Order of Magnitude Estimates in Quantum

As our second step in understanding the principles of quantum mechanics, we'll think about some order of magnitude estimates. These are important for the same reason they always are: they allow quick assessment of models or effects for importance, so that if necessary we can then make more accurate calculations.

The effect we'll focus on is one that may seem surprising. The uncertainty principle doesn't just limit precision in measurement. Remarkably, it also produces a host of other effects, including the appearance of a new type of energy and new forces! We'll explore these principles in a couple of different ways, then look at applications.

Suppose that you confine a particle within a box of size Δx. **Ask class:** according to the uncertainty principle, what is the lower limit on the uncertainty about the momentum of this particle? Since we have $\Delta x \Delta p \gtrsim \hbar$, then the uncertainty in the momentum is $\Delta p \gtrsim \hbar/\Delta x$. So far, so good. However, the next step may not be as obvious: if the magnitude of the momentum itself were to be less than $\hbar/\Delta x$, then we would know the momentum to more than the allowed accuracy of $\hbar/\Delta x$. Therefore, $|p| \gtrsim \hbar/\Delta x$!

If you're not convinced, we can do a little quantum mechanics on the cheap to motivate this further. Suppose as before that we confine a particle within a box of size Δx. Let the box have strong walls that are infinitely thick and high. This means that the particle has zero probability of being outside the box. From the postulates of quantum mechanics, this implies that the squared modulus of the wavefunction is zero outside the box as well. However, the probability must integrate to unity over all space. Therefore, all of the probability has to be confined to the box, within a distance Δx. In addition, further investigation reveals that the probability cannot be discontinuous (this is not something that follows immediately from the axioms we've discussed, but is true anyway). Thus the probability has to vanish at the sides of the box, and must integrate to 1 over the box.

Imagine, then, that the wavefunction can be represented by something like $\sin(x/\lambda)$, where λ is the wavelength of the probability function inside the box and we choose this form because it can have zeros at periodic intervals. **Ask class:** what do these conditions imply about λ? If there is a zero at, say, $x = 0$ and $x = \Delta x$, then we know $\lambda = \Delta x/(\pi n)$, where n is a positive integer. That's the only way to have zeroes at the right places. In particular, it means that the wavelength cannot be any *more* than $\Delta x/\pi$. You may worry that this is the result of a special choice of wavefunctions, but in fact since any function may be represented by the sum of sines and cosines (that is, in a Fourier series), it is roughly the case that no term in that series may have a wavelength longer than $\Delta x/\pi$, otherwise the boundary conditions wouldn't be satisfied.

For our next step, let's pretend that the particle acts like a photon, so we have a definite relation between the wavelength and the momentum. **Ask class:** what is the momentum of a photon with wavelength λ? The momentum is simply $p = h/\lambda$. Therefore, the *minimum* momentum of the particle is $p_{\rm min} = h/(\Delta x/\pi)$. Ignoring factors of π and the like, we again find $p \gtrsim \hbar/\Delta x$. Note that it doesn't make sense to be overly precise at this point, because the true minimum momentum will depend on the shape of the box (or more physically, on the functional form of the confining potential).

Now, of course, there's nothing to prevent the momentum from being *larger* than this value. For a particle in a box, it is perfectly legal for the wavelength of the wavefunction to be smaller than $\Delta x/\pi$, as long as an integral number of wavelengths fit inside the box. However, unlike in classical physics, there is a lower limit to the momentum. Note, incidentally, that the lower limit is proportional to $\hbar$. The appearance of Planck's constant in anything at all tells us that quantum mechanics is important, and to get the classical limit you can set $\hbar \to 0$. Similarly, if you ever see c, the speed of light, you know that relativity is important, and if you ever see G, the gravitational constant, you know that gravity is important. This gives you another way to check your equations quickly.

What other consequences does this have? If a particle has momentum, it has energy. Suppose that the momentum is very nonrelativistic, i.e., $p_{\rm min} \ll mc$, where m is the rest mass of the particle. **Ask class:** what is the kinetic energy of a particle of momentum p? It's $p^2/2m$ in the nonrelativistic limit. Therefore, the minimum energy is $E_{\rm min} \approx p_{\rm min}^2/2m$, or $\sim (\hbar/\Delta x)^2/2m$. **Ask class:** what if the momentum is highly relativistic? Then, as with photons, $E \approx pc$, or $E_{\rm min} \approx \hbar c/\Delta x$. Therefore, even if the particle has no other source of energy (e.g., normal kinetic energy or thermal energy), it will have this energy. This energy, based on the uncertainty principle, is called *Fermi energy*, and is written E_F. Similarly, the minimum momentum is called the Fermi momentum, and written p_F.

What applications does this have? For one, think about states of matter. In normal experience, a substance is a gas when its thermal energy is larger than the Coulomb energy between individual molecules (more or less; there's actually a factor between those energies, but we'll ignore it in this simple treatment). As the substance cools down, there comes a point when the thermal energy is smaller than the Coulomb energy, then the substance becomes a liquid. At even smaller temperatures, the lattice energy (i.e., the energy benefit of arranging molecules in a regular order) is larger than the thermal energy, and the substance becomes a solid. If thermal energy were the only competitor to these effects, then all substances would become solid at a small enough temperature. However, we also have to worry about Fermi energy. Even if the temperature is absolute zero, there is some residual energy left and if that energy is greater than the lattice energy, the substance won't become a solid. This is actually the case for helium at atmospheric pressure. Helium is so symmetric that it has just a tiny lattice energy, which is enough less than the Fermi energy that helium stays a liquid. If the pressure is boosted to about 30 atmospheres, then helium can become a solid because of enhanced lattice energy, but at normal pressures this is dramatic proof of the importance of Fermi energy!

We can therefore, roughly, divide up substances into whether thermal energy or Fermi energy is more important, i.e., whether $kT > E_F$ or $E_F > kT$. If the former is true, especially if $kT \gg E_F$, then we have more or less classical statistics. If $E_F > kT$, especially if $E_F \gg kT$, then quantum statistics dominate and the material is called *degenerate*. If the material is degenerate, then we need to know whether it is relativistic or nonrelativistic. For fully ionized normal material, electrons have a relativistic Fermi energy (i.e., $E_F \sim m_e c^2$) at a density $\rho \sim 10^6$ g cm^{-3}. The boundary scales as m^3, so neutrons and protons have relativistic Fermi energies at much, much, higher densities. Note the distinction: degeneracy depends on the comparison between Fermi energy and temperature, so it can happen whether or not the components are relativistic.

For Perspective: am I degenerate? In the old days we'd figure this out by considering my deeds and bad habits, but now we can answer it mathematically! **Ask class:** what do we need to determine? We need to figure out the Fermi energy of my constituents, then compare it to my thermal energy. **Ask class:** if there are plenty of free particles of all kinds, what kind of particle would be degenerate first? Electrons, because they have lower mass and $E_F \propto 1/m$ for nonrelativistic. **Ask class:** is the nonrelativistic limit the correct one? Yes, because 10^6 g cm^{-3} is the rough boundary, and I'm nowhere near that!

In the examples above we've discussed matter that is completely ionized, so that electrons are free to move around as they will. However, in me the electrons are mostly not free. Instead, typically there are ions. So, let's calculate first what the Fermi energy is assuming the dominant species is a molecule of some sort. What is the most common molecule? Water, of course. Water has an atomic weight 18 times that of hydrogen, or about 20 times that of the neutron, roughly speaking. The critical density at which the Fermi energy becomes relativistic goes like M^3, so for water it is about $20^3 \approx 10^4$ times that for neutrons, or about 6×10^{19} g cm^{-3}. Below this density the Fermi energy is nonrelativistic, and therefore goes like $p^2 \sim n^{2/3}$. At my density of ~ 1 g cm^{-3}, the Fermi energy is therefore $\sim 10^{-13}$ times the rest mass energy of water, or $10^{-13}\times 20$ GeV$=2 \times 10^{-3}$eV. The equivalent temperature for 1 eV is about 10^4 K, so this equates to about 20 K versus about 300 K for the temperature. Sadly, most of my mass is not degenerate! Of course, this is also true for, say, a white dwarf, where the mass is dominated by nondegenerate nucleons but the degenerate electrons provide the pressure.

But there may still be hope for me! Suppose that I have some small fraction of free electrons running around in me. In particular, suppose that there are about 10 electrons per molecule, and that about 1% of molecules have donated 1 electron to the general environment. The density of free electrons is therefore 10^{-3} times the density it would be if all atoms were completely ionized. For the purpose of this calculation, therefore, it's as if I were completely ionized but had a density of about 10^{-3} g cm^{-3}. Using the same approach as before, we know that for electrons the density at which relativistic degeneracy starts is about 10^6 g cm^{-3}, and that below this the Fermi energy scales as $p^2 \sim n^{2/3}$. Therefore, at 10^{-9} of this density the energy is 10^{-6} of the electron rest mass energy, or 0.5 eV. This equates to ∼5000 K, meaning that my electrons would be degenerate by a factor of more than 10! Woohoo! Unfortunately, J. Norman Hansen, professor of chemistry and biochemistry at Maryland, says that in biological systems free electrons essentially don't exist, because as soon as one would be stripped off of a molecule it would go to another one, and hence electrons spend time in one orbital or another. Thus, tragically, I'm not degenerate :).

Let's try another application. In this one, we will derive a maximum mass for white dwarfs and neutron stars, which are supported by degeneracy pressure. What we mean by that is that the Fermi energy is so much larger than the thermal energy in the bulk of the star that we may as well ignore thermal effects. Then, the star is in hydrostatic support with a pressure gradient based on Fermi effects rather than, say, ideal gas pressure.

Suppose there are N particles supplying the pressure in a star of radius R, so that the number density is $n \sim N/R^3$ (note that we are dispensing with factors of order $4\pi/3$). **Ask class:** what is the typical distance between particles? It's about $\Delta x \sim n^{-1/3}$. **Ask class:** therefore, what is the approximate Fermi momentum? Roughly $p_F = \hbar/\Delta x = \hbar n^{1/3}$. **Ask class:** if the material is nonrelativistic and the mass of the particles supplying the Fermi pressure is m, what is the Fermi energy per particle? It is $E_F \approx p_F^2/2m \approx \hbar^2 n^{2/3}/2m \approx \hbar^2 N^{2/3}/(2mR^2)$. We now consider the gravitational energy; note that most of the mass is in baryons (neutrons and protons), even if the particles providing the Fermi energy are electrons. Therefore, the mass per particle of interest is roughly m_B, the mass of a baryon. If the star has mass M and radius R, **Ask class:** roughly what is the gravitational potential energy per particle? It is on the order of $E_G = -GMm_B/R = -GNm_B^2/R$. Therefore, the total energy per degenerate particle in the nonrelativistically degenerate case is

$$E_{\rm tot} \sim \frac{\hbar^2 N^{2/3}}{2mR^2} - \frac{GNm_B^2}{R}\ . \tag{1}$$

The star will minimize its total energy given the constraints, and since the radius is the only free variable here, the radius will change so that E is as low as possible. Note that the positive term goes like R^{-2} whereas the negative term goes like R^{-1}, so the star can't contract indefinitely. Therefore, in the nonrelativistic regime, the star is stable.

What about the relativistic regime? **Ask class:** when the Fermi momentum is relativistic, what is the approximate Fermi energy? It is $E_F \approx p_F c \approx \hbar c N^{1/3}/R$. Then the total energy per relativistically degenerate particle is

$$E_{\rm tot} \sim \frac{\hbar c N^{1/3}}{R} - \frac{G N m_B^2}{R} \ . \tag{2}$$

Now, the radial dependences are the same for both terms. If this energy is positive, the star minimizes its energy by increasing R. In doing so, it eventually becomes nonrelativistic, at which point it becomes stable. However, if the total energy is negative, then the star decreases its energy by decreasing R, making the particles even more relativistic, so the star contracts further, and so on. This is unstable. The stability threshold is therefore reached when $E_{\rm tot} = 0$, which happens when the particle number reaches

$$\begin{aligned} N_{\rm max} &\sim [\hbar c/(G m_B)^2]^{3/2} \sim 2 \times 10^{57} \\ M_{\rm max} &\sim N_{\rm max} m_B \sim 1.5\, M_\odot \ . \end{aligned} \tag{3}$$

This is called the *Chandrasekhar limit*. White dwarfs or neutron stars much more massive than this can't exist. We have cheated a little in the numerical factors, and for neutron stars in particular there are other effects that may move the maximum mass up to $2.2\, M_\odot$ or so, but this is the basic physics.