Abstract

Nuclear Magnetic Resonance (NMR) is an important part of modern life. In medicine it is called Magnetic Resonance Imaging and used as a safer way to see inside of patents because the patent is not exposed to high intensity photons like during X-rays. Additionally, NMR is used in a variety of industries in order to examine materials for imperfections or weaknesses. A third major use of NMR is discovering the chemical makeup and bonds of complex proteins, potential drugs, and industrial materials. Unfortunately, because NMR is based on a quantum mechanical phenomena, it is difficult for a large percentage of people who benefit from NMR to understand how it works. The goal of this program is to explain one of the simplest forms of NMR, continuous wave NMR in order for more people to know the fundamentals of this versatile and increasingly ubiquitous technology.

1 Basics of Nuclear Magnetic Resonance

Every atom is made up of protons, neutrons, and electrons. Electrons have a negative charge and small mass and surround the nucleus in different energy level clouds. Protons have a positive charge and large mass and reside in the nucleus along with the neutrons which have no charge and comparable mass. Particles can be defined by their intrinsic properties, and for many, the intrinsic properties they know of are only charge and mass. NMR depends on a third intrinsic property called spin.

1.1 Spin

Spin is an intrinsic property of each subatomic particle. Note to reader, an object, no matter its composition will be referred to as a particle if that objects constituent particles are not of interest. This means that protons and entire atoms will be referred to as particles depending on the context. Spin, just like charge is quantized, that means that only certain values are allowed to exist. In fact, many more properties such as angular momentum are conserved, but spin quantization is the most will known. Particles are divided in to two categories: Fermions such as electrons, protons, and neutrons which have spins $\hbar/2$, $3\hbar/2$,

... $(2n\hbar+1)/2$ ... and Bosons such as photons and alpha particles which have spins of integer $\hbar$. The spin can be compared to the spin of a globe. This is a limited analogy because while a globe can spin in any direction, a particle can only spin "upish" or "downish" no matter what orientation is chosen to measure a particle's spin. This is because quantum mechanics states that it is impossible to know the exact orientation, position, and momentum of a particle. The only thing that matters to someone trying to understand NMR is that a particle will either have a spin up or spin down.

1.2 Magnetic Dipole Moment

A particle with spin can also posses a magnetic dipole moment if it is made up of charged particles. This is because if a particle has distributed charges and has spin "is spinning", a magnetic field is formed. As a result, the this dipole points in the same direction as the spin, either up or down. Because neutrons are composed of three charged quarks, protons, electrons, and neutrons all have a magnetic dipole moment. The equation for the magnetic moment of a particle is

$$\mu \approx \frac{q\hbar}{2m}$$

where q is the charge of the particle and m is the mass of the particle. In many cases, μ_z,

$$\mu_z = \mu \cdot \mathbf{B}$$

the part of the magnetic moment that is parallel or anti-parallel to an external magnetic field is the only part of μ of interest.

It is this dipole moment that a NMR machine will detect. However, because electrons, protons, and neutrons are Fermions, no two particles can have identical quantum numbers, numbers that function as an address in a given atom. This results in electrons forming energy shells around the nucleus of an atom and protons and neutrons forming energy shells inside of the nucleus. Because of this, particles will pair up with another particle with the almost identical quantum numbers except that one particle will have spin up and the other will have spin down. This pairing causes many dipole moments to cancel each other out.

1.3 Detecting Differences in Spin

One can distinguish between particles with different spins by putting the object of interest in a strong magnetic field. An if a particles spin is parallel to the external field, it will be in a low energy state of $-|\mu_z\mathbf{B}|$ and if the spin is anti-parallel, it will be in a higher energy state of $|\mu_z mathbf B|$ with an energy difference of $\Delta E = 2\mu_z mathbf B|$. This energy difference can be matched to the energy of a photon with frequency

$$f = \frac{\Delta E}{h}$$

where a particle with a parallel spin can absorb a photon of corresponding frequency and flip to the higher energy anti-parallel state. Because each element has a different total μ, each element absorbs a different frequency of radio wave and can be told apart.

In continuous wave NMR, a sample is put in a strong magnetic field and a varying frequency, but constant magnitude radio wave irradiates the sample and decreases in intensity correspond to the number of atoms that absorbed that frequency.

2 Workings of Program

The program created for this project is a real time interactive computer animation (RTICA). It simulates constant wave NMR for a five by five sample of carbon and hydrogen atoms.

2.1 Drawing the Window

This RTICA uses Python with OpenGL to draw the entire window. All drawing is contained in the class plotfunc which uses GL_LINES and G_LPOINTS. The GL_LINES function is used to draw the arrows representing if an atom is in a high or low energy state. For the convenience of those who use the program, a down arrow is an atom in a low energy state (parallel to the external magnetic field) while a up arrow is an atom in a high energy state (anti-parallel to the external magnetic field.) The GL_LINES function is also used to draw the graphs for each row and column. The GL_POINTS function is used to draw circles,one for each element. The program, like many visualizations of elements uses black for carbon and yellow for hydrogen.

2.2 Running the RTICA

The user controls the RTICA using the keyboard. By pressing "r", the program will preform constant wave NMR horizontally and display carbon and hydrogen row counts in each row graph. Likewise, pressing "c" the program will preform constant wave NMR vertically and display carbon and hydrogen column counts in each column graph. Like in real life, preforming NMR will excite all the atoms to the higher energy state and because NMR only counts elements in a low energy state, the spins will need to be redistributed after each test. This is done by pressing "d". Finally, if the user would like a new sample the user should press "n". The program will exit if the escape key is pressed.

The graphs will automatically update after each test, redistribution of spins, and new sample. The vertical bars show what the current test results were and the horizontal lines show what the maximum test results were for all completed tests.

3 Works Cited

Jin, Janming. Electromagnetic Analysis and Design. New York: CRC Press, 1999. Book

www.cis.rit.edu/htbooks/nmr/inside.htm

http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/nmr/nmr1.htm

courses.physics.illinois.edu/phys214/fa2013/syllabus.asp

illinois.edu/about/overview/facts/nobel.html

teaching.shu.ac.uk/hwb/chemistry/tutorials/molspec/nmr1.htm