \left(-d_s^2 + W_0^2 - [d_s, W_0] \right) + \epsilon_{00} \quad (8)$$

$$= \frac{1}{2} \left(-d_s^2 + W_0^2 - W_0' \right) + \epsilon_{00} \quad (9)$$

$$= -\frac{1}{2} d_s^2 + U_0 \quad (10)$$

In the last step we used Eq. 4. This "factorization" of the Hamiltonian with arbitrary potential U_0 is quite analogous to the famous rewriting of the harmonic oscillator problem in terms of raising and lower operators.

Applying H_0 to the ground state gives

$$\left(\frac{1}{2} A_0^\dagger A_0 + \epsilon_{00} \right) \psi_{00} = \epsilon_{00} \psi_{00} \longrightarrow A_0 \psi_{00} = 0 \quad (11)$$

Substituting in for A_0 and solving for ψ_{00} ,

$$(d_s + W_0) \psi_{00} = 0 \longrightarrow \psi_{00} = e^{-\int W_0 ds} \quad (12)$$

We have come full circle, and verified the relationship between the superpotential and the ground-state wavefunction.

Now we form the supersymmetric partner Hamiltonian by switching the order of A_0 and A_0^\dagger :

$$H_1 = \frac{1}{2} A_0 A_0^\dagger + \epsilon_{00} \quad (13)$$

Using the commutation relation $[A_0, A_0^\dagger] = 2[d_s, W_0] = 2W_0'$ gives the explicit relationship

$$V_1 = V_0 + W_0' \quad (14)$$

showing that the two potentials are different (assuming $W' \neq 0$). Nevertheless, their energy levels are degenerate, as we can see by taking

$$H_1 A_0 \psi_{0k} = \left(\frac{1}{2} A_0 A_0^\dagger A_0 + \epsilon_{00} A_0 \right) \psi_{0k} \quad (15)$$

$$= A_0 H_0 \psi_{0k} \quad (16)$$

$$= \epsilon_{0k} A_0 \psi_{0k} \quad (17)$$

Thus $A_0\psi_{0k}$ is an eigenstate of H_1 with eigenvalue ϵ_{0k} . This holds unless $n = 0$, for which we already showed $A_0\psi_{00} = 0$.

Thus we infer that the energy levels of H_1 are identical to those of H_0 , except that there is no state of H_1 with energy ϵ_{00} :

$$\epsilon_{1k} = \epsilon_{0k+1} \quad (18)$$

Furthermore, we can generate the eigenfunctions for H_1 via

$$\psi_{1k} = \frac{A_0\psi_{0k+1}}{\sqrt{2(\epsilon_{0k+1} - \epsilon_{00})}} = \frac{A_0\psi_{0k+1}}{\sqrt{2(\epsilon_{1k} - \epsilon_{00})}} \quad (19)$$

Or, if we like, we can go the other way:

$$\psi_{0k} = \frac{A_0^\dagger\psi_{1k-1}}{\sqrt{2(\epsilon_{0k} - \epsilon_{00})}} = \frac{A_0^\dagger\psi_{1k-1}}{\sqrt{2(\epsilon_{1k-1} - \epsilon_{00})}} \quad (20)$$

Since the k th excited state has k nodes, we see that the operator A_0 produces an eigenstate of H_1 that has one less node, while A_0^\dagger takes us from an eigenstate of H_1 to an eigenstate of H_0 with one more node.

EXERCISE 2: Check that these equations give the correct normalizations for the eigenfunctions.

To summarize, we have shown that the Hamiltonian for motion in any potential can be factorized, and the factorization allows us to form a second potential whose energies are degenerate with the first, except for a missing partner to the ground state. The two Hamiltonians are said to obey a supersymmetry, and the connection between them is the superpotential W_0 .

Note that this process can be repeated. From the ground-state of H_1 , we can find a superpotential W_1 and corresponding A_1 , and generate H_2 whose energy levels are degenerate with H_1 save the missing ground state.... We will do this for the hydrogen atom next.

EXERCISE 3&4: Use the discretized Schrödinger equation method to find the lowest 10 energies for the supersymmetric partner potential of Exercise 1. Do they match with the particle in a box energies?

2 Supersymmetric Hydrogen atom

In atomic units ($r = sa_0$, $a_0 = \hbar^2/me^2$, $\epsilon = \frac{ma_0^2}{\hbar^2}E$), the radial Hamiltonian for the hydrogen atom is

$$H_l = -\frac{1}{2}d_s^2 + \frac{l(l+1)}{2s^2} - \frac{1}{s} \quad (21)$$

Our strategy is this: ~~we will find the energies and wavefunctions for the lowest energy state at each l .~~ From this, we will find the superpotentials W_l and show that each U_l is a supersymmetric partner with U_{l+1} . Thanks to the degeneracies of supersymmetric partners, this will give us the energies of all the states for arbitrary l and k . Using the ground state wavefunctions for each l , we can repeatedly apply the operators A^\dagger to generate the excited state wavefunctions.

For the eigenfunctions to be well-behaved at the origin, $\chi_l \sim s^{l+1}$. (The reason for calling the wavefunctions χ_l instead of $P_l(r)$ will become clear later). Thus a reasonable guess for the ground state wavefunction for arbitrary l is

$$\chi_{l0} = s^{l+1} e^{-bs} \quad (22)$$

Substituting this into Eq. 21 gives $b = 1/(l+1)$, $\epsilon_{l0} = -1/2(l+1)^2$. We now know the ground state wavefunctions, so we can find the superpotentials from Eq. 3:

$$W_l = -d_s \ln \chi_{l0} = \frac{1}{l+1} - \frac{l+1}{s} \quad (23)$$

To test whether or not supersymmetric works here, we check Eq. 14:

$$U_{l+1} = U_l + W'_l \quad (24)$$

$$\frac{(l+1)(l+2)}{2s^2} - \frac{1}{s} = \frac{l(l+1)}{2s^2} - \frac{1}{s} + \frac{l+1}{s^2} \quad (25)$$

which works.

Now that we have shown that each H_l is a superpartner with H_{l-1} , we deduce

$$\epsilon_{l,0} = \epsilon_{l-1,1} = \epsilon_{l-2,2} = \dots = \epsilon_{0,l} = \frac{-1}{2(l+1)^2} \quad (26)$$

or, succinctly,

$$\epsilon_{lk} = \frac{-1}{2(l+k+1)^2} \quad (27)$$

where both l and k go from zero to infinity. This is not the usual way the hydrogen energy level formula is written. It is conventional to define the principal quantum number $n = l + k + 1$, in which case

$$\epsilon_{nl} = \frac{-1}{2n^2} \quad (28)$$

where n goes from 1 to infinity, and l goes from 0 to $n-1$. In this notation, the wavefunctions are $P_{nl} = \chi_{l,n-l-1}$.

We are almost done. We can generate the $k > 0$ wavefunctions using Eq. 20. For example,

$$\chi_{l-1,1} = \frac{A_{l-1}^\dagger \chi_{l0}}{\sqrt{2(\epsilon_{l0} - \epsilon_{l-1,0})}} \quad (29)$$

Since we know the χ_{l0} (Eq. 22), this is a straightforward operation using

$$A_l^\dagger = -d_s + W_l \quad (30)$$

To translate this into principal quantum number language, to calculate the wavefunction for a state of given n and l , we first find $k = n - l - 1$. We calculate $\chi_{n,0}$, then apply k A_l^\dagger operators in succession, the last being A_l^\dagger . Thus, to calculate the 5p wavefunction, we first find the 5g wavefunction $P_{5g} = \chi_{40}$, then apply $A_1^\dagger A_2^\dagger A_3^\dagger$:

$$P_{5p} = \frac{A_1^\dagger}{\sqrt{2(\epsilon_{4,0} - \epsilon_{1,0})}} \frac{A_2^\dagger}{\sqrt{2(\epsilon_{4,0} - \epsilon_{2,0})}} \frac{A_3^\dagger}{\sqrt{2(\epsilon_{4,0} - \epsilon_{3,0})}} \chi_{40} \quad (31)$$

EXERCISE 5&6: Write a Mathematica function to calculate P_{nl} using supersymmetry. Verify its correctness for P_{7d} .
