

Factorisation of Hamiltonians: theory and some applications



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In these notes we shall try to explain the method of factorisation of Hamiltonians as it is a potent technique for finding spectra of 1-dimensional quantum mechanical systems. For some odd reason this technique is not dealt with in the major text books on quantum mechanics, whence the envisaged need for these notes.¹

The outline of these notes, is to start with Dirac's treatment of the quantum harmonic oscillator as it was the first system to be solved by factorisation. Then in sec. (2) we shall outline the idea of factorisation and introduce the notion of a *dual Hamiltonian* and its implications. In secs. (2.1,2.3) and (2.4) we shall apply the factorisation method together with a recurrence relation to obtain the spectrum of some simple 1-dimensional systems. The last section, sec. (3), is devoted to the hydrogen atom and how the method of factorisation is used to obtain the spectrum.

Finally: please have in mind that these notes are work in progress and that comments are welcome.

1 Harmonic Oscillator

As is well-known the harmonic oscillator is a simple physical system whose classical Hamiltonian is given by²

$$\mathcal{H}(p, q) = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 . \quad (1)$$

Before plunging into the quantum harmonic oscillator, we will quickly discuss the classical harmonic oscillator.

In order to find the classical trajectories it is easier to go from the phase-space description in terms of the p and q variables to the configuration space variables \dot{q} and q . This is easily done by the Legendre transform $\mathcal{L}(\dot{q}, q) = \dot{q}p - \mathcal{H}(p, q)$, which leads to the perhaps better known Lagrangean

$$\mathcal{L} = \frac{m}{2} [\dot{q}^2 - \omega^2 q^2] . \quad (2)$$

The Euler-Lagrange equations that follow from the above Lagrangean are

$$\ddot{q} = -\omega^2 q \longrightarrow q(t) = q_0 \cos(\omega t) + (v_0/\omega) \sin(\omega t) , \quad (3)$$

where q_0 , *resp.* v_0 , is the position, *resp.* velocity, at the time $t = 0$. If we impose the, physically reasonable,³ boundary condition $v_0 = 0$, then q_0 is the amplitude of the oscillation. Independently of the chosen boundary conditions, however, it is paramount that the period of the oscillation is $2\pi/\omega$, and therefore follows *Galileo's isochronous law*: the period of oscillation of a pendulum with small amplitude is independent of said amplitude. Finally, the energy of the trajectory is

$$E = \frac{m\omega^2 q_0^2}{2} \geq 0 , \quad (4)$$

and the zero energy trajectory is clearly the one that is not moving at all, *i.e.* $q(t) = 0$.

¹ One exception to this rule is R. Robinett's "*Quantum Mechanics*" [1], Faculty of Science library code K-53-645, who has a small section about factorisation, and you are advised to read it. Needless to say, should you find books dealing with the factorisation of Hamiltonians, I would be very pleased to hear about it.

² The factor of m in the potential term is not usual in classical treatments but will greatly simplify the formulas in the quantum case.

³ Imagine the situation of a pendulum being held fixed at a position q_0 until at $t = 0$ we release it.

Let us then go on and consider the quantum version of the harmonic oscillator described by the Hamiltonian operator

$$H = \frac{P^2}{2m} + \frac{m\omega^2}{2} Q^2 . \quad (5)$$

The first observation is that in the quantum system the energy, *i.e.* the possible eigenvalues of the Hamiltonian operator, cannot be zero: this is easily seen by considering an arbitrary normalised state $|\Psi\rangle$ to calculate

$$E[\Psi] \equiv \langle \Psi | H | \Psi \rangle = \frac{1}{2m} |P|\Psi\rangle|^2 + \frac{m\omega^2}{2} |Q|\Psi\rangle|^2 , \quad (6)$$

which clearly is bigger than or equal to zero. But, in order to attain $E[\Psi] = 0$, the state $|\Psi\rangle$ must satisfy $P|\Psi\rangle = 0$ and $Q|\Psi\rangle = 0$, which is incompatible with the fundamental commutation relation $[Q, P] = i\hbar$. We therefore reach the conclusion that in the quantum harmonic oscillator the energy is bounded from below and is strictly bigger than zero. The question then should be: What is the lowest energy of this system?

There is an algebraic approach to this system, invented by Dirac, which plays a prominent rôle in 20th century physics and it is this rôle that prompts us to re-discuss it.

The gist of Dirac's approach resides in the introduction of the following 2 operators

$$A \equiv \frac{1}{\sqrt{2\hbar m\omega}} P - i\sqrt{\frac{m\omega}{2\hbar}} Q , \quad (7)$$

$$A^\dagger = \frac{1}{\sqrt{2\hbar m\omega}} P + i\sqrt{\frac{m\omega}{2\hbar}} Q . \quad (8)$$

Using these operators we can rewrite the Hamiltonian as

$$H = \frac{\hbar\omega}{2} \left(A^\dagger A + A A^\dagger \right) , \quad (9)$$

which in itself is not too exciting. The excitement starts when we calculate

$$\left[A , A^\dagger \right] = \text{Id} . \quad (10)$$

We can use the above commutation relation to rewrite the Hamiltonian as

$$H = \hbar\omega \left[A^\dagger A + \frac{1}{2} \right] . \quad (11)$$

If we use this last expression to calculate $E[\Psi]$, we see that

$$E[\Psi] = \hbar\omega |A|\Psi\rangle|^2 + \hbar\omega/2 \geq \hbar\omega/2 !!! \quad (12)$$

This result indicates that the lowest energy that can be achieved in this system holds for a normalised state, denominated $|0\rangle$, that satisfies

$$A|0\rangle = 0 , \quad H|0\rangle = \frac{\hbar\omega}{2} |0\rangle , \quad \langle 0|0\rangle = 1 . \quad (13)$$

As any other state necessary has a higher energy we will call the state $|0\rangle$ the *groundstate* or the *vacuum state*.

The reader may feel ill-at-ease with the abstract definition of the groundstate, especially w.r.t. its existence, a situation we propose to ameliorate by discussing the wave-function corresponding to the groundstate: define the corresponding wave-function as $\Psi_0(q) \equiv \langle q|0\rangle$ and use the differential representation of the operators, *i.e.* $Q = q$ and $P = -i\hbar\partial_q$, then you can see that the normalised wavefunction is

$$\Psi_0(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} q^2\right), \quad (14)$$

where, as usual, we chose a possible phase to be unity.

Given that we found the state $|0\rangle$, can we use it to find other states? Well, consider the state

$$A^\dagger|0\rangle, \quad (15)$$

and ask yourself whether it is an eigenstate of the Hamiltonian H . This question is readily answered by calculating

$$\begin{aligned} HA^\dagger|0\rangle &= \hbar\omega \left(A^\dagger A + \frac{1}{2}\right) A^\dagger|0\rangle \\ &= \hbar\omega A^\dagger \left(AA^\dagger + \frac{1}{2}\right) |0\rangle \\ &= \hbar\omega A^\dagger \left[A^\dagger A + [A, A^\dagger] + \frac{1}{2}\right] |0\rangle \\ &= \hbar\omega A^\dagger \left[1 + \frac{1}{2}\right] |0\rangle \\ &= \hbar\omega \left[1 + \frac{1}{2}\right] A^\dagger|0\rangle. \end{aligned} \quad (16)$$

So the state in eq. (15) is indeed an energy eigenstate with an energy $\hbar\omega$ above the groundstate. At this point then we should try to find out whether it can be normalised and whether it is orthogonal to $|0\rangle$. The orthogonality issue is readily clarified once we see that energy eigenstates of different energies are always orthogonal: consider the states $|E\rangle$ and $|E'\rangle$ and calculate

$$\langle E|H|E'\rangle = E' \langle E|E'\rangle \quad (17)$$

$$= \overline{\langle E'|H|E\rangle} = E \langle E|E'\rangle, \quad (18)$$

from which we see that

$$(E' - E) \langle E|E'\rangle = 0 \quad \text{whence if } E' \neq E: \langle E|E'\rangle = 0. \quad (19)$$

A small calculation of $|A^\dagger|0\rangle|^2$ shows⁴ that the state can also be normalised and we must conclude that we found another normalised energy eigenstate, denoted by $|1\rangle$, whose relation to the groundstate is given by

$$|1\rangle \equiv A^\dagger|0\rangle. \quad (20)$$

Observe that in the normalisation of the above state, we took a possible phase to be unity.

⁴ To wit: $|A^\dagger|0\rangle|^2 = \langle 0|AA^\dagger|0\rangle = \langle 0|[A, A^\dagger]|0\rangle = \langle 0|0\rangle = 1$.

Of course we can use the same trick to create state with higher energies. In order to see this, it is handy to introduce an operator $N = A^\dagger A$ whose commutation relation with A and A^\dagger are readily calculated to be

$$[N, A] = -A, \quad (21)$$

$$[N, A^\dagger] = A^\dagger. \quad (22)$$

It is then an easy task to see that

$$N (A^\dagger)^n = (A^\dagger)^n (N + n), \quad (23)$$

which when coupled to $H = \hbar\omega [N + \frac{1}{2}]$ means that the states $(A^\dagger)^n |0\rangle$ are energy eigenstates with energy $\hbar\omega(n + 1/2)$. Normalising these states, and labeling them with the index n , we end up with a countable infinite set of energy eigenstates

$$|n\rangle = \frac{1}{\sqrt{n!}} (A^\dagger)^n |0\rangle \quad \rightarrow \quad \begin{cases} H|n\rangle &= \hbar\omega(n + 1/2) |n\rangle, \\ \langle n|m\rangle &= \delta_{n,m}. \end{cases} \quad (24)$$

Given this set of states we can calculate the action of the operators on them, only to find

$$N|n\rangle = n|n\rangle, \quad (25)$$

$$A|n\rangle = \sqrt{n} |n-1\rangle, \quad (26)$$

$$A^\dagger|n\rangle = \sqrt{n+1} |n+1\rangle. \quad (27)$$

We can imagine the energy spectrum as a ladder with the energy levels being the spokes;⁵ the operator N then gives the number of spokes that one had to climb up from the ground to get to the desired spoke, and correspondingly N receives the name *number operator*. Using the same analogy, the operator A^\dagger pushes you up one spoke and receives the name *ladder-up operator*. Unsurprisingly, the operator A is baptised with the name *ladder-down operator*.⁶

In eq. (14) we defined the wave-function of the groundstate as $\Psi_0(q) = \langle q|0\rangle$, and in this case we want to find the wave-functions for all energy eigenstates. In order to do so, we follow the same steps as needed for the derivation of eq. (14) and start by defining $\Psi_n(q) \equiv \langle q|n\rangle$ and introducing the abbreviation $\mu \equiv m\omega/\hbar$. Then it is an easy calculation to show that

$$\Psi_n(q) = \frac{i^n}{\sqrt{2^n n!}} \left(\frac{\mu}{\pi}\right)^{1/4} \exp(-\mu/2 q^2) \mathbf{H}_n(\sqrt{\mu}q), \quad (28)$$

where \mathbf{H}_n is the n^{th} Hermite polynomial, one representation of which is

$$\mathbf{H}_n(x) = (-1)^n e^{x^2} \partial_x^n e^{-x^2}. \quad (29)$$

The painful properties of the Hermite polynomials such as the orthogonality and completeness relations can be derived quite painlessly from the algebraic approach to the quantum harmonic oscillator.

⁵ Ladder = escalera; spoke = peldaño.

⁶ Similar operators appear in Quantum Field Theory and there they go by the names particle number operator or occupation number (N), (particle) creation operator (A^\dagger) and (particle) annihilation operator (A).

Summarising, we have found a countable infinite number of energy eigenstates, all of which can be created using the operator A repeatedly on the groundstate $|0\rangle$. The remaining question to be answered is whether there are energy eigenstates that were left out in the above analysis. The answer is no, and in order to see this suppose there exists an energy eigenstate $|E\rangle$, that doesn't belong to the set we obtained above, *i.e.* $\nexists_{n \in \mathbb{N}} E = \hbar\omega(n + \frac{1}{2})$. The argument of $A|E\rangle$ being an energy eigenstate with energy $E - \hbar\omega$, however, goes through and we can apply A repeatedly on the state $|E\rangle$ as to end up with a negative energy, leading to a contradiction with the fact that the energy should be positive. We must therefore conclude that the only energy eigenstates of the harmonic oscillator are the ones that were obtained above.

2 Factorisation of Hamiltonians

Dirac's treatment of the harmonic oscillator by factorising the Hamiltonian, leads to the obvious question, one supposedly posed first by Schrödinger in ref. [2], whether all quantum mechanical system can be factorised: for one dimensional systems the answer to this question is, modulo important titbits, affirmative.

Suppose we are given a Hamiltonian operator H that is bounded from below, which is a sound restriction as otherwise the system would be unstable, and that the groundstate $|\Psi_0\rangle$ has energy E_0 . Given this situation we will redefine the Hamiltonian as $H_- \equiv H - E_0 \text{ Id}$, which implies that the energy eigenvalues of H_- is positive semi-definite, *i.e.* $\langle H_- \rangle \geq 0$. The question posed by Schrödinger can then be formulated as:

$$\text{Is there an operator } A \text{ such that } H_- = A^\dagger A ? \quad (30)$$

As the groundstate of the Hamiltonian H_- has zero energy we have that $0 = \langle \Psi_0 | H_- | \Psi_0 \rangle = |A|\Psi_0\rangle|^2$, implying that the groundstate satisfies the equation

$$A|\Psi_0\rangle = 0. \quad (31)$$

In the modern technical language equations such as eq. (31) are called Bogomol'nyi-Prasad-Sommerfield equations, which is usually abbreviated to *BPS equations*.

In order to advance a bit in the direction of demonstrating the feasibility of factorisation, consider the following position-representation of the operators A and A^\dagger :

$$A \equiv i(\partial_q + W(q)) \quad , \quad A^\dagger = i(\partial_q - W(q)) \quad , \quad (32)$$

where W is a real function of q , called the *superpotential*. Using the above representation and defining $\Psi_0 \equiv \langle q | \Psi_0 \rangle$, we can then use the BPS equation, eq. (31), to determine

$$W = -\partial_q [\log(\Psi_0)] \quad , \quad (33)$$

which shows that given a system with a well-defined groundstate, we can always find W .

Conversely, given W we can always find Ψ_0 as

$$\Psi_0(q) \sim \exp(-\chi(q)) \quad \text{where} \quad \partial_q \chi = W. \quad (34)$$

Obviously, for the groundstate to be part of the spectrum of H_- , it must be normalisable which we suppose to be the case:⁷ so we see that the factorisation of Hamiltonians is always possible.

⁷ Observe that if the spectrum of Q , $S(Q)$, is equivalent to \mathbb{R} then this implies drop-off conditions for Ψ_0 .

A related question is whether given a Hamiltonian, the factorisation can be used to find the groundstate: in order to see whether this is possible let us calculate

$$\mathbb{H}_- \Psi = \mathbb{A}^\dagger \mathbb{A} \Psi = -\partial^2 \Psi + [W^2 - \partial W] \Psi, \quad (35)$$

which we can compare to the Schrödinger equation (which we have rescaled with a factor $2m\hbar^{-2}$)

$$-\partial^2 \Psi + V_-(q) \Psi = E \Psi. \quad (36)$$

Now, before going over to identify eq. (35) with eq. (36), let us point out that the quantum mechanical ground energy can be redefined by summing a finite piece without affecting the physics: we used this relation in the beginning of this section when we related \mathbb{H} to \mathbb{H}_- . This then means that in order to make the match we must consider for our factorisation programme the following constraint

$$W^2 - \partial W \equiv V_-(q) = V(q) + V_0, \quad (37)$$

where V_0 is some real constant that we can add to the potential such that the factorisation works: seeing that the factorised Hamiltonian's ground-state energy is zero, you can easily work out that $V_0 = -E_0$. The equation (37) is the *Ricatti equation* and its relation to the 2nd order Schrödinger equation is well-known.

Even though the above is a nice tidbit, which may be helpful to find the groundstate and its energy, it may be that actually finding the function W for a given potential is actually a tremendous, daunting or even impossible task. And even if we are able to find the function W , what can we say about the rest of the energy spectrum?

Well, given eq. (30) we might be curious about the spectrum of the so-called *dual Hamiltonian*

$$\mathbb{H}_+ \equiv \mathbb{A} \mathbb{A}^\dagger = -\partial^2 + V_+(q) \quad \longrightarrow \quad V_+ \equiv W^2 + \partial W. \quad (38)$$

Clearly the possible energy eigenvalues of \mathbb{H}_+ , denoted by \tilde{E} , must be positive semidefinite, and the zero energy solution must satisfy $\mathbb{A}^\dagger |\tilde{\Psi}_0\rangle = 0$; the solution to the resulting differential equation exists and reads

$$\mathbb{A}^\dagger \tilde{\Psi}_0(q) = 0 \quad \longrightarrow \quad \tilde{\Psi}_0(q) \sim e^{\chi(q)}, \quad (39)$$

where χ was defined in eq. (34). Now, if we take $\mathbb{S}(Q) \sim \mathbb{R}$ then, as we imposed the groundstate of \mathbb{H}_- to be normalisable, the state $|\tilde{\Psi}_0\rangle$ is not normalisable, and hence not part of \mathbb{H}_+ 's spectrum.

Consider then an arbitrary \mathbb{H}_- -eigenstate $|E\rangle$ with energy $E > 0$, *i.e.* any energy eigenstate except the groundstate. A small calculation then shows that

$$\mathbb{H}_+ (\mathbb{A}|E\rangle) = \mathbb{A} (\mathbb{H}_-|E\rangle) = E (\mathbb{A}|E\rangle), \quad (40)$$

whence the state $\mathbb{A}|E\rangle$ is an eigenstate of the Hamiltonian \mathbb{H}_+ with the same energy. Of course, for the state $\mathbb{A}|E\rangle$ to be physical it must be normalisable which is luckily no problem: it is easy to see that the corresponding normalised states are given by

$$|\tilde{E}\rangle = E^{-1/2} \mathbb{A}|E\rangle \quad (E > 0), \quad (41)$$

which means that $\mathbb{S}(\mathbb{H}_-)/\{0\} \subseteq \mathbb{S}(\mathbb{H}_+)$.

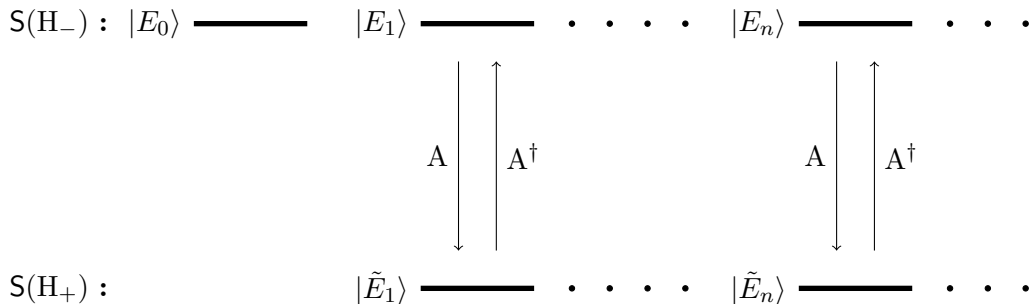


Figure 1: A graphical depiction of the mapping of states derived in this section.

Turning the argument in eq. (40) around we have

$$H_- \left(A^\dagger |\tilde{E}\rangle \right) = A^\dagger \left(H_+ |\tilde{E}\rangle \right) = \tilde{E} A^\dagger |\tilde{E}\rangle \quad (\tilde{E} > 0), \quad (42)$$

so that $S(H_+) \subseteq S(H_-)$. Putting then both things together we must conclude that

$$S(H_+) \cong S(H_-) / \{0\}, \quad (43)$$

or said in words: the spectrum of H_+ consists of all the non-groundstates of H_- .

Summarising the results obtained thus far, we see that given a system with a groundstate, we can always factorise the Hamiltonian, H_- , and define the “dual Hamiltonian” H_+ which is also factorised. The spectrum of the dual Hamiltonian is equal to that of the original Hamiltonian but for the groundstate. As one can imagine, this mapping is useful if the spectrum of the dual Hamiltonian is known as then the problem of finding the spectrum of the original Hamiltonian is solved.

Of course, we might have a small problem if the dual Hamiltonian’s spectrum is not known. But, as the dual Hamiltonian does admit a groundstate, namely the state dual to the first excited state in the original system, the dual Hamiltonian itself must allow for a factorisation and we can imagine using the process of factorisation recursively till we end up with something known. In the following sections we shall apply the technique of factorisation, together with the recurrence, to deduce the spectrum of some easy Hamiltonians.

2.1 The simplest of the pedagogical Pöschl-Teller potentials

Consider the superpotential⁸

$$W = \tanh(q), \quad (44)$$

which using eq. (37) leads to the potential

$$V_-(q) = 2 \tanh^2(q) - 1 = 1 - \frac{2}{\cosh^2(q)}, \quad (45)$$

⁸ One can consider of course the general function $W = A \tanh(\mu q)$ and follow the factorisation reasoning to find the spectrum *etc.* for the resulting family of potentials, which are called Pöschl-Teller potentials. The version we are using here gives easy formulas, is easy to understand and is therefore especially suited for pedagogical purposes.

which is a simple potential whose absolute minimum lies at $q = 0$ with value $V_-(0) = -1$ and asymptotes to $V_-(|q| \rightarrow \infty) = 1$. So the potential has all the necessary ingredients for allowing a discrete spectrum and the question is how many discrete states there are?

From the general discussion, we see that it is worthwhile to investigate the dual Hamiltonian: a small calculation show that

$$V_+(q) = 1 \quad (!!!) \quad (46)$$

So we see that the dual-Hamiltonian is that of a particle in a constant potential, which is equivalent to a free particle whose spectrum is continuous. This then means that the above simple potential has only one discrete energy level whose energy w.r.t. the potential in eq. (45) is zero; Had we chosen the more physically reasonable definition of the potential, namely the one for which $V(|q| \rightarrow \infty) = 0$, which can easily be arranged by adding a constant, then the minimum value of the potential would be -2 and the energy of the bound state would be -1 .

The groundstate is then easily found and is given by the normalised wavefunction

$$\Psi_0 = \frac{1}{\sqrt{2} \cosh(q)}. \quad (47)$$

What happens to the naive groundstate of the dual system given by $A^\dagger \tilde{\Psi} = 0$? Clearly we can solve the differential equation to give $\tilde{\Psi} = \tilde{\psi} \cosh(q)$, where $\tilde{\psi}$ is a complex constant, but can readily convince oneself that it is non-normalisable.

Having dealt with the discrete part of the spectrum, it is then time to turn to its continuous part: from eq. (42) we can see that the correctly normalised state in the original theory is given in terms of the dual theory as

$$|E\rangle = \frac{1}{\sqrt{E}} A^\dagger |\tilde{E}\rangle \quad \text{which for the wavefunctions leads to: } \Psi_E(q) = \frac{1}{\sqrt{E}} A^\dagger \tilde{\Psi}_{\tilde{E}}(q), \quad (48)$$

where in the last equation A^\dagger is the operator in the coordinate representation, see eq. (32), and we defined $\Psi_E = \langle q|E\rangle$ *etc.* As we know, for a free particle the eigenstates are, due to parity invariance of the Hamiltonian, 2-fold degenerate and correspond to momentum eigenstates; in the case at hand this means that the energy eigenstates of the dual theory are given by $\tilde{\Psi}_{\tilde{E}(k)} = (2\pi)^{-1/2} e^{ikq}$ and the corresponding energy is $\tilde{E}(k) = k^2 + 1$. A straightforward application of eq. (48) then leads to the following expression for the wavefunctions of the energy eigenstates in the continuous spectrum

$$\Psi_k(q) = (2\pi(k^2 + 1))^{-1/2} [\tanh(q) - ik] e^{ikq}, \quad (49)$$

whose energy is $k^2 + 1$. As usual for states in the continuous part of the spectrum, the $\Psi_k(q)$ form a δ -orthonormal set, *i.e.* $\langle \Psi_{k'} | \Psi_k \rangle = \delta(k - k')$.

2.2 The pedagogical Pöschl-Teller potentials, self-similarity and recursion

The foregoing example was chosen such that the dual theory's spectrum was known. Normally one is not that lucky and one ends up with a dual theory whose spectrum is also unknown. In that case one can use the fact that the dual Hamiltonian is bounded from below, factorise the dual Hamiltonian and obtain the dual of the dual Hamiltonian. There is of course no guarantee that the thus obtained dual-dual Hamiltonian's spectrum is known, which is however no problem as we know how to deal with such situations: just factorise the dual-dual

Hamiltonian! This just-factorise-the-dual-Hamiltonian approach to solving problems has the obvious drawbacks of being time/work-consuming and of having no guarantee whatsoever that at some point one will end up with a known system.

The time/work-consuming part of the drawbacks can sometimes be overcome, as is the case in some of the standard examples in quantum mechanics. The key to overcome these problems lies in the similarity of the dual Hamiltonian to the original one. It is this self-similarity, as it is called in the literature, that allows one to write down hierarchies of Hamiltonians and to derive recursion relations for the energies of the states and the wave-functions. We shall explain this using a generalisation of the Hamiltonian studied in the foregoing section.

Consider the following generalisation of the prepotential in eq. (44)

$$W^{(n)} = n \tanh(q) \quad (n \in \mathbb{N}^+), \quad (50)$$

for some given $n \geq 2$. With this choice we can calculate the potential V_- and also the corresponding dual potential V_+ to be

$$V_-^{(n)}(q) = n^2 - \frac{n(n+1)}{\cosh^2(q)} = n(n+1) \tanh^2(q) - n, \quad (51)$$

$$V_+^{(n)}(q) = n^2 - \frac{n(n-1)}{\cosh^2(q)} = n(n-1) \tanh^2(q) + n. \quad (52)$$

By direct comparison we can derive the relation⁹

$$V_+^{(n)} = V_-^{(n-1)} + 2n - 1 \quad \longrightarrow \quad H_{\pm}^{(n)} \equiv P^2 + V_{\pm}^{(n)}, \quad (53)$$

What does this recursion relation mean? Well, consider for the moment the case of $n = 2$: in that case the potential $V_+^{(2)}$ is up to a trivial shift in groundstate energy exactly the one in eq. (45), which is the case with $n = 1$, whence the hierarchy of factorisation ends quickly as we already know the spectrum of the dual theory. Since we lose one state in the step to the dual Hamiltonian and the dual theory has 1 state in the discrete spectrum, we must conclude that $H_-^{(2)}$'s discrete spectrum consists of 2 states.

For general n , the discrete spectrum of $H_-^{(n)}$ consists of n states: indeed, starting from the Hamiltonian, we can use eq. (53) to derive the sequence

$$H_-^{(n)} \xrightarrow{\text{step no. } 1} H_+^{(n)} = H_-^{(n-1)} + 2n - 1 \longrightarrow \dots \xrightarrow{\text{step no. } n-1} H_-^{(1)}, \quad (54)$$

where it effectively stops as we know the spectrum of the Hamiltonian $H_-^{(1)}$. From the general discussion we know that every \longrightarrow means the eradication of one state, namely H_- 's groundstate, and since there are $(n-1)$ \longrightarrow 's needed in order to get from n to 1, we see that the spectrum of $H_-^{(n)}$ consists of n discrete states. Of course, there is a continuous spectrum on top of that.

Having given the number of states in the discrete part of the spectrum, we would also like to know the associated energy eigenvalues. These can be derived as follows: let $E_p^{(n)}$ denote the energy eigenvalue of the p^{th} state in the discrete spectrum of the Hamiltonian $H_-^{(n)}$. As we start counting from 0, the groundstate energy is $E_0^{(n)}$ which by construction is $E_0^{(n)} = 0$.

⁹ Remember that we are comparing factorised Hamiltonians to ordinary, albeit rescaled, Hamiltonians of the type displayed in eq. (36). This means that in this formula we are using $P = -i\partial_q$!

Suppose then that we want to know the energy $E_1^{(n)}$, *i.e.* the energy of the first excited state of $H_-^{(n)}$. As we know from the general theory in sec. (2), this energy is exactly the same as the one of the corresponding state for the dual Hamiltonian $H_+^{(n)}$, whence we have $E_1^{(n)} = \tilde{E}_1^{(n)}$. Eq. (53) then means that the state $|\tilde{E}_1^{(n)}\rangle$ is an eigenstate of the Hamiltonian $H_-^{(n-1)}$, in fact its groundstate. W.r.t. to the Hamiltonian $H_-^{(n-1)}$ we would call this state $|E_0^{(n-1)}\rangle$ and a straightforward application of eq. (53) leads to the identity $\tilde{E}_1^{(n)} = E_0^{(n-1)} + 2n + 1 = 2n + 1$, where we used the fact that $E_0^{(n)} = 0$ for all n . Putting all ingredients together we see that $E_1^{(n)} = 2n + 1$.

We can repeat the above steps for an arbitrary energy in the discrete spectrum of $H_-^{(n)}$. Consider the p^{th} state with energy $E_p^{(n)}$. By duality we have that $E_p^{(n)} = \tilde{E}_p^{(n)}$, and by the refactorisation of the dual Hamiltonian, eq. (53), we have that $\tilde{E}_p^{(n)} = E_{p-1}^{(n-1)} + 2n + 1$; the fact that the energy of the $(p-1)^{\text{th}}$ state appears in $E_{p-1}^{(n-1)}$ is due to the fact that the state $|\tilde{E}_1^{(n)}\rangle = |E_0^{(n-1)}\rangle$, *i.e.* we have to take into account that we start counting states from 0 in $H_-^{(n-1)}$'s spectrum. Putting then everything together, we find the recursion relation

$$(p = 1, \dots, n-1) : \quad E_p^{(n)} = E_{p-1}^{(n-1)} + 2n - 1, \quad (55)$$

The above recursion relation can be immediately integrated by using the boundary condition $E_0^{(n)} = 0$ to give

$$E_p^{(n)} = p(2n - p). \quad (56)$$

Observe that the possible energy eigenvalues lie beautifully between the extrema of $V_-^{(n)}$, namely $-n$ and n^2 .

Given that we know the discrete part of the spectrum,¹⁰ we can then ask ourselves about the wavefunctions, which we shall define through $\Psi_p^{(n)}(q) \equiv \langle q | E_p^{(n)} \rangle$. The groundstate wavefunctions are determined as usual by means of the BPS equation (31), but as we are dealing with a family of Hamiltonians, we must take care to use the appropriate As. Introduce the annihilation operators

$$A_{(n)} = i \left(\partial_q + W^{(n)}(q) \right) \xrightarrow{\text{appropriate BPS condition}} A_{(n)} \Psi_0^{(n)}(q) = 0. \quad (57)$$

The normalised solution to the BPS equation reads

$$\Psi_0^{(n)} = \sqrt{\frac{(2n-1)!!}{2^n(n-1)!}} \frac{1}{\cosh^n(q)}, \quad (58)$$

where the normalisation was obtained by using

$$\int_{-\infty}^{\infty} dq \cosh^{-2n}(q) = \frac{2^n(n-1)!}{(2n-1)!} \quad (n \geq 1), \quad (59)$$

and choosing a possible phase to be unity.

¹⁰ Of course, as in the case for $n=1$, the continuous spectrum is two-fold degenerate and is given by states $|k\rangle$ ($|k| > 0$) with energy $E^{(n)}(k) = k^2 + n^2$. The reader is invited to figure this out.

Using these groundstate wavefunctions we can then derive a recursion relation for the wavefunctions: remember that there is mapping taking normalised states of the dual system to normalised non-groundstates in the original theory, see eq. (48). If we combine this with the fact that the refactorisation of the dual system does not change the state, but only the Hamiltonian that acts on them, we must infer that for $p \neq 0$

$$|E_p^{(n)}\rangle = \sqrt{\frac{1}{E_p^{(n)}}} A_{(n)}^\dagger |\tilde{E}_p^{(n)}\rangle = \sqrt{\frac{1}{E_p^{(n)}}} A_{(n)}^\dagger |E_{p-1}^{(n-1)}\rangle. \quad (60)$$

Hitting the above relation with $\langle q|$ and using eq. (56), we find the following recursion relation for the wave functions

$$\Psi_p^{(n)}(q) = \frac{-i}{\sqrt{p(2n-p)}} A_{(n)}^\dagger \Psi_{p-1}^{(n-1)}(q) \quad (p \neq 0), \quad (61)$$

where we have introduced an extra phase-factor, $-i$, as to ensure that the resulting wavefunctions are real. This recursion relation, together with the groundstate wavefunctions in eq. (58) is enough to derive all wavefunctions.

As an example consider the case of $n = 2$, then the two states in the discrete spectrum are $\Psi_0^{(2)}$, given by eq. (58), and $\Psi_1^{(2)}$, which can be generated using eqs. (61) and (47), lead to

$$\Psi_0^{(2)} = \sqrt{\frac{3}{4}} \frac{1}{\cosh^2(q)}, \quad (62)$$

$$\Psi_1^{(2)} = -\sqrt{\frac{3}{2}} \frac{\sinh(q)}{\cosh^2(q)}, \quad (63)$$

which are easily seen to be correctly normalised.

2.3 The trigonometric Pöschl-Teller potential

As a variation on the foregoing subsection, consider the family of prepotentials

$$W^{(n)} = n \tan(q) \quad (n \in \mathbb{N}^+). \quad (64)$$

This prepotential leads automatically to the potential

$$V_-^{(n)} = -n + n(n-1) \tan^2(q), \quad (65)$$

which is naturally defined on the interval $q \in (-\pi/2, \pi/2)$ which we shall take to be the domain of our problem: clearly for $n = 1$ we find a problem with a constant potential on an interval, which is equivalent to the problem of a particle in an infinite square well. From now on we shall consider the case $n \geq 2$.

The potential for $n = 2$ has a minimum at $q = 0$ which lies at $V_-(0) = -2$ and blows up at $q = \pm\pi/2$, which is what we meant when we said that the potential was naturally defined on the interval $(-\pi/2, \pi/2)$. As this potential, for any $n \geq 2$, has no point where it becomes flat or constant, there is an infinite number of discrete states, just as in the case of the particle in a box or the harmonic oscillator. We shall use the method of factorisation to find the energy eigenstates of the associated Hamiltonian. To this end calculate

$$V_+^{(n)} = n + n(n+1) \tan^2(q). \quad (66)$$

As before we can use this form of the potential to derive a recursion relation

$$V_+^{(n)} = V_-^{(n+1)} + 2n + 1, \quad (67)$$

which in itself leads to the recursion relation for the energies

$$E_k^{(n)} = \tilde{E}_k^{(n)} = E_{k-1}^{(n+1)} + 2n + 1. \quad (68)$$

This recursion relations can be integrated immediately by using $E_0^{(n)} = 0$, to give

$$E_k^{(n)} = k(2n + k), \quad (69)$$

which as we suspected has no upper-limit and is, as it should be, bounded from below.

The wavefunction of the groundstate of the Hamiltonian $H_-^{(n)}$ follows easily from eq. (34) and results in¹¹

$$\Psi_0^{(n)} = \sqrt{\frac{(2n)!!}{(2n-1)!! \pi}} \cos^n(q); \quad (70)$$

the normalisation of the wavefunctions being fixed by using the integral

$$\int_{-\pi/2}^{\pi/2} dq \cos^{2n}(q) = \frac{(2n-1)!!}{(2n)!!} \pi, \quad (71)$$

and taking a possible phase to be unity.

From the wavefunction of the groundstates, we can deduce the wavefunctions using relations like (48); for the model with $n = 2$ the normalised wavefunctions of the 4 lowest energy eigenstates are

$$\begin{aligned} \Psi_3^{(2)} &= \sqrt{\frac{16}{3\pi}} \sin(q) \cos^2(q) (8 \cos^2(q) - 5) \\ \Psi_2^{(2)} &= \sqrt{\frac{32}{15\pi}} \cos^2(q) (6 \cos^2(q) - 5) \\ \Psi_1^{(2)} &= \sqrt{\frac{16}{\pi}} \sin(q) \cos^2(q) \\ \Psi_0^{(2)} &= \sqrt{\frac{8}{3\pi}} \cos^2(q) \end{aligned} \quad (72)$$

In the above figure we overlaid the potential, the outer line, with the energy levels, the straight horizontal lines; the wiggly lines around the energy levels are the (real) wavefunctions.

¹¹ Observe that the wave functions naturally satisfy the boundary conditions $\Psi_0^{(n)}(q = \pm\pi/2) = 0$.

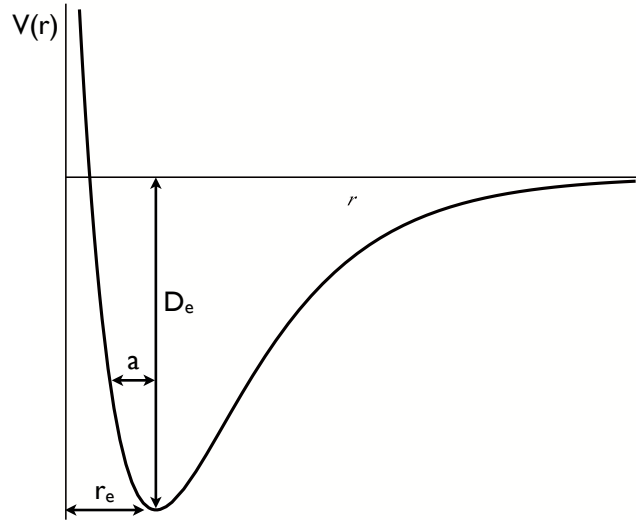


Figure 2: A graphical representation of the Morse potential, indicating the meaning of the parameters a , r_e and D_e .

2.4 Di-atomic molecules and vibrational modes: the Morse Potential

When thinking of a di-atomic molecule, we can envisage the molecule as two bodies connected by some force, and clearly the first image that comes to mind is a spring connecting them. When we then start thinking about the possible states of the molecule we first should think about vibrational modes, perhaps influenced by the image of the molecule as being two bodies connected by a spring. Clearly, we can also think about the rotational modes that are known to occur, but we shall restrict our attention to vibrational modes: seeing the spring analogy, we might be inclined to use the harmonic oscillator potential to approximate the true force between the atoms. Even though this might be a correct approximation for small vibrations, it means that there is no way to break the molecule apart: as we saw, the spectrum of the harmonic oscillator is purely discrete and unbounded from above. In true molecules, however, there is an energy which breaks up the molecule, in the same way atoms have an ionization energy, called the *dissociation energy*. Also, measurements of true di-atomic energy spectrum shows that the energy of the states does not grow linearly with a possible mode number, indicating that the harmonic oscillator is a very bad approximation to the nature of the force between the atoms in di-atomic molecules.

In order to remedy the above, Morse [3] proposed a phenomenological potential of the form

$$V = D_e (1 - \exp(-a(r - r_e)))^2 - D_e , \quad (73)$$

a graphical representation of which is given in fig. (2). As said before we are only interested in vibrational modes, whence we are only interested in wavefunctions that depend only on the distance between the atoms. This means that the problem we have to solve becomes effectively 1-dimensional and in fact can be written as

$$-\frac{\hbar^2}{2m} \partial_r^2 \Psi + V(r)\Psi = E\Psi . \quad (74)$$

If we introduce the following redefinitions

$$\rho = ar \ , \ \lambda = \frac{\sqrt{2mD_e}}{\hbar a} \ , \ \mathcal{E} = \frac{2m}{\hbar^2 a^2} E \ , \quad (75)$$

we can rewrite the problem in eq. (74)

$$-\partial_\rho^2 \Psi + \lambda^2 \left(e^{-2(\rho-\rho_0)} - 2e^{-(\rho-\rho_0)} \right) \Psi = \mathcal{E} \Psi \ . \quad (76)$$

Let us then try to use the factorisation method in order to find the eigenenergies: after some educated guesses one can see that the solution to eq. (37) for the case at hand, is given by

$$W = \lambda - \frac{1}{2} - \lambda e^{-(\rho-\rho_0)} \ , \ V_0 = \left(\lambda - \frac{1}{2} \right)^2 \ . \quad (77)$$

This means that the groundstate energy of the system is given by

$$E_0 = -\frac{\hbar^2 a^2}{2m} \left(\lambda - \frac{1}{2} \right)^2 \ . \quad (78)$$

True to the letter of the factorisation approach, we then consider the dual Hamiltonian and calculate

$$V_+ = W^2 + \partial W = \left(\lambda - \frac{1}{2} \right)^2 - 2\lambda(\lambda - 1) e^{-(\rho-\rho_0)} + \lambda^2 e^{-2(\rho-\rho_0)} \ , \quad (79)$$

which is quite similar to the original Morse potential and we can use the same recursion trick as in sec. (2.2): consider the following family of superpotentials

$$W_{(n)} = \lambda - n - \frac{1}{2} - \lambda e^{-(\rho-\rho_0)} \ , \quad (80)$$

where $n \in \mathbb{N}$. $n = 0$ corresponds to the Morse's potential, albeit with a shifted groundstate energy.

Given the family of superpotentials in eq. (80), one can straightforwardly calculate the associated potentials to be

$$V_-^{(n)} = \left(\lambda - n - \frac{1}{2} \right)^2 - 2\lambda(\lambda - n) e^{-(\rho-\rho_0)} + \lambda^2 e^{-2(\rho-\rho_0)} \ , \quad (81)$$

$$V_+^{(n)} = \left(\lambda - n - \frac{1}{2} \right)^2 - 2\lambda(\lambda - n - 1) e^{-(\rho-\rho_0)} + \lambda^2 e^{-2(\rho-\rho_0)} \ . \quad (82)$$

We can then relate the two potentials by the relation

$$V_+^{(n)} = V_-^{(n+1)} + \left(\lambda - n - \frac{1}{2} \right)^2 - \left(\lambda - n - \frac{3}{2} \right)^2 \ , \quad (83)$$

which automatically leads to the discrete spectrum and the associated energy values for Morse's Hamiltonian, namely

$$E_n = -\frac{\hbar^2 a^2}{2m} \left(\lambda - n - \frac{1}{2} \right)^2 \ . \quad (84)$$

Are we then finished? Well, taking eq. (84) at face-value, the energy spectrum would be unbounded from below, which is clearly impossible. This means that we should restrict n to

$$0 \leq n \leq \lfloor \lambda - \frac{1}{2} \rfloor \ , \quad (85)$$

as then there is a finite number of states in the discrete part of the spectrum, all of which have a negative energy.

Why did the recursion argument fail? The argument failed because we did the recurrency relation without thinking about the spectrum of the dual theories! In fact, one can see that when $n > \lfloor \lambda - \frac{1}{2} \rfloor$ the associated potentials have no global minimum except for the region $r \rightarrow \infty$, whence for those values of n the spectrum is purely continuous and our hierarchy ends. Taking this into account, the method works out just fine.

3 The Hydrogen atom and Hydrogen-like systems

As one knows from classical mechanics the 2-body system with an interaction that depends only on the relative distance between the 2 bodies can be split into two unrelated physical systems, namely one describing the free motion of the centre of mass, and the other one describing the relative motion. Given then the masses m_1 and m_2 of the two bodies, we know that the centre of mass system is governed by the systems total mass $M = m_1 + m_2$, whereas the relative motion is governed by the so-called *reduced mass* μ given by

$$\mu \equiv \frac{m_1 m_2}{m_1 + m_2} . \quad (86)$$

Clearly, if one of the masses is far bigger than the other one then the reduced mass is approximately equal to the smaller one: take for instance $m_1 \gg m_2$ then one sees from the above formula that $\mu = m_2$.¹²

As the dynamics of the centre of mass system is that of a free particle of mass M , its physics is under control and we will from now on only deal with the system of the relative motion. The relevant Hamiltonian is given in terms of the operators \vec{P} and \vec{X} and reads

$$H = \frac{\vec{P}^2}{2\mu} + V(|\vec{X}|) , \quad (87)$$

which is clearly invariant under rotations in \mathbb{R}^3 : we can use the rotational invariance to reduce this system to an effectively 1-dimensional system, which can then be dealt with using the factorisation approach.

In order to reduce the above problem to a 1-dimensional problem, remember that the angular momentum operators L_i in the coordinate-representation are given by $L_i = -i\varepsilon_{ijk}x^j\partial_k$. Using this expression one can see that

$$\vec{L}^2 \Psi = -\vec{x}^2 \vec{\partial}^2 \Psi + \vec{x} \cdot \vec{\partial} (\vec{x} \cdot \vec{\partial} \Psi) + \vec{x} \cdot \vec{\partial} \Psi . \quad (88)$$

If we then introduce the standard spherical coordinate system with $\vec{x}^2 = r^2$, we see that $\vec{x} \cdot \partial = r\partial_r$ and can then reshuffle and rewrite the above expression as

$$-\vec{\partial}^2 \Psi = -\frac{1}{r} \partial_r^2 (r\Psi) + \frac{\vec{L}^2}{r^2} \Psi . \quad (89)$$

¹² If you want to see numbers, you can try to calculate the reduced mass for the sun-earth and the earth-moon system using $m_\odot = 1,99 \cdot 10^{30}$ kg, $m_\oplus = 5,97 \cdot 10^{24}$ kg and $m_\text{L} = 7,34 \cdot 10^{22}$ kg. If you'd like to see things a bit more atom-like you can use $m_p = 938,3$ MeV/ c^2 , $m_n = 939,6$ MeV/ c^2 and $m_e = 511$ keV/ c^2 . Of course, you might also calculate the reduced mass for the positronium which is a bound state of an electron and its anti-particle, the positron, or for muonium, which is a bound state of an anti-muon and an electron and was experimentally found in 1960 [4]. For this last calculation you'll need $m_\mu = 105,7$ MeV/ c^2 .

If we use this result in the eigenvalue problem associated to the Hamiltonian (86), *i.e.* $H\Psi = E\Psi$, and multiply it by $2m\hbar^{-2}$ in order to have nicer formulae, we find that

$$\begin{aligned} \frac{2\mu}{\hbar^2} E \Psi &= -\bar{\partial}^2 \Psi + \frac{2\mu}{\hbar^2} V(r) \Psi \\ &= -\frac{1}{r} \partial_r^2 (r\Psi) + \left[\frac{2\mu}{\hbar^2} V(r) + \frac{\vec{L}^2}{r^2} \right] \Psi. \end{aligned} \quad (90)$$

The key point of the reduction then lies in the fact that the dependency on the spherical coordinates θ and ϕ is hidden in the Casimir operator \vec{L}^2 , and we will just split

$$\Psi = r^{-1} \Phi_l(r) \mathbf{Y}_m^l(\theta, \phi) \quad \text{and use } \vec{L}^2 \mathbf{Y}_m^l = l(l+1) \mathbf{Y}_m^l. \quad (91)$$

Doing so we end up with the following Schrödinger equation for the function Φ_l

$$-\partial_r^2 \Phi_l + \frac{l(l+1)}{r^2} \Phi_l + \frac{2\mu}{\hbar^2} V(r) \Phi_l = \frac{2\mu}{\hbar^2} E \Phi_l, \quad (92)$$

where one should observe that the resulting system does not depend on the magnetic moment quantum number m , indicating that for a given l , the energy state will be $(2l+1)$ -fold degenerate; this degeneracy is due to the fact that the system is spherically symmetric. For the moment we will obviate this degeneracy.

Up to this point our discussion was really only limited by the fact that the potential only depended on the distance between the 2 bodies, implying immediately that in the relative motion system, the potential was going to be spherically symmetric. At this point then, we shall consider the case of an electron ‘circling’ a nucleus of charge Z , meaning that the potential can be written as

$$V(r) = -\frac{Z e^2}{r}. \quad (93)$$

A way to avoid errors during calculations is to deal with the simplest possible expressions, and in this case simpler expressions can be obtained by redefining $r = \lambda\rho$ and $E = E_R \mathcal{E}$ where

$$\lambda = \frac{\hbar^2}{\mu e^2} \quad \text{which is called the Bohr radius,} \quad (94)$$

and

$$E_R = \frac{\mu e^4}{2\hbar^2} \quad \text{is called the Rydberg energy.} \quad (95)$$

The Rydberg energy can also be written as $E_R = \frac{\mu c^2}{2} \alpha$, where we introduced the *fine structure constant*

$$\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}. \quad (96)$$

In terms of the new variables ρ and \mathcal{E} , we can rewrite eq. (92) as

$$\mathbf{H}_{(l)} \Phi_l \equiv \left[-\partial_\rho^2 - \frac{2Z}{\rho} + \frac{l(l+1)}{\rho^2} \right] \Phi_l = \mathcal{E} \Phi_l, \quad (97)$$

which can be thought of as being an ordinary 1-dimensional quantum mechanical system.

In order to find the spectrum of the above Hamiltonian, we shall apply the technique of factorisation of Hamiltonians outlined in sec. (2). To this end consider the prepotential

$$\mathbf{W}_l \equiv \frac{Z}{l+1} - \frac{l+1}{\rho}. \quad (98)$$

Given this prepotential, the calculation of the Hamiltonian (35) and its dual (38) is straightforward and leads to

$$\mathbf{H}_-^{(l)} = -\partial_\rho^2 - \frac{2Z}{\rho} + \frac{l(l+1)}{\rho^2} + \frac{Z^2}{(l+1)^2}, \quad (99)$$

$$\mathbf{H}_+^{(l)} = -\partial_\rho^2 - \frac{2Z}{\rho} + \frac{(l+1)(l+2)}{\rho^2} + \frac{Z^2}{(l+1)^2}, \quad (100)$$

There are two things to observe about the Hamiltonians $\mathbf{H}_\mp^{(l)}$: first of all we have the relation of $\mathbf{H}_-^{(l)}$ with \mathbf{H}_l . This relation is

$$\mathbf{H}_-^{(l)} = \mathbf{H}_l + \frac{Z^2}{(l+1)^2}, \quad (101)$$

which, as the ground-state energy of a \mathbf{H}_- -type factorised Hamiltonian is zero, implies that the groundstate energy of the Hamiltonian \mathbf{H}_l is

$$\mathcal{E}_{0,l} = -\frac{Z^2}{(l+1)^2} \quad \text{which in the original variables reads: } E_{0,l} = -\frac{Z^2}{(l+1)^2} E_R. \quad (102)$$

Clearly, the lowest value of the energy is attained for $l = 0$, which then corresponds to the true groundstate energy of the hydrogen-like atoms. For the hydrogen atom we have $Z = 1$ and $\mu = m_e = 511 \text{ keV}/c^2$, which leads to

$$E_{0,0,0} = -E_R \simeq -13,6 \text{ eV}. \quad (103)$$

The second thing to observe is the relation of the dual Hamiltonian $\mathbf{H}_+^{(l)}$ to $\mathbf{H}_-^{(l+1)}$; this relation is

$$\mathbf{H}_+^{(l)} = \mathbf{H}_-^{(l+1)} + \frac{Z^2}{(l+1)^2} - \frac{Z^2}{(l+2)^2}. \quad (104)$$

Consider for clarity's sake, first the case of $l = 0$. Then as we know the ground-state energy of the Hamiltonian $\mathbf{H}_-^{(0)}$ is $\mathcal{E}_0^{(0)} = 0$. The energy of the first excited state is $\mathcal{E}_1^{(0)}$, which we know to be equal to the energy of the same state of the dual Hamiltonian $\mathbf{H}_+^{(0)}$, whence $\mathcal{E}_1^{(0)} = \tilde{\mathcal{E}}_1^{(0)}$. The recurrency relation in eq. (104) then means that $\tilde{\mathcal{E}}_1^{(0)} = \mathcal{E}_0^{(1)} + Z^2 - \frac{Z^2}{2^2} = Z^2 - \frac{Z^2}{2^2}$, where in the last step we used the fact that the groundstate of any factorised Hamiltonian \mathbf{H}_- has zero energy. Applying the same reasoning to the second excited state we find

$$\begin{aligned} \mathcal{E}_2^{(0)} &= \tilde{\mathcal{E}}_2^{(0)} = \mathcal{E}_1^{(1)} + Z^2 - \frac{Z^2}{2^2} \\ &= \tilde{\mathcal{E}}_1^{(1)} + Z^2 - \frac{Z^2}{2^2} = \mathcal{E}_0^{(2)} + Z^2 - \frac{Z^2}{3^2} \\ &= Z^2 - \frac{Z^2}{3^2}. \end{aligned} \quad (105)$$

It is then a small step to deduce that for the k^{th} state we have

$$\mathcal{E}_k^{(0)} = Z^2 - \frac{Z^2}{(k+1)^2}. \quad (106)$$

At this point the deduction of the energy level of the Hamiltonian $H_-^{(l)}$ should pose no problem and in fact the energy of the k^{th} state is given by

$$\mathcal{E}_k^{(l)} = \frac{Z^2}{(l+1)^2} - \frac{Z^2}{(k+l+1)^2}. \quad (107)$$

The above energy levels fully deplete the discrete part of the spectrum and we can use them to write down the possible energy levels of the original system by remembering eqs. (101) and (95) and that the Hamiltonian H_l lead to an $(2l+1)$ -fold degeneracy in the full system: we see that there are energy levels given by integers $k = 0, 1, \dots, \infty$, $l = 0, 1, \dots, \infty$ and $m = -l, \dots, l$ whose energy is given by

$$E(k, l, m) = -\frac{Z^2}{(k+l+1)^2} E_R, \quad (108)$$

from which the announced $(2l+1)$ -fold degeneracy is obvious as the energies do not depend m . What is perhaps less obvious, but surely well-known, is that there are further degeneracies. Indeed, as one can see we have that $E(1, 0, 0) = E(0, 1, m)$ indicating that there are further degeneracies. The full degeneracy can be highlighted by the introduction of the so-called *principal radial quantum number* n ($n = 0, 1, \dots, \infty$) to write the energy simply as¹³

$$E_{n,l,m} = -\frac{Z^2}{(n+1)^2} E_R, \quad (109)$$

meaning that for a given n the possible pairs of integer number (k, l) have to satisfy $k+l = n$; it immediately implies that for a given n the possible angular momentum quantum numbers are $l = 0, 1, \dots, n$. The total degeneracy of the level n can then be easily calculated by observing that there is no degeneracy due to the number k , leading to an $(n+1)^2$ -fold degeneracy.¹⁴

Using the BPS equation (31) and the relations (41,42), it is a reasonably straightforward yet tedious task to calculate the explicit forms of the wavefunctions. The easiest ones are

$$\Psi_{l,l,m} = [(2l+2)!]^{-1/2} \left(\frac{2Z}{(l+1)\lambda} \right)^{l+3/2} r^l \exp\left(-\frac{Z}{(l+1)\lambda} r\right) \mathbf{Y}_m^l(\theta, \phi). \quad (110)$$

¹³ Observe that in the literature the principal radial quantum number does not start at 0, but rather at $n = 1$. Please keep this in mind when you are comparing books with the present notes.

¹⁴ One can ask oneself the following question: Since the $(2l+1)$ -fold degeneracy was due to the spherical symmetry present in the original system, what is the symmetry reason we end up with an even bigger degeneracy? The clue to finding the responsible symmetry can be found in classical mechanics. In the study of the earth-sun system, or Kepler problems in general, one finds that there exists an extra conserved current due to the so-called Laplace-Runge-Lenz vector, which renders the Kepler problems integrable. The quantum mechanical version of the Laplace-Runge-Lenz vector combines with the spherical symmetry of the hydrogen atom, mathematically this symmetry is described by a group denoted by $SO(3)$, into the bigger symmetry group $SO(4)$, which causes the above degeneracy [5].

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