Chapter 3: atom – a community of electrons

background reading

Al-Khalili, J. (2008), *Quantum*, Phoenix, London.

Atkins, P. (1995), *The Periodic Kingdom: a journey into the land of the chemical elements*, Weidenfeld and Nicholson, London.

von Baeyer, H. (1993), *Taming the Atom: the emergence of the visible microworld*, Viking, London.

Ball, P. (2018), *Beyond Weird*, The Bodley Head, London.

Czerski, H. (2017), *Storm in a Teacup: the physics of everyday life*, Black Swan, Transworld publishers, London.

Emsley, J. (2001), *Nature's Building Blocks*, Oxford University Press.

Feynman, R. (1990), *QED: the strange theory of light and matter*, Penguin, London, chapter 3.

Feynman, R. (1998), *Six Easy pieces: the fundamentals of physics explained*, Penguin, London, chapters 1 and 6.

Orzel, C. (2021), *How to Teach Quantum Physics to your Dog*, Oneworld, London.

Rae, A. (2005), *Quantum Physics: a beginner's guide*, Oneworld Publications, Oxford.

notes

Constructive comments are welcome.

the atom – a conflict of inclinations

"**In the Standard Model**", Randall 2006:156, Lincoln 2012:170, and Feynman 1990:100.

"***photons transmit, or mediate, a force***", Randall 2006:156. It's not easy to explain how the exchange of photons can lead to an attraction or a repulsion. A scenario that is commonly used to explain is to imagine two people on ice skates or in small boats (so there is no friction acting), throwing an object to each other, back and forth. If the object is a heavy ball, this will result in a mutual repulsion and they will drift further apart. This is fairly straightforward, but explaining attraction is more tricky. In this case, we imagine that the two people face away from each other, and each throws a boomerang or a frisbee that loops around to be caught by the other person. This results in a force that draws them together (Randall 2006:156, Lincoln 2012:172).

See also the note to section 1.2.2.

"***exchanging photons***", Feynman 1990:figure 65 shows a proton and an electron continually exchanging photons, very like the exchange of gluons between quarks in protons and electrons.

the electron – both particle and wave

3.1 quantum mechanical tunnelling

3.1.1 principles

"**A quantum entity**", Feynman 1965:7-8, Hey 2003:chapter 5, Rae 2005:50, Tipler 1999:1153, Atkins 2006:286 and Gamow 2006:158.

"**The classical particle**", the wavefunction can't change abruptly, but must be continuous at the edges of the barrier (Atkins 2006:286).

"**This is known as quantum mechanical tunnelling**"; radioactive alpha-decay and nuclear fission are only explicable in terms of quantum tunnelling (Hey 2003:87, Williams 2001:chapter 6), and we make use of quantum tunnelling in the scanning tunnelling microscope (Hey 2003:76, von Baeyer 1993:chapters 4 and 5).

Figure 3.1 is based on Feynman 1965:figure 7-5 and Rae 2005:figure 2.6, using freeze-frames from the simulation, "Quantum tunnelling and wave Packets (1.12)", available at https://phet.colorado.edu/en/simulations/quantum-tunneling. The red waveforms are taken from the simulation, and the barrier and text have been added. This simulation is by PhET Interactive simulations, University of Colorado Boulder, licensed under CC-BY-4.0 (https://phet.colorado.edu).

3.1.2 quantum tunnelling by photons

Figure 3.2 is based on Tipler 1999:figure 15-21. The glass prisms are from a pair of WWII binoculars, pressed together in a vice, with two pieces of wood to act as cushions between the glass and the metal jaws of the vice, and a piece of white paper behind to show the laser light spots. A helium-neon laser in a spirit level provides the light photons, with a wavelength of ~633 nm. The exact critical angle for total internal reflection at the glass/air interface depends on the type of glass used, but is about 42°. The laser was shone from the lower left in each picture. The laser light photons cannot be seen, and so the red lines have been added to show their paths through the prisms. It is important to get the mating prism faces very clean, for even the slightest bit of grease or dust will prevent photon tunnelling. You can then easily enable tunnelling with only light pressure from the vice, and you can apply and relax the pressure, and see the light spot on the right-hand screen appear and disappear.

The situation shown in figure 3.2 is known as "frustrated TIR", or FTIR, and is the optical analogue of quantum tunnelling (Feynman 1964:33-12, Gamow 2006:156, Hey 2003:75, Coon 1966, Zhu 1986, Vörös 2008 and https://en.wikipedia.org/wiki/Evanescent_field). When light is totally internally reflected inside a glass-air interface there is a standing wave that extends a short distance out into the air. This standing wave does not carry any energy, and is called an evanescent wave. If there is a small enough gap, then this evanescent wave can tunnel through it, and the light photons can escape from the glass, and we have FTIR (Feynman 1964:33-12). Coon has observed and counted individual photons that tunnelled through an air gap up to 8 wavelengths wide between a pair of glass prisms (Coon 1966).

We have made very many uses of this seemingly innocuous little feature of the physical world: see https://en.wikipedia.org/wiki/Total_internal_reflection.

The situation in figure 3.2 is a standard physics demonstration: see https://sciencedemonstrations.fas.harvard.edu/presentations/frustrated-total-internal-reflection.

3.1.3 quantum tunnelling by electrons – flash memory

"**However, we all use**", this section on flash memory is based on Bez 2003, Pavan 1997 and Crippa 2008.

Figure 3.3 is greatly simplified, and is based on Bez 2003:figure 7 and Pavan 1997:figures 2 and 13, and also see the Wikipedia article at https://en.wikipedia.org/wiki/Flash_memory. A flash memory cell is a floating-gate metal oxide semiconductor (MOS) transistor. There are two main types of logic gate used in flash memory – NOR gates and NAND gates, and the flash memory cell shown in figure 3.2 is a NOR gate. The quantum tunnelling processes are called hot electron injection for storing electrons on the floating gate, and thereby writing a data bit, and

Fowler-Nordheim tunnelling for removing those electrons, thereby erasing the memory. The voltage differences for writing and erasing are rather complicated, and so I have omitted them from the main text, but Bez and Pavan give typical values.

"**Electrons do occasionally escape**", Bez 2003 states that the normal complement of electrons on the floating gate for logic state *0* is 1,000−10,000, and that 80% of these have to be retained at the end of 10 years. I have taken a middle figure of 6,000, so over 10 years no more than 20% of 6,000 = 1,200 can be lost, which is about 10 per month.

3.2 diffraction

3.2.1 the uncertainty principle and diffraction

Figure 3.4 is based on the standard depiction of single gap diffraction, as shown in Feynman 1965:figure 2-2, Rae 1996:figure 4.1 and Rae 2004:figure 1.5, and see also Herbert 1987, chapter 4.

3.2.2 photon diffraction

Figure 3.5: these and subsequent pictures of laser photon diffraction and interference patterns were taken with a Samsung Galaxy S7 smartphone, SM-G930F. The camera resolution was set at 3.7 MPx (2560 x 1440 pixels), white balance was set at auto, the ISO was set to 400, and exposure times were in the range 1/15 – 1/250 s. The laser source was a Bosch PLL 1P laser spirit level, incorporating a helium-neon laser with a wavelength of about 633 nm, and a power of < 1 mW.

The laser spot diameter was about 3 mm at all distances up to 3 m. The distances from the screen to the single gap was 2.90 m, and to the laser was 3.00 m. The gaps in figure 3.5 were made by a pair of razor blade edges, with the gap widths set by engineering feeler gauges, and so the gap widths are approximate. A steel ruler with a millimetre scale was fixed to the screen just below the diffraction patterns, and included in photographs of them. It was then easy to use the images to measure the width of diffraction patterns to an accuracy of about 1−2 mm. The four laser light patterns shown in the figure are cropped from the original images.

"**The laser used to produce**", if we take the laser power as 1 mW (it is given as < 1 mW), then it will produce photons with a total energy of 1 mJ in 1 second. Each photon has an energy given by:

$E = hf = hc/\lambda = 6.6 \times 10^{-34} \times 3 \times 10^{8}/633 \times 10^{-9} = 3 \times 10^{-19}$ J.

So the laser produces about $1 \times 10^{-3}/3 \times 10^{-19} \approx 3 \times 10^{15} \approx 3{,}000 \times 10^{12}$ photons each second. The laser spot diameter is about 3 mm at all distances, which is an area of ~7 mm^2, so the photon flux is ~400×10^{12}, or 400 trillion photons/mm^2/s.

The area of the 0.05 mm gap that is in the laser beam is ~0.15 mm^2, which makes the number reaching the screen to be ~60×10^{12}/s , and so the number of photons in the diffraction pattern in figure 3.5(d), photographed with a shutter speed of 1/60 s, is ~1×10^{12}, or one trillion.

"**With such a high photon flux**", Rae 2004:11.

"**Halving the gap width**", these diffraction patterns enable a semi-quantitative demonstration of the uncertainty principle, and a rough value of Planck's constant, *h*. If the gap width is *a* m, then the uncertainty in the photon's position is *a*/2. The uncertainty in the photon's momentum is *p*sin*θ*, where *p* is the momentum, and 2*θ* (theta) radians is the angle subtended by the spread out diffraction pattern. The *de Broglie* equation (section 3.4.3) tells us that the photon momentum is *h*/*λ* (see equation 3.2), and this means that the uncertainty in momentum is *h*sin*θ*/*λ*.

So, we can say that the product of the two uncertainties is

$\Delta x\, \Delta p = a/2 \times (h\sin\theta/\lambda)$

For the 0.2 mm gap, with a diffraction pattern width of 16 mm,

$\Delta x\, \Delta p = 0.1 \times 10^{-3} \times (6.6 \times 10^{-34} \times (8 \times 10^{-3}/2.9)/633 \times 10^{-9}) \approx 3 \times 10^{-34}\ \text{Js} \approx h/2$

This calculation is taken from Rae 1996:78, and gives a value of ~*h*/2, rather than *h*/4π.

Figure 3.5 shows that halving the gap width roughly doubles the spread of the diffraction pattern, so calculations with the 0.1 and 0.05 mm gap widths will give the same result.

3.3 photon interference

3.3.1 interference patterns

from one gap to two gaps

Figure 3.6 is based on Feynman 1965:chapter 1, Penrose 2004:figure 21.4 and Bach 2013:figure 2, and also see laser interference patterns in Hey 2003:figure 1.6.

The double gap used for figure 3.6 was made by positioning a pair of razor blades on either side of a single strand of copper conductor wire, diameter of 0.53 ±0.01 mm, measured with a micrometer. The copper wire had been stretched, giving it a small plastic extension, to make it perfectly straight. The gaps on either side of the wire, G_1 and G_2, were initially set at about 0.05 mm wide, using a feeler gauge. This gave only an approximate setting, and the gaps were then made very nearly equal by adjusting the razor blades to make the single gap diffraction patterns of roughly equal width (55 mm for G_1 and 52 mm for G_2). The masks, M_1 and M_2, were another pair of razor blades that could each be positioned over one of the gaps, so that single diffraction patterns could be obtained from each gap. Both masks were removed to get the double-gap interference pattern. The distance from the screen to the double gap was 2.90 m, and 3.00 m to the laser source. Distances on the screen were measured as for the diffraction patterns in figure 3.5.

The laser photon flux was ~400×10^{12}, or 400 trillion photons/mm^2/s (see note to figure 3.5). The area of each gap was ~0.15 mm^2, and the shutter speed was 1/20 s, so the number of photons making each single-gap pattern was ~3×10^{12}, and the number making the double-gap pattern was ~6×10^{12}, or about six trillion.

3.3.2 the principle of the two-gap interference pattern

Figure 3.7 is based on Cox 1996:figure 1.13, Tipler 1999:section 35-3, Hey 2003:figure 1.11, and Carroll 2019:77. The photon interference patterns in (d) and (e) are screenshots from the PhET quantum wave simulation, "Quantum Wave Interference (1.11)", available at https://phet.colorado.edu/en/simulations/quantum-wave-interference. This simulation is by PhET Interactive simulations, University of Colorado Boulder, licensed under CC-BY-4.0 (https://phet.colorado.edu).

The screenshots are from the photon simulation, but the simulations of the behaviour of electrons, neutrons and helium atoms are available, and the patterns are identical.

3.3.3 random single events build up a deterministic interference pattern

"***a piece of the overall interference pattern***", Lindley 1996:55.

"***the dualism between determinism***", "***strictly determined***", and "***objectively random***", are all from Arndt 2009:388.

what is not forbidden will happen

"***if a process is not strictly forbidden, then it must occur***", Freedman 2002:673.

3.3.4 yes, but which gap did the photon actually go through?

"***interference between two different photons***" and "***interferes only with itself***", Dirac 1981:9.

"**So, we can say**", this is why I've avoided the commonly used phrase, "particle-wave", because it includes the word "particle", and so we think in terms of a "thing" which must go through one gap or the other, and this ties our thinking into knots (Cox 2011:24, Al-Khalili 2008:20). Even to say that it behaves sometimes as a particle and sometimes as a wave is misleading: a quantum entity behaves as a particle *and* as a wave *all* of the time.

A variety of careful and ingenious experiments have shown that any attempt to find out if the quantum entity went through one or the other gap results in the interference pattern disappearing and reverting to the single-gap diffraction pattern (Al-Khalili 2008:20, Ball 2018:71, Feynman 1965:1-1).

The two-gap interference pattern is commonly seen as a perfect demonstration of the self-contradictory behaviour of a "particle-wave" (see discussions by Al-Khalili 2008:chapter 1, Penrose 2004:504, Feynman 1965:chapter 1, Ball 2018:65., Cox 2011:20 and 27).

3.4 matter waves

"**Surely a particle of "solid matter"**", Louis de Broglie argued that there should be a symmetry between light and matter, so if light waves can behave like particles, then particles should be able to behave like waves (Orzel 2021:32).

3.4.1 the de Broglie wave equation

"**The de Broglie wave equation**", Tipler 1999:516, Penrose 2004:500, Orzel 2021:32.

Louis de Broglie (1939:166) noted that at the start of the 20th century physics was divided into two camps: (1) the physics of matter, based on the concepts of corpuscles (particles) that obeyed the classical laws of Newtonian mechanics, and (2) the physics of radiation, based on the concepts of undulating waves propagating in a continuous medium. These two systems of physics "*could not remain alien to each other: an amalgamation had to be effected*".

The energy of a quantum entity manifests itself in its mass and in its vibration, so it has both a particle and a wave nature, at the same time, and all the time. If we bring together the concepts of the energy intrinsic in mass, and the energy intrinsic in vibration, then we have:

$$\underbrace{mc^2}_{\text{mass}} = E = \underbrace{hf}_{\text{vibration}}$$

where m (kg) is the mass, c (m/s) is the speed of light, E (J) is the energy, h (Js) is Planck's constant, and f (Hz) is the frequency.

This is how de Broglie derived his equation (de Broglie 1939:171). Alternatively, the de Broglie equation can also be derived from the Schrödinger equation (Atkins 2006:255). Brian Cox shows how the Schrödinger and de Broglie equations are consistent (Cox 1996:25).

"**This equation is named**", the best way to pronounce the name de Broglie is to say something like "de Broy" (Orzel 2021:32).

"***corpuscles and waves***", de Broglie 1939:169.

"**In de Broglie's simple equation**", de Broglie speculated upon the significance of the value of Planck's constant (1939:54): "*If the constant h were infinitely small, the light quanta having the value hf would also be infinitely small, and their number in a ray of given energy would be infinitely great. Everything would then occur as though the rays had a continuous structure, and were of … purely undulatory character … On the other hand, the material corpuscles could in such a case easily be proved to obey exactly the classical laws of the dynamics of the material point, and there would be no need whatever to introduce waves into the Theory of Matter. … But if, on the other hand, Planck's constant were infinitely great then light quanta would be enormous, and their existence would leap to the eye – if I may so put it – of the least attentive physicist. In this case, however, the material corpuscles would never again follow the laws of classical dynamics, and as soon as they began to be investigated at all it would be perceived that a wave must be introduced to predict their motion*".

If Planck's constant, h, has any finite value, then there will be a link between the particle and wave aspects of matter, and the link is only broken if h has a value of zero. Paul Dirac noted that classical mechanics "*is the form which quantum mechanics takes when one makes Planck's constant* $\hbar$ [h-bar, equal to $h/2\pi$] *tend to zero*" (Dirac 2001:1).

Why is the value of h so small? The answer perhaps lies more in the realms of biology than physics. In order to make "*a functioning, intelligent, unit-using creature, you need to put together a lot of atoms. … In the end, the reason that Planck's constant is so small is that we are so big and heavy and slow*" (Susskind 2014:104).

"***a kind of connecting link***", de Broglie 1939:53.

de Broglie wavelengths for different particles

Figure 3.8 compares the *de Broglie* wavelengths for a selection of particles, as has been done by Al-Khalili 2008:49, who compared the *de Broglie* wavelengths of a cow, a C_{60} molecule, and an electron, all moving at a speed of a few m/s. The *de Broglie* wavelengths in figure 3.8 have been calculated using the formula $h = mv\lambda_{dB}$, where h is Planck's constant, with a value of about 6.6×10^{-34} Js. The values shown in the figure are rounded from the calculated values.

In **part (a)** the electron is taken as dimensionless, and $\lambda_{dB} \approx 0.73$ mm, or 730,000 nm.

In **part (b)** the carbon atom has a diameter of ~0.15 nm, and a mass of $\sim 2 \times 10^{-26}$ kg (Atkins 2002:A24), and $\lambda_{dB} \approx 33$ nm.

Human hair diameters can vary between about 20−180 µm, and the average is usually taken as ~75 µm, see https://en.wikipedia.org/wiki/Hair%27s_breadth.

The C_{60} molecule shown in **part (c)** is buckminsterfullerene, CSID:110185, http://www.chemspider.com/Chemical-Structure.110185.html (accessed 08:40, Jun 26, 2023), the diameter is from Nairz 2003:note 33, and $\lambda_{dB} \approx 0.55$ nm.

The particle of soot shown in **part (d)** is the same as in figure 1.4, and $\lambda_{dB} \approx 10^{-9}$ nm.

Things move very fast on the micro-scale, for example, air molecules move at an average speed of around 500 m/s. I've given all the particles the same, very slow velocity so as to show how the *de Broglie* wavelength becomes negligible for something as small as a soot particle. However, the situation shown in figure 1.4 excludes collisions from air molecules, which would set the electron and carbon atom and C_{60} molecule moving at high speeds, and make the soot particle jiggle.

Physics textbooks often give example calculations of the *de Broglie* wavelengths of objects such as particles of dust or baseballs – see, for example, Tipler 1999:516.

3.4.2 quantum interference of electrons

"***the sum of many independent events***", Merli 1976.

"***archetypal example of wave-particle duality***", Rae 1999.

Figure 3.9(a) is from Bach 2013:figure 3. The full paper is available at https://iopscience.iop.org/article/10.1088/1367-2630/15/3/033018/meta, and figure 3 is reproduced here under the terms of the Creative Commons Attribution 3.0 licence (https://creativecommons.org/licenses/by/3.0/). The figure is unchanged except for the addition of the white box in (a) to show the five central bright fringes, and the white circles to mark the electrons in (b) and (c). The small white boxes at the top left of each frame are labels in the original figure.

Electrons were accelerated by a 600 V potential difference, and had a speed of about 15 million m/s, and hence a *de Broglie* wavelength of about 0.05 nanometres. The double slits were each 62 nm wide, and separated by 272 nm, the five central fringes in (a) spanned about 220 µm.

Single electron interference has been demonstrated by Merli 1976, Tonomura 1989 and more recently by Bach 2013, using the classic double slit. Electron self-interference has been much described and discussed, for example, Feynman 1965:chapter 1, Hey 2003:12, Herbert 1987:chapter 4, and Physics World, September 1 2002, available at http://physicsworld.com/cws/article/print/2002/sep/01/the-double-slit-experiment. The video of the build-up of electron self-interference patterns is available at http://www.hitachi.com/rd/portal/research/em/doubleslit.html and also http://physicsworld.com/cws/article/news/2013/mar/14/feynmans-double-slit-experiment-gets-a-makeover.

The image in **figure 3.9(b)** is figure 7 in "Quantum interference experiments with large molecules", by Olaf Nairz, Markus Arndt, and Anton Zeilinger, American Journal of Physics, 2003, volume 71, p. 319−325 (Nairz 2003), and is reproduced here with the permission of the American Association of Physics Teachers.

There is an accompanying erratum note, which states that the molecular velocity was actually 136 m/s.

The molecule count does not go down to zero for two major reasons: because (1) the molecules interact with the porous barrier (a diffraction grating), and (2) the molecules have a small spread of velocities, and therefore a spread of *de Broglie* wavelengths, and so there cannot be complete cancelling out where the path difference is (n+½) wavelengths.

The C_{60} molecules producing the interference pattern in part (b) had a speed of ~136 m/s, which is 136 times faster than the C_{60} molecule shown in figure 3.8, so we would expect the wavelength to be about 136 times smaller, about 0.004 nm.

We check this by using the relation, $h = mv\lambda$, to calculate each molecule's *de Broglie* wavelength as follows …

$\lambda = h/mv = 6.6 \times 10^{-34} / 1.2 \times 10^{-24} \times 136 = 4 \times 10^{-12}$ = 0.004 nm. This is about 250 times smaller than the C_{60} molecule diameter.

The interference pattern is built up by single C_{60} molecules negotiating their way through the interferometer, but, remarkably, we can calculate the spacing of peaks by treating each molecule as if it was a classical wave rolling through the porous barrier and on to the screen. In this case the relationship is $S/D = \lambda/d$, where S is the spacing of peaks in the interference pattern, D is the distance from the diffraction grating to the detector, λ is the wavelength and d is the regular spacing of the gaps in the barrier, with all distances in metres.

We can calculate the spacing of the peaks in the interference pattern as follows …

$S = \lambda D/d = 4 \times 10^{-12} \times 1.2/100 \times 10^{-9} = 48 \times 10^{-6}$ = 48 µm ≈ 0.05 mm, and this is the spacing shown in Nairz 2003:figure 7.

The image in **figure 3.9(c)** is figure 3 in Juffmann 2009, which is "Wave and particle in molecular interference lithography", by T. Juffmann, S. Truppe, P. Geyer, A. Major, S. Deachapunya, H. Ulbricht, and M. Arndt, Physical Review Letters, volume 103, 263601, 2009, © 2009 by the American Physical Society.

The upper image shows individual C_{60} molecules captured on a silicon surface, and imaged in a scanning tunnelling microscope. The molecular density on the screen was 1,166 molecules/µm^2, and the area shown is about 1.3 x 1.5 ≈ 2 µm^2, so I've estimated the number of C_{60} molecules in the pattern as ~2,000.

3.4.3 quantum interference of molecules

"***particle-nature***", Juffmann 2009:caption to fig. 3.

all matter "particles" travel as waves

"**It's found that neutrons, atoms and molecules**", "*All molecular experiments to date have realized single-particle interference, where partial wave functions of one and the same particle interfere and all molecules are prepared in similar – but not necessarily identical – states to add to the same fringe pattern*" (Juffmann 2013:086406).

Interference is usually described and explained in terms of continuous waves, such as water waves and classical light waves (for example, Tipler 1999:sections 16.1, 35.4 and 35.5). Because material "particles" such as electrons, atoms and molecules travel with an associated wavelength set by the *de Broglie* equation, quantum interference is conveniently described in terms of classical wave optics. So, the stream of individual molecules is described as a "*molecular beam*" (Juffmann 2013:5), and is often depicted as a continuous wave, with secondary diffracted wavelets, passing through the interferometer, for example, Hornberger 2003:figure 1 and Hackermüller 2004:figure 1.

Exploring the wave nature of matter is simple in principle, but extremely challenging in practice, and a variety of elaborate experimental arrangements have been devised, which have been reviewed by Arndt 2005, Cronin 2009, Hornberger 2012, and Juffmann 2013.

"***unambiguous signature of a wave***", is from Rae 1999:653.

"**For example, all the textbook experiments**", Gähler 1991. The neutron flux was so low, that on average one neutron passed through the interferometer every two seconds. Neutrons were produced by the fission of uranium nuclei, so while one neutron was passing through the interferometer, the next neutron was still confined in a uranium nucleus.

yes, but which way did the molecule go?

"***completely holistic entities***", and "***describing (or being) just a single particle***", Penrose 2004:512.

"***there is something real about the wave function***", Carroll 2019:79.

"**It's perhaps more helpful**", the simple fact seems to be that one molecule enters the apparatus, and somehow dissociates to travel by two or more paths to appear as one molecule again at the screen. But this is to think of the C_{60} molecule as a particle, a lump of matter. Perhaps we should not ask where the molecule went, but instead focus on what is continuous here, which is the wavefunction.

It may be helpful to think of the biological domain, where we also have examples of transformations and continuity. For example, in its life cycle a butterfly takes the form of an egg, then a caterpillar, then a pupa and finally adult imago (Campbell 2008:689, and see also https://en.wikipedia.org/wiki/Metamorphosis). The physical form undergoes enormous changes, so extreme that it's challenging to see these as the same organism, but underlying the changing physical form is the continuity of the organism's DNA. In the biological case, the DNA connects the changes in the biological entity's physical nature; in the quantum interference case the wavefunction connects the localised and delocalised states of the quantum entity, as it passes through the gaps in the barrier.

“***question is what you believe happens***”, Hossenfelder 2020:136.

from quantum to classical behaviour

“**The de Broglie equation can be derived**”, Atkins 2006:255.

“**Everyday objects don’t behave like C_{60} molecules**”, these examples are perhaps fanciful, but Gamow has discussed how everyday objects, such as billiard balls and gazelles, show quantum mechanical behaviour if the value of Planck’s constant is made very much larger. In these circumstances bullets spread out when they emerge from a rifle barrel (Gamow 1993:chapters 7 and 8).

“***quantum physics is a universal theory***”, Arndt 2005.

“**So, everyday objects**”, there appear to be two main explanations of the non-quantum behaviour of macroscopic objects (Hornberger 2012).

In the text I’ve given the simpler **kinematic** explanation, whereby “*the de Broglie wavelength of macroscopic objects is just way too small for us to have hope to ever resolve it*”. The other is the **decoherence** explanation, which “*points to the fact that quantum observations are usually made on isolated systems”*, and considers the way a quantum entity interacts with its environment while it is in the interferometer (both quotes from Juffmann 2013, section 5.5.4).

There are two ways that a quantum entity that is passing through a porous barrier can interact and become entangled with its environment: (1) by colliding with gas molecules, and (2) by emitting photons. Both of these result in decoherence and the loss of the object’s interference pattern (see reviews by Cronin 2009, Hornberger 2003 and Hornberger 2012 on decoherence by collisions, and Hackermüller 2004 on decoherence by photon emission).

The heart of the decoherence approach “*argues that quantum systems can never be totally isolated from the larger environment and that Schrödinger’s equation must be applied not only to the quantum system but also to the coupled quantum environment. In real life, the ‘coherence’ of a quantum state – the delicate phase relations between the different parts of a quantum superposition – is rapidly affected by interactions with the rest of the world outside the quantum system*” (Hey 2003:177). Through molecular collisions and photon emission the quantum states of a C_{60} molecule and the surrounding molecules become entangled and correlated, thereby in principle providing information on the C_{60} molecule’s location (Hornberger 2012:165). This leads to the localisation of the C_{60} molecule, and the loss of its wave behaviour.

The only way an object can retain its quantum mechanical behaviour, and not lose its coherence, is for it to be isolated from its environment, so that its matter-wave can propagate freely and unperturbed through the interferometer system. Just as the interference pattern is the signature of wave behaviour, its disappearance is the “*signature of decoherence*” (Arndt 2005).

We usually think of quantum descriptions for small matter systems, and classical descriptions for large systems. But Wojciech Zurek sees the difference as being between “*a system that is closed and a system that is open. A completely closed system – one that is interacting with nothing – is represented by the pristine symmetry of the wave function, with every possible state and every possible combination of states in superposition, interfering with one another*” (Johnson 1996:165, based on interviews with Zurek – see his note on p.341). But these superpositions are extremely unstable, and survive only in a closed system. When the system interacts with its environment, such as occurs in an act of measurement, the multiple superpositions are lost, and the system becomes classical. Thus, “*measurement is simply the correlation of two systems, which go away from the encounter with a record of each other*” (Johnson 1996:166).

Erich Joos has given a helpful summary of the decoherence approach (Joos 2006). He points out that we see macroscopic objects by the light they scatter, so they can never be isolated from their environment (Joos 2006:58). After scattering, the light contains information about the object’s position, simply because the state of the environment depends on the object’s position, and it follows that “*there can be no Schrödinger equation for macro-objects*” (Joos 2006:59).

So, the “*properties of the ‘ordinary’ objects of our experience – precisely those that we call macroscopic – are now seen not to be inherent in those objects. Instead, they emerge from, or are* ***created*** *by, irreversible interactions with the environment. … For example, objects appear localized in* ***space****, since these interactions typically depend on* ***position****.*” (Joos 2006:71). Thus, “*classical properties can be seen to emerge from the quantum world* ***only after*** *decoherence has properly been taken into account.*” (Joos 2006:71).

The overall message of decoherence is that “*we do not need classical notions as the starting point for physics. Instead, these emerge through the dynamical process of decoherence from the quantum substrate.*” (Joos 2006:77).

“***undetectably small***”, Atkins 2006:252.

3.5 progressive waves and standing waves

3.5.1 one-dimensional waves in strings

standing waves

See Tipler 1999:chapter 16 on progressive and standing waves.

Figure 3.10 is based on Tipler 1999:figures 15-17, and 16-1 to 16-4.

See HyperPhysics on standing waves at http://hyperphysics.phy-astr.gsu.edu/hbase/Waves/standw.html, and animations of standing waves at https://www.acs.psu.edu/drussell/Demos/superposition/superposition.html .

3.5.2 one-dimensional standing waves in guitar strings

“**Musical instruments are basically devices**”, Tipler 1999:488 and see for example, Joe Wolfe at https://newt.phys.unsw.edu.au/jw/strings.html.

The standing waves shown in **figure 3.11** were plotted in EXCEL, and then inserted in the figure, and the nodes matched up almost exactly with the frets.

Hey 2003:figure 3.7 shows photographs of the first four standing waves in a string. Dan Russell gives animations of standing waves in a fixed string at https://www.acs.psu.edu/drussell/Demos/string/Fixed.html.

“***confined to a limited space are quantized***”, von Baeyer 1993:46.

“**A guitar string can vibrate**“, Dan Russell states that a plucked string will vibrate at many of its natural standing wave frequencies at the same time. Tipler 1999:501 states that in general “*a vibrating system does not vibrate in a single harmonic mode but in a mixture of the allowed harmonics*”.

resonance

“**If you apply a regular push**”, for a summary of the physics of resonance, see Tipler 1999:section 14-5.

one-dimensional standing waves in bathrooms

“**Standing sound waves**“, Dan Russell gives animations of linear standing waves in a room at https://www.acs.psu.edu/drussell/Demos/RoomModes/driving.html.

3.5.3 two-dimensional standing waves in drum skins

Figure 3.12 shows a series of screenshots, taken from Dan Russell's animations of the modes of vibration of a two-dimensional membrane, available at https://www.acs.psu.edu/drussell/Demos/MembraneCircle/Circle.html, and I am grateful for his permission to make use of his work. Professor Russell has provided animations of a wide range of acoustic and vibration phenomena, available at https://www.acs.psu.edu/drussell/demos.html.

For standing wave patterns on other 2−D surfaces, see for example, Tipler 1999:496 (a metal bell), and Hey 2003:58 (a violin and a kettledrum).

To some extent, the vibrations of a circular elastic membrane can be regarded as the two-dimensional analogue of the vibrations of a one-dimensional string. For a discussion of the differences see https://www.acs.psu.edu/drussell/Demos/Membrane-vs-String/Membrane-vs-String.html.

3.6 electron orbitals around a proton

3.6.1 a trapped electron

"***negatively charged electrons***", Mark Leach, in his Chemogenesis Web Book, at https://www.meta-synthesis.com/webbook/34_qn/qn_to_pt.html.

3.6.2 electron orbitals – three-dimensional electron standing waves

"***Atoms contain electrons***", and "***the wave function forms standing waves***", Rae 2005:43 and 42. The quantum mechanical description of an electron in an atom often starts by confining the electron in an imaginary box (see for example, Tipler 1999:chapters 17 and 36, Rae 2005:43 and Atkins 2006:chapter 9). The electron's wavefunction becomes quantized in the same way that the vibrations in a guitar string are quantized.

"***waves that are confined***" and "***music is made possible***", von Baeyer 1993:46.

Figures 3.13−3.15 are based on diagrams in Keeler 2008:sections 2.1 – 2.4 and Atkins 2006:sections 10.1 and 10.2.

To give a visual depiction of the wavefunctions "*it is usual to represent them as standing waves*" (Atkins 2006:333). The depictions of the electron standing waves are based on plots of the radial wave functions of the different hydrogen atomic orbitals, given in Atkins 2006:figure 10.4, and in Keeler 2008:sections 2.2−2.3. The latter figures are available online at http://fdslive.oup.com/www.oup.com/orc/resources/chemistry/keeler2e/student/weblinks/chapter02/hydrogen/weblink2_2.htm.

The electron standing waves shown here were made by reflecting the plots of the radial wave functions in both axes, to make an approximate 2−D representation of a 3−D standing wave. This is the qualitative, visual equivalent of making linear combinations of the wavefunctions, which give "*real standing waves*" (Atkins 2006:333−334). The shapes of the orbitals, the "iso-surfaces", are taken from the same web-page. The standing waves are shaded red and blue, to show a snapshot of one phase in the cycle, to match the orbital shown. The standing waves are shown as a cross-section in the *yz* plane, so you are looking along the *x*-axis. The cross-sections of the 2*s* and 3*s* orbitals are based on http://www.chemtube3d.com/orbitals-s.htm.

The depiction of the orbitals as clouds of electron charge is based on Atkins 2006:figure 10.10 and Tipler 1999:figure 37-9. The square of the wave function gives the probability of "finding the electron" at any location in the orbital, and this gives a measure of the electron charge density (Atkins 2006:331, Tipler 1999:1181). To keep things as simple as possible, I am staying with a qualitative treatment of the wave function: the electron charge density depends on the amplitude of the standing wave, which is itself taken directly from the plot of the wave function.

Figures 3.13−3.15 give no indication of the relative sizes of the different orbitals. The 2*s* and 2*p* orbitals are about the same size, and about five times bigger than the 1*s* orbital. The 3*s*, 3*p* and 3*d* orbitals are of comparable size and about twelve times the size of the 1*s* orbital (Atkins 2006:figure 10.12). The *p* orbitals are shown here with the correct shape, but they are often shown incorrectly, with an elongated shape (Keeler 2008:50).

Figures 3.13−3.15 show the places where the wavefunction is zero as planar nodes and spherical nodes, and I've named them as nodes to be consistent with the 1−D and 2−D standing waves that we've seen earlier. In the literature they are often called "nodal planes", and "radial nodes".

Atomic orbitals can only be fully described and understood through the mathematical wave function – see for example, Keeler 2008:chapter 2, Atkins 2006:chapters 9 and 10, and Tipler 1999:chapter 37. I have attempted to give a qualitative description of atomic orbitals through a description of standing waves in one, two and three dimensions – see for example, Hey 2003:54 and Mark Leach at https://www.meta-synthesis.com/webbook/34_qn/qn_to_pt.html, and the Open University Physics module 10.3, at http://www.physics.brocku.ca/PPLATO/h-flap/phys10_3.html. This, I hope, gives the reader a "feel" for the shapes of atomic orbitals, and some appreciation of the rationale underlying *s*, *p* and *d* orbitals. This is enough to make sense of the periodic table and the fundamentals of the rôle of molecular orbitals in chemical bonding.

the quantum mechanical description of the atom

This section is based on Keeler 2008:chapters 2 and 16, Atkins 2006:chapter 10, Tipler 1999:sections 37-3 and 37-4, and the Open University Physics module 10.3, at http://www.physics.brocku.ca/PPLATO/h-flap/phys10_3.html.

The behaviour of an electron in an atom is described by the Schrödinger wave equation for electrons confined in a volume of three-dimensional space around the nucleus. The Schrödinger equation "*constitutes the principal mathematical tool for describing the atom. It is only a mild exaggeration to say that theoretical atomic physics is the study of solutions to the Schrödinger equation*" (von Baeyer 1993:45).

The solutions of the Schrödinger equation give electron wave functions, from which the atomic orbitals are derived. For an electron, the wave function is a mathematical function of the electron's position in relation to the nucleus, as given by the three-dimensional coordinates *x*, *y* and *z*. At any point in 3−D space the wave function has a numerical value, which can be positive or negative, or zero.

The square of the wave function is a measure of the probability of "finding the electron" in a particular location around the nucleus, which is known as the electron density. Because the square of any number, positive or negative, must be positive, there can be no negative probabilities, and the electron density must be zero or positive. Another way to view this is to consider the orbital as being filled by a "cloud" of electron charge, with the density of the charge cloud corresponding to the square of the wave function.

The atomic orbitals that electrons can form are specified by four quantum numbers: the principal quantum number (n), the orbital angular momentum quantum number (l), the magnetic quantum number (m_l) and the spin quantum number (m_s). These quantum numbers obey the following rules …

1) The principal quantum number, n, has integer values in the series 1, 2, 3 … .
2) The orbital angular momentum quantum number, l, has integer values from 0 to $n-1$.
3) The magnetic quantum number, m_l, has integer values from $-l$ to $+l$.
4) The spin quantum number, m_s, can be either +½, often called "spin up", or –½, called "spin down".

A "hydrogenic atom" is an atom with only one electron, and can be described by the first three quantum numbers. We will go on later to look at poly-electron atoms, which are the elements of the periodic table. The spin quantum number becomes relevant in poly-electron atoms, in which there can be more than one electron in an orbital.

Each electron orbital in a hydrogenic atom has a unique set of values of the first three quantum numbers, n, l and m_l, and these specify the energy and three-dimensional shape of the orbital.

The energy of an orbital in a hydrogenic atom depends only on the value of the principal quantum number, n, and it is common to group orbitals with the same value of n into shells. Shells are often referred to by capital letters, so the series of four shells for which n has the values 1 to 4 are known as the *K*, *L*, *M*, and *N* shells.

Within a given shell, orbitals with different values of l form a series of sub-shells, which are also referred to by lower-case letters, and the series of four sub-shells for which l has the values 0 to 3 are known as the *s*, *p*, *d* and *f* sub-shells.

The principal quantum number, n, decides the number of possible values of l and of m_l. For example, if $n = 3$, then there can be three values of l (0, 1 and 2), and five values of m_l (−2, −1, 0, +1 and +2). So in general, for any value of n there are n possible values of l, from zero up to n–1, and ($2n$−1) possible values of m_l (n−1 negative values, n−1 positive values, and zero).

For $n = 1$, there is only one *s* sub-shell, with $l = 0$, containing one orbital, with $m_l = 0$, and this is known as the 1*s* orbital.

For $n = 2$, there are two sub-shells, an *s* sub-shell with one orbital (as for $n = 1$), and a *p* sub-shell ($l = 1$), containing three orbitals ($m_l = -1, 0, +1$), so there are one 2*s* and three 2*p* orbitals, making a total of four.

For $n = 3$, there are three sub-shells, an *s* sub-shell with one orbital (as for $n = 1$), a *p* sub-shell with three orbitals (as for $n = 2$), and a *d* sub-shell ($l = 2$), with five orbitals ($m_l = -2, -1, 0, +1, +2$), making a total of nine orbitals, one 3*s*, three 3*p* and five 3*d* orbitals.

There are yet more shells than this, with values of n up to 7. Generally, the number of orbitals in an electron shell with principal quantum number n is n^2.

The numbers of the different types of nodes in hydrogenic orbitals follows a set of simple rules (Keeler 2008:62):

1) the total number of internal planar and spherical nodes is (n–1)

2) the total number of planar nodes is l

3) the number of spherical nodes is (n–1–l)

This last rule simply follows from the first two, and is equivalent to saying that the number of spherical nodes is the total number of nodes minus the number of planar nodes.

relating the standing wave harmonics to quantum numbers

The standard quantum mechanical description of atomic orbitals is not appropriate to the readers I am writing for, and to be honest, it is beyond me, too. What I think that you, the reader, need to know is that an atom comprises a number of orbitals that are at a series of energy levels, have particular shapes, and are filled in a particular sequence. With this, you can understand how the periodic table of the elements emerges (in this chapter), and the basis for chemical bonds between atoms in molecules (in the next).

Fundamentally, atomic orbitals are three-dimensional electron standing waves. Accordingly, I have described standing waves in one and two dimensions, in which a physical medium is undergoing periodic displacement, and used these to prepare the reader for atomic orbitals, in which the wave function has no simple physical meaning.

Wave functions are usually expressed in spherical polar coordinates, using the angle θ (theta) to the *z*-axis, and the angle ϕ (phi) to the *x*-axis, rather than the cartesian coordinates, *x*, *y* and *z* (for conversion of polar to cartesian coordinates see Tipler 1999:1176). With spherical coordinates, the quantum number associated with the distance from the nucleus, *r*, is *n*; the quantum number associated with θ is the orbital angular momentum quantum number, *l*; and the quantum number associated with ϕ is the magnetic quantum number m_l (Tipler 1999:1177).

Each wave function can now be expressed in terms of a radial part, which depends on the quantum numbers n and l, and an angular part, which depends on the quantum numbers l and m_l. Usually the wave functions are shown as the radial part plotted against two axes, in only one quadrant, with only positive values of the two coordinates. Sometimes two wave function plots are put "back-to-back" to show the orbital across the full width of the atom (for example, Keeler 2008:chapter 2).

In figures 3.13−3.15, I have taken the plot of the orbital's wave function, extended the axes to include negative values, and reflected the wave function in both axes, to make a "standing wave" in all four quadrants, that can be related to the one- and two-dimensional standing waves seen earlier. The shapes of the atomic orbitals, and their number and types of internal nodes can be related to these standing waves.

The total number of nodes in the 3−D electron standing waves, including the imprecise boundary node, is the same as the principal quantum number, *n*, and this matches rule 1, given above. All standing waves have at least one boundary node, and a possible number of internal nodes, that can be spherical and centred on the nucleus, or planar and passing through the nucleus. The nodes that I call spherical, because that is their complete shape, are called radial nodes in the quantum mechanical description, because they are at a constant distance from the nucleus. Planar nodes are sometimes called angular nodes, because they are at a constant angle to one of the three axes (Keeler 2008:48).

The number of planar nodes that pass through the nucleus is the same as the orbital angular momentum quantum number, *l*, that decides the shape of the orbital, and this matches rule 2, given above. When $l = 0$, then the orbital is spherical, and the most probable location at which the electron may be found is at the nucleus itself. All orbitals with $l > 0$ have zero amplitude at the nucleus, and consequently zero probability of finding the electron there.

The *s*-type orbitals ($l = 0$) have no planar nodes, the *p*-type orbitals ($l = 1$) have one planar node, the *d*-type orbitals ($l = 2$) have two, and the *f*-type orbitals ($l = 3$) have three planar nodes. So, as the value of *l* increases from 1 (*p*-type) to 2 (*d*-type) to 3 (*f*-type) the electron charge is more and more excluded from the vicinity of the nucleus (Atkins 1995:118).

Each of the four types of orbitals can incorporate a number of spherical nodes, which leaves their overall shape unchanged, and "moves" them up to the next shell. So, for example, the three 2*p* orbitals with an extra spherical node become three 3*p* orbitals, with the same overall shape, but with each orbital lobe sub-divided by the new spherical node. We know that a 3*p* orbital has one boundary node and one planar node, so its number of spherical (radial) nodes must be 3–1–1 = 1, which matches rule 3, given above.

It is easy to see that there are three *p*-type orbitals, each lying along one of the three axes. However, it is not easy to see how there come to be five *d*-type orbitals, in one of which the planar nodes have come together to make a double cone. I have tried to relate this in a simple visual way to the other four *d*-type orbitals, in which there are two planar nodes at right angles to each other.

There are a number of websites available for viewing atomic orbitals:

Jonathan Gutow, at https://cms.gutow.uwosh.edu/gutow/Orbitals/Cl/Cl_AOs.shtml

Mark Winter’s orbital viewer, “Orbitron”, at https://winter.group.shef.ac.uk/orbitron/

Mark Leach, has a gallery of Orbitron atomic orbitals, at https://www.meta-synthesis.com/webbook/35_pt/pt_database.php?PT_id=261.

David Manthey’s Orbital Viewer, at https://www.orbitals.com/orb/ov.htm.

Nick Greeves, of the University of Liverpool, at http://www.chemtube3d.com/orbitals-s.htm.

James Keeler and Peter Wothers, provide resource material at http://fdslive.oup.com/www.oup.com/orc/resources/chemistry/keeler2e/student/weblinks/chapter02/hydrogen/weblink2_2.htm.

the single 1s orbital

“**Because the standing w**ave”, it is usual to set this boundary to contain a certain proportion of the electron charge, commonly 90%.

“***the electron should not be thought***”, Rae 2005:59.

“**We can imagine**”, Atkins 2006:331.

“***the cloud is densest***”, Atkins 1995:109.

“***useful to think of the electron***”, Tipler 1999:1181.

“***if we actually look for the electron***”, Rae 2005:61. The density of the electron “cloud” is commonly interpreted as a depiction of where it is likely for the electron to be found (Atkins 1995:110). Mathematically, the probability of finding the electron at any particular location in its orbital is given by the square of the wave function (Atkins 1995:110, Atkins 2006:256, Keeler 2008:37, Rae 2005:59). I am keeping to a qualitative, visual description of electron orbitals.

the 2s and 2p orbitals

the 3s, 3p and 3d orbitals

reviewing orbitals

3.6.3 *the hydrogen atom*

“**The hydrogen atom**”, the hydrogen atom is described by Atkins 2006:320, Atkins 2002:23, Feynman 1965:chapter 19, Keeler 2008:44, Rae 1996:52, Rae 2005:56, and Tipler 1999:1178.

“**In the hydrogen atom all the sub-shells**”, wave functions which are different but have the same energy are described as degenerate, so the 3*s*, 3*p* and 3*d* are degenerate orbitals. In atoms with more than one electron the orbitals are not degenerate (Keeler 2008:46).

“***the electron has less energy***”, Feynman 1965:2-6.

Figure 3.16: the thumbnail images of the hydrogen atomic orbitals are those used in Keeler 2008:chapter 2, and have been taken from their on-line resource materials at http://fdslive.oup.com/www.oup.com/orc/resources/chemistry/keeler2e/student/weblinks/chapter02/hydrogen/weblink2_2.htm.

The diameter of the *n* = 1 shell is taken as twice the Bohr radius, equal to 2 x 53 = 106 pm (Atkins 2006:324), and compared to the *n* = 1 shell, the *n* = 2 shell is about 5 times bigger, and the *n* = 3 shell is about 12 times bigger (Atkins 2006:figure 10.12).

atoms are indestructible by everyday energies

“**It takes an energy of 6–8 million eV**”, Williams 2001:83.

“**In general, events involving electrons**”, Weinberg 1993:61, Heyde 1998:figure 1.3. It seems that Isaac Newton understood the hierarchy of energies: “*the smallest particles of matter may cohere by the strongest attractions, and compose bigger particles of weaker virtue; and many of these may cohere and compose bigger particles whose virtue is still weaker; and so on for divers successions, until the progression end in the biggest particles on which the operations in chemistry and the colours of natural bodies, depend, and which, by adhering, compose bodies of sensible magnitude*” (Brewster 1855).

“**It is only stars**”, Bertulani 2007, section 12.4.

3.7 *electron communities – building up the periodic table*

“**We now have 82 electron communities**”, in this section I am going to build up the periodic table of the stable elements, using only atomic numbers, which will be in **bold**. This will reveal the underlying electronic pattern more clearly, and we will not have the distraction of the names of the elements. I am ignoring isotopes here, because they have identical chemical properties, though their physical properties can differ slightly, because of their different atomic masses.

3.7.1 *the first ten atoms*

“**An electron in an orbital**”, Keeler 2008:64.

“**This is the only way that two electrons**”, paired electrons have a combined spin angular momentum of zero, because the spin of one electron is cancelled by the spin of the other (Atkins 2006:337).

Figure 3.17: the thumbnail icons of the hydrogen atomic orbitals are the same as figure 3.16.

the Pauli exclusion principle

“**This is known as the Pauli exclusion principle**”; and another way to state this is: “*no two electrons in an atom can have the same set of four quantum numbers*” (Atkins 2002:36).

“***an extraordinarily deep principle***”, Atkins 1995:116. The Pauli exclusion principle is a special case of the more general Pauli principle, which distinguishes between fermions and bosons (Atkins 2006:338, Feynman 1965:chapter 4).

planar nodes

“**Figure 3.16 shows all orbitals**”, for explanations of charge screening, penetration and planar nodes, see Atkins 1995:chapter 10, Atkins 2006:section 10.4, and Keeler 2008:section 2.6.2.

three key principles

“**The first three atoms reveal**“, the first principle is known as the *aufbau* or “building-up” principle, and the second is the Pauli exclusion principle.

“**However, the 2*p* orbitals**“, this is an example of Hund’s rule, which states that an atom adopts a configuration with the greatest number of unpaired electrons (Atkins 2006:341). Keeler 2008:83 point out that the common explanation that the electrons go into different orbitals to stay as far apart as possible is incorrect.

consequences of the exclusion principle

"**This is a hydrogen molecule**", Rae 2005:figure 3.1.

"**Figure 3.18 shows us how**", strictly speaking, an atom is a discrete electron community around a nucleus. Once an atom shares one or more electrons with another atom, then it is no longer an atom, and instead, it is a nucleus in a larger community of nuclei and electrons, which may be a molecule or a crystal. This might sound pedantic, but it helps us focus on the community of electrons, which is the key principle at this level in the hierarchy. In the next level molecules are called communities of atoms for simplicity, but in fact they are larger communities of electrons.

"***a stubborn insistence***", Carroll 2019:34.

"***So now we understand***", Feynman 1965:2-6.

"***responsible for the stability of matter***", Feynman 1965:4−13.

"***the key to the structure of complex atoms***", Atkins 2006:337.

Figure 3.18 is based on Feynman 1965, figures 4-11 to 4-13. This diagram just introduces the concept of a shared electron orbital encompassing two nuclei, and so the orbitals in (a) and (b) are just shown as partially overlapping, and are not drawn the correct shape; that will come in the next chapter.

3.7.2 orbital energy levels in atoms

Figure 3.19 is based on Atkins 2002:figure 1.35, Han 1990:figures 4-5 and 4-6, and on a diagram by Jim Clark, at https://www.chemguide.co.uk/atoms/properties/atomorbs.html#top. Orbitals fill in the order of the sum (*n* + *l*), sometimes known as Madelung's rule, and the inset box is based on a diagram by Mark Leach at https://www.meta-synthesis.com/webbook/35_pt/pt_database.php?PT_id=228.

The sequence shown in figure 3.19 shows the electron configurations of neutral atoms, each one with its full complement of electrons. So, we see that once the 4*s* orbital is full, with atoms **19** and **20**, then the 3*d* orbital starts filling, from atoms **21−30**.

However, this is the order for complete neutral atoms, and is not the same order in which orbitals may be filled in an individual atom. For explanations of this, see Atkins 2006:342, Jim Clark at https://www.chemguide.co.uk/atoms/properties/3d4sproblem.html, and Eric Scerri at http://ericscerri.blogspot.com/2012/06/trouble-with-using-aufbau-to-find.html.

3.7.3 the complete periodic table

"**We're now ready to understand** ", we now see a hydrogen atom as the first element in the periodic table, in which one atom stands for all, because all hydrogen atoms are identical. But why should this be so?

John Barrow has observed that "*elementary particles come in populations of universally identical particles*. … *We do not know why particles are identical in this way*" (Barrow 1992:197). Going further, even if our world comprises populations of identical elementary particles, these could not come together to make larger systems unless their energy is quantised in some way. "*In a Newtonian world, all physical quantities, like energy and spin, can take on any values whatsoever. … Hence, if one were to form a 'Newtonian hydrogen atom' by setting an electron in circular orbit around a single proton then the electron could move in a closed orbit of any radius because it could possess any orbital speed. As a result, every pair of electrons and protons that came together would be different. The electrons would find themselves in some randomly different orbit. The chemical properties of each of the atoms would be different and their sizes would be different. … There could not exist a well-defined element called hydrogen with universal properties, even if there existed universal populations of identical electrons and protons. Quantum mechanics shows us why there are identical collective structures. The quantization of energy allows it to come only in discrete packets, and so when an electron and a proton come together there is a single state for them to reside in. … This universal state is what we call the hydrogen atom. … Thus the quantization of energy lies at the root of the repeatability of structure in the physical world and the high fidelity of all identical phenomena in the atomic world*" (Barrow 1992:197).

"**The orbitals are filled**", Feynman 1965:19-15 discusses the build-up of the periodic table in terms of electron orbitals.

Figure 3.20 broadly follows the general arrangement of the periodic table that is found in chemistry texts and authoritative web-sites, such as WebElements, at https://www.webelements.com/periodic_table_image.html.

The way the modern arrangement is derived is explained at https://www.meta-synthesis.com/webbook/35_pt/pt_database.php?PT_id=14., and this page gives access to the thousands of versions of the periodic table that have been made.

The positions of hydrogen (atom **1**) is different in different versions of the periodic table (see, for example, Atkins 1995:90). Hydrogen can be in group ***I*** because has one electron in an *s* orbital, or it can go in group ***VII*** because it is one electron short of a full shell. Helium (atom **2**) is very commonly put on the right, above atom **10**, because it has a full electron shell, but it can also go in group ***II*** because it has a full *s* orbital. In figure 3.20 I have put both atoms together in groups ***I*** and ***II***, along with the other *s*-block elements.

I have used the traditional group numbers, from ***I*** to ***VIII***, because they give the numbers of electrons in the *s* and *p* orbitals in the outer shell, and because this numbering "*captures more directly the rhythms of chemistry*" (Atkins 1995:93).

The pattern in the *d*-block is broadly that the *d* orbitals are being filled, one shell behind the *s* orbitals. But the *d* and *s* orbitals are so close in energy that the sequence of orbital filling is not straightforward (see for example Atkins 2002:39).

trends and patterns in the periodic table

"**With just a handful of concepts**", this is a re-wording of Atkins 1995:122: "*There are few views in the kingdom more awesome than the one we have just seen. … Now, with an astonishing meagreness of concepts – atomic orbitals, the exclusion principle, and the consequences of penetration and shielding – we have arrived at the kingdom's rationalization*".

3.8 electron transitions between energy levels – spectra

3.8.1 energy transitions in the hydrogen atom – the hydrogen spectrum

"**But the excited state is not stable**", the excited electron typically stays at the higher energy level for about 10 ns (10^{-8} s) before spontaneously dropping back to a lower level (Tipler 1999:1030, Han 1990:97).

"**The total energy of the two emitted photons**", this is the Ritz combination principle, whereby the photon frequency for a single multi-level transition equals the sum of the photon frequencies of a series of intermediate energy level transitions (Atkins 2006:321 and see also Feynman 1963:38-7).

Figure 3.21 is based on Hey 2003:figure 4.14 and on Tipler 1999:figure 33-3(c) and (d), which show resonance absorption and fluorescence.

Photon energies in Joules can be calculated using the formula $E = hc/\lambda$, and converted to eV by dividing by 1.6 x 10^{-19}, which is the size of the electron charge in Coulombs. So a photon at the red end of the visible spectrum has a wavelength of about 700 nm, and an energy of 1.8 eV, while a photon at the violet end has a wavelength of about 400 nm and an energy of about 3.1 eV. Beyond this, lies the ultra-violet, with photon energies up to 100 eV or more.

Figure 3.21 illustrates the principles of the emission spectrum of hydrogen, and in fact of any atom or molecule (Hey 2003:63, Tipler 1999:1170 and Atkins 2002:20).

3.8.2 a continuous spectrum from an incandescent lamp

"**Atoms are excited**", Tipler 1999:1030.

"**The closely spaced tracks**", a standard music CD has tracks spaced about 1,600 nm apart, a distance comparable with the wavelengths of visible light. Consequently, a CD can act as a diffraction grating, and spread out light into a spectrum (Tipler 1999:1130, Feynman 1990:chapter 2). The pitch, the spacing between adjacent tracks, on a standard compact disc, is 0.0016 mm, or 1,600 nm, giving about 600 tracks/mm – https://en.wikipedia.org/wiki/Compact_disc.

Figure 3.22 was taken with a Canon PowerShot A640, set at f/5 and 1/160 sec.

3.8.3 the mercury spectrum

The spectrum in **figure 3.23** is from an IKEA 5W model K205 CFL, photographed with a Samsung SM-G970U1 smartphone, set at ISO 50, F1.5, and a shutter speed of 1/750 seconds.

An excited mercury atom emits photons in the UV region of the spectrum, and these are unwanted because they are harmful, as well as being outside our visible range. So the inside of the CFL is coated with a phosphor, a material that absorbs the high energy UV photons and emits lower energy photons in the visible spectrum – rather like breaking down a £1 coin into small change. Different phosphors are blended to give an overall "white" light with different degrees of warmth. The spectrum shown in figure 3.23 is the pure mercury spectrum of yellow/orange, green and deep blue, with the addition of red from the phosphor.

The main mercury spectral lines are given at https://en.wikipedia.org/wiki/Mercury-vapor_lamp. A nice mercury/phosphor spectrum is available at https://commons.wikimedia.org/wiki/File:Leuchtstoff_spektrum.jpg.

If you shine the light from a CFL through a narrow slit, then you can produce a spectrum showing all the colours, major and minor, as in the beautiful image shown here.

3.8.4 the sodium spectrum

"**In a sodium street light**", atoms in the vapour state are well separated, and collisions are rare compared with atoms in a solid. If we can excite atoms in a vapour, then we can see the electrons making transitions between discrete levels.

The sodium spectrum shown in **figure 3.24(a)** was taken from the sodium street light conveniently sited across the road from the house where we lived in 2008, and photographed with a tripod-mounted Canon PowerShot A640, at f3.5 and 2 sec exposure.

Figure 3.24(b) shows a simple Grotrian diagram of energy transitions for sodium, based on Clugston 2000:43 and Cox 1996:figure 5.1. This shows only the three most prominent lines, but other transitions occur (Cox 1996:figure 5.1).

A Grotrian diagram summarises the energy levels and the permitted electron transitions between them (Atkins 2006:335, and http://hyperphysics.phy-astr.gsu.edu/hbase/Atomic/grotrian.html. Only some of the possible transitions are permitted, decided by the spins of the electron and photon. A photon has an intrinsic spin angular momentum corresponding to $s = 1$. The change in angular momentum of the electron as it transits from one orbital to another must tally with the angular momentum carried away by the photon. So an electron in a *d* orbital ($l = 2$) cannot make a transition to an *s* orbital ($l = 0$), because the photon cannot carry away enough angular momentum. Likewise, an electron cannot make a transition from one *s* orbital to another because there is no change in angular momentum to match the angular momentum carried away by the photon (Atkins 2006:335).

3.8.5 the visible everyday world

"***active, dynamic systems***", von Baeyer 1993:xix.

3.9 review of Level 3

3.9.1 the everyday world of atoms

"***dressed with electrons***", Bertulani 2007:22.

"***If, in some cataclysm***", Feynman 1998:4.

3.9.2 the exclusion principle

"**For example, a carbon atom**", the atomic diameter is about 150 pm (Atkins 2002:appendix 2D) and the nuclear diameter is about 5 fm (Mackintosh:50, and see back to figure 2.7).

"**The exclusion principle**", Atkins 1995:116, Atkins 2006:337.

"**It's not a force**", Bertulani 2007:section 12.11.

"***moves matter at a specific place***", Davies 2006:39.

3.9.3 endless, reversible interactions

"***be dislodged from molecules***", Atkins 1992:11.

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