for the 21st Century

# Unit 6: Macroscopic Quantum Systems



© Mike Matthews, JILA.

#### Unit Overview

The fundamentals of quantum mechanics that we met in Unit 5 characteristically appear on microscopic scales. Macroscopic quantum systems in which liquids, or electric currents, flow without friction or resistance have been known since the early part of the previous century: these are the superfluids and superconductors of traditional condensed matter physics that are discussed in Unit 8. In this unit we focus on an entirely new state of matter only recently created in the laboratory: this is the gaseous macroscopic quantum mechanical system known as a Bose-Einstein Condensate, or BEC. These quantum gases show the full panoply of quantum wave behavior as the individual particles of Unit 5, but now on a size scale visible to the naked eye because many millions, to many billions, of atoms occupy exactly the same quantum state, and thus form a coherent quantum whole. The quantum nature of a BEC can be directly visualized as the quantum effects are not hidden within liquids or solids as is the case with the more traditional superfluids and superconductors. Rather, they may be actually photographed, as the gas itself is a naked macroscopic quantum system. This unit starts by introducing the basic principles necessary to understand BECs, then details how the cooling and trapping introduced in Unit 5 led to the creation and subsequent manipulation of these quantum gases. Finally, we will see how atomic gases of ultra-cold fermions have evolved, in direct analogy to the Cooper paring needed to form bosonic pairs of electrons in superconductors, to molecular BECs, formed from pairs of the fermionic atoms.

#### Content for This Unit

#### Sections:

1.	Introduction	3
2.	Early Models of the Atom	10



3.	The Quantum Atom	.17
4.	Spin, Bosons, and Fermions	.21
5.	Composite Bosons and Fermions	.28
6.	Gaseous Bose-Einstein Condensates	34
7.	Phase Control and New Structures	. 39
8.	Making BECs from Fermi Gases	. 46
9.	Conclusions and a Look Ahead	.49
10.	Further Reading	. 51
	Glossary	52



# Section 1: Introduction

The quantum theory that evolved at the beginning of the 20th century is a strange creature: It assigns particulate properties to light—long thought to consist of waves—and, astonishingly, wave properties to individual fundamental particles that have definite masses. This seeming confusion between waves and particles never seems to bother us in ordinary life, where particles (such as grains of rice or baseballs) are simply particles, and what comes out of a flashlight or laser pointer can be focused or even diffracted, thereby revealing the wave-like properties we associate with light. Of course, large numbers of particles acting in collusion can create waves as a possible collective motion—on the surface of the ocean, for example. And a slinky or violin string can display wave properties, to the surprise of no one. But these are classical, not quantum, waves, a distinction we will make clear in this unit.



Figure 1: Some of the first experimental evidence for a gaseous macroscopic quantum state. Source: © Mike Matthews, JILA.

We typically view quantum mechanics as applying only to the fundamental particles or fields of Units 1 and 2, and not to the objects we find in a grocery store or in our homes. If large objects like baseballs and our dining tables don't behave like waves, why do we bother about their possible quantum nature? More practically, we can ask: If we are supposed to believe that ordinary objects consist of wave-like quantum particles, how does that quantum nature disappear as larger objects are assembled from smaller ones? Or, more interestingly: Are there macroscopic objects large enough to be visible to the naked eye that still retain their quantum wave natures? To answer these questions, we need the rules for building larger objects out of smaller ones, and the means of applying them. The rules are of a highly quantum nature; that is, they have no counterpart at all in classical physics, nor are they suggested by the behavior of the ordinary material objects around us. But in surprising ways, they lead to macroscopic quantum behavior, as well as the classical world familiar to all of us.



To interpret these rules, we need to understand two critical factors. First, particles of all types, including subatomic particles, atoms, molecules, and light quanta, fall into one of two categories: fermions and bosons. As we shall see, the two play by very different rules. Equally important, we will introduce the concept of pairing. Invoked more than a century ago to explain the creation of molecules from atoms, this idea plays a key role in converting fermions to bosons, the process that enables macroscopic quantum behavior. This unit will explore all these themes and Unit 8 will expand upon them.

### Building up atoms and molecules



#### Classical Pairing in DNA

The concept of pairing is not restricted to simple chemical bonds and the conversion of fermions to bosons. Pairs also occur at higher levels of molecule formation. In the Watson-Crick model of DNA, the molecules in each strand of the double helix are made up of four distinct groups of molecules denoted by A, G, C, and T; A and T form pairs, as do G and T. In cell division, one strand creates the template for correct formation of second strand. The proper pairings A, T and C, G allow transmission of genetic information when cells replicate.

DNA is tightly coiled in the nucleus of a cell. Stretched out, some chromosomes may contain DNA molecules whose lengths extend from ten centimeters to over one meter. These are indeed macroscopic single molecules. But at room temperature they have no special quantum properties, even though it is the quantum nature of the electrons in the A, G, C, and T that determine the forces between them. So although pairs are indeed ubiquitous, the chemical pairing of DNA is a "classical pairing," not the quantum pairing that can make bosons out of paired fermions.

We start with the empirically determined rules for building atoms out of electrons, protons, and neutrons, and then move on to the build-up of atoms into molecules. The quantum concept of the Pauli exclusion principle plays a key role in this build-up (or, in the original German, *aufbau*). This principle prevents more than one fermion of the same fundamental type from occupying the same quantum state, whether that particle be in a nucleus, an atom, a molecule, or even one of the atom traps discussed in Unit 5. But the exclusion principle applies only to *identical* fermions. Electrons, neutrons, and protons are all fermions; but, although all electrons are identical, and thus obey an exclusion principle, they certainly differ from neutrons or protons, and these non-identical fermions are not at all restricted by the presence of one another. Chemists and physicists understood the exclusion principle's empirical role in constructing the periodic table well before the discovery of the quantum theory of Unit 5; but they did not understand its mathematical formulation or its theoretical meaning.

Particles of light, or photons, are of a different type altogether: They are bosons, and do not obey the exclusion principle. Thus, identical photons can all join one another in precisely the same quantum state; once started, in fact, they are actually attracted to do so. This is the antithesis of the exclusion principle. Large numbers of such photons in the same quantum state bouncing back and forth between



two mirrors several inches or even many meters apart create an essential part of a laser that, in a sense, is a macroscopic quantum system with very special properties.



medium. Source: © William P. Reinhardt.

Lasers are everywhere in our technology, from laser pointers to surgical devices and surveying equipment, to the inner workings of CD and DVD players. Laser light sent from telescopes and reflected from mirrors on the Moon allows measurement of the distance between the Earth and Moon to better than one millimeter, allowing tests of gravitational theory, measurement of the slowly increasing radius of the moon's orbit around the Earth, and even allows geophysicists to observe the day-to-day motion of the continents (actually the relative motion of plate tectonics) with respect to one another: A bright light indeed. In addition to being bright and intense, laser light is *coherent*. Not only do all the particulate photons wave with the same wavelength (or color), but they are also shoulder to shoulder in phase with one another. This phase coherence of very large numbers of photons is a quantum property that follows from their bosonic nature. Yet, it persists up into the macroscopic world.

### Superfluids and superconductors

Are there other macroscopic quantum systems in which actual particles (with mass) cooperate in the same coherent manner as the photons in a laser? We might use the molecules we will build up to make a



dining room table, which has no evident quantum wave properties; so perhaps quantum effects involving very large numbers of atoms simply don't persist at the macroscopic level or at room temperature. After all, light is quite special, as particles of light have no mass or weight. Of course, we fully expect light to act like a wave, it's the particulate nature of light that is the quantum surprise. Can the wave properties of massive particles appear on a macroscopic scale?

The surprising answer is yes; there are macroscopic quantum systems consisting of electrons, atoms, and even molecules. These are the superfluids and superconductors of condensed matter physics and more recently the Bose condensates of atomic and molecular physics. Their characteristics typically appear at low (about 1–20 K), or ultra-low (about 10<sup>-8</sup> K and even lower) temperatures. But in some superconductors undamped currents persist at rather higher temperatures (about 80 K). These are discussed in Unit 8.

Superfluids are liquids or gases of uncharged particles that flow without friction; once started, their fluid motion will continue forever—not a familiar occurrence for anything at room temperature. Even superballs eventually stop bouncing as their elasticity is not perfect; at each bounce, some of their energy is converted to heat, and eventually they lie still on the floor.



produce dramatic images. Source: © Left: Wikimedia Commons, Creative Commons Attribution 3.0 Unported License. Author: Jan Ainali, 12 February 2008. Right: NIH.

Superconductors have this same property of flowing forever once started, except that they are streams of charged particles and therefore form electric currents that flow without resistance. As a flowing current generates a magnetic field, a superconducting flow around a circle or a current loop generates a possibly very high magnetic field. This field never dies, as the super-currents never slow down. Hospitals everywhere possess such superconducting magnets. They create the high magnetic fields that allow the diagnostic procedure called MRI (Magnetic Resonance Imaging) to produce images of the brain or other



soft tissues. This same type of powerful superconducting magnetic field is akin to those that might levitate trains moving along magnetic tracks without any friction apart from air resistance. And as we saw in Unit 1, physicists at CERN's Large Hadron Collider use superconducting magnets to guide beams of protons traveling at almost the speed of light.

Thus, there *are* large-scale systems with quantum behavior, and they have appropriately special uses in technology, engineering, biology and medicine, chemistry, and even in furthering basic physics itself. How does this come about? It arises when electrons, protons, and neutrons, all of which are fermions, manage to arrange themselves in such a way as to behave as bosons, and these composite bosons are then sucked into a single quantum state, like the photons in a laser.

## Pairing and exclusion

What is required to create one of these composite quantum states, and what difference does it make whether the particles making up the state are fermions or bosons? Historically, the realization that particles of light behaved as bosons marked the empirical beginning of quantum mechanics, with the work of Planck, Einstein, and, of course, Bose, for whom the boson is named. In Unit 5, we encountered Planck's original (completely empirical) hypothesis that the energy at frequency in an equilibrium cavity filled with electromagnetic radiation at temperature T should be nhv, where h is Planck's constant, v is the photon frequency, and n is a mathematical integer, say 0, 1, 2, 3.... Nowadays, we can restate the hypothesis by saying that n photons of energy hv are all in the same quantum mode, which is the special property of bosons. This could not happen if photons were fermions.

Another, at first equally empirical, set of models building up larger pieces of matter from smaller came from Dmitri Mendeleev's construction and understanding of the periodic table of the chemical elements. American chemist G. N. Lewis pioneered the subsequent building up of molecules from atoms of the elements. His concept that pairs of electrons form chemical bonds and pairs and octets of electrons make especially stable chemical elements played a key role in his approach. This same concept of pairing arises in converting fermions into the bosons needed to become superconductors and superfluids, which will be our macroscopic quantum systems.

Group I	Group II	Group III	Group IV	Group V	Group VI	Group VII	Group VIII
H							
Li	Ве	в	с	N	0	F	
Na	Mg	AI	Si	Р	s	сі	
K Cu	Ca Zn		Π	V As	Cr Se	Mn Br	Fe Co Ni
Rb Ag	Sr Cd	Y In	Zr Sn	Nb Sb	Mo Te	́ і	Ru Rn Pd

Austrian theorist Wolfgang Pauli took the next step. The theoretical development of modern quantum mechanics by Heisenberg and Schrödinger allowed him to make a clear statement of the exclusion principle needed to build up the periodic table of elements. That principle also made clear the distinction between fermions and bosons as will be discussed in Section 4. But first, we will address how models of atomic structure were built, based on the discovery of the electron and the atomic nucleus. Then we will follow the quantum modeling of the atom, explaining these same empirical ideas once the quantum theory of Unit 5 is combined with Pauli's exclusion principle.



# Section 2: Early Models of the Atom

The foundation for all that follows is the periodic table that Russian chemist Dmitri Mendeleev formulated by arranging the chemical elements in order of their known atomic weights. The table not only revealed the semi-periodic pattern of elements with similar properties, but also contained specific holes (missing elements, see Figure 4) that allowed Mendeleev to actually predict the existence and properties of new chemical elements yet to be discovered. The American chemist G. N. Lewis then created an electron shell model giving the first physical underpinning of both Mendeleev's table and of the patterns of chemical bonding. This is very much in the current spirit of particle physics and the Standard Model: symmetries, "magic numbers," and patterns of properties of existing particles that strongly suggest the existence of particles, such as the Higgs boson, yet to be discovered.



Figure 5: The father and son of chemical periodicity: Mendeleev and Lewis. Source: © Left: Wikimedia Commons, Public Domain. Right: Lawrence Berkeley National Laboratory.

## J. J. Thomson

When Mendeleev assembled his periodic table in 1869, he was the giant standing on the shoulders of those who, in the 6 decades before, had finally determined the relative masses of the chemical elements, and the formulae of those simple combinations of atoms that we call "molecules." In this arduous task, early 19th century chemists were greatly aided by using techniques developed over several millennia by the alchemists, in their attempts to, say, turn lead into gold. This latter idea, which nowadays seems either antiquated or just silly, did not seem so to the alchemists. Their view is reinforced by the realization that even as Mendeleev produced his table: *No one had any idea what the chemical elements, or atoms as we now call them, were made of.* Mendeleev's brilliant work was empiricism of the highest order.



John Dalton, following Democrates, had believed that they weren't made of anything: Atoms were the fundamental building blocks of nature, and that was all there was to it.



**Figure 6:** Plum pudding (or raisin scone) model of the atom. **Source:** © William P. Reinhardt, 2010.

This all began to change with J. J. Thomson's discovery of the electron in 1897, and his proposed atomic model. Thomson found that atoms contained electrons, each with a single unit of negative charge. To his great surprise he also found that electrons were very light in comparison to the mass of the atoms from which they came. As atoms were known to be electrically neutral, the rest of the atom then had to be positively charged and contain most of the mass of the atom. Thomson thus proposed his plum pudding model of the atom.

## Rutherford and Lewis

Thomson's model was completely overthrown, less than 15 years later, by Ernest Rutherford's discovery that the positive charge in an atom was concentrated in a very small volume which we now call the "atomic nucleus," rather than being spread out and determining the size of the atom, as suggested by Thomson's model. This momentous and unexpected discovery completely reversed Thomson's idea: Somehow, the negatively charged electrons were on the *outside* of the atom, and determined its volume, just the opposite of the picture in Figure 6. How can that be?

The fact that electrons determine the physical size of an atom suggested that they also determine the nature of atomic interactions, and thus the periodic nature of chemical and physical interactions as



for the 21st Century



A start had already been made. In 1902, when Rutherford's atomic nucleus was still almost a decade in the future, American chemist G. N. Lewis, had already proposed an empirically-developed shell model to explain how electrons could run the show, even if he was lacking in supplying a detailed model of how they actually did so.

He suggested that the first atomic shell (or *kernel* as he originally called it) held two electrons at maximum, the second and third shells a maximum of eight, and the fourth up to 18 additional electrons. Thus, for neutral atoms and their ion, the "magic numbers" 2, 8, 8, and 18 are associated with special chemical stability. Electrons in atoms or ions outside of these special closed shells are referred to as valence electrons, and determine much of the physical and chemical behavior of an atom. For example, in Unit 8, we will learn that atoms in metallic solids lose their valence electrons, and the remaining ionic cores form a metallic crystal, with the former valence electrons moving freely like water in a jar of beads, and not belonging to any specific ion. In doing so, they may freely conduct electrical currents (and heat), or under special circumstances may also become superconductors, allowing these free electrons to flow without resistance or energy dissipation.

Lewis also assumed that chemical bonding took place in such a way that stable molecules had fully filled shells, and that they formed these full shells by sharing electrons in pairs. The simplest example is the

formation of the hydrogen molecule. He denoted a hydrogen atom by H•, where the • is the unpaired electron in the atom's half-filled first shell. Why two atoms in a hydrogen molecule? The answer is easy in Lewis's picture: H•H. This pair of dots denotes that two shared electrons form the bond that holds the  $H_2$  molecule together, where the subscript means that the molecule consists of two hydrogen atoms. As there are now no longer any unpaired electrons, we don't expect to form  $H_3$  or  $H_4$ . Similarly, helium, which already has the filled shell structure He•, has no unpaired electrons to share, so does not bond to itself or to other atoms.

for the 21st Century



Next, Lewis introduced his famous counting rule (still used in models of bonding in much of organic chemistry and biochemistry): As the electrons are shared in overlapping shells, we count them twice in the dot picture for H<sub>2</sub>, one pair for each H atom. Thus, in the Lewis manner of counting, each H atom in H<sub>2</sub> has a filled shell with two electrons just like Helium: He<sup>‡</sup>. Here, we have the beginning of the concept of pairs or pairing, albeit in the form of a very simple empirical model. Such pairings will soon dominate all of our discussion.

#### How can those tiny electrons determine the size of an atom?

Lewis's model implies certain rules that allow us to understand how to build up an atom from its parts, and for building up molecules from atoms, at least for the electrons that determine the structure of the periodic table and chemical bonding. Another set of such rules tells us how to form the nucleus of an atom from its constituent neutrons and protons. The formation of nuclei is beyond the scope of this unit, but we should note that even these rules involve pairing.

We can take such a blithe view of the structure of the nucleus because this first discussion of atoms, molecules, solids, and macroscopic quantum systems involves energies far too low to cause us to worry about nuclear structure in any detail. It is the arrangement of and behavior of the electrons with respect to a given nucleus, or set of nuclei, that determines many of the properties of the systems of interest to us. However, we should not forget about the nucleus altogether. Once we have the basic ideas involving the structure of atoms and molecules at hand, we will ask whether these composite particles rather than their constituent parts are bosons or fermions. When we do this, we will suddenly become very interested in certain aspects of the nucleus of a given atom. But, the first critical point about the nucleus in our initial discussion involves its size in comparison with that of the atom of which it is, somehow, the smallest component.

for the 21st Century



Although it contains almost all of the atom's mass and its entire positive electrical charge, the nucleus is concentrated in a volume of 1 part in 10<sup>15</sup> (that's one thousand trillion) of the physical volume of the atom. The size of the atom is determined by the electrons, which, in turn, determine the size of almost everything, be it solid or liquid, made of matter that we experience in daily life. For example, the volume of water in a glass of water is essentially the volume of the atoms comprising the water molecules that fill the glass. However, if the water evaporates or becomes steam when heated, its volume is determined by the size of the container holding the gaseous water. That also applies to the gaseous ultra-cold trapped atoms that we first met in Unit 5 and will encounter again later in this unit as Bose-Einstein condensates (BECs). They expand to fill the traps that confine them. How is it that these negatively charged and, in comparison to nuclei, relatively massless electrons manage to take up all that space?



### Atoms and their nuclei

The atomic nucleus consists of neutrons and protons. The number of protons in a nucleus is called the atomic number, and is denoted by Z. The sum of the number of protons and neutrons is called the mass number, and is denoted by A. The relation between these two numbers Z and A will be crucial in determining whether the composite neutral atom is a boson or fermion. The volume of a nucleus is approximately the sum of the volumes of its constituent neutrons and protons, and the nuclear mass is approximately the sum of the masses of its constituent neutrons and protons. The rest of the atom consists of electrons, which have a mass of about 1/2,000 of that of a neutron or proton, and a negative charge of exactly the same magnitude as the positive charge of the proton. As suggested by its name, the neutron is electrically neutral. The apparently exact equality of the magnitudes of the electron and proton charges is a symmetry of the type we encountered in Units 1 and 2.

## Do electrons have internal structure?

Now back to our earlier question: How can an atom be so big compared to its nucleus? One possibility is that electrons resemble big cotton balls of negative charge, each quite large although not very massive, as shown in Figure 10 below. As they pack around the nucleus, they take up lots of space, leading to the very much larger volume of the atom when compared to the volume of the nucleus.



Figure 10: A cotton ball model of an atom. Source: © William P. Reinhardt.

However, there is a rather big problem with the simple cotton ball idea. When particle physicists try to measure the radius or volume of an individual electron, the best answer they get is zero. Said another way, no measurement yet made has a spatial resolution small enough to measure the size of an individual electron thought of as a particle. We know that electrons are definitely particles. With modern technology we can count them, even one at a time. We also know that each electron has a definite amount of mass, charge, and—last, but not at all least, as we will soon see—an additional quantity called spin. In spite of all this, physicists still have yet to observe any internal structure that accounts for these properties.

for the 21st Century

It is the province of string theory, or some yet-to-be created theory with the same goals, to attempt to account for these properties at length scales far too small for any current experiments to probe. Experimentalists could seek evidence that the electron has some internal structure by trying to determine whether it has a dipole moment. Proof of such a moment would mean that the electron's single unit of fundamental negative charge is not uniformly distributed within the electron itself. Since the Standard Model introduced in Unit 1 predicts that the electron doesn't have a dipole moment, the discovery of such an internal structure would greatly compromise the model.

For now, though, we can think of an electron as a mathematical point. So how do the electrons take up all the space in an atom? They certainly are not the large cotton balls we considered above; that would make everything too simple, and we wouldn't need quantum mechanics. In fact we do need quantum mechanics in many ways. Ironically, the picture that quantum mechanics gives, with its probability interpretation of an atomic wavefunction, will bring us right back to cotton balls, although not quite those of Figure 10.



Section 3: The Quantum Atom



As we learned in Unit 5, quantum theory replaces Bohr's orbits with standing, or stationary state, wavefunctions. Just as in the Bohr picture, each wavefunction corresponds to the possibility of having the system, such as an electron in an atom, in a specific and definite energy level. As to what would happen when an atom contained more than one electron, Bohr was mute. Astronomers do not need to consider the interactions between the different planets in their orbits around the Sun in setting up a first approximation to the dynamics of the solar system, as their gravitational interactions with each other are far weaker than with the Sun itself. The Sun is simply so massive that to a good first approximation it controls the motions of all the planets. Bohr recognized that the same does not apply to the classical motion of electrons in the next most complex atom: Helium, with a charge of +2 on its nucleus and two moving electrons. The electrons interact almost as strongly with each other as with the nucleus that holds the whole system together. In fact, most two-electron classical orbits are chaotically unstable, causing theoretical difficulties in reconciling the classical and quantum dynamics of helium that physicists have overcome only recently and with great cleverness.

Perhaps surprisingly, the energy levels described by Schrödinger's standing wave picture very quickly allowed the development of an approximate and qualitative understanding of not only helium, but most of the periodic table of chemical elements.

www.learner.org

### Energy levels for electrons in atoms

What is the origin of the Lewis filled shell and electron pair bonding pictures? It took the full quantum revolution described in Unit 5 to find the explanation—an explanation that not only qualitatively explains the periodic table and the pair bond, but also gives an actual theory that allows us to make quantitative computations and predictions.

When an atom contains more than one electron, it has different energies than the simple hydrogen atom; we must take both the quantum numbers n (from Unit 5) and I (which describes a particle's quantized angular momentum), into account. This is because the electrons do not move independently in a manyelectron atom: They notice the presence of one another. They not only affect each other through their electrical repulsion, but also via a surprising and novel property of the electron, its spin, which appeared in Unit 5 as a quantum number with the values  $\pm 1/2$ , and which controls the hyperfine energies used in the construction of phenomenally accurate and precise atomic clocks.

The effect of electron spin on the hyperfine energy is tiny, as the magnetic moment of the electron is small. On the other hand, when two spin-1/2 electrons interact, something truly incredible happens if the two electrons try to occupy the same quantum state: In that case, one might say that their interaction becomes infinitely strong, as they simply cannot do it. So, if we like, we can think of the exclusion principle mentioned in the introduction to this unit as an extremely strong interaction between identical fermions.



for the 21st Century

We are now ready to try building the periodic table using a simple recipe: To get the lowest energy, or ground state of an atom, place the electrons needed to make the appropriate atomic or ionic system in their lowest possible energy levels, noting that two parallel spins can never occupy the same quantum state. This is called the Pauli exclusion principle. Tradition has us write spin +1/2 as  $\uparrow$  and spin -1/2 as  $\downarrow$ , and these are pronounced "spin up" and "spin down." In this notation, the ground state of the He atom would be represented as n = 1 and  $\uparrow \downarrow$ , meaning that both electrons have the lowest energy principal quantum number n = 1, as in Unit 5, and must be put into that quantum state with opposite spin projections.

Quantum mechanics also allows us to understand the size of atoms, and how seemingly tiny electrons take up so much space. The probability density of an electron in a helium atom is a balance of three things: its electrical attraction to the nucleus, its electrical repulsion from the other electron, and the fact that the kinetic energy of an electron gets too large if its wavelength gets too small, as we learned in Unit 5. This is actually the same balance between confinement and kinetic energy that allowed Bohr, with his first circular orbit, to also correctly estimate the size of the hydrogen atom as being 10<sup>5</sup> times larger than the nucleus which confines it.

#### Assigning electrons to energy levels past H and He

Now, what happens if we have three electrons, as in the lithium (Li) atom? Lewis would write Li•, simply not showing the inert inner shell electrons. Where does this come from in the quantum mechanics of the *aufbau*? Examining the energy levels occupied by the two electrons in the He atom shown in Figure 12 and thinking about the Pauli principle make it clear that we cannot simply put the third electron in the n = 1 state. If we did, its spin would be parallel to the spin of one of the other two electrons, which is not allowed by the exclusion principle. Thus the ground state for the third electron must go into the next lowest unoccupied energy level, in this case n = 2, l = 0.

for the 21st Century



Using the exclusion principle to determine electron occupancy of energy levels up through the lithium (Li), sodium (Na), and potassium (K) atoms, vindicates the empirical shell structures implicit in the Mendeleev table and explicit in Lewis's dot diagrams. Namely Li, Na, and K all have a single unpaired electron outside of a filled (and thus inert and non-magnetic) shell. It is these single unpaired electrons that allow these alkali atoms to be great candidates for making atomic clocks, and for trapping and making ultra-cold gases, as the magnetic traps grab that magnetic moment of that unpaired electron.

Where did this magical Pauli exclusion principle come from? Here, as it turns out, we need an entirely new, unexpected, and not at all intuitive fundamental principle. With it, we will have our first go-around at distinguishing between fermions and bosons.



# Section 4: Spin, Bosons, and Fermions

In spite of having no experimentally resolvable size, a single electron has an essential property in addition to its fixed charge and mass: a magnetic moment. It may line up, just like a dime store magnet, north-south or south-north in relation to a magnetic field in which it finds itself. These two possible orientations correspond to energy levels in a magnetic field determined by the magnet's orientation. This orientation is quantized in the magnetic field. It turns out, experimentally, that the electron has only these two possible orientations and energy levels in a magnetic field. The electron's magnetic moment is an internal and intrinsic property. For historical reasons physicists called it spin, in what turned out to be a bad analogy to the fact that in classical physics a rotating spherical charge distribution, or a current loop as in a superconducting magnet, gives rise to a magnetic moment. The fact that only two orientations of such a spin exist in a magnetic field implies that the quantum numbers that designate spin are not integers like the quantum numbers we are used to, but come in half-integral amounts, which in this case are  $\pm 1/2$ . This was a huge surprise when it was first discovered.



What does this mean? A value of 1/2 for the spin of the electron pops out of British physicist Paul Dirac's relativistic theory of the electron; but even then, there is no simple physical picture of what the spin corresponds to. Ask a physicist what "space" spin lives in, and the answer will be simple: Spins are mathematical objects in "spin space." These spins, if unpaired, form little magnets that can be used to trap and manipulate the atoms, as we have seen in Unit 5, and will see again below. But spin itself has much far-reaching implications. The idea of "spin space" extends itself into "color space," "flavor space,"



"strangeness space," and other abstract (but physical, in the sense that they are absolutely necessary to describe what is observed as we probe more and more deeply into the nature of matter) dimensions needed to describe the nature of fundamental particles that we encountered in Units 1 and 2.

## Spin probes of unusual environments



#### Atoms, Nuclei, and Nomenclature

The nuclei of atoms never come into contact with one another at the relatively low energies and moderate temperatures that correspond to our everyday experience. But those conditions do not apply to detonation of nuclear bombs or in nuclear reactors: here nuclei are in direct contact and either split or join together, releasing enormous amounts of energy. Atomic energy and atomic bombs involve the properties of nuclei rather their atoms. But in the 1940s, when they were being developed, scientists and politicians were afraid to use the word nucleus in public, fearing that nobody would know what that meant; so they stuck with the somewhat more familiar word atom. This type of fiction continues today. Because the phrases nuclear energy and nuclear reactors tend to make people nervous, hospitals using the diagnostic tool MRI (Magnetic Resonance Imaging) that involves direct probing of atomic nuclei choose not to mention that nuclei are involved. MRI is a technique that American physicists Ed Purcell and Bob Pound, who invented it, called NMR, for Nuclear Magnetic Resonance. Chemists, biophysicists, and biologists who use the technology to determine how proteins work, for example, call it NMR. But nonscientists who are afraid of nuclei don't want to hear anything about them, so NMR becomes MRI when doctors use it to image soft tissues in the body.

Is spin really important? Or might we just ignore it, as the magnetic moments of the proton and electron are small and greatly overwhelmed by their purely electrical interactions? In fact, spin has both straightforward implications and more subtle ones that give rise to the exclusion principle and determine whether composite particles are bosons or fermions.

The more direct implications of the magnetic moments associated with spin include two examples in which we can use spins to probe otherwise hard-to-reach places: inside our bodies and outer space. It turns out that the neutron and proton also have spin-1/2 and associated magnetic moments. As these magnetic moments may be oriented in only two ways in a magnetic field, they are usually denoted by the ideograms  $\uparrow$  and  $\downarrow$  for the spin projections +1/2 (spin up) and -1/2 (spin down). In a magnetic field, the protons in states  $\uparrow$  and  $\downarrow$  have different energies. In a strong external magnetic field, the spectroscopy of the transitions between these two levels gives rise to Nuclear Magnetic Resonance (NMR), a.k.a. MRI in medical practice (see Figure 3). Living matter contains lots of molecules with hydrogen atoms, whose nuclei can be flipped from spin up to spin down and vice versa via interaction with very low energy electromagnetic radiation, usually in the radiowave regime. The images of these atoms and their



interactions with nearby hydrogen atom nuclei provide crucial probes for medical diagnosis. They also support fundamental studies of chemical and biochemical structures and dynamics, in studies of the folding and unfolding of proteins, for example.

Another example of the direct role of the spins of the proton and electron arises in astrophysics. In a hydrogen atom, the spin of the proton and electron can be parallel or anti-parallel. And just as with real magnets, the configuration  $(p(\uparrow)e(\downarrow)$  has lower energy than  $p(\uparrow)e(\uparrow)$ . This small energy difference is due to the hyperfine structure of the spectrum of the hydrogen atom reviewed in Unit 5. The photon absorbed in the transition  $p(\uparrow)e(\downarrow) \rightarrow p(\uparrow)e(\uparrow)$  or emitted in the transition  $p(\uparrow)e(\downarrow)$  has a wavelength of 21 centimeters, in the microwave region of the electromagnetic spectrum. Astronomers have used this 21 centimeter radiation to map the density of hydrogen atoms in our home galaxy, the Milky Way, and many other galaxies.



## Electrons are fermions

However, there is more: That a particle has spin 1/2 means more than that it has only two possible orientations in a magnetic field. Fundamental particles with intrinsic spin of 1/2 (or any other half-integer



spin, such as 3/2 or 5/2 or more whose numerators are odd numbers) share a specific characteristic: They are all fermions; thus electrons are fermions. In contrast, fundamental particles with intrinsic spin of 0, 1, 2, or any integral number are bosons; so far, the only boson we have met in this unit is the photon.

Is this a big deal? Yes, it is. Applying a combination of relativity and quantum theory, Wolfgang Pauli showed that identical fermions or bosons in groups have very different symmetry properties. No two identical fermions can be in the same quantum state in the same physical system, while as many identical bosons as one could wish can all be in exactly the same quantum state in a single quantum system. Because electrons are fermions, we now know the correct arrangement of electrons in the ground state of lithium. As electrons have only two spin orientations,  $\uparrow$  or  $\downarrow$ , it is impossible to place all three electrons in the lowest quantum energy level; because at least two of the three electrons would have the same spin, the state is forbidden. Thus, the third electron in a lithium atom must occupy a higher energy level. In recognition of the importance of spin, the Lewis representation of the elements in the first column of the periodic table might well be  $H\uparrow$ ,  $Li\uparrow$ ,  $Na\uparrow$ ,  $K\uparrow$ , and  $Rb\uparrow$ , rather than his original  $H\bullet$ ,  $Li\bullet$ ,  $Na\bullet$ ,  $K\bullet$ , and  $Rb\bullet$ . The Pauli symmetry, which leads to the exclusion principle, gives rise to the necessity of the periodic table's shell structure. It is also responsible for the importance of Lewis's two electron chemical pair bond, as illustrated in Figure 16.



The Pauli rules apply not only to electrons in atoms or molecules, but also to bosons and fermions in the magnetic traps of Unit 5. These may be fundamental or composite particles, and the traps may be

macroscopic and created in the laboratory, rather than electrons attracted by atomic nuclei. The same rules apply.

for the 21st Century

Conversely, the fact that bosons such as photons have integral spins means that they can all occupy the same quantum state. That gives rise to the possibility of the laser, in which as many photons as we wish can bounce back and forth between two mirrors in precisely the same standing wave quantum state. We can think of this as a macroscopic quantum state. This is certainly another example of particles in an artificial trap created in the laboratory, and an example of a macroscopic quantum state. Lasers produce light with very special and unusual properties. Other bosons will, in fact, be responsible for all the known macroscopic quantum state are the real subject of this and several subsequent units.

#### Photons are bosons

When Max Planck introduced the new physical constant h that we now call Planck's constant, he used it as a proportionality constant to fit the data known about blackbody radiation, as we saw in Unit 5. It was Albert Einstein who noted that the counting number n that Planck used to derive his temperature dependent emission profiles was actually counting the number of light quanta, or photons, at frequency v, and thus that the energy of one quantum of light was hv. If one photon has energy hv, then n photons would have energy  $n_{hv}$ . What Planck had unwittingly done was to quantize electromagnetic radiation into energy packets. Einstein and Planck both won Nobel prizes for this work on quantization of the radiation field.

What neither Planck nor Einstein realized at the time, but which started to become clear with the work of the Indian physicist Satyendra Bose in 1923, was that Planck and Einstein had discovered that photons were a type of particle we call "bosons," named for Bose. That is, if we think of the frequency as describing a possible mode or quantum state of the Planck radiation, then what Planck's nhv really stated was that any number, n = 0, 1, 2, 3..., of photons, each with its independent energy hv could occupy the same quantum state.



for the 21st Century

In the following year, Einstein also suggested in a second paper following the work of Bose, that atoms or molecules might be able to behave in a similar manner: Under certain conditions, it might be possible to create a gas of particles all in the same quantum state. Such a quantum gas of massive particles came to be known as a Bose-Einstein condensate (BEC) well before the phenomenon was observed. Physicists observed the first gaseous BEC 70 years later, after decades of failed attempts. But, in 1924, even Einstein didn't understand that this would not happen for just any atom, but only for those atoms that we now refer to as bosons. Fermionic atoms, on the other hand, would obey their own exclusion principle with respect to their occupation of the energy levels of motion in the trap itself.



Section 5: Composite Bosons and Fermions



#### Gained in Translation



Source: © Wikimedia Commons, Public Domain.

In 1923 Satyendra Nath Bose, an Indian physicist working alone, outside of the European physics community, submitted a short article to a leading British physics journal. The article presented a novel derivation of the Planck distribution and implicitly introduced the concept of equal frequency photons as identical bosons. After the editors rejected the paper, Bose sent it to Einstein. Einstein translated the paper into German and submitted it for publication in a leading German physics journal with an accompanying paper of his own. These two papers set the basis for what has become called Bose-Einstein statistics of identical bosons. In his own accompanying paper, Einstein pointedly remarks that Bose's paper is of exceptional importance. But he then indicates that it contains a great mystery, which he himself did not understand. Perhaps the larger mystery is why Einstein, the first person to use the term quantum in his realization that Planck's E=nhv was the idea that light came in packets or quanta" of energy, didn't put the pieces together and discover modern quantum theory five years before Heisenberg and Schrödinger.

Whether atoms and molecules can condense into the same quantum state, as Einstein predicted in 1924, depends on whether they are bosons or fermions. We therefore have to extend Pauli's definition of bosons and fermions to composite particles before we can even talk about things as complex as atoms being either of these. As a start, let's consider a composite object made from two spin-1/2 fundamental particles. The fundamental particles are, of course, fermions; but when we combine them, the total spin is



either 1/2+1/2=1 or 1/2-1/2=0. This correctly suggests that two spin-1/2 fermions may well combine to form a total spin of 1 or 0. In either case, the integer spin implies that the composite object is a boson.

Why the caveat "may well"? As in many parts of physics, the answer to this question depends on what energies we are considering and what specific processes might occur. We can regard a star as a structureless point particle well described by its mass alone if we consider the collective rotation of billions of such point masses in a rotating galaxy. However, if two stars collide, we need to consider the details of the internal structure of both. In the laboratory, we can think of the proton (which is a composite spin-1/2 fermion) as a single, massive, but very small and inert particle with a positive unit charge, a fixed mass, and a spin of 1/2 at low energies. But the picture changes at the high energies created in the particle accelerators we first met in Unit 1. When protons moving in opposite directions at almost the speed of light collide, it is essential to consider their internal structures and the new particles that may be created by the conversion of enormous energies into mass. Similarly two electrons might act as a single boson if the relevant energies are low enough to allow them to do so, and if they additionally have some way to actually form that composite boson; this requires the presence of "other particles," such as an atomic nucleus, to hold them together. This also usually implies low temperatures. We will discuss electrons paired together as bosons below and in Unit 8. A hydrogen atom, meanwhile, is a perfectly good boson so long as the energies are low compared to those needed to disassemble the atom. This also suggests low temperatures. But, in fact, Einstein's conditions for Bose condensation require extraordinarily low temperatures.



Source: © CERN.



#### Helium as boson or fermion

When is helium a boson? This is a more complex issue, as the helium nucleus comes in two isotopes. Both have Z = 2, and thus two protons and two electrons. However, now we need to add the neutrons. The most abundant and stable form of helium has a nucleus with two protons and two neutrons. All four of these nucleons are spin-1/2 fermions, and the two protons pair up, as do the two neutrons. Thus, pairing is a key concept in the structure of atomic nuclei, as well as in the organization of electrons in the atom's outer reaches. So, in helium with mass number A = 4, the net nuclear spin is 0. Thus, the <sup>4</sup>He nucleus is a boson. Add the two paired electrons and the total atomic spin remains 0. So, both the nucleus and an atom of helium are bosons.



The chemical symbol He tells us that Z = 2. But we can add the additional information that A = 4 by writing the symbol for bosonic helium as <sup>4</sup>He, where the leading superscript 4 designates the atomic number. This extra notation is crucial, as helium has a second isotope. Because different isotopes of the same element differ only in the number of neutrons in the nucleus, they have different values of A. The second stable isotope of helium is <sup>3</sup>He, with only one neutron. The isotope has two paired protons and two paired electrons but one necessarily unpaired neutron. <sup>3</sup>He thus has spin-1/2 overall and is a composite fermion. Not surprisingly, <sup>3</sup>He and <sup>4</sup>He have very different properties at low temperatures, as we will discuss in the context of superfluids below.

#### Atomic bosons and fermions

More generally, as the number of spin-1/2 protons equals the number of spin-1/2 electrons in a neutral atom, any atom's identity as a composite fermion or boson depends entirely on whether it has an odd or



even number of neutrons, giving a Fermi atom and a Bose atom, respectively. We obtain that number by subtracting the atomic number, Z, from the mass number, A. Note that A is not entirely under our control. Experimentalists must work with the atomic isotopes that nature provides, or they must create novel ones, which are typically unstable; which isotopes these are depends on the rules for understanding the stability of nuclei. A difficult task as neutrons and protons interact in very complex ways, which befits their composite nature, and are not well represented by simple ideas like the electrical Coulomb's Law attraction of an electron for a proton.



We are now in a position to understand why one would need bosonic atoms to make a BEC: Fermions cannot occupy the same macroscopic quantum state, but bosons can. And, we know how to recognize which atoms will actually be bosons. The first atomic gaseous Bose-Einstein condensates were made in Boulder, Colorado, using rubidium (Rb) atoms; in Cambridge, Massachusetts, using atomic sodium (Na); and in Houston, Texas, using atomic lithium (Li). These three elements are members of the alkali metal family, and share the property of having a single (and thus unpaired) electron outside a fully closed shell of electrons. These unpaired outer shell electrons with their magnetic moments allow them to be caught in a magnetic trap, as seen in Unit 5. If we want gases of these atoms to Bose condense, we must think counterintuitively: We need isotopes with odd values of A, so that the total number of spin-1/2 fermions —protons, electrons, and neutrons—is even. These alkali metals all have an odd number of protons, and



a matching odd number of electrons; therefore, we need an even number of neutrons. This all leads to A being an odd number and the alkali atom to being a boson. Thus the isotopes <sup>7</sup>Li, <sup>23</sup>Na, and <sup>87</sup>Rb are appropriate candidates, as they are composite bosons.



# Section 6: Gaseous Bose-Einstein Condensates



What does it take to form a gaseous macroscopic quantum system of bosonic atoms? This involves a set of very tricky hurdles to overcome. We want the atoms, trapped in engineered magnetic or optical fields, to be cooled to temperatures where, as we saw in Unit 5, their relative de Broglie wavelengths are large compared with the mean separation between the gaseous atoms themselves. As these de Broglie waves overlap, a single and coherent quantum object is formed. The ultimate wavelength of this (possibly) macroscopic quantum system is, at low enough temperatures, determined by the size of the trap, as that sets the maximum wavelength for both the individual particles and the whole BEC itself.

Einstein had established this condition in his 1924 paper, but it immediately raises a problem. If the atoms get too close, they may well form molecules: Li<sub>2</sub>, Rb<sub>2</sub>, and Na<sub>2</sub> molecules are all familiar characters in the laboratory. And, at low temperatures (and even room temperatures), Li, Na, and Rb are all soft metals: Cooling them turns them into dense hard metals, not quantum gases. Thus, experiments had to start with a hot gas (many hundreds of degrees K) and cool the gases in such a way that the atoms didn't simply



condense into liquids or solids. This requires keeping the density of the atomic gases very low—about a million times less dense than the density of air at the Earth's surface and more than a billion times less dense than the solid metallic forms of these elements.

		Bosons
Figure 22: Atoms in a Bose condensate at 0 K	Figure 22: Ato	burns in a Bose condensate at 0 K

Stating all this in terms of bosonic atoms in quantum energy levels, rather than overlapping de Broglie waves, leads to the picture shown in Figure 22. Here, we see the energy levels corresponding to the quantum motion of the atoms in the magnetic (or optical) trap made in the laboratory for collecting them. As the temperature cools, all of the bosonic atoms end up in the lowest energy level of the trap, just as all the photons in an ideal laser occupy a single quantum state in a trap made of mirrors.

#### The role of low temperature

The fact that gaseous atoms must be quite far apart to avoid condensing into liquids or solids, and yet closer than their relative de Broglie wavelengths, requires a very large wavelength, indeed. This in turn requires very slow atoms and ultra-cold temperatures. Laser cooling, as discussed in Unit 5, only takes us part of the way, down to about 10<sup>-6</sup> (one one-millionth) of a degree Kelvin. To actually achieve the temperature of 10<sup>-8</sup> K, or colder, needed to form a BEC, atoms undergo a second stage of cooling, ordinary evaporation, just like our bodies use to cool themselves by sweating. When the first condensates were made, no temperature this low had ever been created before, either in the laboratory or in nature. Figure 23 illustrates, using actual data taken as the first such condensate formed, the role of evaporative cooling and the formation of a BEC.





The process, reported in *Science* in July 1995, required both laser cooling and evaporative cooling of <sup>87</sup>Rb to produce a pretty pure condensate. Images revealed a sharp and smoothly defined Bose-Einstein condensate surrounded by many "thermal" atoms as the rubidium gas cooled to about 10<sup>-8</sup> K. By "pretty pure," we mean that a cloud of uncondensed, and still thermal, atoms is still visible: These atoms are in many different quantum states, whereas those of the central peak of the velocity distribution shown in Figure 23 are in a single quantum state defined by the trap confining the atoms. Subsequent refinements have led to condensates with temperatures just above 10<sup>-12</sup> K—cold, indeed, and with no noticeable cloud of uncondensed atoms. That tells us that all these many thousands to many millions of sodium or rubidium atoms are in a single quantum state.

## The behavior of trapped atoms

How do such trapped atoms behave? Do they do anything special? In fact, yes, and quite special. Simulations and experimental observations show that the atoms behave very much like superfluids. An initial shaking of the trap starts the BEC sloshing back and forth, which it continues to do for ever longer-times as colder and colder temperatures are attained. This is just the behavior expected from such a gaseous superfluid, just as would be the case with liquid helium, <sup>4</sup>He.

The extent of the oscillating behavior depends on the temperature of the BEC. A theoretical computer simulation of such motion in a harmonic trap at absolute zero—a temperature that the laws of physics prevent us from ever reaching—shows that the oscillations would never damp out. But, if we add heat to the simulation, little by little as time passes, the behavior changes. The addition of increasing amounts of the random energy associated with heat causes the individual atoms to act as waves that get more and more out of phase with one another, and we see that the collective and undamped oscillations now begin to dissipate. Experimental observations readily reveal both the back-and-forth oscillations—collective and macroscopic quantum behavior taking place with tens of thousands or millions of atoms in the identical quantum state—and the dissipation caused by increased temperatures.

for the 21st Century



This loss of phase coherence leads to the dissipation that is part of the origins of our familiar classical world, where material objects seem to be in one place at a time, not spread out like waves, and certainly don't show interference effects. At high temperatures, quantum effects involving many particles "de-phase" or "de-cohere," and their macroscopic quantum properties simply vanish. Thus, baseballs don't diffract around a bat, much to the disappointment of the pitcher and delight of the batter. This also explains why a macroscopic strand of DNA is a de-cohered, and thus classical, macroscopic molecule, although made of fully quantum atoms.

Gaseous atomic BECs are thus large and fully coherent quantum objects, whereby coherent we imply that many millions of atoms act together as a single quantum system, with all atoms in step, or in phase, with one another. This coherence of phase is responsible for the uniformly spaced parallel interference patterns that we will meet in the next section, similar to the coherence seen in the interference of laser light shown in the introduction to this unit. The difference between these gaseous macroscopic quantum systems and liquid helium superfluids is that the quantum origins of the superfluidity of liquid helium are



hidden within the condensed matter structure of the liquid helium itself. So, while experiments like the superfluid sloshing are easily available, interference patterns are not, owing to the "hard core" interactions of the helium atoms at the high density of the liquid.



# Section 7: Phase Control and New Structures

We have mentioned several times that laser light and the bosonic atoms in a gaseous BEC are coherent: The quantum phase of each particle is locked in phase with that of every other particle. As this phase coherence is lost, the condensate is lost, too. What is this quantum phase? Here, we must expand on our earlier discussion of standing waves and quantum wavefunctions. We will discuss what is actually waving in a quantum wave as opposed to a classical one, and acknowledge where this waving shows up in predictions made by quantum mechanics and in actual experimental data. Unlike poetry or pure mathematics, physics is always grounded when faced with experimental fact.

#### Imaginary Numbers and Quantum Waves

What do complex numbers have to do with waves? We can describe familiar waves such as those on the ocean in terms of trigonometric sines and cosines. But quantum waves are neither sines nor cosines; they are complex linear combinations of the two. We need this combination to account for the fact that, while wave amplitudes are definitely time-dependent, the probability densities of quantum mechanical stationary states don't depend on time at all, which is why we call them stationary states. How does this happen, and where do the complex numbers and functions come from? It turns out that the time-dependent part of the wave amplitude is a (complex) linear combination: cosine(Et/h) + i sine(Et/h), where i is  $\sqrt{-1}$ , t is the time, and E the energy of the quantum stationary state. A compact representation of this sum of real and imaginary sines and cosines is given by a remarkable, and intriguing formula due to the great Swiss mathematician Euler:  $\varphi = \cos(\varphi) + i \sin(\varphi)$ . Physicist Richard Feynman often called this Euler formula one of the most unexpected and amazing results in all of mathematics; for example, if we choose  $x = \pi$ , we find that hat = 0, which, improbably at first sight, relates the five most fundamental numerical constants in all of mathematics: 0, 1, i, e and  $\pi$ . Here e is the base of natural logarithms,  $\pi$  the ratio of the circumference of a circle to its diameter, and i the square root of -1. Thus, we can now honestly state what is waving as time passes.

Like vibrating cello strings or ripples in the ocean, quantum wavefunctions are waves in both space and time. We learned in Unit 5 that quantum mechanics is a theory of probabilities. The full story is that quantum wavefunctions describe complex waves. These waves are sometimes also called "probability amplitudes," to make clear that it is not the wavefunction itself which is the probability. Mathematically, they are akin to the sines and cosines of high school trigonometry, but with the addition of i, the square root of -1, to the sine part. So, the wave has both a real part and an imaginary part. This is represented mathematically as  $e^{i\phi}$  (see sidebar), where the  $i\phi$  is called the "complex phase" of the wavefunction.





The probability density (or probability distribution), which tells us how likely we are to detect the particle in any location in space, is the absolute value squared of the complex probability amplitude, and as probabilities should be, they are real and positive. What is this odd-sounding phrase "absolute value squared"? A particle's probability density, proportional to the absolute value of the wavefunction squared, is something we can observe in experiments, and is always measured to be a positive real number. Our detectors cannot detect imaginary things. One of the cardinal rules of quantum mechanics is that although it can make predictions that seem strange, its mathematical description of physics must match what we observe, and the absolute value squared of a complex number is always positive and real. **\*** See the math

What about the stationary states such as the atomic energy levels discussed both in this unit and in Unit 5? If a quantum system is in a stationary state, nothing happens, as time passes, to the observed



probability density: That's, of course, why it's called a stationary state. It might seem that nothing is waving at all, but we now know that what is waving is the complex phase.

For a stationary state, there is nothing left of the underlying complex waving after taking the absolute value squared of the wavefunction. But if two waves meet and are displaced from one another, the phases don't match. The result is quantum interference, as we have already seen for light waves, and will soon see for coherent matter waves. Experimentalists have learned to control the imaginary quantum phase of the wavefunction, which then determines the properties of the quantum probability densities. Phase control generates real time-dependent quantum phenomena that are characteristic of both BECs and superconductors, which we will explore below.

## Phase imprinting and vortices

When does this hidden phase that we don't see in the experimentally measurable probability density become manifest? The simplest example is in interference patterns such as those shown in Figure 26. Here, the phase difference between two macroscopic quantum BECs determines the locations of the regions of positive and negative interference. So, situations do exist in which this mysterious phase becomes actual and measurable: when interference patterns are generated.



But, there is more if we fiddle with the overall phase of a whole superfluid or superconductor with its many-particle macroscopic wavefunction. Imprinting a phase on such a system can create moving dynamical structures called vortices and solitons. Both signify the existence of a fully coherent, macroscopic many-particle quantum system.



A phase can be "imprinted" by rotating such a macroscopic quantum system. This creates vortices as we see in the density profile calculated in Figure 27. Physicists have observed such vortices in liquid superfluids, gaseous BECs, and superconductors. All have the same origin.



We can obtain a physical picture of what's happening if we examine the phase of the underlying macroscopic wavefunction. That's difficult to do experimentally, but easy if we use a computer calculation to generate the coherent many-body macroscopic wavefunction, as Figure 27 illustrates. Here, unlike in an experimental situation, we fully know the phase of the wavefunction because we have programmed it ourselves. We can then calculate its absolute value squared if we like, which gives the resulting probability density that an experiment would observe. If we calculate the phase in a model of a circulating BEC, superfluid, or superconducting current, and compare it to the observable probability density, we find the phase changes periodically as you trace a circle around what appear to be holes in the probability density, as you can see in Figure 27. Each hole is a tiny quantum whirlpool, or vortex; the lines of phase radiating outward indicate that the quantum fluid is circulating around these holes.

### Solitons: waves that do not decay

Clearly, then, altering the phase of a macroscopic wavefunction may have dramatic effects. Another such effect is the creation of the special nonlinear waves called "solitons," which physicists have observed in BECs following a phase imprinting. Solitons are a very special type of wave. They can, and do, pass right though each other without dissipating. And if they are in a superfluid (a gaseous atomic BEC in this case), they will carry on this oscillatory motion forever. These are called "density notch solitons," and are created by phase imprinting on part of a condensate. The process both creates and drives the motion of the solitons, just as circular phase imprints both create and maintain superfluid vortices.

for the 21st Century



The vortices and solitons are both highly unusual persistent defects in the quantum wavefunction. Were these systems not macroscopic superfluids, such defects would just disappear and dissipate of their own accord. Try to make a hole in a tub of water and watch it fill in. (On the other hand, lumps of water can propagate without dispersion: Think of tsunamis, where, in exactly the right circumstances, lumps of water can move across a whole ocean.) The same would happen to a quantum bump or dip in the density corresponding to one or a few quantum particles in free space: The wavefunction would spontaneously disperse. It is the collective and coherent nature of the many-particle BEC that allows these nonlinear wave structures to persist. Of course, if you can create a whirlpool as the bath tub drains, it will persist; but such a classical whirlpool has nothing to do with the phase of the liquid water, phase being a purely quantum concept as we apply it here.



for the 21st Century

Figure 29: The formation of vortices in this BEC shows that it is a superfluid. Source: © Martin Zwierlein.

The vortices and solitons we describe are all consistent with the idea that all the particles are in a single quantum state. These highly dilute gaseous condensates are essentially 100 percent pure, in the sense that all the particles occupy a single quantum state in the trap—although, to be sure, the quantum state wavefunction distorts as the trap is filled. The simple tools developed here have their limitations. They apply to dilute atomic gases, but cannot deal with a more traditional liquid such as <sup>4</sup>He in its superfluid state. Owing to the very strong interactions between the helium atoms at the much higher density of the liquid, the condensate is only about 10 percent pure condensate. This does not affect its remarkable properties as a superfluid, but certainly makes its theoretical description more difficult. In fact, it makes the quantitative description of the coherent quantum wavefunction a tremendously exciting exercise in computational physics.

www.learner.org



# Section 8: Making BECs from Fermi Gases

We have discussed the fact that a neutral atom of <sup>7</sup>Li is a boson. That's because the neutral atom's three protons, three electrons, and four neutrons add up to an even number of spin-1/2 fermions, thus giving the atom an integral total spin. <sup>7</sup>Li is the predominant isotope of lithium that occurs naturally on Earth. However, the isotope <sup>6</sup>Li accounts for about 7 percent of naturally occurring lithium. This isotope has an odd number of spin-1/2 fermion constituents: three protons, three neutrons, and three electrons, and is thus a fermionic atom. What happens to this fermionic isotope of Li if you trap it and cool it down? Rather than Bose condensing like <sup>7</sup>Li, it fills in the energy levels in the trap just like electrons fill in the energy levels of an atom. A fermionic gas in which the lowest energy levels are occupied with one particle in each level is called "degenerate." One can thus envisage making an ultra-cold degenerate Fermi gas from <sup>6</sup>Li, and researchers in the laboratory have actually done so.



Cooling Fermi gases in that way is far more difficult than making an atomic gaseous BEC. Once physicists learned to make them, gaseous BECs immediately became commonplace. Part of the advantage of making a BEC is the bosonic amplification—the effect of sucking all the bosons into the same quantum state that we encountered in our earlier discussion of lasers. The word "laser" is actually an acronym for "light amplification through stimulated emission of radiation." Once a single quantum state begins to fill up with bosons, others, miraculously, want to join them.

This is not at all the case with fermions, as their exclusion principle dictates entirely the opposite behavior. In fact, once a cold and partly degenerate Fermi gas begins to form, many of the energy levels are occupied but a (hopefully) small fraction are not. It then becomes very difficult to further cool the Fermi system. As most levels are already full, only the few empty ones are available to accept another atomic fermion. If these are few and far between, it takes a lot of time and luck to have a Fermi particle lose—through evaporative cooling, say—just the right amount of energy to land in one of the unoccupied energy levels. The other levels are blocked by the exclusion principle. Unsurprisingly called "Pauli blocking," this is a real impediment to making gaseous macroscopic, fully degenerate cold Fermi gases from fermionic atoms. Experimentalists often co-condense <sup>6</sup>Li with <sup>7</sup>Li and allow the <sup>7</sup>Li BEC to act as a refrigerator to cool the recalcitrant <sup>6</sup>Li atoms into behaving.

#### Pairing fermions to make bosons

for the 21st Century

In the style of earlier parts of this unit, we can represent fermionic <sup>6</sup>Li as <sup>6</sup>Li↑, with the ↑ now representing the atom's outer unpaired electron. Here we can, at last, illustrate the pairing of fermions to give bosons—the analog of the Cooper pairing of electrons in a superconducting metal that Unit 8 will develop fully. Combine two fermions and you get a boson. This is simple numerics: Doubling an odd number produces an even number. So, for our example, the molecule <sup>6</sup>Li<sub>2</sub> must be a boson whether it exists in the higher energy level <sup>6</sup>Li↑↑<sup>6</sup>Li or the lower energy <sup>6</sup>Li↓↑<sup>6</sup>Li. Now you can see why, in a chapter about macroscopic quantum states, we started off with a discussion of simple molecules. We should note, conversely, that combining two bosons just gives another boson, as the number of spin-1/2 particles is still even.



Figure 31 indeed shows that fermionic atoms can pair and become molecular bosons, which can then condense into a molecular BEC. This is evident from the striking similarity of the interference patterns shown in Figures 26 and 31. Two overlapping degenerate Fermi gases would not create such macroscopic interference patterns because those wavefunctions have no intrinsic phase relationships, in contrast to the BEC wavefunctions. Molecular BECs, especially if the molecules are polar and can communicate with one anther through long-range forces, are of special interest as being quantum information storage devices, as individual molecules can potentially be addressed via their many internal degrees of freedom.



# Section 9: Conclusions and a Look Ahead

Macroscopic quantum fluids, or superfluids, can be formed from cold bosons. Many types of composite entities fulfill the basic bosonic requirement of integral spin. So, the gaseous quantum superfluid can consist of bosonic atoms, and quite newly bosonic molecules, all of which contain an even overall number of spin-1/2 fermions, be they electrons, protons, or neutrons. All are uncharged superfluids. In the dilute gaseous superfluid phase, they display fully quantum properties, such as interference on the length scale of around a millimeter, which are visible to the naked eye. So, they are certainly macroscopic. Dense liquid superfluids such as <sup>4</sup>He, of course, contain many more atoms than gaseous BECs in laboratory traps, and have a myriad of unusual properties. But, they do not directly display their fundamental quantum nature quite so directly, even though it underlies their superfluid behavior.



Figure 32: A fountain of superfluid <sup>4</sup>He Source: © Peter Taborek, Low Temperature Materials Laboratory, University of California, Irvine.

Two fermions can pair to make a boson: This allows fermionic <sup>3</sup>He to become a superfluid, albeit at a much lower temperature than its bosonic neighbor <sup>4</sup>He. The pair interaction between these <sup>3</sup>He atoms is far too weak to allow formation of molecules in the liquid, so the pair formed is rather ephemeral, and is best described in analogy to what happens to electrons in a superconductor rather than atoms in <sup>4</sup>He.

Famously, and unexpectedly, even two electrons can pair in a metallic free-electron "sea" to make a composite boson inside a superconductor. This seems odd at first, as these electrons have like charges and thus repel each other. Thus, their pairing is not at all like making bosonic <sup>6</sup>Li<sub>2</sub> from fermionic <sup>6</sup>Li, as those atoms actually attract and form molecules in physical space. The pairing of electrons to make



bosonic pairs of electrons, called "Cooper pairs," is indeed more complex. It does not even take place in the three-dimensional coordinate space in which we live. Rather, the pairing occurs in a more abstract "momentum" space. We leave that description to Unit 8, simply noting that it is yet another example of the pairing concepts that we have introduced here. And, because a bosonic pair of electrons carries two units of negative electrical charge, the Bose condensate of such paired electrons is not only a superfluid, but also a superconductor.



# Section 10: Further Reading

- Eric A. Cornell and Carl E. Weimann, "The Bose-Einstein Condensate" *Scientific American*, March 1998.
- Eric A. Cornell, Carl E. Weimann, Wolfgang Ketterle: Nobel Prize Lectures, available at http:// nobelprize.org/nobel\_prizes/physics/laureates/2001/index.html.
- Wolfgang Ketterle, "How are temperatures close to absolute zero achieved and measured?" *Scientific American.com, Ask the Experts*, January 19, 2004, found here: http://www.scientificamerican.com/article.cfm?id=how-are-temperatures-clos.
- Carlos A.R. Sa de Melo, "When fermions become bosons: Pairing in ultracold gases" *Physics Today*, Oct. 2008, p. 45–51.
- Eric R. Scerri, "The Periodic Table, Its Story and Significance" Oxford University Press, 2007.
- Charles Townes, "How the Laser Happened: Adventures of a Scientist" Oxford University Press, 2002.



## Glossary

alkali metals: The alkali metals are the chemical elements in the first column of the periodic table. They all have one valence electron. Alkali metals are commonly used atoms in atomic physics experiments for several reasons. Their structure is relatively simple and provides energy states that are convenient for laser cooling. Many of their transition frequencies match convenient laser sources. Also, the single valence electron's magnetic moment allows the atoms to be easily trapped using magnetic fields, which is convenient for the evaporative cooling process necessary to reach ultracold temperatures.

atomic number: The atomic number of an atom, denoted by Z, is the number of protons in its nucleus. The atomic number of an atom determines its place in the periodic table, and thus which chemical element it is.

blackbody: A blackbody is an object that absorbs all incident electromagnetic radiation and re-radiates it after reaching thermal equilibrium. The spectrum of light emitted by a blackbody is smooth and continuous, and depends on the blackbody's temperature. The peak of the spectrum is higher and at a shorter wavelength as the temperature increases.

Bose-Einstein condensate: A Bose-Einstein condensate, or BEC, is a special phase of matter in which the quantum mechanical wavefunctions of a collection of particles line up and overlap in a manner that allows the particles to act as a single quantum object. The electrons in a superconductor form a BEC; superfluid helium is an example of a liquid BEC. BECs can also be created from dilute gases of ultracold atoms and molecules.

boson: A boson is a particle with integer, rather than half-integer, spin. In the Standard Model, the forcecarrying particles such as photons are bosons. Composite particles can also be bosons. Mesons such as pions are bosons, as are <sup>4</sup>He atoms. See: fermion, meson, spin.

complex: In the context of physics and math, the term complex refers to the presence of complex numbers and is not a synonym of complicated. Thus, a "complex wave" is a mathematical function that describes a wave that can take on complex number values.

complex number: A complex number is a composite of a real number and an imaginary number, and can be written in the form a+bi where a and b are real numbers and i is the square root of -1.



counting number: The counting numbers are the integers greater than zero: 1, 2, 3.

de Broglie wavelength: A particle's de Broglie wavelength,  $\lambda$ , is defined as Planck's constant divided by the particle's momentum, *p*:  $\lambda = h/p$ . The de Broglie wavelength is named after Louis de Broglie, the French physicist who first suggested that it might be useful to describe particles as waves. A relativistic electron has a de Broglie wavelength of around a nanometer, while a car driving down the highway has a de Broglie wavelength of around  $10^{-38}$  meters. Quantum mechanical effects tend to be important at the scale of an object's de Broglie wavelength; thus we need to describe electrons quantum mechanically, but classical physics is adequate for cars and most other macroscopic objects.

electric dipole moment: The electric dipole moment of a system with two electric charges is defined as the product of the two charges divided by the distance between them. It is a vector quantity, with the positive direction defined as pointing from the (more) negative charge toward the (more) positive charge. The electric dipole moment of a more complicated system of charges is simply the sum of the moments of each pair of charges.

fermion: A fermion is a particle with half-integer spin. The quarks and leptons of the Standard Model are fermions with a spin of 1/2. Composite particles can also be fermions. Baryons, such as protons and neutrons, and atoms of the alkali metals are all fermions. See: alkali metal, baryon, boson, lepton, spin.

ground state: The ground state of a physical system is the lowest energy state it can occupy. For example, a hydrogen atom is in its ground state when its electron occupies the lowest available energy level.

harmonic trap: A harmonic trap is a trap in which the trapped objects (e.g., atoms) are pushed toward the center of the trap with a force proportional to their distance from the center of the trap. The motion of particles in a harmonic trap is analogous to the motion of a mass attached to a spring around the spring's equilibrium position. It is convenient to use harmonic traps in experiments because it is straightforward to calculate the motion of particles in analogy to the mass on a spring.

hyperfine structure: When the nucleus of an atom has a nonzero magnetic moment, some of the energy levels that electrons can occupy in the atom are very finely spaced. The arrangement of these finely spaced levels is called "hyperfine structure." The difference in energy between hyperfine levels typically



corresponds to a microwave photon frequency or light with a wavelength on the order of centimeters. The energy levels in the cesium atom used to define the second are hyperfine levels.

ion: An ion is an atom with nonzero electrical charge. A neutral atom becomes an ion when one or more electrons are removed, or if one or more extra electrons become bound to the atom's nucleus.

isotope: Different atoms of a chemical element in the periodic table all have the same number of protons, but may have a different number of neutrons in their nuclei. These different versions of the same element are called isotopes. The number of neutrons is not simply random, however—the nucleus will only be stable for combinations of protons and neutrons. Most chemical elements have several stable isotopes. For example, lithium (A=3) has two stable isotopes, one with three neutrons in the nucleus (<sup>6</sup>Li) and one with four (<sup>7</sup>Li). See: atomic number, mass number.

macroscopic: A macroscopic object, as opposed to a microscopic one, is large enough to be seen with the unaided eye. Often (but not always), classical physics is adequate to describe macroscopic objects, and a quantum mechanical description is unnecessary.

magnetic moment: The magnetic moment (or magnetic dipole moment) of an object is a measure of the object's tendency to align with a magnetic field. It is a vector quantity, with the positive direction defined by the way the object responds to a magnetic field: The object will tend to align itself so that its magnetic moment vector is parallel to the magnetic field lines. There are two sources for a magnetic moment: the motion of electric charge and spin angular momentum. For example, a loop of wire with a current running through it will have a magnetic moment proportional to the current and area of the loop, pointing in the direction of your right thumb if your fingers are curling in the direction of the current. Alternatively, an electron, which is a spin-1/2 fermion, has an intrinsic magnetic moment proportional to its spin.

mass number: The mass number (or atomic mass number) of an atom, denoted by A, is the total number of nucleons (protons+neutrons) in its nucleus. Sometimes, the mass number of an atom is written as a superscript to the left of its chemical symbol (e.g., <sup>6</sup>Li) to show which isotope is being discussed. See: atomic number, isotope.

Pauli exclusion principle: The Pauli exclusion principle states that no two identical fermions can occupy the same quantum state. It plays an important role in determining the structure of atoms and atomic nuclei, as well as how electrons behave in metals and semiconductors.

phase: In physics, the term phase has two distinct meanings. The first is a property of waves. If we think of a wave as having peaks and valleys with a zero-crossing between them, the phase of the wave is defined as the distance between the first zero-crossing and the point in space defined as the origin. Two waves with the same frequency are "in phase" if they have the same phase and therefore line up everywhere. Waves with the same frequency but different phases are "out of phase." The term phase also refers to states of matter. For example, water can exist in liquid, solid, and gas phases. In each phase, the water molecules interact differently, and the aggregate of many molecules has distinct physical properties. Condensed matter systems can have interesting and exotic phases, such as superfluid, superconducting, and quantum critical phases. Quantum fields such as the Higgs field can also exist in different phases.

for the 21st Century

phase coherence: If we think of a wave as having peaks and valleys with a zero-crossing between them, the *phase* of the wave is defined as the distance between the first zero-crossing and the point in space defined as the origin. Two waves are *phase coherent* (or simply *coherent*) if the distance between their respective peaks, valleys, and zero-crossings is the same everywhere.

photon: Photons can be thought of as particle-like carriers of electromagnetic energy, or as particles of light. In the Standard Model, the photon is the force-carrier of the electromagnetic force. Photons are massless bosons with integer spin, and travel through free space at the speed of light. Like material particles, photons possess energy and momentum.

Planck's constant: Planck's constant, denoted by the symbol h, has the value 6.626 x  $10^{-34}$  m<sup>2</sup> kg/s. It sets the characteristic scale of quantum mechanics. For example, energy is quantized in units of h multiplied by a particle's characteristic frequency, and spin is quantized in units of h/2 $\pi$ . The quantity h/2 $\pi$  appears so frequently in quantum mechanics that it has its own symbol:  $\hbar$ .

plum pudding model: The Plum Pudding Model is a model of atomic structure proposed by J.J. Thomson in the late 19th century. Thomson had discovered that atoms are composite objects, made of pieces with positive and negative charge, and that the negatively charged electrons within the atom were very small compared to the entire atom. He therefore proposed that atoms have structure similar to a plum pudding, with tiny, negatively charged electrons embedded in a positively charged substrate. This was later shown to be incorrect.



polar: A polar molecule has a nonzero electric dipole moment, so it has a side that is positively charged and a side that is negatively charged.

probability density: The exact location of a quantum mechanical particle is impossible to know because of the Heisenberg uncertainty principle. Rather than specifying the location of a particle such as an electron, quantum mechanics specifies a wavefunction. The probability density, which is a mathematical function that specifies the probability of finding the particle at any location in space, is the square of the wavefunction (technically, its absolute value squared).

real number: Real numbers are most easily defined by contrast to what they are not: imaginary numbers. The set of real numbers includes counting numbers, integers, rational numbers that can be written as fractions, and irrational numbers such as  $\pi$ . They can be thought of as all the points on a number line stretching from negative infinity to infinity.

shell model: The shell model of atomic structure is based on the notion that electrons in an atom occupy "shells" that can fill up, so only a certain number of electrons will fit in a given shell. G. N. Lewis found this idea useful in explaining the chemical properties of different elements. Lewis's shell model is consistent with the Bohr model of the atom in which electrons are thought of as orbiting the nucleus. The "shells" are three-dimensional counterparts of two-dimensional circular orbits with different radii. Although we now know that the Bohr model of the atom is not correct, the concept of shells is still sometimes used to describe the arrangement of electrons in atoms according to the Pauli exclusion principle.

soliton: A soliton is a stable, isolated wave that travels at a constant speed. As a soliton travels, its shape does not change and it does not dissipate. If it collides with another wave, it emerges from the collision unscathed. In a sense, it is a wave that behaves like a particle. Solitons have been predicted and observed in nearly every medium in which waves propagate, including fluids such as water, transparent solids such as optical fibers, and magnets.

standing wave: A standing wave is a wave that does not travel or propagate: The troughs and crests of the wave are always in the same place. A familiar example of a standing wave is the motion of a plucked guitar string.

valence electron: A valence electron is an electron in the outermost shell of an atom in the Lewis model, or in the orbital with the highest value of the principal quantum number, *n*, in the quantum mechanical description of an atom. The valence electrons determine most of the chemical and physical properties of



the atom. It is the valence electrons that participate in ionic and covalent chemical bonds, and that make the primary contributions to an atom's magnetic moment.

vortex: A vortex is a region in which a fluid or gas flows in a spiral toward the vortex center. The speed of fluid flow is fastest at the center of the vortex, and decreases with distance from the vortex center. Tornados and whirlpools are examples of vortices. Quantized vortices will appear in a superfluid when it is rotated fast enough, and quantized vortices will form in the electron gas inside a type-II superconductor when it is placed in a strong enough magnetic field.