

Proposition 4.3

- (i) $N \geq 0$.
 (ii) $\sigma(N) = \sigma_p(N) = \{0, 1, 2, 3, \dots\}$ and each eigenvalue has multiplicity 1.

Proof: (i) is easy: $(f, Nf) = (f, a^* a f) = (af, af) = \|af\|^2 \geq 0$.

We now prove (ii). We know from Theorem 4.2 that $\sigma(N) = \sigma_p(N)$.

Observe that $Nf = 0 \iff af = 0$: The implication $\implies$ is obvious, and the converse follows from the proof of (i). Next, consider the function $f_0(x) = \pi^{-1/4} e^{-\frac{1}{2}x^2}$:

$$af_0 = \frac{1}{\sqrt{2}} (X - iP)f_0 = \frac{1}{\sqrt{2}} \pi^{1/4} \left(x + \frac{d}{dx}\right) e^{-\frac{1}{2}x^2} = 0.$$

Then f_0 is eigenvector of N with eigenvalue 0. It follows from the theory of ODEs that f_0 is the unique solution of $f'_0 = -x f_0$ (fixing e.g. $f_0(0) = \pi^{-1/4}$), so 0 has multiplicity 1.

Next, let $f_n = c_n (a^*)^n f_0$. We have

$$\begin{aligned} Nf_n &= c_n \underbrace{N(a^*)^n f_0}_{N a^* (a^*)^{n-1} f_0} = c_n a^* (N+1) (a^*)^{n-1} f_0 \\ &= c_n (a^*)^2 (N+2) (a^*)^{n-2} f_0 \\ &= \dots = c_n (a^*)^n (N+n) f_0 \stackrel{Nf_0=0}{=} n c_n (a^*)^n f_0. \end{aligned}$$

Then f_n is eigenvector of N with eigenvalue n .

(29)

Now suppose that $Nf = \lambda f$ with $\lambda \neq 0$. Then af is a (non-zero) eigenvector of N with eigenvalue $\lambda - 1$:

$$Na f = a(N-1)f = (\lambda - 1)af,$$

and $\|af\|^2 = (f, Nf) = \lambda \|f\|^2 \neq 0$ by the proof of (i).

Consequently, if λ is an eigenvalue that is not an integer, then $\lambda - 1, \lambda - 2, \lambda - 3, \dots$ are eigenvalues. Eigenvalues cannot be negative since $N \geq 0$, so that $\sigma_p(N) = \{0, 1, 2, \dots\}$.

There remains to show that each eigenvalue has multiplicity 1. We know it for 0. If f_n and g_n are orthogonal eigenvectors with eigenvalue n , then af_n, ag_n are orthogonal eigenvectors with eigenvalues $n-1$. Then $a^* f_n, a^* g_n$ are orth. eigenvectors with eig. 0, which is impossible. Hence n has multiplicity 1.

□

Exercise 10. Show that $c_n = \frac{1}{\sqrt{n!}}$ in order that $\|f_n\| = 1$.

Hint: Write $\|f_n\|^2 = (f_0, a^n (a^*)^n f_0)$ and use $aa^* = a^*a + 1$ repeatedly.

We have proved:

Theorem 4.4. The spectrum of $H = \frac{1}{2}(-\Delta + x^2)$ is $\sigma(H) = \sigma_p(H) = \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots\}$ where each eigenvalue has multiplicity 1.

(30)

Remark: The eigenvectors are related to Hermite polynomials

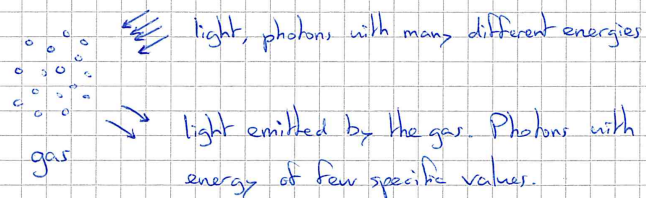
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} = e^{\frac{1}{2}x^2} \left(x - \frac{d}{dx}\right)^n e^{-\frac{1}{2}x^2}.$$

5. THE HYDROGEN ATOM

5.1 Background.

The system consists of one proton and one electron. The mass of the proton is about 1836 times larger than that of the electron, so it is essentially infinite — that is, the proton is a fixed classical particle, and the electron is a quantum particle.

Experiments of atomic emissions:



Thus elements are characterised by their spectrum. The mathematician Balmer, confident that there was mathematical beauty behind all things, looked for a formula for the

Four rays of energy of visible light of hydrogen. His formula, proposed in 1885 (he was 60, and this is his only work that is still remembered!) was extended by Rydberg. The possible energies are of the form $\frac{me^4}{2\hbar^2} \left(\frac{1}{n^2} - \frac{1}{l^2}\right)$ where $n < l$ are integers. Experiments were then conducted in order to detect further rays, and they were successful! It took a while to find an explanation.

Here is the common explanation. At rest the electron of a hydrogen atom occupies the ground state, i.e. the eigenstate of the corresponding Schrödinger operator with the lowest eigenvalue. When it receives light, the electron may absorb a photon and reach an eigenstate with higher eigenvalue. This is an unstable state and the electron eventually relaxes to an eigenstate with less energy, emitting a photon with precisely the energy difference. This photon is what is detected. We shall see that the point spectrum of the Hamiltonian for the hydrogen atom consists of all numbers of the form

$$-\frac{me^4}{2\hbar^2} \frac{1}{n^2},$$

with $n=1, 2, 3, \dots$, and m is the mass of the electron and e the charge.