

### The wavefunction

(with apologies to lovers of “Frère Jacques”)

What is waving, what is waving?

I don't know, I don't know!

Probability is, probability is.

That is so, yes that's so.

## Chapter 5

# THE QUANTUM PROPERTIES OF NATURE — PART TWO

### 1. QUANTUM PARTICLES AND UNCERTAINTIES

#### *Particle attributes of the wavefunction*

The first hint of the particle aspects of electromagnetic waves was found by Max Planck at the beginning of the twentieth century, although he did not recognize it as such at the time. (Albert Einstein was the one who recognized the significance of Planck's discovery.) In the course of his work, he discovered an extremely small constant of nature that we refer to as *Planck's constant*, which is denoted by the letter  $h$ . In Standard International (SI) units this number is roughly 6 *divided by* the enormous number  $10^{34}$  (1 followed by 34 zeros) and is written  $6 \times 10^{-34}$ . It is about 3/5 of a billionth of a trillionth of a trillionth, by far the smallest physical number we know.

For a simple sinusoidal wavefunction, it has been found that the momentum of the quantum particle described by this wave is Planck's constant *divided by* the wavelength\*; thus, *a short wavelength corresponds to a high momentum*. The particle's energy is Planck's constant *times* the frequency, so that *a high frequency corresponds to a high energy*. Since high momentum implies high energy, these quantum-particle relationships are consistent with the fact that short wavelengths correspond to high frequencies, as we saw in the previous chapter.

For actual particles, which do not extend over all of space, the wavefunction cannot be a simple sinusoidal wave (which does). Instead the wavefunction may be understood as a sum of sinusoidal waves of different wavelengths that destructively interfere outside the region occupied by the particle. In Fig. 5.1 we see how even two waves of slightly different wavelengths can be in phase in one region but out of phase in others.

Actually, the two waves in Fig. 5.1 come back into phase again further out in both directions. For complete destructive interference *everywhere* outside the

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\*commonly referred to as “the DeBroglie wavelength” of the particle.

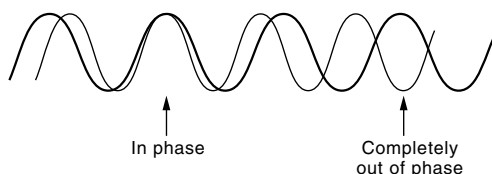


Fig. 5.1. A comparison of two waves of different wavelength — the darker one has the longer wavelength. Notice how they go increasingly out of phase the further away from the in-phase region we look.



Fig. 5.2. A wavepacket, that is essentially zero outside the region shown.

central region, we need an infinite number of waves, one for each wavelength in a (continuum) spread of values. Such sums are often referred to as *wavepackets* and they look roughly like the waveform shown in Fig. 5.2.

Let us explore this notion of a sum of sinusoidal waves and its consequences:

### *Uncertainty relations*

As we have already discussed, in a quantum mechanical world, measurements are not as simple as our intuition expects. We have already seen that a measurement of the location of an electron as it goes through a two-slit barrier has a dramatic effect on the subsequent behavior of that electron. For example, consider a place on the screen that corresponds to a dark line when the slit detector is off, i.e., when no sidewise position measurement is made at the barrier. That place is dark because no electron goes to that position on the screen. With the position detector on, however, the interference pattern disappears so that that position is no longer dark — some electrons *do* arrive at that place on the screen. Those electrons thus have completely different behavior than they would have had were the detector left off. The detector’s measurement of their sidewise position along the barrier evidently changed the sidewise speed or momentum with which they subsequently traveled. In fact, some electrons have their momenta changed by large amounts, some by small amounts, and some not at all; individual changes are uncontrollable and unpredictable. It is very similar to trying to confine a water wave to a small region; it becomes very choppy. The smaller the region of space we confine the electron to, the more “choppy” is the momentum distribution of its wavefunction, which gives the relative probabilities for different possible values of the electron’s momentum. Thus, *the smaller we make the position uncertainty of the particle, the greater is its momentum uncertainty.* In order for the particles’ sidewise momenta to remain zero,

we would need to remove the barrier altogether, which amounts to complete uncertainty of their sidewise positions. This and many other more detailed experiments confirm this quantum-correlation between position uncertainty and momentum uncertainty. This relationship is referred to as *the Heisenberg uncertainty principle*. It should be noted that this quantum-correlation of position and momentum measurements is usually not observable for macroscopic-size objects. This is so because the quantum-correlation of the uncertainties depends on Planck's constant, which is a very tiny number; the accuracy of usual measurements on macroscopic systems is not good enough to get the uncertainties down to that level. It is only when we can measure properties of small numbers of particles, or particles that are all in exactly the same quantum state, that quantum mechanical uncertainty relations become evident.

In summary, we can say that the uncertainty principle arises in a natural way in quantum mechanics, since particles are described by wavefunctions. In the case of a sinusoidal wave, *the momentum of the particle is determined by the wavelength* of the wavefunction. In the three-dimensional space of our universe, a sinusoidal wavefunction extends over all of space in every direction; consequently, it does not describe a particle at all! In order to describe a particle *localized* in some region of space, the wavefunction must have waves of *different* wavelengths, which can destructively interfere outside that region — *the smaller the region, the larger the required spread of wavelengths*. But a spread in wavelengths corresponds to a spread in the momentum distribution contained in the wavefunction. Thus, the uncertainty principle results from: (1) the property possessed by waves, that a localized wave must contain sinusoidal waves over a *spread* of wavelengths — the smaller the region of localization, the wider the spread; and (2) the quantum mechanical connection between wavelength and momentum.

#### Uncertainty

And built into nature, we can see  
uncertainty, uncertainty.

It's hard believing we're not free  
of uncertainty, uncertainty.

It doesn't impugn our ability,  
this uncertainty, uncertainty,  
but nature's teaching humility  
with uncertainty, uncertainty.

You can measure the position.  
You can measure the position.  
You can measure the position,  
with the very best precision!

You can measure the momentum.  
You can measure the momentum.  
You can measure the momentum,  
So precise, with great invention!

But not both!

### *Interchange — Independent or Quantum-conjugate*

Let us now imagine a chef at work. She is preparing several dishes, but we only need to look at a couple of them to learn the concepts we are after. She is preparing a salad; see how she puts the dressing on top and then tosses the salad. Suppose she had *interchanged* the order of those operations, tossing the salad first and then putting the dressing on top. The result would be completely different! I don't know about you, but I prefer my dressing mixed in! The two operations we have witnessed, putting dressing on top and tossing the salad, are obviously not independent of one another, since the order in which they are performed is crucial. We can say that in some sense these two operations are *related*.

Now watch as the chef butters the croissants. Does it matter that she put them on the platter before buttering? What if she would have buttered them on the table and then put them on the platter; if we had looked away until they were sitting there beautifully buttered, could we have detected which was done first? Before you answer, I must caution you that these are croissants that do not make crumbs when being buttered and she is an *expert* butterer. No, the interchange of these two operations, putting them on the platter and buttering would have no effect. These two operations are completely *independent* of one another.

Let us now consider an extremely simple experimental setup. Suppose we have only one narrow slit in a barrier. A beam of quantum particles is incident on it and a screen is placed several feet away on the other side. The quantum particles' distribution as they emerge from the slit will have a wavelike probability that behaves like a classical wave (including interference). There will be a pattern with an unexpectedly wide bright region in the center of the screen — much wider than the width of the slit itself; it is caused by the interference of the (probability) waves “coming” from different locations across the width of the slit. It is called a diffraction pattern because it looks as if the beam were *diffracted* or bent outward by the edges of the slit. Figure 5.3 shows such a diffraction pattern.

If we measured the sidewise momenta of the beam particles *before* they reached the slit, we would find them to be zero or very very small (zero within experimental error); after all, it is a beam of particles moving *toward* the barrier. However, after they go through the open slit, some of the particles acquire sidewise momenta, as is evidenced by their arrival at widely dispersed regions on the screen. (In fact, their position on that screen can be used as a measure of their sidewise momenta.) So a measurement of their sidewise momenta, *after* their sidewise position was determined to be within the slit opening (since they did go through it), gives a completely different result than would be obtained by the measurement of zero for their sidewise momenta made *before* they reached the slit. The shorthand expression of this relationship between position and momentum (in the same direction) is to say that they are a *quantum-conjugate pair of measurements — the order of their*

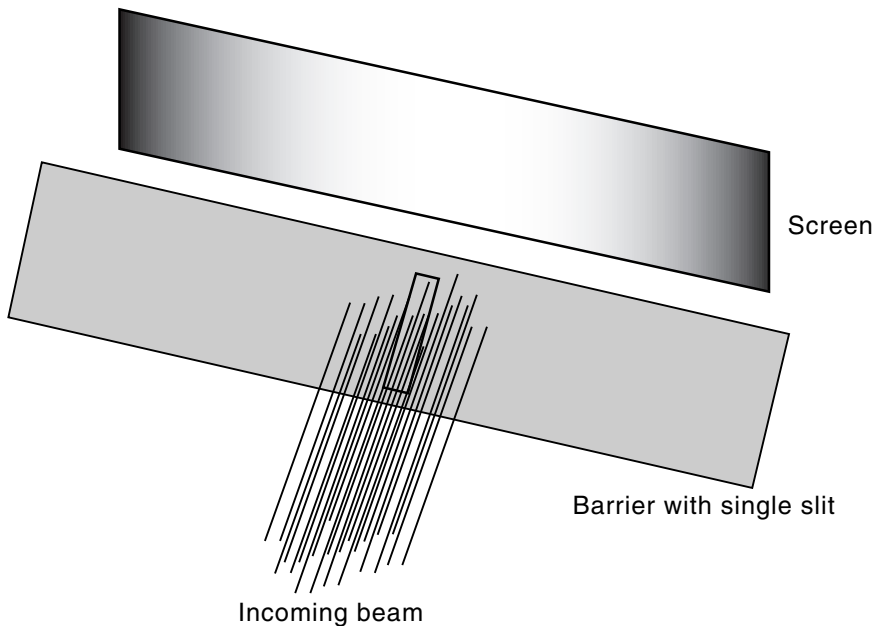


Fig. 5.3. A single-slit diffraction pattern.

*measurements determines the result.\** More generally, the effect that a measurement has on the subsequent behavior of a particle implies that successive measurements of quantum-conjugate properties may give markedly different results, depending on the order in which the measurements are made. Furthermore, the mathematics shows that quantum-conjugate pairs of observables, like position and momentum, must obey an uncertainty relation — the smaller the uncertainty in the measurement of one of them, the wider the spread of the other.

#### Quantum-conjugate Measurements

A young physicist claimed he'd observed  
two quantities (that are conserved).  
That that clashed with the theory,  
Made the referee leery.  
Was the paper's rejection deserved?

To indicate that the interchange of two operations is undetectable, we say that they *commute* (with one another); this has nothing to do with traveling — a completely different meaning of the word. If two operations are quantum-conjugate then they do not commute. Therefore, we can say that the position and momentum

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\*Technically, the designation “quantum-conjugate” requires more than the fact that the result of successive measurements depends on order, but the distinction is of no importance here. The pair position & momentum do indeed form a quantum-conjugate pair.

operators do not commute. We shall encounter other sets of operators that do not commute as we approach *gauge theories* in our travels.

Quantum-conjugate

do they *commute*?  
they do *commute*,  
NOT!

An uncertainty relation exists also for energy and lifetime. The quantum mechanical argument is somewhat analogous to the one we just looked at for position and momentum. The energy associated with a particle is directly related to the frequency of the (probability) wave describing that particle. However, a (sinusoidal) wave of one frequency oscillates forever. For a wave to die out with time, it must have sinusoidal waves of different frequencies in it to interfere with one another. The shorter the time of its existence (referred to as its *lifetime*), the wider the spread of frequencies that must be present to accomplish the cancellation. Thus lifetime and frequency have an uncertainty relation connecting them, in the same way that position and momentum do. In this quantum world of ours, however, the frequency of the wavefunction is directly related to the energy of the corresponding particles. For particles at rest, their energy is characterized by their (rest) masses (recall  $E = mc^2$ ) so that we have *an uncertainty relation between lifetime and mass!* Among its consequences is the fact that particles that have finite lifetimes will not have definite masses. Instead, if we measure the individual masses of a collection of such particles, we will find a *distribution* of values; they will not all have the same mass! The distribution will be large in the center, i.e., most such particles will have masses close to that central value; however, some may have masses quite different from that value. The shorter the lifetime, the wider the mass spread.

***Quantum sizes of particles***

The wavefunction of a particle is not located solely at a point; it takes up a finite region of space, as all waves, including wavepackets, do. Therefore, a particle sitting at a point in space has an effective size, which is not infinitesimal. The lower the mass of the particle, the larger its effective size.

Quantum Rebel

A particle 's spread like a wave  
that *no* point can ever enslave.  
So *quantum* in manner, it taunts,  
as classical notions it flaunts.  
No matter how we may enjoin 't,  
the point is it can't be a point!

## 2. QUANTIZATION

### *Quantized energy levels*

Our first inkling of the quantized structure of atoms resulted from observations of light emerging from them. Many different experiments showed that when atoms are heated, bombarded, or jolted with electricity, they emit certain definite colors of light. Each type of atom has its own spectrum of colors which, unlike the colors of the rainbow, are isolated (discrete) and distinct rather than continuous gradations of color. Different colors correspond to different frequencies, so that the frequencies of the emerging light do not form a continuum but instead are quantized. Studies of light emerging from hot objects and from atoms eventually led to the development of quantum mechanics, one quarter of the way into the twentieth century. The detailed predictions of quantum mechanics have been checked very many times, and applications of that theory have led to a large number of technological developments as well. These include the transistor and all the subsequent electronic technology based on it. Quantum mechanics has revealed the structure and behavior of molecules, knowledge that has led to many medical achievements including the determination of the causes of diseases, the invention of new medications, the creation of tracers and other diagnostic tools, all the way to genetics (and genetic treatments). A large number of developments in chemistry and its industrial applications have also been made.

We shall soon see that the *wavelike* character of the particles of nature leads to the quantization of their energies in matter and ultimately to the stability of matter. In order to explore this matter (definitely a pun), let us first consider a familiar classical wave: the wave that we set up when we pluck a string of a guitar or violin (or *your* favorite stringed instrument). We hear a definite tone. In addition, there are overtones of it that give the instrument its distinctive sound — a different relative-loudness distribution of the overtones for different instruments. (That is why a note plucked on the violin sounds different from the same one plucked on the guitar.) The point is that there are only certain definite pitches excited when we pluck the string; referring to the frequency associated with the perceived tone as  $f$ , ideally we also excite some amount of the frequencies *2 times  $f$*  (the first overtone), *3 times  $f$* , *4 times  $f$* , etc. For actual strings, the frequencies of the overtones may be slightly different, but nevertheless their frequencies are *quantized*. They are restricted to certain definite isolated (discrete) values; they do not have a continuum of possible values.

When we are dealing with the *wavefunctions* that describe particles, the frequencies correspond to their allowed energies. For electrons in an atom (or a solid, etc.), we have a situation analogous to a string of an instrument and the result is that only certain allowed energy states exist for the electrons; *their energies are quantized*.

Quantization in My House

A half a step you can't alight;  
 you cannot walk down less.  
 And *more* may still not be just right.  
 Exactly one? Oh, yes!  
 Or two or three or four or five,  
 or six or seven; more?  
 Well reaching twelve you will arrive  
 right at the basement floor!

***Quantized spin***

The quantization that results because of the wave nature of particles is not restricted to energies but also appears in the intrinsic angular momenta of particles known as spin, as we have already discussed in Chapter 2. Furthermore, the orientation of the spin is quantized as well. In particular, particles that have spin  $\frac{1}{2}$ , like electrons (and all the other fundamental matter particles), have only two possible orientations of their spin — they can be rotating clockwise (called spin down) or counter-clockwise (called spin up) about any direction chosen for the measurement. Thus, for a spin  $\frac{1}{2}$  particle, we have two possible states for every state that it would have if it had no spin. *Massless* gauge particles like the photon and its cousins also have two possible orientations of their spin.

***The Pauli (pronounced Powli) Exclusion Principle***

Quantum theory also teaches us that fermions — e.g. electrons and, in fact, all of the fundamental matter particles (leptons and quarks) — have a solitary nature. In fact, they obey a strict *exclusion principle* — once a fermion is in a particular physical state, all other *identical* fermions are excluded from it. Thus, this Pauli Exclusion Principle shows that no two identical fermions can be in the same state.

KEEP OUT

You cannot come in here, I say,  
 although there is no sign.  
 I need my state; I will not sway.  
 This state is solely mine!  
 And if you think I'm being mean  
 and selfish as can be,  
 I ask, "Haven't you *ever* seen,  
 the FERMION DECREE?"  
 THOU SHALT NOT SHARE YOUR STATE 's the rule;  
 we may not share at all!  
 Now don't get angry, please stay *cool*;  
 but just respect my "wall."

### *A classical cataclysm*

In classical electrodynamics, it is shown that a *charged* particle radiates electromagnetic energy as its momentum changes (direction and/or size). Charged particles moving around the oval beam paths in accelerators display this property very dramatically, producing radiation (called synchrotron radiation) that has been put to medical and other important uses. Similarly, in a classical world, the electrons circling the nucleus in an atom would emit a steady stream of electromagnetic waves. This continual loss of energy would cause them to spiral down into the nucleus. In this manner, all classical atoms would collapse shortly after they are made! Of course, the very fact that we *exist* shows that such cataclysmic collapses do not occur. After all, we and everything around us are *made* of (uncollapsed) atoms. In other words, *the fact that we exist to create and consider the classical theory of nature precludes its validity.*

### *The classical cataclysm averted and chemistry explained*

It is the fact that the allowed energies of electrons in atoms are quantized, along with the Pauli Exclusion Principle, that explains the stability of atoms — their violent collapse is averted. Envision a skyscraper shaped like an ice cream cone with the bottom broken off, containing no stairs and no basement, as shown in Fig. 5.4.

The floors have corridors that circle around the cone back onto themselves. The ground floor has one corridor and successive floors have more and more (concentric) corridors. The different floors correspond to different allowed energies of the electrons in an atom; they are referred to as *energy levels*. Like the floors of any skyscraper, they are not a continuous set, but are spaced instead — the allowed energy levels are quantized. An electron on a particular floor will be spread out throughout a particular corridor like a wave (or like cotton candy), but no electron can exist between floors. An electron can make a transition to a lower floor by

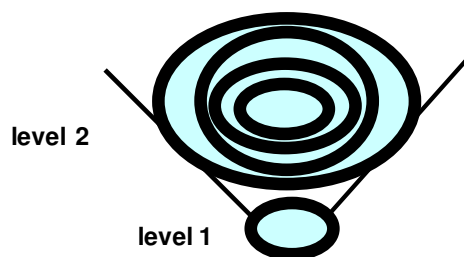


Fig. 5.4. A *simplified* representation of the energy levels, and the corresponding states, of an atom (showing the lowest two levels). As we go up this ‘energy-level skyscraper,’ there are more and more ‘corridors’ (shown as **black** ovals) representing the possible states of the electron. Each oval represents two states, one corresponding to spin up and the other to spin down.

coalescing long enough to enter the elevator. (This “coalescing” to enter an elevator is only meant metaphorically. The actual process cannot be followed that closely.) In this *particle-like* condition, the electron will give off energy in the form of a photon and wind up on a lower floor (a state of lower energy) where it will again spread out in one corridor. To go up, the electron must obtain the extra energy required to reach a higher floor. This may be accomplished by having a photon close enough for the electron to absorb it. It is significant for the stability of atoms that there is a ground floor, below which the electron cannot go — the atom will not collapse! Furthermore, only two electrons (spin up and spin down) can exist at the same time in any corridor, due to the exclusion principle.

*The number of electrons in a neutral atom equals the number of protons in the nucleus*, for the charges of the atom must add to zero. In an unexcited atom, the electrons *fill* the lower levels (floors), the more electrons, the higher the top of the *filled* states. Different elements (i.e., atoms) have different numbers of protons and that same number of electrons. Consequently, the electrons in one element fill to a different level, or a different corridor on the same level, from those in another element. All of the chemical properties of different elements result from this because chemical interactions and also the behavior of bulk material depend on interactions of the outer (highest energy) electrons of one atom with those of another. For example, hydrogen, with one electron behaves very differently in chemical reactions than does oxygen with eight, just because the other seven electrons of oxygen must all be in *different* states. A successful explanation of chemical behavior, even of organic molecules (that make up living organisms), has come from quantum mechanics.

In order that our skyscraper analogy be more faithful or realistic, we must imagine that the cone-skyscraper itself is invisible — we “see” only the electrons. Furthermore, the skyscraper would have to have an infinite number of floors, which are far apart near the bottom but are closer and closer together as we approach the roof, even though the roof is only a finite distance above the ground — impossible for an actual skyscraper, even an invisible one, but ordinary for an atom. Yes, there are, indeed, an infinite number of bound states bunched up like that. (In practice, any electrons near the top, i.e., that are very loosely bound, are so easily pulled away from the atom that they behave as if they are free.) Looking down from a helicopter, we see a two-dimensional pattern that looks somewhat like the electron distribution in an atom. (This metaphorical skyscraper is not a completely accurate representation of an atom. The wavefunctions are actually spread beyond their “corridors,” and the atom is a more complicated *three-dimensional* object.)

### 3. QUANTUM FIELDS

As we have already seen, when electromagnetic waves (light, etc.) are sent through a two-slit barrier, they produce an interference pattern looking like that expected for a *classical wave*. However, when we use *extremely dim* light and a screen made

of small sensitive detectors, we find that the light does not spread out across the screen as a classical wave would. Instead, one tiny detector at a time receives light, just as for electrons. Thus, we verify that light and all electromagnetic waves are made of particles — photons. It is apparent, from the *interference* pattern (made of spots) that builds as more and more photons reach the screen, that the individual photons must be conforming to a probability distribution much as the electrons did in a similar interference experiment. Photons are *quantum particles* whose wavelike characteristics have been apparent to us for about two centuries; however, it wasn't until the first part of the twentieth century that we realized that electromagnetic “waves” were actually composed of photons. Even fairly dim light corresponds to so many billions of photons that we cannot distinguish the individual flashes; that is why this point-like behavior of light was not seen before the development of very sensitive detectors.

The first evidence of the inadequacy of classical electromagnetic theory to account for the behavior of electromagnetic waves was found in the study of electromagnetic radiation from hot objects (technically called “black-body radiation”). At the beginning of the twentieth century, Max Planck found that the relative intensities (brightnesses) of the different frequencies contained in blackbody radiation could be understood only if that electromagnetic radiation were being emitted in *quantized* amounts. After subsequent elaboration by Einstein and others, over a period of about fifteen years, it was understood that electromagnetic waves were actually made of photons; the quantized amounts of radiation were the energies of the individual photons. Each photon has an energy equal to the *product* of Planck's minute constant ( $h$ ) *with* the frequency ( $f$ ) of the wave associated with that photon. Consequently, the electromagnetic energy of frequency  $f$  in an electromagnetic “wave” must be the *product* of the number of photons *times* the tiny energy of each one ( $hf$ ). Thus the energy of an electromagnetic wave of frequency  $f$  is quantized in units of  $hf$  (just as prices in the supermarket are quantized in units of pennies). Each photon of frequency  $f$  carries the same (tiny) amount of energy, whether the light is dim or bright — *the more intense* the radiation *the more photons* present. Since Planck's constant  $h$  is an incredibly small number, it is understandable that this quantization was not noticed earlier.

Let us now enlarge our electromagnetic vocabulary: An electromagnetic wave has a definite strength and direction for the electric disturbance and a definite strength and direction for the magnetic disturbance *at each point in space*. The situation is somewhat analogous to the lawn in front of my house. At each point on the lawn, there is a blade of grass with a definite height pointing in a definite direction. (Those places that are bare have a blade of height zero.) The height corresponds, in this analogy, to the strength of the electric or magnetic disturbance under consideration and the direction corresponds to its direction. This analogy to a *field* of grass leads to the characterization of the electric disturbances as an electric *field*, and the magnetic disturbance as a magnetic *field*; the wave, containing

both, is referred to as an electromagnetic *field*. (We also use “electromagnetic field” generically to refer to either one or any possible combination of electric and magnetic fields.) Although my lawn is a two-dimensional field, *electromagnetic fields* exist in three-dimensions, and so *are three-dimensional fields*.

Since electromagnetic waves are made of photons, we conclude that the electromagnetic field (a wave) plays a (roughly) similar role for them as does the wavefunction for electrons. Thus, the electromagnetic field is a *quantum field*. The behavior of this quantized field is explained by a quantum field theory called *quantum electrodynamics* (QED). The birth pangs of the photon concept lasted about two decades from Planck’s 1901 discovery, and it wasn’t until the 1940s that the complete theory of quantum electrodynamics was successfully formulated.

Let us review the essential features of the electromagnetic field. The energy of the electromagnetic field is not spread out like a classical wave, but instead is concentrated in quantized *bundles* — the photons. For a given frequency, each photon has the same tiny amount of energy. Strong fields have very many photons, each with that tiny amount of energy, and weaker fields have correspondingly fewer photons. The photons follow probabilities that are determined by the electromagnetic fields.