

# IL027

## COMPUTING MODELLING FOR ALL.

### QUANTUM MECHANICS

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*"I think I can safely say that nobody understands quantum mechanics"* - Richard Feynman<sup>1</sup>

In this part of IL027, we're going to look at some of the rules of *Quantum Mechanics*, and use these rules as a context for writing code to solve simple quantum-mechanical modelling problems. The activities of this part of IL027 are organized as follows:

- **Lecture 1:** We will go through some of the basic ideas of quantum mechanics, including why we need quantum mechanics, and how some example quantum-mechanical systems behave.
- **Lecture 2:** This will be computer-based (*e.g.* JuliaBox), and will walk through the solution of the Schrödinger equation for simple 1-dimensional systems using the discrete variable representation (DVR).
- **Assignment:** This will build on the methods discussed in Lecture 2, and will focus on calculating properties of a particle tunnelling in a 1-dimensional double-well potential.

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### *Failures of Classical Mechanics*

By the beginning of the 20th Century, classical mechanics, as laid out by Isaac Newton from mid-17th century onwards, was the dominant scientific paradigm. Along with Maxwell's treatment of electrostatics, classical (or Newtonian) mechanics is enormously successful in describing many of the physical phenomena in the world around us.<sup>2</sup> There are two particularly important features of classical mechanics which, as we'll see later, are contrary to the ideas of quantum mechanics:

1. The current state of a system can be described by the set of positions  $\mathbf{r}$ , and momenta  $\mathbf{p}$  of all the particles.<sup>3</sup>
2. The energy of a system can change *continuously*. For example, a tennis ball could be at rest (so its kinetic energy is zero), or could be accelerated to 100 mph (where the kinetic energy is definitely not zero).

<sup>1</sup> Feynman was a giant of 20th century physics; he predicted quantum computing, invented nanotechnology, and developed quantum electrodynamics. He worked on the Manhattan project, played the bongos, witnessed the first ever detonation of a nuclear bomb while hiding in his truck, took LSD as a means of investigating consciousness while a professor at Caltech, and used the money from his Nobel prize to buy a beach house; I highly recommend reading more about this extraordinary man.

<sup>2</sup> Reminder: Newton's second law,  $F = ma$ , tells us that a force on a particle gives it an acceleration; this can be used to generate particle trajectories.

<sup>3</sup> A *system* here is just a collection of discrete objects, like tennis balls, atoms or electrons. If we have  $N$  such objects, each moving in 3-dimensions,  $\mathbf{r}$  and  $\mathbf{p}$  will both be *vectors* of length  $3N$ .

### Classical mechanics begins to fail

Early in the 20th century, a series of experimental observations emerged which classical mechanics failed to explain. Although many experiments are now known to verify the predictions of quantum mechanics, we will consider three specific examples.

#### Photoelectric effect

When ultraviolet light falls on a metal surface, it is found that electrons are emitted; the energy of the incident light is transferred to the electrons in the metal surface, which can then escape. In this experiment, two observations clearly suggest that something is amiss with classical theory:

1. Classical electromagnetic theory predicted that the kinetic energy of the ejected electrons should increase if the intensity of the light was increased. *In the experiments, the kinetic energy of the ejected electrons did not change at all when the intensity of the light was changed!*
2. Classical physics predicts that electrons should be ejected from the metal for *any* frequency of radiation, as long as the intensity is large enough. *In the experiments, it was found that electrons are only emitted if the frequency of the radiation is above some threshold frequency,  $\nu_0$ , which depends on the metal.*

Einstein solved this mystery. He proposed that the radiation exists as small packets of energy, called *photons*, each carrying an energy  $E = h\nu$ , where  $\nu$  is the frequency and  $h$  is a constant, called *Planck's constant*.<sup>4</sup> With this simple idea, Einstein was then able to explain the photoelectric effect; for example, Einstein showed that conservation-of-energy can be used to explain why there is a threshold frequency for each metal.<sup>5</sup>

The amazing conclusion from these experiments and their interpretation is that light must be considered as both a wave *and* a discrete particle; this is referred to as wave-particle duality.

#### Diffraction of electrons

Bragg discovered that X-rays could be diffracted by a crystal in 1913; when illuminated with X-rays, a crystal produces a characteristic pattern of reflected X-rays, depending strongly on both the wavelength of the radiation and the angle of incidence. Bragg reasoned that strong *diffraction peaks* are observed when X-rays are scattered from different planes of the crystal lattice such that they can interfere constructively. This Bragg condition gives rise to the well-known relation<sup>6</sup>

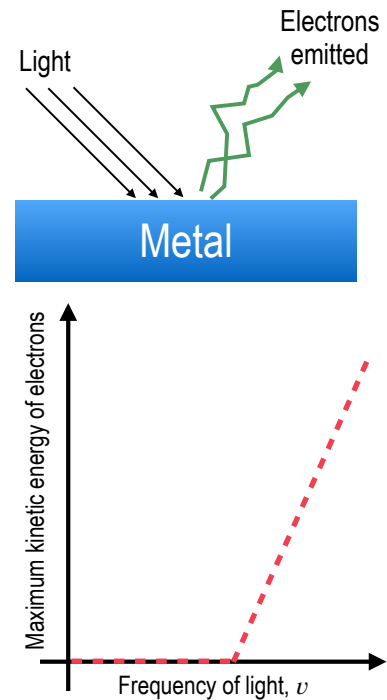


Figure 1: Observation of the photoelectric effect

<sup>4</sup>  $h = 6.626 \times 10^{-34}$  Js

<sup>5</sup> Einstein showed that the energy of the emitted electrons follows the relation  $E = h\nu - \phi$ , where  $\nu$  is the frequency of the radiation and  $\phi$  is the work function, a characteristic of the metal. The threshold frequency occurs when  $E = 0$ , such that  $h\nu = \phi$ .

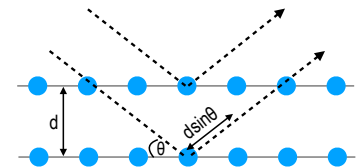


Figure 2: Bragg's law for diffraction from a crystal lattice. If the lattice spacing is  $d$  and the angle of incidence is  $\theta$ , the difference in the distance travelled by beams scattered from adjacent planes is  $2d \sin \theta$ .

<sup>6</sup>  $\lambda$  is the X-ray radiation wavelength and  $n$  is any integer.

$$n\lambda = 2d\sin\theta,$$

which tells us when we should expect constructive interference (and hence a scattered X-ray peak).<sup>7</sup>

All of the above is based on the assumption that X-rays are electromagnetic *waves*. So, imagine everybody's surprise when Thomson and Davisson demonstrated that *electrons* also form interference patterns when they are scattered by thin metal films! In other words, Thomson and Davisson's experiments demonstrated that electrons can behave like waves - at the time, this was a perplexing concept, and an observation that classical mechanics had no way of explaining (Fig. 3).

In fact, a few years before Thomson and Davisson's electron diffraction experiment, Louis de Broglie had hypothesised that electrons should also exhibit wave properties, and proposed that the *de Broglie wavelength* of a particle should be given by

$$\lambda = \frac{h}{p},$$

where  $p$  is the momentum of the particle.<sup>8</sup> The Thomson and Davisson electron diffraction experiments confirmed that electrons can indeed behave like waves (another example of wave-particle duality), and also found that the wavelength of the electrons matched de Broglie's predictions.

### Discrete atomic spectra

A third observation which couldn't be explained by classical physics was the appearance of atomic emission spectra. When subjected to high temperatures, atoms emit light with a characteristic spectrum (Fig. 4). Each type of atom emits light with a distinct set of *discrete* frequencies; in other words, we observe *line spectra*.

The appearance of these spectra defied explanation until Johannes Rydberg<sup>9</sup> work demonstrated that, for hydrogen, the frequencies of *all* of the lines in the emission spectrum were given by the simple relation

$$\tilde{\nu} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right),$$

where  $n_1$  and  $n_2$  are integers (with  $n_2 > n_1$ ) which characterise the final and initial state of the system.<sup>10</sup> Although the Rydberg formula was successful in describing the frequencies of lines in the hydrogen emission spectrum, the fact that it was controlled by two integer values seemed hard to explain. Niels Bohr provided a simple explanation of the hydrogen emission spectrum, and also derived the Rydberg formula.<sup>11</sup> To do this, Bohr assumed that the electron in hydrogen acted

<sup>7</sup> William Lawrence Bragg was just 25 years old when he was awarded the Nobel prize in Physics in 1915, along with his father William Henry Bragg.

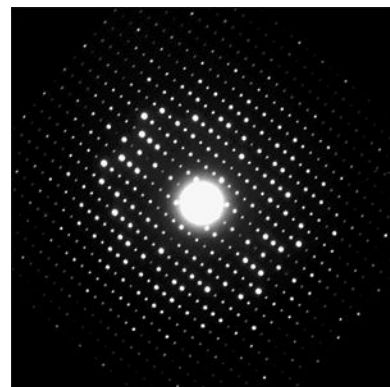


Figure 3: Typical electron diffraction pattern for an inorganic crystalline solid. The sharp peaks are scattered *electrons*, with the scattering behaviour being predicted by Bragg's law for *waves*.

<sup>8</sup>  $p = mv$ , where  $m$  is the particle mass and  $v$  is the speed (or velocity, if one is interested in the momentum vector).

<sup>9</sup> Rydberg was a Swedish physicist whose contributions to quantum theory were somewhat overlooked in his lifetime. Amazingly, he was not given a full-time professorship at a university until he was 54 years old, and would often work as an actuary to make ends meet.

<sup>10</sup>  $R_H$  is now known as the Rydberg constant with a value of  $109,677.581 \text{ cm}^{-1}$ .

<sup>11</sup> Bohr received a Nobel prize in physics in 1922 for his work on atomic structure, and would later play an important role in supporting the establishment of CERN, birthplace of the internet and home of the Large Hadron Collider.

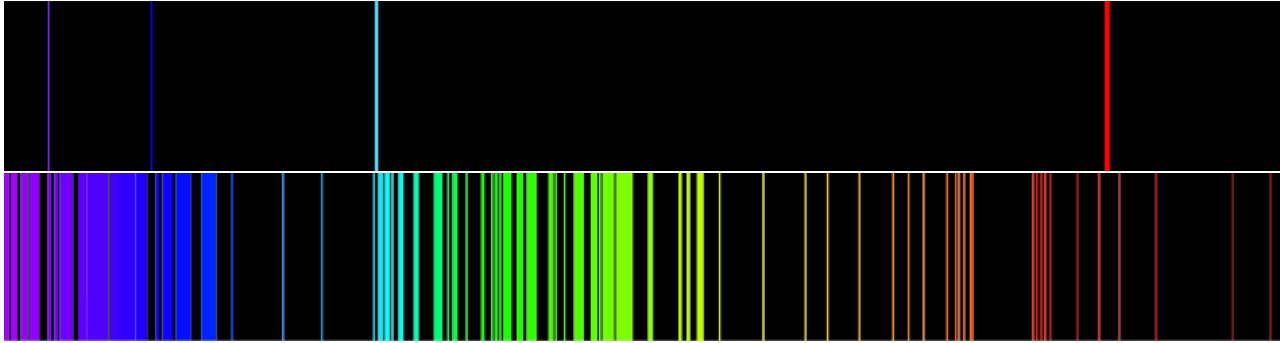


Figure 4: Atomic emission spectra of H (upper) and Fe (lower), showing sharp lines corresponding to discrete energy changes upon emission of light.

like a *wave* (again, wave-particle duality) as it orbited the proton. Assuming that the electron has a wavelength given by the de Broglie formula, Bohr postulated that the electron will exist in orbits which can accommodate the electron wavelength, such that

$$n\lambda = 2\pi r$$

where  $r$  is the radius of orbit. In this picture, it is found that the allowed radii of electron orbits are *quantized*; in other words, only certain radii are allowed, because otherwise the electron wavelength cannot be accommodated. Following this idea through, Bohr then showed that the emission spectrum of hydrogen arises from the electron “hopping” between different orbits. Because the orbits are quantized, then the energy changes allowed as the electron hops between different orbits must also be quantized, giving rise to the observed line spectrum.

Unfortunately, although Bohr’s model was capable of fully explaining the emission spectrum of hydrogen, it fails for all other atoms (even helium, with just two electrons). It also failed to describe the spectra which arise when a magnetic field is applied to the atoms. So, although the idea of quantization (or discrete energy changes) appears to be important, the simplicity of Bohr’s model did not stand up to scrutiny; further work was needed...

### *Some conclusions so far...*

We've seen three examples where classical physics fails to explain experiments. It is worth noting that:

- the above examples (as well as those considered in the questions below) are all related to microscopic (or atomic-level) phenomena; in other words, although the results of classical mechanics seem to be sufficient to explain *macroscopic* phenomena, classical predictions break down at the smaller scales associated with atoms, molecules and electrons.
- the idea of *quantization* is emerging. Notice that Einstein assumed that photons exist as *discrete* packets of energy, and the atomic spectrum of hydrogen could be described by assuming that only *discrete* energy changes are allowed; we can say that energy is *quantized* in these cases.

Overall, the conclusion early in the 20th century was that a new set of laws were required to describe the behaviour of particles at the atomic-scale, and these new rules are what we call *quantum mechanics*.

### *Quantum mechanics*

Quantum mechanics is not something that scientists have *derived* from first principles. Instead, quantum mechanics should be viewed as a set of *postulates*<sup>12</sup> which we believe to be true. All of the experiments performed to date lead us to believe that these postulates are an accurate description of the behaviour of matter at the atomic-scale; the fact that quantum mechanics cannot be “derived” from some more fundamental principles does not change the fact that it works in describing chemistry!<sup>13</sup>

In what follows, we will simply state the important postulates of quantum mechanics; later, we will see what these imply when applied to study various physical systems.

<sup>12</sup> A postulate is an idea or concept which we can assume to be true to enable us to discuss or explain something. In this case, we assume that the postulates of quantum mechanics are true, so that we can use quantum mechanics to describe chemistry.

<sup>13</sup> In fact, this is not weird at all! Remember that Newton's second law of motion,  $F = ma$ , is really just an empirical relation which explains real-world observations for macroscopic system (*i.e* if you push a light object, it accelerates faster than when you push a heavy object!)

### The postulates of quantum mechanics

**Postulate 1:** A system at time  $t$  is described by a *wavefunction*,  $\psi(\mathbf{r}, t)$ , which depends on all positions of the particles in the system.<sup>14</sup>

**Postulate 2:** The wavefunction  $\psi(\mathbf{r}, t)$  evolves according to the time-dependent Schrödinger equation. For a single particle of mass  $m$  moving in 1-dimension, this is given by<sup>15</sup>

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x)\psi(x, t). \quad (1)$$

where  $V(x)$  is the potential energy of the system. For shorthand, we usually define the Hamiltonian operator as<sup>16</sup>

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x),$$

so the time-dependent Schrödinger equation can be written

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H}\psi(x, t). \quad (2)$$

**Postulate 3:** The wavefunctions and corresponding total energies of the *allowed* states of a quantum-mechanical system are those which obey the time-independent Schrödinger equation:

$$\hat{H}\psi(x) = E\psi(x). \quad (3)$$

If a wavefunction  $\psi(x)$  obeys this equation, it corresponds to an allowed quantum state of the system!

**Important:** Any quantum-mechanical system will support several allowed quantum states,  $\psi_i(x)$ , each of which obeys Eq. 3, but with a different energy  $E_i$ .

Because Eq. 3 has the form of an *eigenproblem*, the solutions  $\psi(x)$  are often referred to as *eigenvectors* and the energies are referred to as *eigenvalues*.

**Postulate 4:** The probability of finding a particle at a particular position  $x$  at some time  $t$  is proportional to  $|\psi(x, t)|^2$ .

**Important:** This probabilistic behaviour is completely different from classical mechanics! In the classical world, we know exactly where a particle is (*i.e.* it has a position); in the quantum world, we only know the probability of a particle being at a particular position!

<sup>14</sup> So, for a system of one particle moving in one dimension  $x$ , we have  $\psi(x, t)$ . For a water molecule, with 3 nuclei and 10 electrons moving in 3-dimensions, the full wavefunction of the system depends on  $3 \times 13 = 39$  positions.

<sup>15</sup>  $\hbar = h/2\pi = 1.054 \times 10^{-34}$  Js. This constant, namely Planck's constant divided by  $2\pi$ , appears so frequently in quantum mechanics that it has its own symbol,  $\hbar$  (pronounced "h bar").

<sup>16</sup> This is the Hamiltonian for one particle moving in one-dimension.

**Postulate 5:** Observables can be calculated from wavefunctions as *expectation values*, given by

$$\langle A \rangle = \frac{\int \psi^*(x) \hat{A} \psi(x) dx}{\int \psi^*(x) \psi(x) dx}$$

where  $\hat{A}$  is the quantum operator for the observable of interest. For example, the position expectation value is given by:<sup>17</sup>

$$\langle x \rangle = \frac{\int \psi^*(x) x \psi(x) dx}{\int \psi^*(x) \psi(x) dx}$$

<sup>17</sup> It turns out that the position operator is just the position itself:  $\hat{A} = x$ .

As another example, the momentum operator in the  $x$ -direction is

$$p_x = -i\hbar \frac{d}{dx},$$

so the  $x$ -momentum expectation value is

$$\langle p_x \rangle = -i\hbar \frac{\int \psi^*(x) \frac{d\psi(x)}{dx} dx}{\int \psi^*(x) \psi(x) dx}$$

*What do wavefunctions look like?*

It turns out that there are really only a few simple systems for which we can *analytically* solve the time-independent Schrödinger equation (Eq. 3) to get the allowed eigenfunctions  $\psi_i$  and eigenvalues  $E_i$ . However, these simple model systems are enormously useful in helping us to interpret experiments, particularly spectroscopic experiments which tell us about vibrational and rotational motion of molecules.

Here, we'll just look at some of the features of three quantum-mechanical problems which we can solve exactly.

*A particle trapped in a box*

**System:** Particle of mass  $m$  trapped in a box between  $x = 0$  and  $x = L$ .

The potential  $V(x)$  is zero inside the box, and is infinite outside the box.

**Hamiltonian:** The Hamiltonian inside the box is:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

**Eigenstates:** The allowed wavefunctions which satisfy  $\hat{H}\psi_n(x) = E_n\psi_n(x)$  are given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$$

Here,  $n$  is a *quantum number*; the geometry of the problem means that  $n$  can only take *integer* values:

$$n = 1, 2, 3, 4, \dots$$

Figure 2 shows the particle-in-a-box eigenstates for  $n = 1 - 4$ .

**Eigenvalues:** The energies of each eigenstate  $\psi_n(x)$  are given by

$$E_n = \frac{n^2 h^2}{8mL^2}.$$

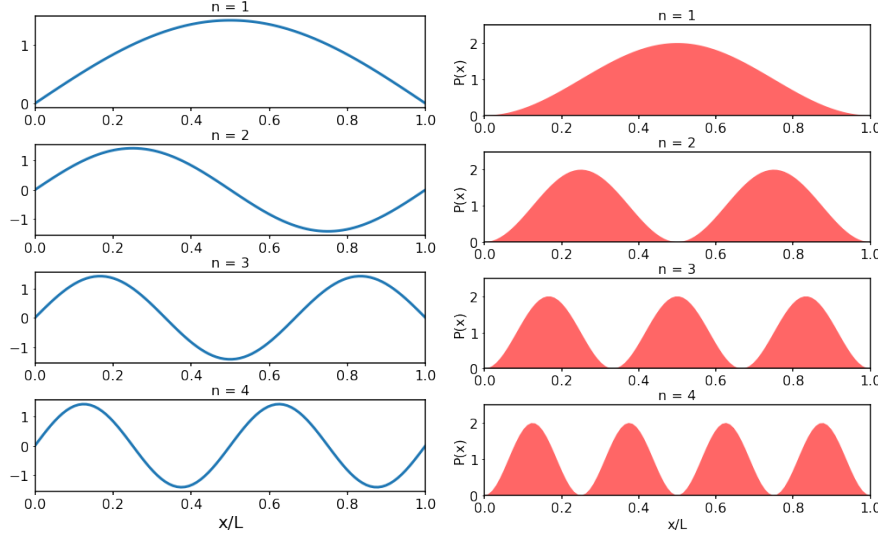


Figure 5: The left-hand figure shows the first 4 eigenstates  $\psi_n(x)$ ; the right-hand column shows the corresponding probability distributions  $|\psi_n(x)|^2$ .

### A particle in a harmonic well

**System:** Particle of mass  $m$  moving in a harmonic potential with the form  $V(x) = \frac{1}{2}kx^2$ . Here,  $k$  is the spring constant, related to the mass and natural frequency  $\omega$  by  $\omega = \sqrt{\frac{k}{m}}$ .

**Hamiltonian:** The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

**Eigenstates:** The eigenstates for the harmonic oscillator are defined by a quantum number  $n = 0, 1, 2, 3, 4, \dots$

The first 4 eigenstates are<sup>18</sup>

$$\begin{aligned} \psi_0(y) &= N_0 e^{-\frac{1}{2}y^2} \\ \psi_1(y) &= N_1 y e^{-\frac{1}{2}y^2} \\ \psi_2(y) &= N_2 (2y^2 - 1) e^{-\frac{1}{2}y^2} \\ \psi_3(y) &= N_3 (2y^3 - 3y) e^{-\frac{1}{2}y^2}. \end{aligned} \tag{4}$$

<sup>18</sup> Note that  $y = \sqrt{\frac{m\omega}{\hbar}}x$ , a change of variable which makes the resulting eigenfunction equations easier to look at.

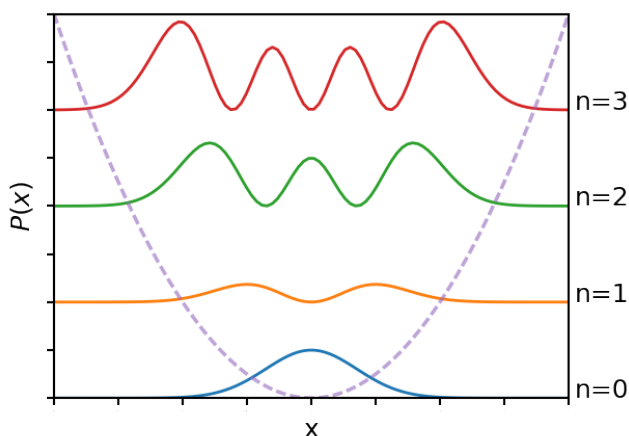


The constants  $N_{0-3}$  are just normalization constants<sup>19</sup>

Most generally, it is found that the structure of the harmonic oscillator eigenstates is

$$\psi_n(y) = N_n H_n(y) e^{-\frac{1}{2}y^2}.$$

In other words, they are products of a *Gaussian* function, multiplied by a function  $H_n(y)$  which is a *Hermite* polynomial.<sup>20</sup> Figure 6 shows the harmonic oscillator probability distributions for  $n = 0 - 3$ .



<sup>19</sup> If you're interested:  $N_0 = \frac{1}{\pi^{1/4}}$ ,  $N_1 = \frac{\sqrt{2}}{\pi^{1/4}}$ , and the other are equally obtuse numbers.

<sup>20</sup> Hermite polynomials can be looked up in tables. The first few are:

- $H_0(y) = 1$
- $H_1(y) = y$
- $H_2(y) = y^2 - 1$
- $H_3(y) = y^3 - 3y$
- $H_4(y) = y^4 - 6y^2 + 3$
- $H_5(y) = y^5 - 10y^3 + 15y$
- $H_6(y) = y^6 - 15y^4 + 45y^2 - 15$
- $H_7(y) = y^7 - 21y^5 + 105y^3 - 105y$
- $H_8(y) = y^8 - 28y^6 + 210y^4 - 420y^2 + 105$

Figure 6: Probability distributions  $|\psi_n(x)|^2$  for the first 4 harmonic oscillator eigenstates.

**Eigenvalues:** The energies of each eigenstate  $\psi_n(y)$  are given by

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

Note that this implies that the lowest energy level  $E_0 = \frac{1}{2}\hbar\omega$ ; this is called the *zero-point energy*. It is an interesting quirk of nature that this ZPE can never be removed from a chemical bond! Even at a temperature of zero Kelvin, chemical bonds still have some vibrational energy! <sup>21</sup>

<sup>21</sup> It turns out that ZPE plays subtle yet important effects in the properties of water; without ZPE, the melting point of water would be about 4 K higher, and much more of the Earth's surface would be covered in ice!

### A hydrogen atom

**System:** Hydrogen is the simplest atom; it has one proton and one electron, and these interact via Coulomb's law.

**Hamiltonian:** The Hamiltonian for the combined electron and proton nucleus is: <sup>22</sup>

$$\hat{H} = -\frac{\hbar^2}{2m_N}\nabla_N^2 - \frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{e^2}{4\pi\epsilon_0 r}.$$

The first term is the (3-d) kinetic energy of the nucleus, the second term is the (3-dimensional) kinetic energy of the electron and the final term is the Coulombic attraction between the nucleus (charge  $+e$ ) and electron (charge  $-e$ ).

It is more straightforward to assume that the nucleus is fixed in position at the origin, and then to solve the remaining Schrödinger equation for the motion of the electron in the Coulomb field of the nucleus.

**Eigenstates:** The solutions of the hydrogen atom Schrödinger equation for the electron are called *atomic orbitals*; if you know anything about chemistry, you'll recognise these, but you might not have previously appreciated where they came from.

We won't give explicit forms here, but the hydrogen atom eigenfunctions are usually written in spherical coordinates  $(r, \theta, \phi)$  and always take the form

$$\psi_{nlm_l}(r, \theta, \phi) = R_{nl}(r)Y_{lm_l}(\theta, \phi).$$

The radial solution  $R_{nl}(r)$  tells us how the wavefunction changes as we move away from the nucleus,<sup>23</sup> whereas the angular solution  $Y_{lm_l}(\theta, \phi)$  tells us about the angular distribution of the electron around the nucleus. Note that the quantum state of the electron is defined by 3 quantum numbers,  $n$ ,  $l$  and  $m_l$ .

Isosurfaces for some of these solutions are shown in Fig. 7.

**Eigenvalues:** The energy eigenvalues for the hydrogen atom only depend on the quantum number  $n$ . They are given by:

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2}.$$

It turns out that the form of this equation is exactly the same as that determined by Rydberg when trying to explain the discrete atomic emission spectrum of hydrogen!

<sup>22</sup> The electron and the proton have kinetic energy in each of the 3 directions of Cartesian space; we use the short-hand  $\nabla^2 = \frac{\partial^2}{\partial^2 x} + \frac{\partial^2}{\partial^2 y} + \frac{\partial^2}{\partial^2 z}$

<sup>23</sup> In general,  $R_{nl}(r)$  is a Laguerre polynomial multiplied by an exponential function.

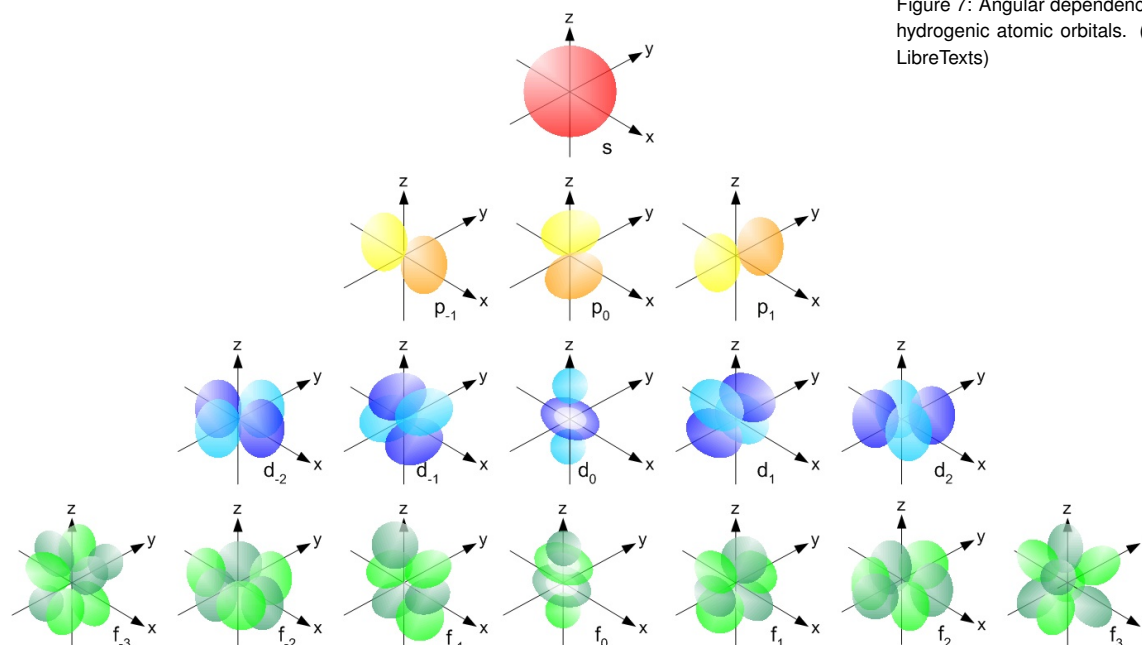


Figure 7: Angular dependence of the first few hydrogenic atomic orbitals. (see: Chemistry LibreTexts)

### Beyond simple models

Solving the Schrödinger equation for the hydrogen atom is tough; solving it analytically for anything with more electrons is impossible!

This is a shame, because we know that the Schrödinger equation tells us about the allowed states of a quantum system; for atoms and molecules with more than one electron (*e.g.* anything interesting), the solutions of the Schrödinger equation would tell us about the energy levels of the molecule, and the distribution of electrons. These things would in turn help us to understand the chemical properties of these molecules.

Fortunately, there are ways forward. In particular, the *variational principle* tells us how to find good *approximate* solutions to the Schrödinger equation for many-electron atoms and molecules. Furthermore, employing the concept of *linear Combination of Atomic Orbitals*, we can use the atomic orbitals predicted for hydrogen to try to understand how these combine to make *molecular orbitals* describing the distribution of electrons in molecules.

Based on such ideas, computational methods like Hartree-Fock theory, Density Functional Theory and coupled-cluster methods can be used to calculate the energies and other electronic properties of atoms and molecules<sup>24</sup>. If you'd like to know more, there are a wide range of (free) codes which can perform these calculations, including ORCA

<sup>24</sup> Including proteins, given enough computational power!

and  $\psi - 4$ . Have a go yourself!

### Summary

In this introductory lecture, we explored the experimental results of the early 20th century which led scientists such as Einstein, Bohr, Schrödinger and Heisenberg to formulate a new set of rules describing the behaviour of microscopic systems. These new rules, which became known as quantum mechanics, fully describe the behaviour of atoms, molecules and electrons. In fact, Paul Dirac once famously said:

*“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”<sup>25</sup>*

So, quantum mechanics is all we need to describe chemistry, although the application of the rules of quantum mechanics to understand chemistry is very challenging....

<sup>25</sup> Born in Bristol, and awarded the Nobel prize with Schrödinger in 1933, Paul Dirac later held the Lucasian Chair in mathematics at Cambridge, the same position held by Isaac Newton and Stephen Hawking. He was a notoriously difficult man; Einstein once wrote “I have trouble with Dirac. This balancing on the dizzying path between genius and madness is awful.”