Chapter 3

Uncertainty principle

Now it is *Amperé's hypotheis* that the source of all magnetic fields is the motion of charges. In particular, magnetic dipole moments arise from the circulation of charge. Thus, there must be a relation between a mechanical property of the atom, referring to that circulation, and the magnetic dipole moment of the atom. That mechanical property is the angular momentum (or *spin*) of the atom, $\mathbf{J}$. We can anticipate that $\boldsymbol{\mu}$ is proportional to $\mathbf{J}$, or

$$\boldsymbol{\mu} = \gamma \mathbf{J}, \tag{3.1}$$

where the constant of proportionality γ is called the *gyromagnetic ratio.* (An example of this was given in Problem 3, Assignment 1.)

The startling conclusion of the Stern-Gerlach experiment that for Ag atoms μ_z takes on only 2 values, means that J_z take on only two discrete values as well, for Ag atoms:

$$\mu_z = \gamma J_z \Rightarrow J_z = \pm |J_z|. \tag{3.2}$$

The magnitude of the two values must be the same, since there is no fundamental difference between up and down. The result of the Stern-Gerlach experiment means that there is a natural unit of angular momentum, here given by the difference of the two physical values of the spin:

$$(J_z)_+ - (J_z)_- = \hbar = \frac{h}{2\pi}, \tag{3.3}$$

where Planck's constant (1900), also called the quantum of action, has the experimental value

$$\hbar = 1.0545717 \times 10^{-27}\,\text{erg sec}. \tag{3.4}$$

(Action is a quantity which has dimensions of [energy×time] = [momentum× distance], that is, it has units g-cm^2/s. Angular momentum has the same dimensions.) $(J_z)_+ - (J_z)_-$ is the same for all atoms for which J_z can take on only two values. This reflects the universality of angular momentum, the properties of which make fundamental reference to three-dimensional space, as we will see later.

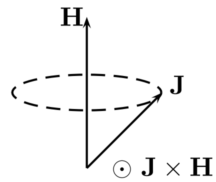

Figure 3.1: If γ is positive, the torque exerted on a magnetic dipole by a fixed magnetic field $\mathbf{H}$ causes the angular momentum $\mathbf{J}$ to precess in a clockwise (negative) sense around the direction of $\mathbf{H}$, keeping a constant angle with respect to $\mathbf{H}$.

Since, for a "two-level" atom

$$(J_z)_+ = -(J_z)_-, \tag{3.5}$$

we see that

$$(J_z)_\pm = \pm\frac{1}{2}\hbar. \tag{3.6}$$

We therefore call this a spin-1/2 atom.

How big is a typical gryromagnetic ration?

$$\gamma = \frac{(\mu_z)_+}{(J_z)_+} \sim \frac{10^{-20}\text{erg/G}}{10^{-27}\text{erg s}} = 10^7\,\text{G}^{-1}\text{s}^{-1}. \tag{3.7}$$

Since this is a large number, it means that it takes a very weak field to make an atomic dipole precess. Consider the torque exerted on an atom by an applied magnetic field,

$$\boldsymbol{\tau} = \boldsymbol{\mu}\times\mathbf{H} = \gamma\mathbf{J}\times\mathbf{H} = \frac{d\mathbf{J}}{dt}, \tag{3.8}$$

since, according to Newton, the torque gives the time rate of change of the angular momentum. This equation implies that $\mathbf{J}$ precesses around a constant magnetic field: $\mathbf{J}$ sweeps around $\mathbf{H}$, at a constant rate, keeping a fixed angle with respect to $\mathbf{H}$, as sketched in Fig. 3.1.

Adopt a coordinate system in which $\mathbf{H}$ lies along the z-axis. Then, our equation of motion reads

$$\frac{dJ_z}{dt} = 0, \quad \frac{dJ_x}{dt} = \gamma J_y H, \quad \frac{dJ_y}{dt} = -\gamma J_x H. \tag{3.9}$$

Convert this system of first order equations into a single second-order one:

$$\frac{d^2J_x}{dt^2} = \gamma\frac{dJ_y}{dt}H = -\gamma^2H^2J_x. \tag{3.10}$$

If at $t=0$, $J_y = 0$, the solution is

$$J_x = A\cos\omega t, \quad J_y = -A\sin\omega t, \tag{3.11}$$

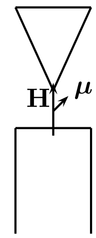

Figure 3.2: An atom with dipole moment $\boldsymbol{\mu}$ polarized at an angle θ with respect to the field of a Stern-Gerlach apparatus.

where the precession frequency is

$$\omega = \gamma H. \tag{3.12}$$

If $\gamma > 0$, the precession is clockwise, that is, in the negative sense. The angle through which the dipole precesses in a time t is $\phi = \omega t = \gamma H t$. If the atom has speed v and passes through a magnet of length ℓ, $t = \ell/v$, and

$$\phi = \gamma H \frac{\ell}{v}. \tag{3.13}$$

How large a field is required to induce a precession through one radian $= 57°$? Take $\ell = 1$ cm, $v \sim 10^4$ cm/s, $\gamma \sim 10^7$; then it would take a field of only $h \sim 10^{-3}$ G, which is very weak indeed, considering that the earth's field is ~ 1 G.

We are trying to learn how to construct a new mechanics, by exploiting the paradoxes which emerge when classical mechanics is applied to atomic physics. We'll see one such paradox by considering the repeated Stern-Gerlach experiment in another way.

Supose we have selected atoms in a first measurement which have a definite orientation of the magnetic moment. Send these atoms into a second Stern-Gerlach apparatus. In the second apparatus, $\mathbf{H}$ is not parallel to $\boldsymbol{\mu}$, so $\boldsymbol{\mu}$ will precess about $\mathbf{H}$, as sketched in Fig. 3.2. Suppose that we choose matters so that the precession is through a multiple of 2π; then when the atom leaves the magnetic field of the second apparatus it will have the same orientation as when it entered the field. Now send this beam of atoms through a third apparatus, oriented in the same direction as the dipoles. All the atoms should be deflected "up" relative to that magnet.

Is this really what happens? No! In fact, we already know how to figure out what happens. The second apparatus splits the beam into two, with probability of deflecting up equal to $\cos^2\theta/2$ and probability of deflecting down equal to $\sin^2\theta/2$. Now keep these two beams together and inject it into the third apparatus. The third apparatus splits *each* beam into two again. The probability of the atoms coming out of the third apparatus with the orientation they had upon entering the second apparatus is

$$p_{32}(+,+) = p_3(+,+)p_2(+,+) + p_3(+,-)p_2(-,+)$$

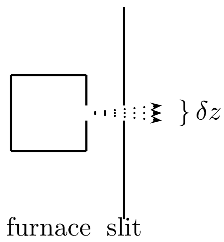

Figure 3.3: Atomic beam emerging from the furnace, collimator arrangement. Note that there is a spread in the z position of the atoms, δz.

$$= \cos^2\frac{\theta}{2}\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\sin^2\frac{\theta}{2} = \cos^4\frac{\theta}{2} + \sin^4\frac{\theta}{2}$$
$$= \left(\frac{1+\cos\theta}{2}\right)^2 + \left(\frac{1-\cos\theta}{2}\right)^2 = \frac{1+\cos^2\theta}{2} < 1. \qquad (3.14)$$

We cannot predict the outcome for a single atom; some of the atoms are deflected "down" by the second apparatus. Of course, if the second apparatus were not present, the third apparatus would deflect all atoms "up." An intermediate measurement has changed the outcome!

What do we learn from this failure of the classical analysis? We assumed we could precisely control how the dipole precesses. We see this is not true provided the Stern-Gerlach experiment acts as we assumed to split the beam. Now, note that we connot control the position of the beam exactly, as shown in the sketch of the atoms leaving the furnace, Fig. 3.3. There is a spread in the z position of the beam, δz. The defining aperture cannot be of zero size, otherwise no beam will get through. But recall that $H_z(z)$ inside the Stern-Gerlach apparatus depends on position, so the different atoms in the beam will experience slightly different fields, depending on their z position:

$$\delta H_z = \frac{\partial H_z}{\partial z}\delta z. \qquad (3.15)$$

This means that the different atoms will precess by different amounts:

$$\delta\phi = \gamma\frac{\partial H_z}{\partial z}\delta z\frac{\ell}{v}. \qquad (3.16)$$

Also, the atoms are not moving exactly along the same line, so they will have a small spread in the z-component of momentum, δp_z.

To perform the Stern-Gerlach experiment, the transfer of momentum due to the inhomogeneity of the field must be much larger than this, at least

$$(\Delta p_z)_+ - (\Delta p_z)_- > \delta p_z, \qquad (3.17)$$

where $(\Delta p_z)_\pm$ is the momentum acquired by the upward- and downward-deflected beams respectively, in the Stern-Gerlach apparatus due to the inhomogeneous magnetic field. Since this momentum is [(2.17)]

$$\Delta p_z = \mu_z \frac{\partial H_x}{\partial z} \frac{\ell}{v}, \tag{3.18}$$

and

$$\mu_z = \gamma J_z, \quad (J_z)_+ - (J_z)_- = \hbar, \tag{3.19}$$

we have

$$(\Delta p_z)_+ - (\Delta p_z)_- = \gamma \frac{\partial H_z}{\partial z} \frac{\ell}{v} \hbar. \tag{3.20}$$

Comparing this with the spread in precession angles, we see

$$\hbar \delta\phi = [(\Delta p_z)_+ - (\Delta p_z)_-]\, \delta z > \delta p_z \delta z \tag{3.21}$$

for the Stern-Gerlach experiment to work. Now, classically $\delta p_z \delta z$ could be as small as you please. But we know $\delta\phi$ cannot be arbitrarily small, in fact, it must be that $\delta\phi \sim 1$. This suggests that

$$\delta p_z\, \delta z \gtrsim \hbar. \tag{3.22}$$

This is the famous (Heisenberg) *uncertainty relation*. We cannot perform measurement of z, p_z together with arbitrary precision.

This all comes back to the process of defining a beam by a slit. If $\delta\theta$ is the angular spread of the beam emerging from the collimating slit,

$$\delta p_z = p\, \delta\theta, \tag{3.23}$$

if the particles all emerge from the oven with momentum p. So the uncertainty relation reads

$$\delta z\, \delta\theta \gtrsim \frac{\hbar}{p}. \tag{3.24}$$

The smaller the slit (the smaller δz) the larger the divergence angle ($\delta\theta$). This is reminiscent of the *diffraction* phenomena occuring with waves. With a wave of wavelength λ impinging on a slit of width δz, the diffraction angle is

$$\delta\theta \sim \frac{\lambda\!\!\!^{-}}{\delta z}, \quad \lambda\!\!\!^{-} = \frac{\lambda}{2\pi}. \tag{3.25}$$

So we see that particles, to some extent, act like waves. The "wavelength" of the particles is

$$\lambda\!\!\!^{-} = \frac{\hbar}{p}, \quad \lambda = \frac{h}{p}. \tag{3.26}$$

This is the *de Broglie wavelength*.

Classically, the concepts of particles and waves are at the extremes—the epitome of localized and distributed objects. In the atomic world we must transcend both the particle and wave pictures.

From the uncertainty principle we can now offer a hueristic explanation for the stability of atoms. Consider a hydrogen atom, which consists of an electron, with charge $-e$ and a very heavy nucleus, of charge $+e$. If the mass of the electron is m, and the motion of the nucleus is neglected, the energy of the atom is

$$E = \frac{p^2}{2m} - \frac{e^2}{r}. \tag{3.27}$$

If the classical idea that the electron radiates its energy away were true, the electron would fall in toward the nucleus, and the energy would become more and more negative. (Recall that ignoring radiation, the virial theorem says $E = \bar{V}/2$.) But in real atoms, the energy is bounded from below. The reason for this is the uncertainty relation. It is not too much of a stretch of the imagination to suppose for the radial components,

$$\delta r\, \delta p_r \gtrsim \hbar, \tag{3.28}$$

or for typical atomic values

$$p_r \sim \frac{\hbar}{r}. \tag{3.29}$$

Then the energy is roughly

$$E \sim \frac{1}{2m}\left(\frac{\hbar}{r}\right)^2 - \frac{e^2}{r}, \tag{3.30}$$

and for small enough r, the kinetic energy dominates as shown in Fig. 3.4. What is the minimum energy, $E_{\rm min}$? It is obtained by differentiating E with respect to r:

$$0 = \frac{\partial E}{\partial r} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{r^2}, \tag{3.31}$$

which give the minimum radius $r = \hbar^2/me^2$, or the minimum energy

$$E_{\rm min} = -\frac{1}{2}\frac{me^4}{\hbar^2}. \tag{3.32}$$

This turns out to be nearly exact for the ground state of the H atom.

There is another simple, but misleading, picture of atoms, in terms of de Broglie waves. When the electron moves in a circular orbit about the nucleus, there is a wave associated with it. For these pictures to be compatible, there must be an integral number of wavelengths in one circuit, otherwise the waves will destructively interfere. Thus

$$2\pi r = n\lambda, \quad n = 1, 2, 3, \ldots, \tag{3.33}$$

or

$$r = \frac{n\lambda}{2\pi} = n\bar{\lambda} = n\frac{\hbar}{p}, \tag{3.34}$$

or

$$rp = n\hbar. \tag{3.35}$$

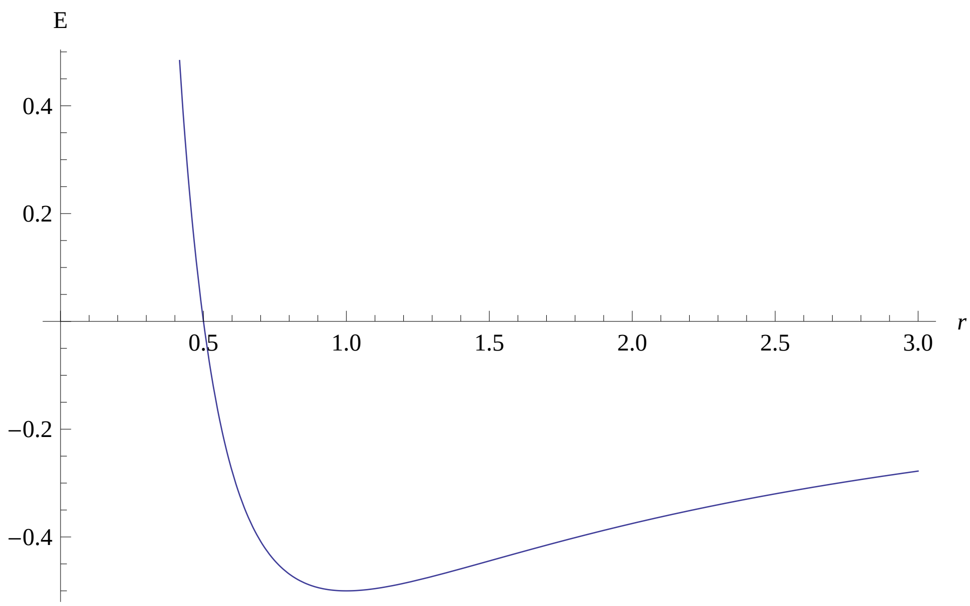

Figure 3.4: The energy estimate given by Eq. (3.30), showing that the energy of an electron in an atom is bounded from below. In this graph, the units adopted are $m = \hbar = e = 1$, which are sometimes called atomic units.

Since rp is the orbital angular momentum, this says angular momentum comes in units of $\hbar$, which is consistent with what we learned from the Stern-Gerlach experiment. (This justifies saying $\lambda = h/p$ exactly.)

Now calculate the energy:

$$E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{1}{2m}\frac{n^2\hbar^2}{r^2} - \frac{e^2}{r}. \tag{3.36}$$

This generalizes the picture seen in Fig. 3.4. The condition for equilibrium is $E = E_{\text{min}}$, where E_{min} is determined from

$$0 = \frac{\partial E}{\partial r} = -\frac{n^2\hbar^2}{mr^3} + \frac{e^2}{r^2}, \tag{3.37}$$

which has solution

$$r = \frac{n^2\hbar^2}{me^2}, \tag{3.38}$$

so we see the virial theorem result again,

$$E_{\text{equil}} = -\frac{1}{2}\frac{e^2}{r} = -\frac{me^4}{2n^2\hbar^2}, \quad n = 1, 2, 3, \ldots. \tag{3.39}$$

This is Bohr's famous formula (1913). He assumed that the angular momentum was an integral multiple of $\hbar$. Here, we've advanced beyond Bohr by introducing the wave picture.

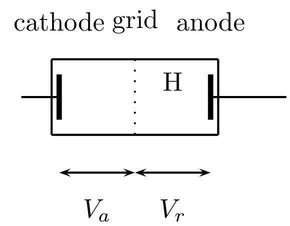

Figure 3.5: A accelerating voltage V_a accelerated electrons through a chamber containing hydrogen gas. The electrons pass through a grid, following which they experience a small retarding voltage V_r. The current passing through the chamber is measured as a function of accelerating voltage.

According to this result, the H atom assumes only these discrete energy values, these *energy levels*, and no others. Direct evidence for this picture was provided by Franck and Hertz in 1914. (They were aware of Bohr's work, but uninfluenced by it.) They accelerated electrons through an electric field in the presence of H gas, as shown in Fig. 3.5. Because of the hydrogen gas, electrons undergo collisions with the gas and lose energy. If the electron does not have enough kinetic energy to overcome the retarding voltage, it will not reach the anode. As V_a increase, the current increases, as more electrons have sufficient energy. But then at a certain critical energy, the current suddenly drops. Why? Because the electrons now have enough energy to excite the gas atoms to the $n = 2$ level. The current increases again for larger V_a, but at a still higher energy, there is again a sudden drop in current, when the electrons have sufficient energy to excite the atoms to the $n = 3$ level. See Fig. 3.6 for a sketch of the result. In order to excite atoms from the $n = 1$ to the $n = 2$ level, the energy of the electron had to be at least

$$E_{\rm el} = E_2 - E_1 = \left(\frac{1}{4} - 1\right) E_1 = \frac{3}{4}(-E_1), \tag{3.40}$$

which is a positive quantity since E_1 is negative. Finally, there is enough energy to drive the electron out of the atom, to ionize it. Then the electrons knocked out of the atoms give a greatly increased current. This ionization energy is

$$E_{\rm ion} = 0 - E_1 = \frac{me^4}{2\hbar^2}. \tag{3.41}$$

This provides a direct experimental method of measuring $\hbar$. (The treatment is approximate, since the nuclear motion is ignored—see homework.) Measurements give for the ionization energy of H the value $E_{\rm ion} = 13.61$ eV. Here we have introduced the convenient energy unit, the electron volt, abbreviated eV, which is the energy acquired by an electron accelerated through a potential of 1 V. Since from deflection and oil-drop experiments we knew that the mass of the electron is

$$m = 9.10938215(45) \times 10^{-31}\,\text{kg}, \tag{3.42}$$

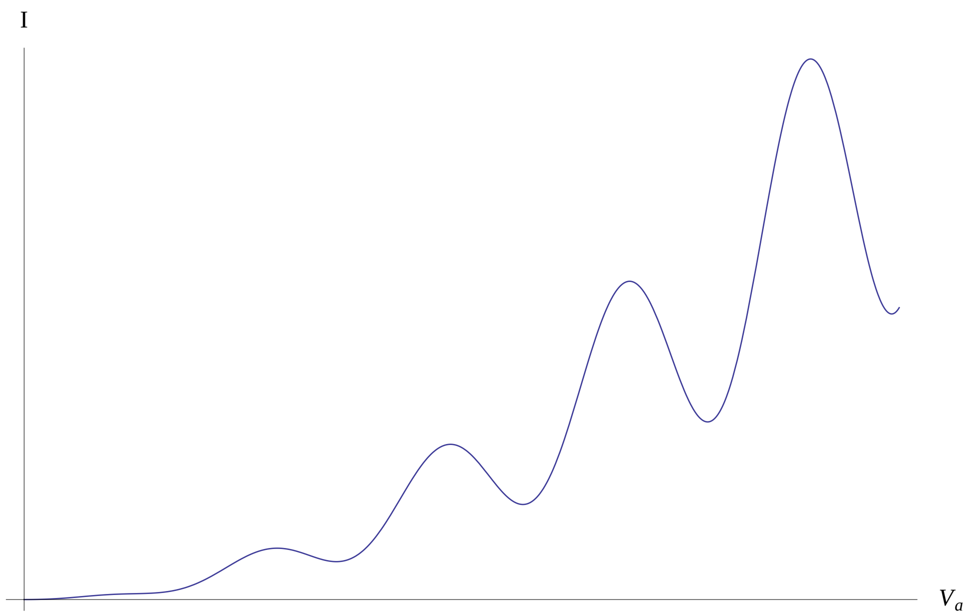

Figure 3.6: The current flowing through the Franck-Hertz chamber as a function of the accelerating voltage. Sharp dips occur at certain critical voltages, corresponding to the energies required to excite the atoms in the gas to higher energy levels.

which is most conveniently given in terms of the equivalent rest energy,

$$mc^2 = 0.510998910(13)\,\mathrm{MeV}. \tag{3.43}$$

Here the speed of light is *defined* as

$$c = 299792458\,\mathrm{m/s} \tag{3.44}$$

exactly. The electronic charge is

$$e = 1.602176487(40) \times 10^{-19}\,\mathrm{C} = 4.80320427(12) \times 10^{-10}\,\mathrm{esu}. \tag{3.45}$$

Since the above formula is given in Gaussian units (there are factors of $4\pi\epsilon_0$ in SI), we have

$$\hbar^2 = \frac{0.5110 \times 10^6\,\mathrm{eV}}{2 \times 13.61\,\mathrm{eV}} \frac{(4.803 \times 10^{-10}\,\mathrm{esu})^4}{(2.998 \times 10^{10}\,\mathrm{cm/s})^2}, \tag{3.46}$$

and taking the square root,

$$\hbar = 1.054 \times 10^{-27}\,\mathrm{erg\ s}, \tag{3.47}$$

to be compared to the best current value

$$\hbar = 1.054571628(53) \times 10^{-34}\,\mathrm{J\ s}. \tag{3.48}$$

(The numbers are the current best values with the uncertainty in the last digits indicated.)

The Franck-Hertz experiment directly demonstrates the reality of the discreteness of the energy levels in atoms. Yet it is much more precise to determine these levels by measuring the energy released as light when the atom returns to the ground, $n = 1$, state.

This picture not only gives the energies, but the atomic distance scale: the radius of the nth Bohr orbit is

$$r = n^2 a_0, \tag{3.49}$$

where a_0 is the Bohr radius, the radius of the first Bohr orbit,

$$a_0 = \frac{\hbar^2}{me^2} = 5.2917720859(36) \times 10^{-11}\,\mathrm{m}. \tag{3.50}$$

The 10^{-8} cm scale of atoms was known in the 19th century.

It is important to note that what we have done here, although it leads to correct results, is still not a consistent theory. Quantum mechanics lies ahead. But a kernel of truth is here, although what Bohr did was a mass of contradictions.